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PREFACE

Dr. Cristián Andrés Quintero

Universidad de Mendoza | Universidad Juan Agustín Maza



This book is the culmination of the Second Southern Science Conference, held from November 7th to 9th, 2024, in Mendoza, Argentina. The event marked two significant milestones: the 64th anniversary of the Universidad de Mendoza, a prestigious institution of higher education, and the 20th anniversary of Periódico Tchê Química, a publication devoted to advancing scientific and technological knowledge across various fields.

Organized jointly by the Universidad de Mendoza (Argentina) and Universidade de Vassouras (Brazil), the conference embraced a hybrid format, allowing for both in-person and virtual participation. This approach facilitated the inclusion of participants from 14 countries across 4 continents. Live-streamed main conferences and asynchronous video presentations for poster sessions expanded the conference's reach and accessibility.

Covering several areas, such as Food Production and Security, Energy Production and Sustainability, Drug Production and Development, Production Without Waste, Science Education, Environmental Sciences and Resource Management, One Health Approach, being environmental and health sciences were the most represented during the conference.

A unique feature of the event was the series of interviews conducted by Dr. Luis de Boni with invited speakers. These interviews provided insights into the speakers' current research, personal motivations, and future aspirations, offering attendees a glimpse of the individuals behind the science.

The success of this conference was made possible through the collaborative efforts of numerous institutions. In addition to the Universidad de Mendoza and Universidade de Vassouras, key support came from the University of Ilorin (Nigeria), INFIQC-CCT CONICET Córdoba (Argentina), KVANTUM Technology & Innovation (Brazil), Ilia State University (Georgia), Araucária – Scientific Association (Brazil), Conecta Mais WebTV (Brazil), University of Misan (Iraq), IFPA-Instituto Federal Pará (Brazil), IFRJ-Instituto Federal Rio de Janeiro Campus Duque de Caxias (Brazil), Universidad Juan Agustín Maza (Argentina), IFSP-Instituto Federal São Paulo Campus Cubatão (Brazil), and LITE – UFPI-Laboratório de Inovação Tecnológica e Empreendedorismo (Brazil). The dedicated efforts of a 30-person organizing committee, supported by staff from Vassouras and Mendoza, alongside 50 researchers from 10 countries who formed the scientific committee, ensured the high quality of the presentations and the smooth execution of the conference.

With 66 papers, over 30 keynote presentations, and contributions from more than 250 authors, the conference showcased a strong presence of Latin American researchers. This achievement highlights the importance of regional collaboration and sets a clear trajectory for future editions. The hybrid format proved to be an effective means of fostering global connections while enriching the scientific dialogue with diverse perspectives. The in-person sessions, meanwhile, offered a valuable platform for exchanging ideas, discussing the unique challenges faced by different scientific communities, and establishing new collaborations.

In the following pages, you will find QR codes providing access to the official conference website and the YouTube channel, where you can explore video posters and speaker interviews. We hope this book serves as both a record of the conference's achievements and a source of inspiration for future scientific endeavors.

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The committees participated in organizing the conference and the book.

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THE IMPACT OF VITAMIN D AND INTERLEUKIN-6 AS RISK FACTORS ASSOCIATED WITH DEPRESSION ADOLESCENTS

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ABSTRACT

Background: Adolescents face an increased risk of depression due to hormonal fluctuations and the impact on physiological and immunological biomarkers, which are associated with a heightened risk of symptoms of depression during puberty. **Aims:** investigate the roles of interleukin-6 (IL-6) and vitamin D (Vt.D) as influential factors in increasing the risk of depression among adolescents. **Methods:** Cross-sectional study of 130 adolescents aged 12 to 18, between November 2023 and February 2024. This study examined serum IL-6 and Vt.D levels. Additionally, the calculation relies on the Beck Depression Inventory to measure the severity of depression. **Results:** Adolescents have a significant increase in depression symptoms, with 59.2% showing signs of depression. Depressed adolescents show a significant increase ($p<0.001$) in IL-6 and decreased Vt. D levels compared to non-depressed individuals. Depression scores were significantly correlated positively with IL-6 levels and negatively with Vt. D levels and Linear regression analysis exhibit a significant positive predictor of IL-6 (B: 4.430; 95% CI: 3.023 to 5.836). Vt. D is a significantly negative predictor (B: -0.145; 95% CI: -0.220 to -0.071) associated with depression scores. They highly predicted depression in adolescents with deficiency Vt. D (OR: 24.4, $p<0.001$), and depressed severity increased with no take Vt. D supplement (OR: 1.769, p=004), more than those who had taken Vt. D Supplement (OR: 0.571, p=0.207). **Discussion:** Vitamin D affects serotonin synthesis by a unique biological mechanism, Serotonin is always involved in the pathophysiology of depression. Vitamin D may have a neuroprotective effect on the inflammatory process in the body. To support immunomodulation, lead to increase in inflammatory cytokines and vitamin which was suppresses the synthesis of inflammatory cytokines such as IL-6 by monocytes. **Conclusions:** The likelihood of severe adolescent depression was found to be associated with elevated IL-6 levels and a deficiency in Vitamin D, serving as available predictors.

Keywords: *Deficiency Vt.D, IL-6, Adolescent depression, and Depress scores*

1. INTRODUCTION

Adolescents are more susceptible to mental health problems during the formative and tumultuous years of adolescence due to changes in physiology, psychosocial development, and cognitive processes, Depression is the fourth most common cause of illness and disability among adolescents, and mental health issues account for 16% of the worldwide burden of disease and damage among this population (Shorey *et al*; 2022). Depression is one of the most common mental illnesses in the world, affecting many people's quality of life (Harsanyi *et al*., 2023). Depression is characterized by the dysregulation of the hypothalamus-pituitary-adrenal (HPA) or hypothalamus-pituitary-gonadal (HPG) axes, as well as other factors such as brain serotonin depletion, the impact of inflammation, and the immune system response (Troubat *et al*; 2021). It may result from low serotonin levels, which are influenced by low vitamin D levels (Kaviani *et al*., 2020). Serotonin (5-HT) is a vital neurotransmitter in the central nervous system as well as a regulatory hormone that regulates a wide variety of physiological functions. Perhaps the most classically defined roles of 5-HT are central to mood, sleep, and anxiety management and peripheral to gastrointestinal motility modulation. Vitamin D, a steroid hormone, plays a vital role in maintaining bone and calcium homeostasis, as noted by Giustina *et al*. in 2020 and Di Molfetta *et al*. in 2024.

2. MATERIALS AND METHODS

2.1. Materials

This cross-sectional study was performed based on ethical clearance in line with the Declaration of Helsinki and verbal agreement from the study subjects' parents, which comprised one hundred and thirty (130)

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adolescents (males and females) with ages ranging from (12-18) years. Samples were collected from different areas in the center and districts of Al-Najaf al-Ashraf City, Iraq. It was conducted from the first of November 2023 to the end of January 2024. Based on the study's experimental design and the formal data for every participant, The participants were healthy, all samples suffering from incurable diseases, cancer patients, tumors, endocrine disorders, mental and physical disabilities, and deaf and mute patients were excluded. The adolescents answered a questionnaire that included the Beck Depression Inventory to determine the degree of depression for each adolescent.

2.2. Methods:

The collected blood was divided into two parts. Approximately 2 mL" and put in an EDTA tube (ethylene diamine tetra acetic acid). In contrast, the other part (3ml) was put in gel tubes for serum separation, centrifuged at 3000 rpm for 5 minutes to separate the serum, and transferred to new Eppendorf tubes and stored at -20 °C until the measurement IL-6 (No.E0090Hu) and Vt. D (No.E1546Hu levels by ELISA according to the kit supplied by (the Bioassay Technology Laboratory Company).

2.3. Statistical analysis:

All data were statistically analyzed by IBM SPSS 26 (SPSS Inc., Chicago, IL). Nominal data was reported by frequencies and percentages with the use of the chi-square test. The normal distribution used the Kolmogorov-Smirnov test. Numerical data were expressed as mean ± standard deviation (SD), an independent t-test between two groups, and an ANOVA with Tukey`s post hoc test for comparison among groups. Median (IQR) interquartile range for continuous variables with non-normal, distribution and Kruskal-Wallis test for among groups. Pearson's or Spearman Rho coefficient correlation tests between serum levels of IL-6 and Serotonin with depressive scores. Linear and logistic nominal regression analyses were performed to predict the of risk depression. The significant level was considered as p-value <0.05.

3. RESULTS AND DISCUSSION:

3.1. Distribution of All Studied Categories in Adolescent Students.

The statistical analysis in Table (1) indicated that 130 adolescent students were enrolled aged (12-18), with (mean ± SD) 14.85±2.19. The results showed a significant increase (p=0.035) in number and percentage 77(59.2%) students had depression symptom median (IQR) of scores about 16(13_21.5), and 53(40.8%) adolescents with non-depressed (scores 5(2.5_7), who considered as controls group, a statistically significant in depressed scores (p<0.001).

The study included 64(49.2%) males and 66 (50.8%) females of total adolescent students; Significant increases were observed in depressed females 46 (59.7%) more than males 31 (40.3%) p=0.014. A significant (p<0.001) increase in mean BMI of depressive adolescents (23.3±4.3 kg/m^2), when compared with (20.21±4.39 kg/m^2). While, BMI categories showed depressive adolescents with underweight (20.8%), less than non-depressive (41.5%), but groups with normal weight (50.6%), overweight and obesity about (19.5%), and (9.1%), depressed highest than non-depressive-adolescents-about (45.3%), (7.5%), and (5.7%), respectively, with significant differences p=0.039. Depressed adolescents have a significant (p<0.001) increase in levels of IL-6 (pg/mL), (Mean:1.85, median (IQR): 1.8(1.3-2.24) and decreased Vt. D (ng/mL) (Mean: 22.32; median (IQR): 18.8(13.1_28.9) as compared with non-depressed (Mean: 1.17; median (IQR): 1.22(0.77-1.43) and 50.54; 52.22(42.2_62.4), respectively.

3.2. Vitamin D Association with Depressive Status

The findings in Table (2) suggested that Depressive adolescents who 49 (63.6%) Deficiency Vt. D (14.14±4.28) has mean scores of (20.29±5.77), a significant difference (p < 0.001) more than 15 (19.5%) who Insufficiency (28.17±1.63) with mean scores (13.53±3.58) and 13(16.9%) Sufficiency Vt. D (46.38±9.23) with mean scores of (12.69±1.25) as compared with vitamin D status 2 (3.8%), 5 (9.4%), and 46 (86.8%) in non-depressive adolescents respectively.

3.3. IL-6 Association with Vt. D status

Serum levels of IL-6 in depressive adolescents with Deficiency Vt. D has a significant increase mean of about (2.08±0.76) than adolescents with Insufficiency Vt. D (1.48±0.35), p=0.003, and Sufficiency Vt. D (1.39±0.43), p=0.001 to compare with (1.23±0.65), (1.41±0.49), and (1.14±0.46) in non-depressive groups respectively (p=482). Figure (1)

3.4. Correlations and Regression Analysis of Vt. D and IL-6 levels with depression scores

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Statistics results reported Depression scores were reverse significant correlated (p<0.0001) with levels of Vt. D (r= -0.786), Figure (2). At the same time, were significantly positively correlated (p<0.0001) with levels of IL-6 (r=0.751), Figure (3). IL-6 was significantly negatively correlated (p<0.0001) with levels of Vt. D (r= -0.570). Figure (4). The results showed in Table (3) that Age (year) was not a significant predictor of depression scores (B: 0.231; p= 0.234; 95% CI: -0.153 to 0.616), and BMI (B: -0.172; 0.079; 95% CI: -0.365 to 0.021). IL-6 exhibits a highly significant positive predictor (B: 4.430; p<0.001; 95% CI: 3.023 to 5.836). At the same time, Vt. D showed highly significantly negative predictors. (B: -0.145; p<0.001; 95% CI: -0.220 to -0.071).

3.5. Logistic Regression analysis to predict the risk factors associated with depression.

Nominal Regression analysis in Table (4), The risk of depression associated with females (OR: 2.33; p=0.002), is higher than males (OR: 0.939; p=0.803). Those overweight adolescents and obese were highest predicted to be more depressive (OR: 3.750, p=0.019; and OR: 2.333, p=0.022), than normal weight and underweight (OR:1.625, p=0.061; and OR: 0.727, p=0.332), respectively. The risk of depression was elevated in adolescents with no Vt. D Supplement (OR: 1.769, p=004), more than those who had taken Vt. D Supplement (OR: 0.571, p=0.207). There was Highly predicted depression in adolescents with deficiency Vt. D (OR: 24.4, p<0.001), as compared with insufficiency (OR: 3.00, p=0.033), but no effects in and sufficiency adolescent and (OR:0.283, p<0.001). adolescent (OR: 486, p=0.015).

Table (1). *Distribution of All Studied Categories in Adolescent Students.*

Variables	Categories	Depressive	Non-Depressive	p-value
Age (year)		14.94±2.2	14.72±2.2	0.579
Studied samples		77 (59.2%)	53 (40.8%)	X^2=4.431 0.035*
Depression Scores		17.69±5.97 16(13.21.5)#	4.98±2.74 5(2.5.7)#	<0.001**
Types of Depression	Simple	35 (26.9%)	-	X^2=6.338 0.042*
	Mild	25 (19.2%)	-	
	Severe	17 (13.1%)	-	
Sex	Male	31(40.3%)	33 (62.3%)	X^2= 6.081 0.014*
	Female	46 (59.7%)	20 (37.7%)	
BMI (kg/m^2)	Mean ± SD	23.3±4.3	20.21±4.39	<0.001**
	Underweight Normal weight Overweight Obesity	16 (20.8%) 39 (50.6%) 15 (19.5%) 7 (9.1%)	22 (41.5%) 24 (45.3%) 4 (7.5%) 3 (5.7%)	X^2=8.341 0.039*
IL-6(pg/ml)		1.85±0.72 1.8(1.3-2.24)#	1.17±0.47 1.22(0.77-1.43)#	<0.001**
Vt.D (ng/mL)		22.32±13.21 18.8(13.1_28.9)#	50.54±14.85 52.22(42.2_62.4)#	<0.001**
Vt. D Supplement	Yes	8 (10.4%)	14 (26.4%)	X^2=5.734 0.017*
	No	69 (89.6%)	39 (73.6%)	
Vt. D Status	Deficiency	49 (63.6%)	2 (3.8%)	X^2= 4.54 <0.001**
	Insufficiency	15 (19.5%)	5 (9.4%)	
	Sufficiency	13 (16.9%)	46 (86.8%)	

Significant differences at p-value. **<0.01, *<0.5. X2: Chi-Square test. #: Median (IQR). BMI: (body mass index)

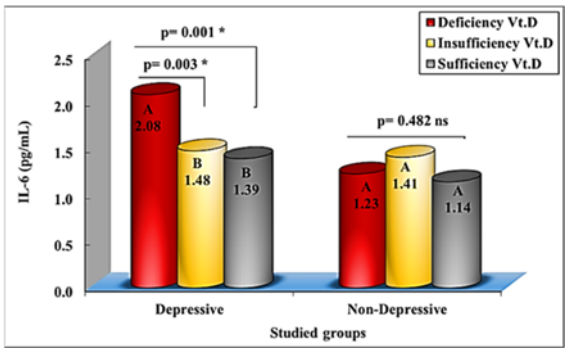


Figure (1): *Serum IL-6 levels in depressive adolescents according to Vt. D status*
Deafferent letters Significant differences at p-value<0.05. ns: non-significant.

Table (2). *Depression Scores Association with Vt. D status*

Vt. D status	Depression Scores		p-value
	Depressive	Non-Depressive	
Deficiency Vt. D	49 (63.6%) 20.29±5.77	2 (3.8%) 8.5±0.71	<0.001**
Insufficiency Vt. D	15 (19.5%) 13.53±3.58	5 (9.4%) 7±1.22	
Sufficiency Vt. D	13 (16.9%) 12.69±1.25	46 (86.8%) 4.61±2.71	

Significant differences at p-value **<0.01, p*<0.05. data of Depression Scores expressed as Mean ± SD

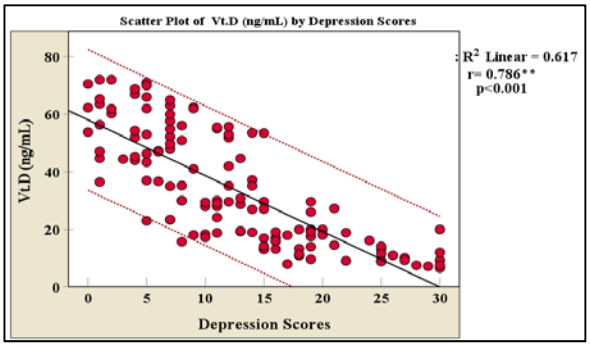


Figure (2). Pearson Correlation of Vt. D with depression scores
The separated red line is a 95% confidence interval

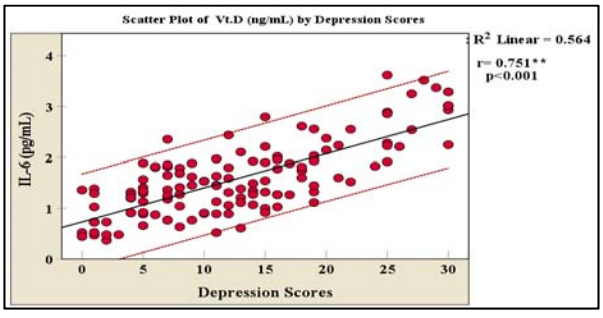


Figure (3). *Pearson Correlation of IL-6 with depression scores.*
The separated red line is a 95% confidence interval.

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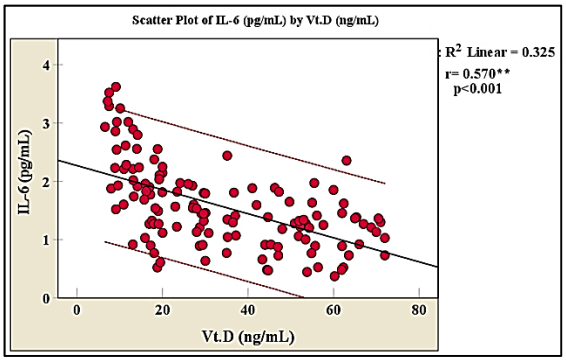


Figure (4). *Pearson Correlation of IL-6 with Vt. D* ***The separated red line is a 95% confidence interval***

Table (3). *Linear regression analysis to predict risk factors associated with the depression scores.*

Predicts parameters	B	SE	p-value	95.0% CI
(Constant)	13.265	4.108	0.002	5.076 to 21.455
Age (year)	0.231	0.193	0.234	-0.153 to 0.616
BMI (kg/m^2)	-0.172	0.097	0.079	-0.365 to 0.021
IL-6 (pg/mL)	4.430	0.706	<0.001	3.023 to 5.836
Vt.D (ng/mL)	-0.145	0.037	<0.001	-0.220 to -0.071

Significant differences at p-value *<0.05, p **<0.01. B: Unstandardized Coefficients (effect size). SE: standard error. CI: Confidence Interval. Dependent Variable: depression Scores.

Table (4). *Nominal Regression analysis to predict the categories of risk factors associated with depressive status.*

Predicts [a]		B	p-value	OR	95% CI
Sex	Male	-0.063	0.803	0.939	0.575 to 1.534
	Female	0.833	0.002	2.300*	1.361 to 3.888
BMI Categories	Underweight	-0.318	0.332	0.727	0.382 to 1.385
	Normal weight	0.486	0.061	1.625	0.977 to 2.702
	Overweight	1.322	0.019	3.750*	1.245 to 11.299
	Obesity	0.847	0.220	2.333	0.603 to 9.023
Vt.D Supplement	Yes	-0.560	0.207	0.571	0.240 to 1.362
	No	0.571*	0.004	1.769	1.195 to 2.620
Vt. D_ Status	Deficiency	3.199	0.0001	24.50**	5.96 to 100.74
	Insufficiency	1.099	0.033	3.00 *	1.09 to 8.254
	Sufficiency	-1.264	0.0001	0.283**	0.153 to 0.523

Significant differences at p-value *<0.05, p<0.01. a: The category references are non-depressive. 95% Confidence Interval for OR**

4. CONCLUSIONS:

Decreased vitamin D and elevated IL-6 levels may indicate a relationship between immune dysregulation and vitamin D metabolism, The likelihood of severe adolescent depression was found to be associated with IL-6 especially with vitamin D deficiency, serving as available predictors of severity of depression.

5. DECLARATIONS

5.1. Acknowledgments

The author thanks all adolescents who participated in this study.

5.5. Open Access

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Southern Science Conference, 2024.

THE IMPACT OF VITAMIN D AND INTERLEUKIN-6 AS RISK FACTORS ASSOCIATED WITH DEPRESSION ADOLESCENTS

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September/2024

INTRODUCTION

Adolescents are more susceptible to mental health problems during the formative and tumultuous years of adolescence due to changes in physiology, psychosocial development, and cognitive processes, Depression is the fourth most common cause of illness and disability among adolescents, and mental health issues account for 16% of the worldwide burden of disease and damage among this population. Depression is one of the most common mental illnesses in the world, affecting many people's quality of life. Depression is characterized by the dysregulation of the hypothalamus-pituitary-adrenal (HPA) or hypothalamus-pituitary-gonadal (HPG) axes, as well as other factors such as brain serotonin depletion, the impact of inflammation, and the immune system response.

BACKGROUND

It may result from low serotonin levels, which are influenced by low vitamin D levels (Kaviani et al., 2020). Serotonin (5-HT) is a vital neurotransmitter in the central nervous system as well as a regulatory hormone that regulates a wide variety of physiological functions. Perhaps the most classically defined roles of 5-HT are central to mood, sleep, and anxiety management and peripheral to gastrointestinal motility modulation. Vitamin D, a steroid hormone, plays a vital role in maintaining bone and calcium homeostasis, as noted by Giustina et al. in 2020 and Di Molfetta et al. in 2024. It is significant for various physiological and pathological processes, including the modulation of the immune and inflammatory systems, neuroendocrine function, and cardiovascular health, as mentioned by Valer-Martinez et al. in 2023. Vitamin D is essential for the control of the serotonergic pathway as well as the generation of melatonin, showing the role of vitamin D not only in sleep but also in mood regulation (Huiberts et al., 2021), and new research emphasizes its critical role in neurodevelopment (Todisco et al., 2020). Interleukin 6 (IL-6) is a cytokine produced from T cells, macrophages, and adipocytes, which can function as either an anti- or pro-inflammatory cytokine and be released into the bloodstream in response to an immunologic stimulation. In depression, cytokine responses to infections and stressors are increased. Responses, when combined with other risk factors, result in extended inflammatory processes, dysregulation of many axes, stress, pain, mood changes, anxiety, and depression, (Harsanyi et al., 2023). Depression and neurosis are diseases that currently affect most young people and affect their social behavior. To achieve this goal.

AIM

This study aimed to investigate the roles of interleukin-6 (IL-6) and vitamin D (Vt.D) as influential factors in increasing the risk of depression among adolescents

METHODOLOGY

The adolescents answered a questionnaire that included the Beck Depression Inventory to determine the degree of depression for each adolescent. Five ml of venous blood samples were obtained from every adolescent for hematological and biochemical screening tests. The collected blood was divided into almost (2ml) and put in an EDTA tube (ethylene diamine tetra acetic acid), while the other part (3ml) was put in gel tubes for separates of serum, centrifuged at 3000 rpm for 5 minutes to completely separate the serum which preserved in new Eppendorf tubes and stored at -20 °C until the measurement IL-6 and Vt. D) by ELISA according to the kit that is supplied by (the Bioassay technology laboratory company), This kit is an Enzyme-Linked immunosorbent Assay(ELISA). the plate has been pre-coated with human antibody. The sample is added and binds to antibodies coated on the wells. And then biotinylated Human Antibody is added and binds to the sample Then Streptavidin-HRP is added and binds to the Biotinylated antibody. After incubation, unbound Streptavidin-HRP is washed away during a washing step. Substrate solution is added and color develops proportionately to the amount of the tested marker. The reaction is terminated by the addition of an acidic stop solution and absorbance is measured at 450nm,

RESULTS AND DISCUSSION

1. Distribution of All Studied Categories in Adolescent Students.

The statistical analysis in Table (4.1) indicated that 130 adolescent students were enrolled aged (12-18), with (mean ± SD) 14.85±2.19. The results showed a significant increase (p=0.035) in number and percentage 77(59.2%) students had depression symptom median (IQR) of scores about 16(13_21.5), and 53(40.8%) adolescents with non-depressed (scores 5(2.5_7), who considered as controls group, a statistically significant in depressed scores (p<0.001). As well the Beck depression scale the results indicated that depressive adolescents who had simple type scores were 35(26.9%), with a mean (of 12.57±1.72), mild was 25(19.2%) and mean about (18.44±1.89), and 17(13.1%) severe depression mean was (27.12±2.29), from these results, it was confirmed that there is a significant difference (p=0.042).

The study included 64(49.2%) males and 66 (50.8%) females of total adolescent students; Significant increases were observed in depressed females 46 (59.7%) more than males 31 (40.3%) p=0.014. A significant (p<0.001) increase in mean BMI of depressive adolescents (23.3±4.3 kg/m2), when compared with (20.21±4.39 kg/m2). While, BMI categories showed depressive adolescents with underweight (20.8%), less than non-depressive (41.5%), but groups with normal weight (50.6%), overweight and obesity about (19.5%), and (9.1%), depressed highest than non-depressive-adolescents-about (45.3%), (7.5%), and (5.7%), respectively, with significant differences p=0.039. Depressed adolescents have a significant (p<0.001) increase in levels of IL-6 (pg/mL), (Mean:1.85, median (IQR): 1.8(1.3-2.24) and decreased Vt. D (ng/mL) (Mean: 22.32; median (IQR): 18.8(13.1_28.9) as compared with non-depressed (Mean: 1.17; median (IQR): 1.22(0.77-1.43) and 50.54; 52.22(42.2_62.4), respectively. According to Vt. D Status, depressive adolescents had deficiency Vt. D 49(63.6%) and Insufficiency Vt. D 15(19.5%) more than non-depressed students 2(3.8%), and 5(9.4%), but who with Sufficiency Vt. D about 13(16.9%) depressive, lowest 46(86.8%) in non-depressive groups, these results showed a significant difference (p<0.001).

Table (1). Distribution of All Studied Categories in Adolescent Students.

Variables	Categories	Depressive	Non-Depressive	p-value
Age (year) #		14.94±2.2	14.72±2.2	0.579
Studied samples		77 (59.2%)	53 (40.8%)	X^2=4.431 0.035*
Depression Scores #		17.69±5.97 16(13_21.5)	4.98±2.74 5(2.5_7)	<0.001**
Types of Depression #	**Simple**	35 (26.9%)	-	X^2=6.338 0.042*
	Mild	25 (19.2%)	-	
	Severe	17 (13.1%)	-	
Sex	**Male**	31(40.3%)	33 (62.3%)	X^2= 6.081 0.014*
	Female	46 (59.7%)	20 (37.7%)	
BMI (kg/m^2)#	**Mean ± SD**	23.3±4.3	20.21±4.39	<0.001**
	Underweight	16 (20.8%)	22 (41.5%)	X^2=8.341 0.039*
	Normal weight	39 (50.6%)	24 (45.3%)	
	Overweight	15 (19.5%)	4 (7.5%)	
	Obesity	7 (9.1%)	3 (5.7%)	
IL-6(pg/ml) #		1.85±0.72 1.8(1.3-2.24)	1.17±0.47 1.22(0.77-1.43)	<0.001**
Vt. D (ng/mL) #		22.32±13.21 18.8(13.1_28.9)	50.54±14.85 52.22(42.2_62.4)	<0.001**
Vt. D Supplement	**Yes**	8 (10.4%)	14 (26.4%)	X^2=5.734 0.017*
	No	69 (89.6%)	39 (73.6%)	
Vt. D Status	**Deficiency**	49 (63.6%)	2 (3.8%)	X^2= 4.54 <0.001**
	Insufficiency	15 (19.5%)	5 (9.4%)	
	Sufficiency	13 (16.9%)	46 (86.8%)	

Significant differences at p-value. **<0.01, *<0.5 X2: Chi-Square test, BMI: (body mass index)

2. Vitamin D Association with Depressive Status

The findings in Table (2) suggested that Depressive adolescents who 49 (63.6%) Deficiency Vt. D (14.14±4.28) has mean scores of (20.29±5.77), a significant difference ($p < 0.001$) more than 15 (19.5%) who Insufficiency (28.17±1.63) with mean scores (13.53±3.58) and 13(16.9%) Sufficiency Vt. D (46.38±9.23) with mean scores of (12.69±1.25) as compared with vitamin D status 2 (3.8%), 5 (9.4%), and 46 (86.8%) in non-depressive adolescents respectively.

Table (2). Depression Scores Association with Vt. D status

Vt. D status	Depression Scores (Mean ± SD)		p-value
	Depressive	Non-Depressive	
Deficiency Vt. D	49 (63.6%) 20.29±5.77	2 (3.8%) 8.5±0.71	**<0.001****
Insufficiency Vt. D	15 (19.5%) 13.53±3.58	5 (9.4%) 7±1.22	
Sufficiency Vt. D	13 (16.9%) 12.69±1.25	46 (86.8%) 4.61±2.71	

Significant differences at p-value **<0.01, p*<0.05.

3. IL-6 Association with Vt. D status

Serum levels of IL-6 in depressive adolescents with Deficiency Vt. D has a significant increase mean of about (2.08±0.76) than adolescents with Insufficiency Vt. D (1.48±0.35), p=0.003, and Sufficiency Vt. D (1.39±0.43), p=0.001 to compare with (1.23±0.65), (1.41±0.49), and (1.14±0.46) in non-depressive groups respectively (p=482). Figure (1)

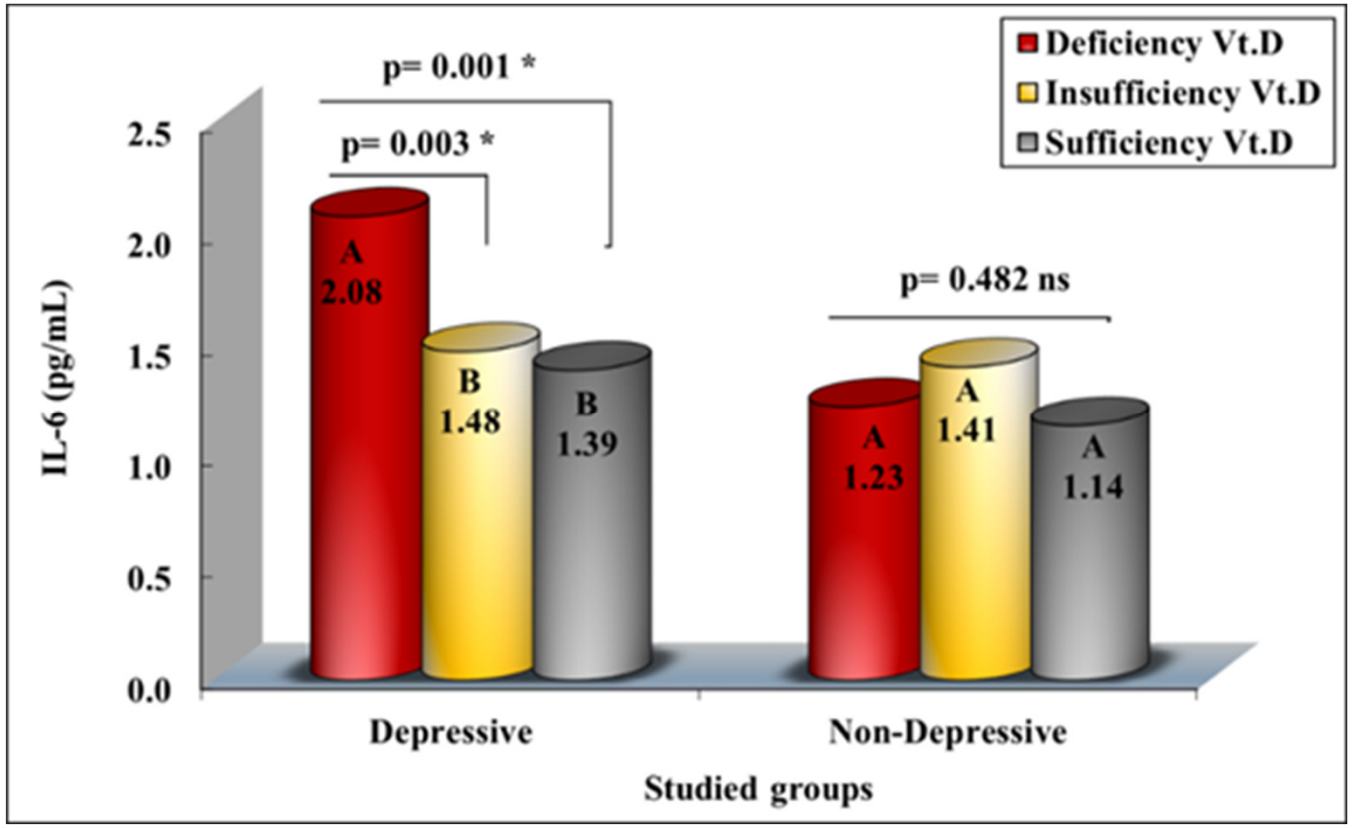


Figure (1): Serum IL-6 levels in depressive adolescents according to Vt. D status Deafferent letters Significant differences at p-value<0.05. ns: non-significant.

4. Correlations and Regression Analysis of Vt. D and IL-6 levels with depression scores

Statistics results reported Depression scores were reverse significant correlated ($p<0.0001$) with levels of Vt. D ($r= -0.786$), Figure (2). At the same time, were significantly positively correlated ($p<0.0001$) with levels of IL-6 ($r=0.751$), Figure (3). IL-6 was significantly negatively correlated ($p<0.0001$) with levels of Vt. D ($r= -0.570$). Figure (4). The results showed in Table (3) that Age (year) was not a significant predictor of depression scores (B: 0.231; p= 0.234; 95% CI: -0.153 to 0.616), and BMI (B: -0.172; 0.079; 95% CI: -0.365 to 0.021). IL-6 exhibits a highly significant positive predictor (B: 4.430; $p<0.001$; 95% CI: 3.023 to 5.836). At the same time, Vt. D showed highly significantly negative predictors. (B: -0.145; $p<0.001$; 95% CI: -0.220 to -0.071).

Table (3). Linear regression to predict risk factors associated with the depression scores.

Predicts parameters	B	SE	p-value	95.0% CI
(Constant)	13.265	4.108	0.002	5.076 to 21.455
Age (year)	0.231	0.193	0.234	-0.153 to 0.616
BMI (kg/m^2)	-0.172	0.097	0.079	-0.365 to 0.021
IL-6 (pg/mL)	4.430	0.706	<0.001	3.023 to 5.836
Vt.D (ng/mL)	-0.145	0.037	<0.001	-0.220 to -0.071

Significant differences at p-value *<0.05, p **<0.01.

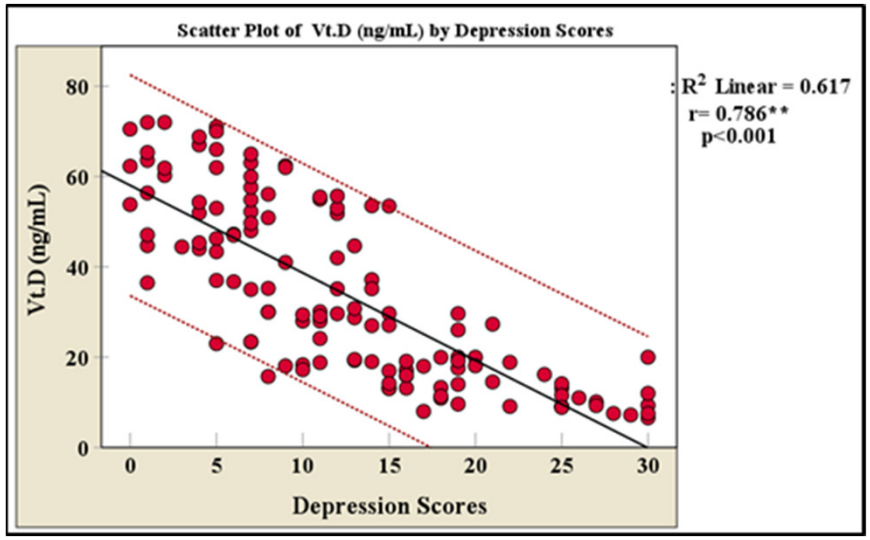


Figure (2). Correlation of Vt. D with depression scores

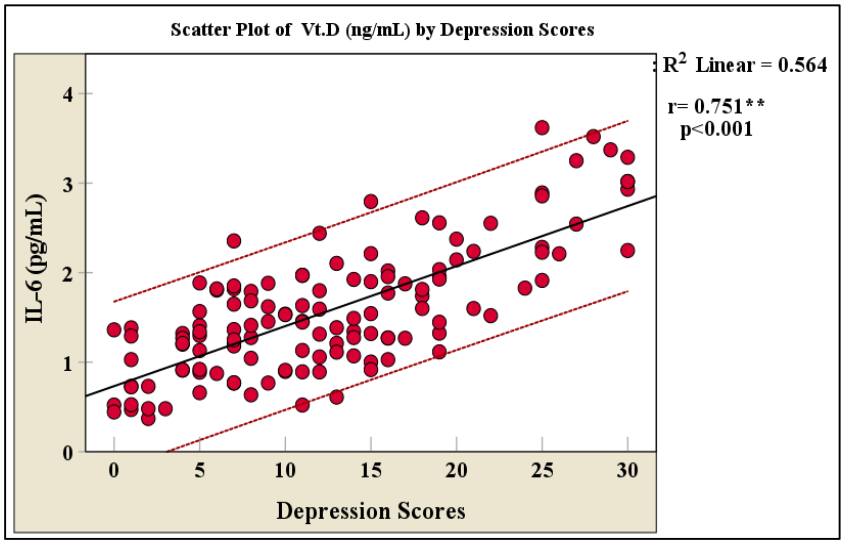


Figure (3). Correlation of IL-6 with depression scores

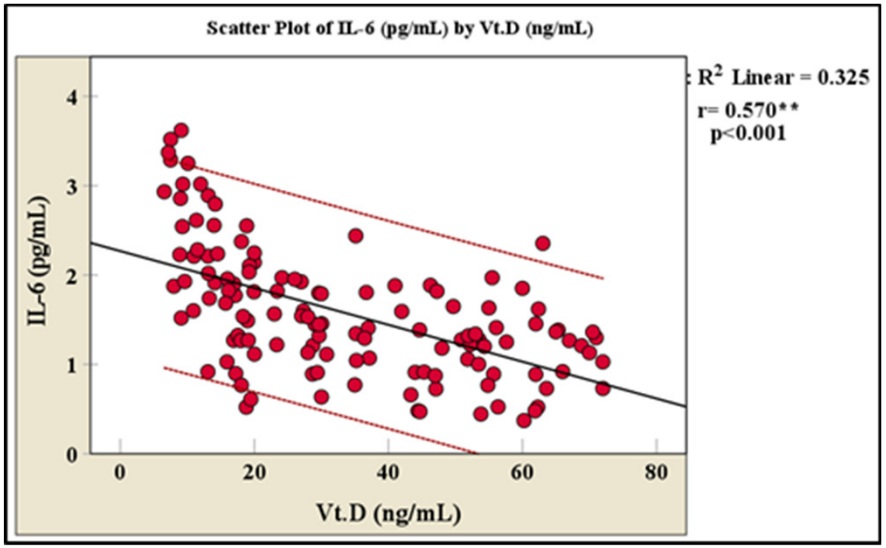


Figure (4). Correlation of IL-6 with Vt. D

Logistic Regression analysis to predict the risk factors associated with depression.

Nominal Regression analysis in Table (4), The risk of depression associated with females (OR: 2.33; p=0.002), is higher than males (OR: 0.939; p=0.803). Those overweight adolescents and obese were highest predicted to be more depressive (OR: 3.750, p=0.019; and OR: 2.333, p=0.022), than normal weight and underweight (OR:1.625, p=0.061; and OR: 0.727, p=0.332), respectively. The risk of depression was elevated in adolescents with no Vt. D Supplement (OR: 1.769, p=004), more than those who had taken Vt. D Supplement (OR: 0.571, p=0.207). There was Highly predicted depression in adolescents with deficiency Vt. D (OR: 24.4, p<0.001), as compared with insufficiency (OR: 3.00, p=0.033), but no effects in and sufficiency adolescent and (OR:0.283, p<0.001). adolescent (OR: 486, p=0.015).

Table (4). Nominal Regression analysis to predict the categories of risk factors associated with depressive status.

Predicts [a]		**B**	**p-value**	**OR**	**95% CI**
Sex	**Male**	-0.063	0.803	0.939	0.575 to 1.534
	Female	0.833	0.002	2.300*	1.361 to 3.888
BMI Categories	**Underweight**	-0.318	0.332	0.727	0.382 to 1.385
	Normal weight	0.486	0.061	1.625	0.977 to 2.702
	Overweight	1.322	0.019	3.750*	1.245 to 11.299
	Obesity	0.847	0.220	2.333	0.603 to 9.023
Vt.D Supplement	**Yes**	-0.560	0.207	0.571	0.240 to 1.362
	No	0.571*	0.004	1.769	1.195 to 2.620
Vt. D_ Status	**Deficiency**	3.199	0.0001	24.50**	5.96 to 100.74
	Insufficiency	1.099	0.033	3.00 *	1.09 to 8.254
	Sufficiency	-1.264	0.0001	0.283**	0.153 to 0.523

Significant differences at p-value *<0.05, p<0.01. a: The category references are non-depressive. 95% Confidence Interval for OR**

CONCLUSIONS

Decreased vitamin D and elevated IL-6 levels may indicate a relationship between immune dysregulation and vitamin D metabolism, The likelihood of severe adolescent depression was found to be associated with IL-6 especially with vitamin D deficiency, serving as available predictors of severity of depression.

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II SOUTHERN SCIENCE CONFERENCE
2024 - VIRTUAL CONFERENCE AND IN PERSON EDITION

AN INTERACTIVE CHEMISTRY GAME FOR EDUCATIONAL ENGAGEMENT

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ABSTRACT

This project aimed to develop an interactive chemistry game accessible on mobile devices and computers to make learning basic chemistry concepts more engaging for students. The game was created using HTML, CSS, and JavaScript, ensuring cross-platform compatibility. Initial tests showed that the game successfully captured students' interest with its intuitive interface and appealing design. While the game proved attractive to young students and encouraged exploration of chemical concepts in a playful manner, areas for improvement were identified, including expanding educational content and providing more detailed user feedback. The game's flexibility in access and positive reception by test users highlight its potential as an educational tool for teaching chemistry. With further enhancements, this game could become a valuable resource in chemistry education, leveraging widespread mobile device usage to transform these devices into productive learning tools.

Keywords: *Interactive Learning, Chemistry Education, Mobile Gaming, Educational Technology, Game-Based Learning.*

1. INTRODUCTION

This project, born from a family initiative to create educational tools, explores the potential of educational games in learning. Authors like Vieira (2016), Tupin, Borges, and Duarte (2021), Lima & Mesquita (2008), Silva, Nogueira, & Souza (2012), and De Souza and Rua (2010) have demonstrated the educational value of such games in promoting engagement and understanding complex concepts.

While mobile phones as educational tools have limitations, Hamari *et al*. (2016) note that challenging games can enhance learning through engagement. When used appropriately, mobile devices can transform screen time into productive educational experiences.

Research by Wouters *et al*. (2013) and Connolly *et al*. (2012) provides evidence of the positive cognitive and motivational effects of serious games across various disciplines. Sung and Hwang (2013) and Tsai & Tsai (2020) further support the effectiveness of game-based learning in science and chemistry education.

This project aims to develop an interactive game to assist in chemistry education, offering a resource that both entertains and educates, inspiring students to explore new concepts engagingly.

2. MATERIALS AND METHODS

2.1. Materials

Computer:
Model: Intel Core i7
Operating System: Windows 11
Code Editor: Sothink HTML Editor

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DOI: 10.48141/SSCON_02_2024.pdf

Artificial Intelligence Resources:
ChatGPT: Used to generate and correct code by leveraging pattern analysis in existing code.
Google Gemini: Employed to generate and refine code and provide insights and suggestions.
Perplexity AI: Utilized to generate code snippets and offer real-time coding assistance.
Claude AI: Applied to generate, correct, and optimize code through advanced machine learning techniques.

2.2. Methods

The game implements a column correlation system for inorganic chemical compounds, matching formulas with names. This method was chosen to aid memorization and understanding of chemical formulas while promoting interactive learning.

Developed using HTML for structure, CSS for styling, and JavaScript for functionality, the game ensures accessibility, visual appeal, and interactivity. JavaScript enables column correlation, instant feedback, and learning reinforcement.

Initial testing was conducted to ensure smooth functionality across mobile devices and computers. The integration of modern technologies and agile practices, along with AI assistance for code generation and correction, resulted in a timely, robust educational tool meeting established objectives.

2.2.1. Game description

a) Splash Screen (figure 1): The game opens with a language selection screen, enhancing accessibility and providing a personalized experience for diverse users.



Figure 1. *Language selection screen.*

b) Avatar Creation Screen (Figure 2): Players can create a customized avatar, enhancing engagement and fostering a deeper connection with the game.



Figure 2. Avatar selection screen

C) Column Matching Game Screen (Figure 3): The main gameplay features a column-matching system for various chemical functions (acids, bases, salts, oxides, or mixed). This allows players to focus on specific areas or challenge themselves with broader topics.

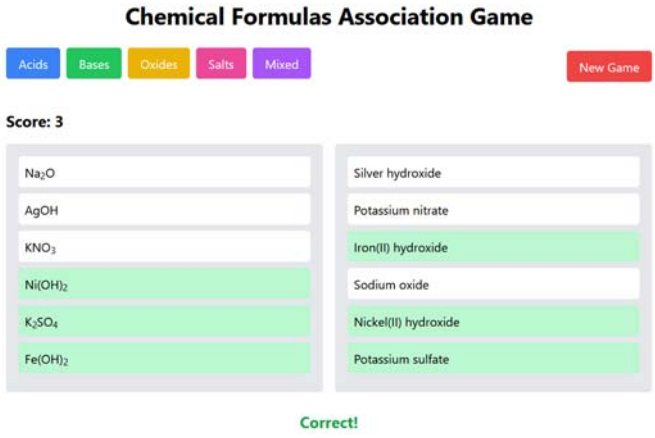


Figure 3. Collum correlation game.

c.1) Auditory and written feedback reinforces learning by indicating correct and incorrect matches.

c.2) A scoreboard tracks correct matches, adding competition and motivation.

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c.3) Players can start a new game or select a different chemical function upon completion.

These features create an engaging, educational experience supporting chemistry learning through interactivity and immediate feedback. To have a simple game experience, please visit: https://acaria.org/codes/code14.htm.

3. RESULTS AND DISCUSSION:

The game works well on Firefox across devices, ensuring wide accessibility. Testers appreciated the intuitive interface, engaging design, avatar customization, and immediate feedback. The language selection (English/Portuguese) and scoreboard function correctly, broadening the game's reach and motivating players. Avatar creation, though simple, enhances engagement. These results suggest the game effectively meets its objectives as an engaging educational tool for chemistry, suitable for various educational settings.

Improvements needed:

a) Enhance mobile interface for better user experience
b) Implement result-sharing feature to boost engagement and competition
c) Add timer to scoreboard to evaluate and challenge response times
d) Include the avatar into the game

These enhancements would increase accessibility, user engagement, and game complexity.

4. CONCLUSIONS:

The developed code created a simple game reinforcing basic chemical concepts (acids, salts, bases, oxides) by associating formulas with compound names. This interactive format enhances memorization and engagement, making learning more accessible. The game's success suggests it can be a valuable complementary tool in chemistry education.

5. DECLARATIONS

5.1. Acknowledgments

The author thanks his daughter for the motivation to make the mobile phone an increasingly useful tool in education.

5.2. Open Access

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Southern Science Conference, 2024.

An Interactive Chemistry Game for Educational Engagement

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September/2024

INTRODUCTION

- Family initiative to create educational tools
- Potential of educational games in learning
- Mobile devices as educational tools

BACKGROUND

- Widespread use of mobile devices among students offers new opportunities for education
- Traditional chemistry learning can be challenging and often viewed as abstract by students
- Educational games have shown potential in enhancing engagement and understanding
- Previous studies (e.g., Hamari et al., 2016; Tsai & Tsai, 2020) demonstrate positive impacts of game-based learning in science education
- There's a growing need for innovative, accessible tools to complement traditional chemistry teaching methods

AIM

- To introduce an interactive chemistry game designed for mobile devices and computers
- To demonstrate how this game reinforces fundamental chemical concepts through engaging gameplay

METHODOLOGY

Development Platform:
- Computer: Intel Core i7, Windows 11
- Code Editor: Sothink HTML Editor

Programming Languages:
- HTML: For structuring game content
- CSS: For styling and visual design
- JavaScript: For game logic and interactivity

AI-Assisted Development:
- ChatGPT: Code generation and correction
- Google Gemini: Code refinement and suggestions
- Perplexity AI: Real-time coding assistance
- Claude AI: Code optimization

Game Design Approach:
- Column correlation system for inorganic chemical compounds
- Matching formulas with compound names
- Focus on basic concepts: acids, salts, bases, oxides

Key Features Implemented:
- Language selection (English/Portuguese)
- Avatar customization
- Immediate feedback system
- Scoreboard for tracking progress

Testing:
- Cross-platform functionality (mobile and computer)
- User experience evaluation
- Performance assessment on Firefox browser

RESULTS

Functionality:
- Successful cross-platform compatibility (mobile and computer)
- Smooth performance on Firefox browser

User Interface:
- Intuitive and engaging design
- Positive reception of avatar customization feature

Educational Impact:
- Effective reinforcement of basic chemical concepts
- Enhanced memorization through interactive format

User Experience:
- Immediate feedback system well-received
- Language selection (English/Portuguese) functioning correctly
- Scoreboard feature increased motivation and engagement



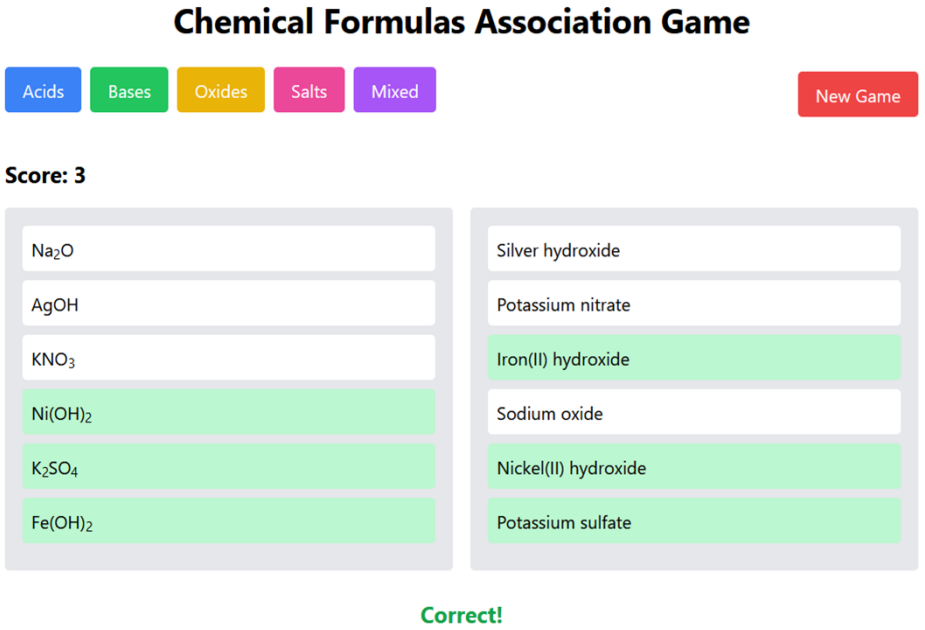
RESULTS

Learning Outcomes:

- Successful exploration of chemical concepts in a playful manner
- Increased student interest in chemistry topics

Overall Reception:

- Testers expressed satisfaction with the game experience
- Positive indication of the game's potential as an educational tool



DISCUSSION

Achievements:
• Successfully created an engaging, interactive chemistry learning tool
• Demonstrated potential of mobile devices for educational purposes
• Positive user feedback validates the game-based learning approach

Limitations:
• Mobile interface requires further optimization
• Current version focuses on basic concepts only

Areas for Improvement:
• Enhance user interface for better mobile experience
• Implement result-sharing feature to boost engagement
• Add timer to scoreboard for speed challenges
• Integrate avatar more deeply into gameplay

Educational Implications:
• Game shows promise as a complementary tool in chemistry education
• Interactive format may help overcome perceived difficulty of chemistry

Broader Impact:
• Demonstrates potential of transforming screen time into productive learning
• Could serve as a model for developing similar games in other subjects
Future Research:
• Conduct more extensive user testing in formal educational settings
• Explore expansion of content to cover more advanced chemistry topics
• Investigate long-term impact on student performance and interest in chemistry

CONCLUSIONS

- Successfully developed an interactive chemistry game accessible on mobile devices and computers
- Game effectively reinforces basic chemical concepts (acids, salts, bases, oxides) through engaging gameplay
- Interactive format enhances memorization and student engagement in chemistry learning
- Positive user feedback indicates the game's potential as a valuable complementary tool in chemistry education
- Project demonstrates the feasibility of transforming mobile devices into productive learning tools
- Further enhancements and testing can increase the game's effectiveness and broaden its educational impact

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II SOUTHERN SCIENCE CONFERENCE
2024 - VIRTUAL CONFERENCE AND IN PERSON EDITION

ANALYSIS OF THE RELIABILITY OF TRADITIONAL PHYSICS AND CHEMISTRY TESTS ACCORDING TO PRE-SERVICE SECONDARY SCHOOL TEACHERS

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ABSTRACT

Background: Assessment is a key aspect of science education. Often, the rigidity and difficulty in implementing changes to the types of assessment tools used in science departments at secondary schools pose an obstacle to updating the teaching teaching methods. **Aims:** To demonstrate the low reliability of traditional science tests widely used in high schools. **Methods:** The study involves 70 pre-service Physics and Chemistry teachers from the University of Valencia. Two tools were used: a 9th-grade test with typical errors and a questionnaire to analyze error correction and perception. **Results:** Pre-service teachers identified procedural, calculation, and unit conversion errors as the most common student mistakes. The average score was 4.95. **Discussion:** Pre-service teachers ranked errors by importance; conceptual mistakes rated highest (35.38%). Future teachers would apply penalties between 20% and 100% of the question's value, averaging 64%. **Conclusions:** Different decisions were made regarding error weight and repetition during grading for the same test, suggesting the need for alternative assessment tools.

Keywords: Evaluation, Physics and Chemistry, Tests, Typical errors

1. INTRODUCTION

In Physics and Chemistry Education, traditional exams are commonly used to evaluate student learning at the end of instructional sequences. However, these assessments primarily certify knowledge rather than enhance learning, as they do not directly impact the learning process (Brandsfor et al., 2000). The way evaluation is conducted influences students' study methods (Crooks, 1988), often leading them to prepare for exams instead of genuinely learning the subject. While summative assessments aim to measure learning outcomes, they often rely on retention-based tests, lacking transfer assessments that yield better results (Arancibia-Herrera et. al., 2019). In the area of science education, there is a conception that it is easier to evaluate student learning with greater objectivity and precision due to the nature of the knowledge to be evaluated (Alonso et. al., 1992). In some way, the elitist vision of science learning continues to persist, assuming that a percentage of students will not be able to achieve the planned objectives and therefore the method or evaluation instruments have no influence on these results (Gil et al., 1991). But there is evidence about using formative assessment in science education leads to higher efficacy in developing students' inquiry skills, especially in lower performing students (Ganajová, 2021).

This study aims to demonstrate the reliability of traditional exams used in Secondary Physics and Chemistry. We assume the definition from Hector Ruiz (2020) explaining that a reliable instrument is one that provides a replicable and consistent qualification. We analyze their consistency to highlight the need for alternative assessment tools. The science learning process itself, which serves as a provisional indicator intended to promote student self-regulation (Sanmartí, 2010) and therefore cannot be based just on terminal assessments but must be incorporated into the entire process in order to know where and why errors occur and how to correct them (Sanmartí, 2020). Confusion between formative and summative purposes can lead to assessment not fulfilling a truly formative

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role in learning (Taras, 2008). Assessment evidences must be useful for making decisions about the next steps to continue with the learning process (William, 2011), but this does not happen when it only serves to grade.

2. MATERIALS AND METHODS

2.1. Materials

The study developed two instruments: (1) a Physics and Chemistry test for third year of compulsory secondary education (9th grade) featuring common errors, and (2) an online questionnaire for gathering correction data and error importance perceptions. The test consists of 8 standard questions taken from exams used on 5 different secondary schools on courses 21-11 and 22-23 designed by active teachers, including 2 theoretical and 6 practical questions, with a focus on typical mistakes made by students. The mistakes were selected from the most commun ones taking into account the descripcion of 3 expert teachers. The ad hoc questionnaire includes 13 items across 4 sections: participant demographics, numerical grading of the test, perceived importance of errors, and weighting of specific common errors.

2.2. Methods

In the "Learning and Teaching in Physics and Chemistry" module of the Secondary Master's program at UV, an activity is conducted during the third session. Prior to this, pre-service teachers learned about evaluation types, LOMLOE (Spanish education law) changes in assessment, and various evaluation tools for Physics and Chemistry. Students are then tasked with individually correcting the provided exam (described earlier) within approximately 30 to 45 minutes. The average time for this correction was 40 minutes. After completing the correction, they are required to respond to the previously mentioned questionnaire to gather insights on their evaluation perceptions and practices.

2.2.1. Test characteristics

As we can see on Table.1 each question of the test included a typical Student mistake on the answer.

3. RESULTS AND DISCUSSION:

3.1. Results

Grading of the Test

Participants first had to decide how to quantify each of the 8 exam questions. A notable 93% assigned equal value to all questions, while only 4 varied their scores: 3 assigned a higher value to P1 (theoretical), and 1 did the same for P4 (Uniformly Accelerated Motion - UAM). Among the 70 corrections, one was discarded for being unreliable due to high scores across all questions. The remaining 69 yielded an average score of 4.95 out of 10, with a maximum of 8 and a minimum of 3. The Distribution is shown in Figure 1.

Common Student Errors

Pre-service Physics and Chemistry teachers identified the most frequent errors made by secondary students as procedural and calculation mistakes, followed by unit conversion errors. Conceptual errors and misunderstandings of questions were also noted.

3.2. Discussions

The pre-service teachers identified the most common errors made by secondary students in Physics and Chemistry exams as follows: procedural or calculation errors were noted by 27.50% of participants, while errors in unit conversions were recognized by 26.90%. Conceptual errors were mentioned by 15.09%, errors in understanding the question by 10.24%, and errors in formula application by 10.24% as well. Lastly, 9.70% identified errors related to explanations.

4. CONCLUSIONS:

The study reveals low reliability in the evaluation instrument used, as participants showed inconsistent grading. This highlights the need for alternative assessment methods in secondary Physics and Chemistry. On the teachers trainning propuse, if we give them the evidence of the need to use other kind of evaluatioon intruments we can improve their learning competences and push them to introoduce formative assessment classroom techniques that has shown statistically significant increase in students' scores in chemistry

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(Babinčáková, 2020). Future research could benefit from applying this approach to active teachers.

5. DECLARATIONS

5.1. Study Limitations

The study could be expanded with other examples of Physics and Chemistry exams.

5.5. Open Access

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Table 2. *Test created with typical mistakes*

Type of question	**Error in the answer**
P1- Theoretical question about the stages of the Scientific Method	Missing information. The answer presents correct but incomplete information.
P2- Calculation question related to gas laws	Error in the change of units
P3- Calculation question about abundance of isotopes	Error in the justification of the answer. It is not explained.
P4- Calculation question related to a MRUA movement	Calculation error
P5- Calculation question about electrical charge of atoms	The procedure followed to obtain the answer is not shown.
P6- Complete a table about particles that form chemical elements	Confusion between two columns of the table
P7- Calculation question about MRU	Incomplete answer
P8- Chemical nomenclature	Confuses nomenclatures with correct answer

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Southern Science Conference, 2024.

ANALYSIS OF THE RELIABILITY OF TRADITIONAL PHYSICS AND CHEMISTRY TESTS ACCORDING TO PRE-SERVICE SECONDARY SCHOOL TEACHERS

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September/2024

ABSTRACT

Background: Assessment is a key aspect of science education. Often, the rigidity and difficulty in implementing changes to the types of assessment tools used in science departments at secondary schools pose an obstacle to updating the teaching teaching methods. **Aims:** To demonstrate the low reliability of traditional science tests widely used in high schools. **Methods:** The study involves 70 pre-service Physics and Chemistry teachers from the University of Valencia. Two tools were used: a 9th-grade test with typical errors and a questionnaire to analyze error correction and perception. **Results:** Pre-service teachers identified procedural, calculation, and unit conversion errors as the most common student mistakes. The average score was 4.95. **Discussion:** Pre-service teachers ranked errors by importance; conceptual mistakes rated highest (35.38%). Future teachers would apply penalties between 20% and 100% of the question's value, averaging 64%. **Conclusions:** Different decisions were made regarding error weight and repetition during grading for the same test, suggesting the need for alternative assessment tools

Keywords: ***Evaluation, Physics and Chemistry, Tests, Typical errors***

INTRODUCTION

•Assessment is a key aspect of science education and is especially important in the teaching and learning processes that take place in secondary school classrooms. The rigidity and difficulty in applying changes in the types of assessment instruments is an obstacle to updating the teaching methods that are intended to be put into practice. The LOMLOE has had an impact on assessment and has therefore generated controversy in the educational world.

- The way in which assessment processes are applied has an influence on the students' learning process because it conditions the way they organize their studies (Crooks, 1988) among other effects.

BACKGROUND

- Summative assessments based on final exams are the most widespread in secondary school classrooms and aim to analyse student performance by monitoring the proposed objectives and the time spent as an intended guarantee of objectivity and rigorous obtaining of evidence (Arancibia-Herrera et. al., 2019) but they do not usually include transfer tests, with a more competency-based approach that are the ones that offer the best results according to research (Brandsfor et al., 2000).

AIM/OBJETIVE/PURPOSE

Based on the concept that a reliable instrument is one that provides a replicable and consistent qualification (Ruiz, 2020), the aim is to analyze the consistency and replicability of these tests to demonstrate the need to incorporate other instruments in the evaluation processes in the subjects of Physics and Chemistry.

METHODOLOGY

The research is framed in a positivist paradigm with an exploratory design with representative sampling and with the function of collecting and interpreting data by the researcher.

Sample: A total of 70 secondary school teachers in training (36 girls and 34 boys) who are studying the Physics and Chemistry specialty of the Secondary Education Master's Degree at the University of Valencia participated. Of the total number of participants, 57.14% come from the Chemistry degree or bachelor's degree, 18.57% from Physics, 17.14% from Chemical Engineering and the remaining 7.14% come from Biotechnology, Biochemistry or Pharmacy.

Instruments: Two different instruments are designed for the study: (1) Physics and Chemistry test solved at 3rd ESO level with common errors and (2) Ad hoc form for collecting information on the correction of the test and perceptions on the importance of errors.

Procedure: Within the Evaluation block of the Teaching and Learning subject, after an introductory session on evaluation, students are asked to correct the same test (1) and, after said correction, they are asked to answer the form (2).The results obtained are analyzed in a subsequent session.

RESULTS AND DISCUSSION

Type of question	Error in the answer
P1- Theoretical question about the stages of the Scientific Method	Missing information. The answer presents correct but incomplete information.
P2- Calculation question related to gas laws	Error in the change of units
P3- Calculation question about abundance of isotopes	Error in the justification of the answer. It is not explained.
P4- Calculation question related to a MRUA movement	Calculation error
P5- Calculation question about electrical charge of atoms	The procedure followed to obtain the answer is not shown.
P6- Complete a table about particles that form chemical elements	Confusion between two columns of the table
P7- Calculation question about MRU	Incomplete answer
P8- Chemical nomenclature	Confuses nomenclatures with correct answer

Table.1 Test created with typical mistakes on the answer

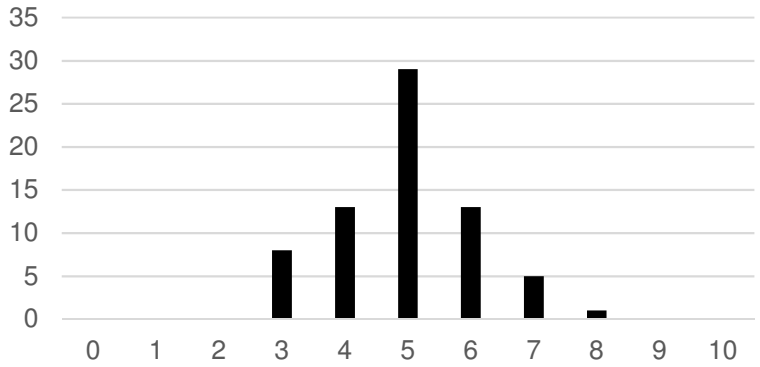


Figure 1. Distribution of the grades obtained in the 69 corrections made of the same test.

% of teachers in training who consider the error to be the most common	
Procedural or calculation errors (E1)	27.50%
Error in changing units (E2)	26.90%
Conceptual errors (E3)	15.09%
Error in understanding the statement (E4)	10.24%
Error in applying formulas (E5)	10.24%
Error in explanation (E6)	9.70%

Table.2 % of teachers in training who consider the error to be the most common

Level of importance of errors: When teachers in training are asked what type of error they consider most important, their answers show the following order (from most important to least important):

E3 (*35.38%*) > *E4* (*24.62%*) > *E2* (*16.92%*) > *E1* (*15.38%*) > *E5* (*4.62%*) > *E6* (*1.54%*)

CONCLUSIONS

- The low reliability of the instrument designed for the research has been confirmed due to the lack of consistency in the grades assigned by the participants. Being an instrument commonly used in secondary schools for the Physics and Chemistry subject of 3rd ESO, this lack of reliability shown to future teachers may be a facilitating element for the introduction of other assessment instruments in their teaching plans.

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ANTIBACTERIAL ACTIVITY OF CLOVE ESSENTIAL OIL (*SYZYGIUM AROMATICUM*) AGAINST STRAINS OF *ESCHERICHIA COLI*, *PSEUDOMONAS AERUGINOSA*, AND *SALMONELLA* SSP

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ABSTRACT

Introduction: Clove (*Syzygium aromaticum*), a member of the Myrtaceae family, is cultivated in various regions of Asia, Africa, and the West. Its primary compound, eugenol, imparts a distinctive aroma and flavor while exhibiting bactericidal properties. **Objective:** This study evaluated the antibacterial activity of clove essential oil against *Escherichia coli*, *Pseudomonas aeruginosa*, and *Salmonella spp.*, isolated from food and water. **Methods:** The essential oil was extracted from dried flower buds using hydrodistillation with a Clevenger apparatus. The antimicrobial activity of the oil and the susceptibility of the strains to commercial antibiotics were assessed using the disk diffusion method. **Results and Discussion:** The essential oil from *Syzygium aromaticum* demonstrated high antibacterial activity against two of the three tested strains (*Escherichia coli* and *Salmonella spp.*) while exhibiting moderate efficacy against *Pseudomonas aeruginosa*. **Conclusions:** The microbiological study revealed that clove essential oil possesses significant antibacterial activity against the tested strains, with eugenol being the primary contributor to this effectiveness.

Keywords: *Essential Oil. Syzygium Aromaticum. Clove. Eugenol. Antibacterial Activity*

1. INTRODUCTION

The Clove (*Syzygium aromaticum*), part of the *Myrtaceae* family, is cultivated in various regions of Asia, Africa, and South America (Ferrão, 1993). The dried flower buds, known as cloves, are highly valued in cooking for their intense aroma and distinctive flavor, primarily due to eugenol, a phenolic compound that accounts for up to 95% of the oil extracted from the leaves (Gomes *et al*., 2018; Raina *et al*., 2001). Eugenol is also widely used in dentistry, serving as a key component in sealants and oral antiseptics, demonstrating significant bactericidal activity (Chong *et al*., 1997; Kaplan *et al*., 1999; Shapiro *et al*., 1994). The growing demand for essential oils from cloves has driven research into their extraction and commercial applications (Clifford *et al*., 1999; Rovio *et al*., 1999).

Additionally, eugenol is a precursor in the synthesis of other phenolic compounds and is investigated in toxicological studies (Priefert *et al*., 2001). Therefore, this study aims to evaluate the antibacterial activity of the essential oil extracted from the dried flower buds of Clove (*Syzygium aromaticum*) against strains of Escherichia coli, Pseudomonas aeruginosa, and Salmonella spp.

2. MATERIALS AND METHODS

This study was conducted at the Laboratory of Analytical Chemistry Research (LPQA) of the Analytical Center, as well as at the Physical Chemistry and Microbiology Laboratory of the Technological Pavilion at the Federal

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University of Maranhão (UFMA) and at the Analytical Center of the State University of Campinas (Unicamp-SP).

2.1. Materials

The reagents used in this study were of analytical grade: Müller Hinton Agar (500 g, Himedia), BHI Agar (500 g, Himedia), and eugenol standard (99%, Sigma).

2.2. Methods

2.2.1. Collection of Clove Fruits

The clove fruits used in this research were sourced from the informal market associated with the Reviver project in São Luís. The selected material was placed in sealed plastic bags and stored in a dry, ventilated area. The dried flower buds were ground using a mill, and the resulting material was stored in a polyethylene container for subsequent essential oil extraction.

2.2.2. Extraction, Treatment, and Storage of Essential Oil

For the extraction of essential oil from *Syzygium aromaticum*, a Clevenger extractor was employed, connected to a 1000 mL round-bottom flask and a heating mantle. Approximately 69 grams of dried clove flower buds were combined with 200 mL of distilled water. The heating mantle was activated to maintain a constant temperature of 100°C. After 5 hours, the distillation process was completed, and the essential oil was collected. To dry the oil, anhydrous sodium sulfate was used for percolation. These procedures were performed in triplicate, and the samples were stored in glass containers under refrigeration to minimize potential loss of volatile components (Gomes *et al*., 2019).

2.2.3. Antibacterial Activity Testing

The strains of *Escherichia coli, Salmonella spp.,* and *Pseudomonas aeruginosa* utilized in this study were obtained from food samples provided by the Microbiology Laboratory of the Food and Water Quality Control Program (PCQA) at the Federal University of Maranhão. The antibacterial activity of the essential oil and eugenol standard was assessed using the disk diffusion method as recommended by the Clinical and Laboratory Standards Institute (2005(Novacosk and Torres, 2006)). Bacterial cultures were inoculated into BHI broth (Brain and Heart Infusion) and incubated at 37°C for 24 hours. Subsequently, dilutions were made to obtain a standardized suspension corresponding to a 0.5 McFarland standard (10^8 microorganisms/mL). A 0.1 mL inoculum from each bacterial culture was swabbed onto the surface of Mueller Hinton Agar plates. Small filter paper discs (6 mm in diameter), each impregnated with 75 µL of the essential oil and the eugenol standard, were gently pressed onto the agar surface. The plates were then incubated at 37°C for 24 hours, and the inhibition zones were measured using a calibrated ruler certified by INMETRO (National Institute of Metrology, Quality and Technology).

3. RESULTS AND DISCUSSION:

The antibacterial activity of clove essential oil *Syzygium aromaticum* was analyzed using the disk diffusion method, involving strains of *Escherichia coli, Salmonella spp*., and *Pseudomonas aeruginosa*, as illustrated in Table 1. The strains of *Escherichia coli* and *Salmonella*, isolated from food, showed sensitivity to the essential oil, with inhibition halos of 16 mm and 18 mm, respectively. In contrast, the *Pseudomonas aeruginosa* strains, isolated from water, did not respond to the essential oil.

The positive results of both clove oil and the standard eugenol align with previous studies. (Novacosk and Torres, 2006) identified that among five essential oils extracted from medicinal plants, those exhibiting the highest antimicrobial activity were rich in alcohols, phenols, and aldehydes. Additionally, (Asolini *et al*., 2006) reported antimicrobial activity in all phenolic compounds extracted from ten plants used in teas. According to (Alzoreky and Nakahara, 2003)) inhibition halos smaller than 12 mm are not indicative of antibacterial activity. However, for essential oils containing eugenol as the main component, their efficacy as antibacterial agents is recognized when the inhibition halo reaches between 8 mm and 10 mm, as demonstrated by (Cimanga *et al*., 2002; Farago *et al*., 2004; Moreira *et al*., 2005).

It is important to consider that the diffusion rate of substances in agar can influence the zone of inhibition of bacterial growth. The essential oil, due to its viscosity and low polarity, may have its diffusion impeded. Therefore, any halo obtained, even if small, suggests the presence of antibacterial activity in the oil, as indicated by (Fonseca *et al*., 2006; Glisic *et al*., 2007).

The results concerning the antibacterial activity of clove essential oil and the standard eugenol against the strains of *E. coli* and the strain isolated from lettuce revealed inhibition halos

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considered sensitive. (Matan *et al*., 2006) highlight that the active compounds present in oils rich in eugenol and other aldehydes can interfere with the synthesis of bacterial enzymes and damage the structure of bacterial cell walls. Essential oils containing eugenol, such as cinnamon oil, also demonstrated comparable inhibitory potential against *E. coli* strains. Although specific photochemical analysis of the studied oils was not conducted, the presence of active compounds and eugenol as the principal component likely contributed to the significant antibacterial activity observed (Scherer *et al*., 2009; Silvestri *et al*., 2010).

Clove essential oil and its principal component, eugenol, demonstrated antimicrobial activity against the gram-negative strains *Salmonella spp*. and *Salmonella* isolated from sururu (*Mytella guyanensis*). The inhibition halos measured were 15 mm for both the oil and eugenol. Notably, when tested against Salmonella isolated from food (sururu), an even greater inhibition was observed, with a value of 18 mm.

According to Cimanga *et al*. (2002), essential oils that yield inhibition halos below 10 mm are considered inactive, while those between 10 mm and 15 mm are classified as active. In the case of the essential oil from the dried flower buds of *Syzygium aromaticum*, excellent antibacterial activity was observed for two of the three tested strains (*Escherichia coli and Salmonella spp*.), with inhibition halos equal to or exceeding 15 mm. For the *Pseudomonas aeruginosa* strains, the oil showed a halo of 12 mm, classified as moderately active.

The mechanism by which essential oils combat bacteria is not yet fully understood. Studies suggest that their action begins at the cell membrane due to the lipophilic and volatile properties of these oils (Stammati *et al*., 1999). (Burt, 2004) emphasizes that the synergistic interaction of the oil's components is what makes it effective as an antibacterial agent. This synergy justifies the activity of the essential oil against the tested bacteria, and the efficiency gain is attributed to the other components of the oil.

4. CONCLUSIONS

The essential oil of *Syzygium aromaticum* (clove) demonstrated significant antibacterial activity against two of the three tested strains, specifically *Escherichia coli* and *Salmonella spp*. At the same time, it showed moderate activity against *Pseudomonas aeruginosa*. These results suggest that clove may serve as a natural and cost-effective alternative for food preservation, as well as being effective in combating certain diseases.

5. DECLARATIONS

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Table 1. *Sensitivity of Escherichia coli, Salmonella spp., and Pseudomonas aeruginosa strains to the essential oil of Syzygium aromaticum and the standard eugenol, using the disk diffusion method. Source: the author.*

Components	***E.coli (mm)***		***Salmonella spp* (mm)**		***Pseudomonas aeruginosa (mm)***	
	Standard	**Lettuce**	**Standard**	***Mytella guyanensis***	**Standard**	**Water**
Essential oil	16	16	15	18	12	-
Eugenol	19	16	15	18	12	12

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ANTIBACTERIAL ACTIVITY OF CLOVE ESSENTIAL OIL (SYZYGIUM AROMATICUM) AGAINST STRAINS OF ESCHERICHIA COLI, PSEUDOMONAS AERUGINOSA, AND SALMONELLA SSP

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November/2024

INTRODUCTION



Clove (*Syzygium aromaticum*)

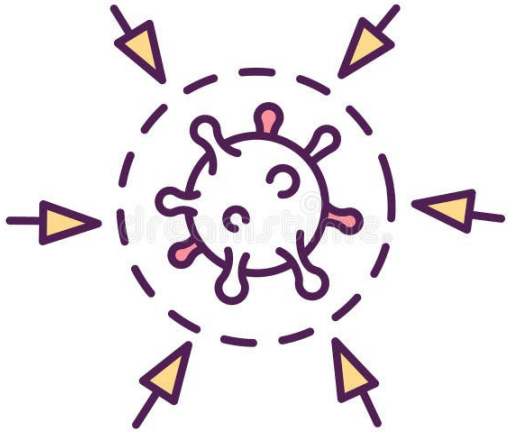
Clove is a medicinal plant that has been used for centuries in various cultures for medicinal and culinary purposes.



BACKGROUND



Clove essential oil has been studied for its antibacterial and antifungal activity. Recent studies have shown that clove essential oil is effective against pathogenic bacteria, including *Escherichia coli, Pseudomonas aeruginosa* and *Salmonella* ssp.



OBJETIVE



To evaluate the antibacterial properties of clove essential oil and its potential applications in food and personal care products.

METHODOLOGY



The study was carried out using the disk diffusion method to evaluate the antibacterial activity of clove essential oil. The bacteria used were *Escherichia coli, Pseudomonas aeruginosa* and *Salmonella* ssp.

Details of the methodology

Essential oil extraction

Chemical composition analysis

Preparation of bacteriaDisk

diffusion test

RESULTS AND DISCUSSION



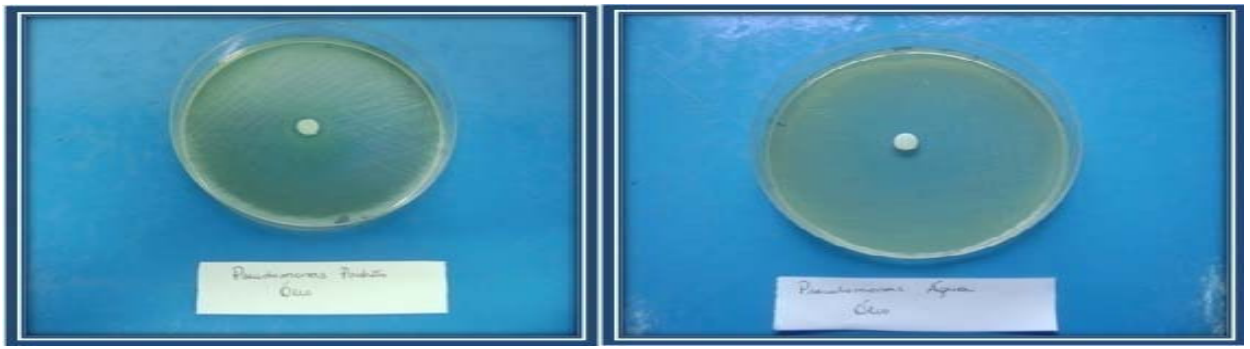
Sensitivity of Escherichia coli, Salmonella spp and Pseudomonas aeruginosa strains to the essential oil of Syzygium aromaticum and the eugenol standard, using the disk diffusion method.

Componentes	*E.coli (mm)*		*Salmonella spp* (mm)		*Pseudomonas aeruginosa (mm)*	
	Padrão	Alface	Padrão	Sururu (*Mytella guyanensis*)	Padrão	Água
Óleo Essencial	16	16	15	18	12	-
Eugenol	19	16	15	18	12	12

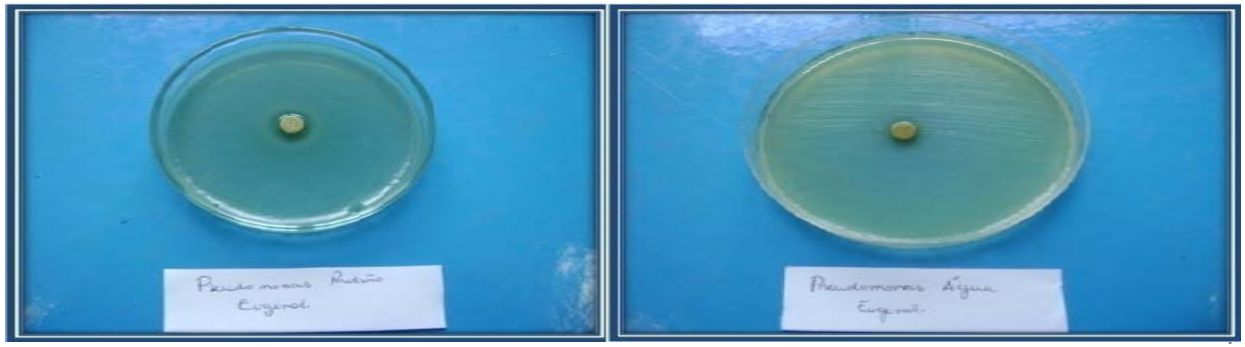
RESULTS AND DISCUSSION



Comparison of the antibacterial activity of the essential oil against standard *Pseudomonas aeruginosa* and *Pseudomonas aeruginosa* strains isolated from water



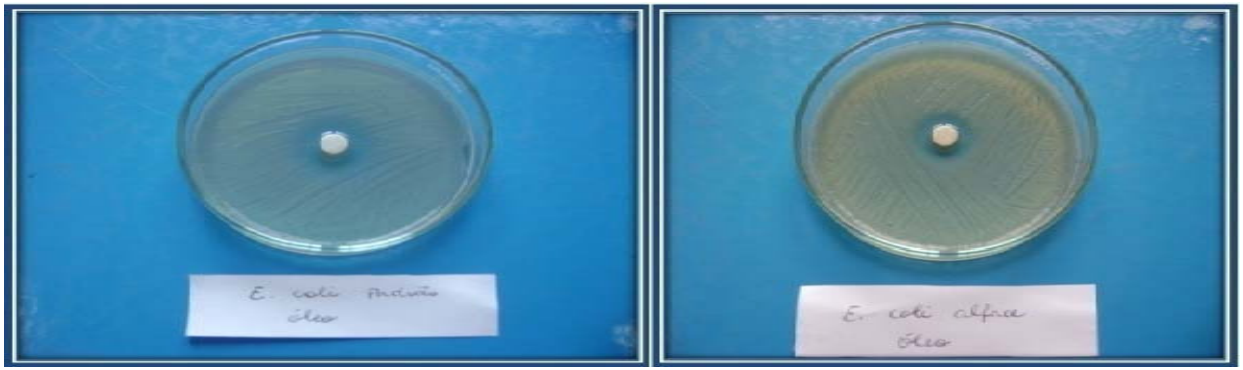
Comparison of the antibacterial activity of eugenol against standard *Pseudomonas aeruginosa* and *pseudomonas aeruginosa* strains isolated from water.



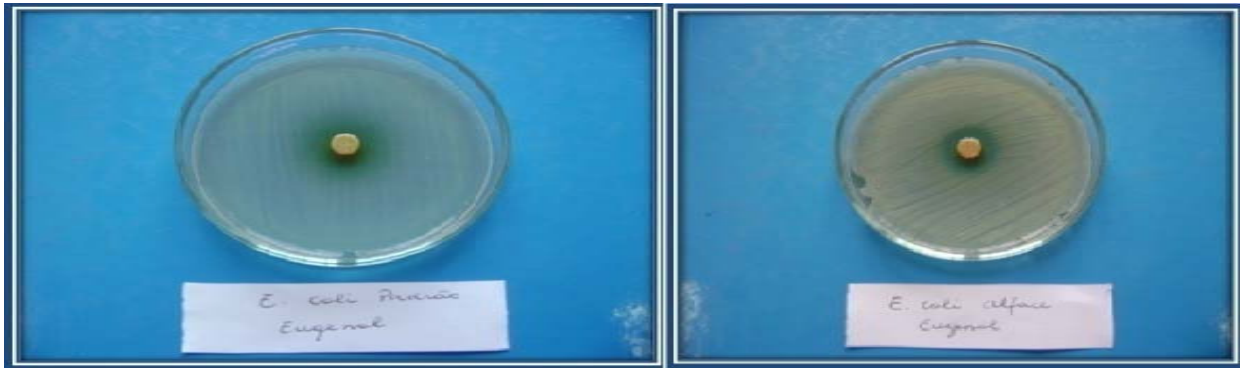
RESULTS AND DISCUSSION



Comparison of the antibacterial activity of the essential oil against standard *E.coli* strains and *E.coli* isolated from water.



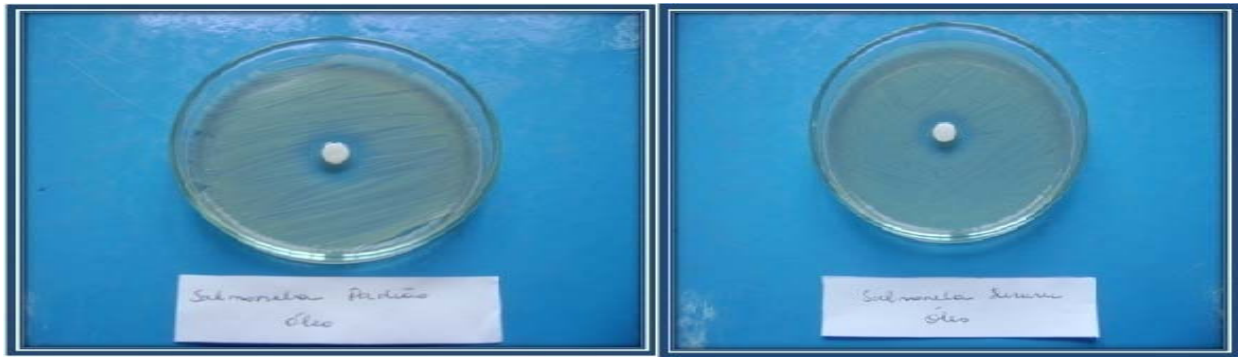
Comparison of the antibacterial activity of eugenol against standard *E.coli* strains and *E.coli* isolated from water



RESULTS AND DISCUSSION



Comparison of the antibacterial activity of the oil against standard *Salmonella* ssp and *Samonella* strains isolated from sururu (*Mytella guyanensis*)



Comparison of the antibacterial activity of eugenol against standard *Salmonella* ssp and *Samonella* strains isolated from sururu (*Mytella guyanensis*)



CONCLUSIONS



Clove essential oil is a natural and low-cost alternative for preserving food and combating illnesses. The results of the study demonstrated that Clove essential oil has significant antibacterial activity against the bacteria tested.

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ASSESSING THE AWARENESS OF MARATHON AND ULTRAMARATHON ATHLETES ABOUT THEIR DENTAL HEALTH BASED ON THE SPECIALISED QUESTIONNAIRE

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ABSTRACT

The marathon, originating from the Greek Μαραθώνιος, is a long-distance foot race covering 42.195 km, typically run on roads but also possible on trails. This study aimed to assess the level of awareness of marathon athletes about their own dental health. A survey was administered to 40 amateur athletes who engage in long-distance running and participate in marathons. These athletes had varying fitness levels and had been involved in distance running for over a year. Results indicated that the greatest influence on the oral hygiene of athletes was exerted by the amount of running performed per month. Increasing monthly running volume may have a negative impact on the oral hygiene scores of marathon athletes. Anthropometric data, as well as oral hygiene products and methods, were also considered. The study concludes that the influence of running volume per month on oral hygiene may be indirect for several reasons, suggesting a complex relationship between endurance running and dental health. This research highlights the need for further investigation into the specific mechanisms by which intensive physical activity might affect oral health in endurance athletes.

Keywords: *cyclic sport, marathon athletes, dental health of athletes, level of home hygiene***.**

1. INTRODUCTION

The marathon (from Greek Μαραθώνιος) is a long-distance foot race with a distance of 42.195 km (c. 26 mi 385 yd), usually run as a road race, but the distance can be covered on trail routes. The marathon can be completed by running or with a run/walk strategy. Carbohydrates that a person eats are converted by the liver and muscles into glycogen for storage. Glycogen burns rapidly to provide quick energy. Runners can store about 8 MJ or 2,000 kcal worth of glycogen in their bodies, enough for about 30 km/18–20 miles of running (Ramagoni et al., 2014).

To assess the level of awareness of marathon and ultramarathon athletes about their own dental health to identify factors in their sports activities that most influence the level of oral hygiene.

2. MATERIALS AND METHODS

2.1. Materials

The survey was administered to 40 amateur athletes who engage in long-distance running and participate in marathons. The athletes had different levels of fitness and had been engaged in distance running for more than a year (Marks et al., 2015)..

2.2. Methods

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A computer program was used: “Program for assessing the dental status of marathon and ultramarathon athletes.” This program includes a number of questions about one’s own awareness of oral health, cariogenic factors and the need for dental treatment, sports achievements, and the nature of nutrition during the preparatory and competitive period.

2.2.1. Ethical Considerations

Permission from the Local Ethics Committee at the Sechenov First Moscow State Medical University of the Ministry of Health of the Russian Federation (Sechenov University) No. 23-22 dated 11/17/2022. All the surveyed track and field athletes were provided with signed, informed voluntary consent.

3. RESULTS AND DISCUSSION:

3.1. Results

It was found that the greatest influence on the level of oral hygiene of athletes was exerted by the amount of running performed per month. With monthly running volume values ranging from 251 km to 300 km, the hygiene level indicator was low at 42.9% in the study group of respondents. With values of this indicator from 351 km to 400 km, the hygiene level was low in 100% of cases (Maruyama et al., 2023).

3.2. Discussions

Increasing monthly running volume may have a negative impact on the oral hygiene scores of marathon athletes. Anthropometric data, as well as oral hygiene products and methods used by respondents at home, did not have a statistically significant impact on the hygiene level indicator.

4. CONCLUSIONS:

The more athletes train, the less time they have for proper home care. The more they exercise, the more they consume carbohydrate foods to replenish energy losses. The more they train, the greater the level of overtraining they may experience.

5. DECLARATIONS

5.1. Study Limitations

It was concluded that there are many factors in the successful completion of the marathon.

5.2. Acknowledgements

Sports medicine and the physiology of cyclic sports are areas for detailed study.

5.3. Funding source

It is necessary to study the health of athletes to create preventive measures..

5.4. Competing Interests

The authors declare no competing interests.

5.5. Open Access

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6. HUMAN AND ANIMAL-RELATED STUDIES

6.1. Ethical Approval

The Local Ethics Committee at the Sechenov First Moscow State Medical University No. 23-22 dated 11/17/2022.

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6.2. Informed Consent

All the surveyed track and field athletes were provided with signed, informed, voluntary consent to conduct research.

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ASSESING THE AWARENESS OF MARATHON AND ULTRAMARATHON ATHLETS ABOUT THEIR DENTAL HEALTH BASED ON THE SPECIALIZED QUESTIONNAIRE

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November/2024

INTRODUCTION

The development of aerobic capabilities at long and ultra-long distances requires significant physiological resources from the human body.

Increased physical activity, as well as emotional stress associated with competition, are an integral part of contests such as marathons and ultramarathons.

Poor dental health in athletes can negatively impact training, performance and well-being both in everyday life and during the training and competition phases.

In this regard, dental diseases can have a negative impact on the performance of track and field athletes, as has been shown in regional studies in different countries.

BACKGROUND

The marathon (from Greek Μαραθώνιος) is a long-distance foot race with a distance of 42.195 km (c. 26 mi 385 yd),[1] usually run as a road race, but the distance can be covered on trail routes. The marathon can be completed by running or with a run/walk strategy.

OBJETIVE

- To assess the level of awareness of marathon and ultramarathon athletes about their own dental health based on a questionnaire
- To identify factors in their sports activities that most influence the level of oral hygiene.

METHODOLOGY

To conduct the study, we received permission from the Local Ethics Committee at the Sechenov First Moscow State Medical University of the Ministry of Health of the Russian Federation (Sechenov University) No. 23-22 dated 11/17/2022.
All the surveyed track and field athletes were provided with signed informed voluntary consent to conduct research.

METHODOLOGY

The survey was administered to 40 amateur athletes who engage in long-distance running and participate in marathons. The athletes had different levels of fitness and had been engaged in distance running for more than a year.

A computer program was used: “Program for assessing the dental status of marathon and ultramarathon athletes.” This program includes a number of questions about one’s own awareness of oral health, cariogenic factors and the need for dental treatment, sports achievements, and the nature of nutrition during the preparatory and competitive period.

RESULTS AND DISCUSSION

It was found that the greatest influence on the level of oral hygiene of athletes was exerted by the amount of running performed per month. With monthly running volume values ranging from 251 km to 300 km, the hygiene level indicator was low at 42.9% in the study group of respondents. With values of this indicator from 351 km to 400 km, the hygiene level was low in 100% of cases.

RESULTS AND DISCUSSION

Index	Categories	Running volume per month								p
		0-50 km	51-100 km	101-150 km	151-200 km	201-250 km	251-300 km	301-350 km	351-400 km	
Level of oral hygiene	Low level	1 (12,5)	0 (0,0)	0 (0,0)	1 (12,5)	3 (100,0)	3 (42,9)	0 (0,0)	2 (100,0)	< 0,001*
	Average level	2 (25,0)	2 (40,0)	5 (83,3)	7 (87,5)	0 (0,0)	4 (57,1)	1 (100,0)	0 (0,0)	
	High level	5 (62,5)	3 (60,0)	1 (16,7)	0 (0,0)	0 (0,0)	0 (0,0)	0 (0,0)	0 (0,0)	

CONCLUSIONS

Increasing monthly running volume may have a negative impact on the oral hygiene scores of marathon athletes. Anthropometric data, as well as oral hygiene products and methods used by respondents at home, did not have a statistically significant impact on the hygiene level indicator.

CONCLUSIONS

Naturally, the influence of this indicator may be indirect for several reasons.

1. The more athletes train, the less time they have for proper home care.
2. The more they exercise, the more they consume carbohydrate foods to replenish energy losses.
3. The more they train, the greater the level of overtraining they may experience, which is accompanied by xerostomia and corresponding changes in the oral cavity.

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PRIVACY-PRESERVING DATA ANONYMIZATION TOOL FOR MEDICAL DATA

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ABSTRACT

Background: Medical institutions collect vast amounts of sensitive patient data for personalized treatments and health trend analysis. However, this raises concerns regarding the privacy of patient data, as it contains sensitive and confidential information. **Aims:** Develop an anonymization tool using diverse techniques to protect data while preserving its utility. **Methods:** A Python-based data anonymization tool for medical datasets supporting both categorical and numerical data is developed. It employs various methods, including data perturbation, binning, scaling, transformation, and differential privacy. **Results:** The tool was able to anonymize the sensitive data, both categorical and numerical, while at the same time preserving its utility for further analysis. **Discussion:** The Privacy-Preserving Data Anonymization Tool advances sensitive medical data management by anonymizing both categorical and numerical data using various techniques while retaining data utility. **Conclusions:** The Anonymization Tool addresses patient data privacy concerns by balancing data utility with privacy, enabling secure medical data use in research.

Keywords: *anonymization, privacy-preservation, medical dataset, data utility, data analytics*.

1. INTRODUCTION

Medical institutions collect sensitive patient information, including personal identification, medical histories, and genetic data, to enable personalized treatments and analyze health trends. However, this raises privacy concerns due to unauthorized access, data breaches, and misuse, which can undermine patient trust, especially amid rising cyberattacks on healthcare facilities. Additionally, ethical issues arise as patients may be unaware of how their data is used. Strong privacy protections and ethical standards are essential to safeguard patient confidentiality and maintain trust.

To create a Privacy-Preserving Anonymization tool for medical datasets, employing various techniques to effectively obscure individual patient identities while protecting sensitive data (Majeed & Lee, 2021; Marques & Bernardino, 2020).

2. MATERIALS AND METHODS

2.1. Materials

The tool was developed on a Windows environment using Python version 3.12.2, chosen for its extensive data processing capabilities. Key libraries include Pandas for data manipulation, NumPy for numerical computations, Scikit-learn for machine learning algorithms, and Faker for generating synthetic data. Jupyter Notebook version 7.1.3 was used to program the tool. For the dataset synthetic data was generated using Faker. The dataset contained 25 attributes and 1500 records.

2.2. Methods

The privacy-preserving anonymization tool utilizes several methods to protect sensitive patient data (Murthy et al., 2019). Data Perturbation adds noise to obscure individual

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identification (Dhawas et al., 2024). Data Binning groups continuous data into categories to reduce granularity. Scaling and transformation adjust value ranges, while Differential Privacy ensures minimal impact from individual data changes, introducing controlled randomness. These techniques collectively safeguard patient privacy while maintaining data utility.

2.2.1. Data Perturbation

Data Perturbation enhances privacy by adding noise or modifying data values, preventing individual identification while maintaining the dataset's statistical properties (Muralidhar & Sarathy, 1999; Kargupta et al., 2003). This approach allows meaningful analysis without compromising the confidentiality of sensitive information.

2.2.2. Data Binning

Data Binning anonymizes sensitive continuous data by grouping it into discrete categories, such as age ranges. This method obscures individual identities while preserving analytical utility, making it crucial for maintaining privacy in sensitive datasets.

2.2.3. Scaling and Transformation

Scaling and transforming anonymized data by adjusting value ranges to obscure original representations while maintaining relationships (Evans, 2005; Sedgwick, 2012). These techniques prevent sensitive information exposure, enabling meaningful analysis and protecting individual privacy in datasets (Ahasn et al., 2021; Sharma, 2022).

2.2.4. Differential Privacy

Differential privacy (Dwork, 2006; Friedman & Schuster, 2010; Geng & Viswanath, 2016) is a powerful data anonymization technique that adds controlled randomness to ensure individual data inclusion or exclusion minimally affects overall analysis, safeguarding personal identities while enabling valuable insights in sensitive contexts.

3. RESULTS AND DISCUSSION:

3.1. Results

The privacy-preserving anonymization tool implemented several methods: Data Perturbation added noise proportional to input values, set to 10%, preserving statistical characteristics for aggregate analysis. Data Binning grouped sensitive attributes into broader ranges, retaining trends while preventing identification. Scaling and transformation applied Min-Max Scaling to normalize data to a specific range, Standardization (adjusting data to a mean of 0, and standard deviation of 1), and Log Transformation to handle outliers and skewness. Differential privacy was used in the Laplace Mechanism to add controlled noise, ensuring strong privacy guarantees while maintaining data utility and statistical integrity. All methods effectively obscured critical details while preserving data usability.

3.2. Discussions

Each anonymization technique has distinct advantages and disadvantages: Data Perturbation: Protects privacy and preserves data utility but can introduce bias and is irreversible. Data Binning: Simplifies data and improves stability but may result in information loss. Scaling and Transformation: Normalizes data for analysis but may reduce interpretability. Differential Privacy: Ensures strong privacy but involves noise addition, complexity, and trade-offs in data accuracy.

4. CONCLUSIONS:

The Privacy-Preserving Data Anonymization Tool successfully addresses patient data privacy concerns by balancing data utility with privacy. Through techniques like data perturbation, binning, scaling, transformation, and differential privacy, the tool anonymizes sensitive medical data while retaining its analytical value, which is crucial for medical research and personalized healthcare applications.

However, some limitations of the study should be acknowledged (Olatunji et al., 2022). The tool's performance was tested on a limited set of medical datasets, and the scalability to larger, more diverse datasets remains to be explored. Additionally, while the tool implements various anonymization techniques, it does not account for the evolving nature of privacy threats, particularly those posed by advanced machine learning and re-identification techniques. Future work should

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focus on expanding the tool's adaptability to a broader range of medical data types, as well as enhancing its robustness against emerging privacy risks.

Future research could explore integrating the anonymization tool with other privacy-enhancing technologies such as homomorphic encryption and federated learning to provide even greater levels of security. Additionally, more extensive testing with real-world medical datasets, including longitudinal data, could provide insights into the tool's effectiveness in long-term privacy protection while maintaining data utility. This would further strengthen the tool's application in diverse healthcare environments, including cross-institutional data sharing for collaborative research.

5. DECLARATIONS

5.1. Study Limitations

Operating System Dependency, Library Version Constraints, and Noise Calibration Challenges.

5.2. Acknowledgements

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5.3. Funding source

This research was funded by the authors.

5.4. Competing Interests

The authors declare no potential conflict of interest in this publication.

5.5. Open Access

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PRIVACY-PRESERVING DATA ANONYMIZATION TOOL FOR MEDICAL DATA

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INTRODUCTION

- Medical institutions collect sensitive patient information, including personal identification, medical histories, and genetic data, to enable personalized treatments and analyze health trends.
- However, this raises privacy concerns due to unauthorized access, data breaches, and misuse, which can undermine patient trust, especially amid rising cyberattacks on healthcare facilities.
- Additionally, ethical issues arise as patients may be unaware of how their data is used. Strong privacy protections and ethical standards are essential to safeguard patient confidentiality and maintain trust.

OBJECTIVE

To create a Privacy-Preserving Anonymization tool for medical datasets, employing various techniques to effectively obscure individual patient identities while protecting sensitive data.

METHODOLOGY

- The privacy-preserving anonymization tool utilizes several methods to protect sensitive patient data.
- Data Perturbation adds noise to obscure individual identification.
- Data Binning groups continuous data into categories to reduce granularity.
- Scaling and Transformation adjust value ranges.
- Differential Privacy ensures minimal impact from individual data changes, introducing controlled randomness.
- These techniques collectively safeguard patient privacy while maintaining data utility.

RESULTS AND DISCUSSION

- The privacy-preserving anonymization tool implemented several methods:
- Data Perturbation added noise proportional to input values, set to 10%, preserving statistical characteristics for aggregate analysis.
- Data Binning grouped sensitive attributes into broader ranges, retaining trends while preventing identification.
- Scaling and Transformation applied: Min-Max Scaling to normalize data to a specific range, Standardization (adjusting data to a mean of 0, and standard deviation of 1), and Log Transformation to handle outliers and skewness.
- Differential Privacy used the Laplace Mechanism to add controlled noise, ensuring strong privacy guarantees while maintaining data utility and statistical integrity.
- All methods effectively obscured critical details while preserving data usability.

CONCLUSIONS

- The study implemented different data anonymization techniques that safeguard individual privacy while preserving the utility of data.
- Different options for anonymizing data were explored in a manner that the data is useful for analysis despite anonymization.
- For this, four different methods of anonymization were implemented – data perturbation, data binning, scaling and transformation and differential privacy.
- Each of these technique is has unique strengths that is applicable to specific contexts and requirements.
- By implementing these techniques strategically, organizations can not only comply with data protection regulation but also foster trust among the stakeholders.
- As data continues to be crucial in driving innovation and decision-making, anonymization strategies ensure that privacy remains of greatest importance without compromising the potential of data-driven insights.

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RECOVERY STUDIES OF MICROBIOLOGICAL SAMPLING METHODS TO SUPPORT CLEANING VALIDATION IN THE PHARMACEUTICAL INDUSTRY

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ABSTRACT

This present work describes recovery studies for direct and indirect sampling methods in combination with microbiological enumeration test methods for bioburden determination on the shared manufacturing equipment surfaces in support of cleaning validation. The swab and rinse sampling methods were developed in order to obtain a suitable recovery (>35 %) for five challenge Gram-negative rod, Gram-positive cocci, yeast, mold and spore former microorganisms and three types of equipment material (plastic, glass, and stainless steel) in this study. The swabbing involved moistening the swab with sterile saline and swabbing the area (100 cm^2) to be sampled in an overlapping zigzag pattern. Rinse sampling was performed using a separate sampling rinse with a fixed volume of water for injection from a piece of equipment. The swab and rinse samples were tested using the plate count and membrane filtration methods, respectively. The recovery rate is higher for the swab sampling method (60.5 %) compared to the rinsing method (46.8 %). The combination of the developed sampling and the microbiological enumeration test methods gives a good recovery (>36.17%) with high precision (RSD<19.25%). The proposed methodology can be used to perform cleaning validation successfully.

Keywords: *Recovery, Sampling, Cleaning Validation, Bioburden*

1. INTRODUCTION

In the pharmaceutical industry, cleaning validation is a critical component of an effective quality assurance system to ensure compliance with the requirements of good manufacturing practice (GMP) and has the largest opportunity to prevent patient risk by assuring that there is no cross-contamination/contamination of drug products with variety substances such as contaminants associated with other active ingredients, cleaning and biocide agents, airborne materials, and microbial bioburden as well (Rubashvili, Karukhnishvili & Makharadze, 2020; Rubashvili, 2022).

This present work is dedicated to the development and validation of sampling methods to demonstrate a suitable methodology in order to perform cleaning validation at an appropriate level in compliance with GMP requirements and confirm that pharmaceutical formulations produced on shared pharmaceutical facilities are free from the risk of microbiological contamination. The paper describes recovery studies for direct and indirect sampling methods in combination with microbiological enumeration test methods for bioburden determination on the shared

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manufacturing equipment surfaces in support of cleaning validation.

2. MATERIALS AND METHODS

Swab and rinse sampling methods available to conduct cleaning validation were used in this study. The swabbing is a direct method and a subjective manual procedure that involves physical interaction between the swab and the equipment surface and varies from sampler to sampler. The surface was successively wiped with one sterile swab (10 cm, small woven, polyester) moistened with the sterile saline solution. The scheme of the swabbing procedure is shown in Figure 1. Rinse sampling is an example of indirect sampling, as any remaining surface residue is not taken directly from the equipment surface. A separate sampling performed it rinse with a fixed volume of water for injection (WFI) from a piece of equipment (Rubashvili *et al.*, 2020).

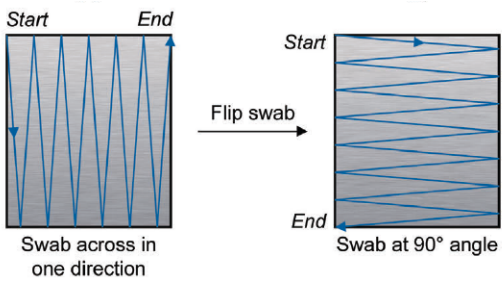


Figure 1. *Swabbing technique*

Properly cleaned and sterilized coupons, which are pieces of three different materials (plastic, glass, and stainless steel) representing equipment to be sampled, were used. A coupon typically 10×10 cm (100 cm^2) was representative of a standard sample size for smaller irregular surfaces and larger flat surfaces. A commercial disinfectant-detergent containing quaternary ammonium salts (0.25 % solution) and sterile 70 % isopropanol is used for cleaning and disinfection of selected coupons.

The study was carried out in a clean environment, such as within a biosafety cabinet (Thermo Scientific). For spiking (inoculation) of challenge microorganisms on test coupons, the working bacterial and fungi cultures were prepared. These cultures included a Gram-negative rod, Gram-positive cocci, yeast, mold, and spore former microorganisms - *Staphylococcus aureus ATCC 6538, Pseudomonas aeruginosa ATCC 9027; Candida albicans ATCC 2091; Escherichia coli ATCC 8739, Bacillus subtilis ATCC 6633*. The bacterial suspensions were adjusted to a value absorption of 0.2 by buffer diluent (0.05 % polysorbate 80 solutions) using a UV-Vis spectrophotometer – Shimadzu UV-1800 at 550 nm. The fungi suspensions were also adjusted to 5.0 McF standard by buffer diluent using a Biosan Den-1 densitometer. Using a standard serial dilution method, the inoculum solution of each challenge microorganism was prepared in the sterile saline from the suspensions. Each type of coupon surface was inoculated (spiked) with 100 µL (100 CFU) of the inoculum's solution using a micropipette so as to spread the solution onto the coupon. After drying the surface, the swab sampling was performed according to the swab procedure. The obtained swab samples in triplicate were tested using the plate-count method. Additionally, blank, swab negative, and positive control samples were prepared in duplicate (n=2). After incubation, the number of CFU per plate was enumerated, and the average number of CFU and the recovery rate % for each test microorganism were calculated.

For rinse sampling, using sterile forceps, aseptically, the surface area of the inoculated coupon (10^3 CFU) was rinsed with approximately 100 mL of the sterile WFI in a sterile beaker and then transferred and diluted to volume with the same diluent to 100 mL in a sterile flask, mixed well. The obtained rinse samples were tested using the membrane filtration method. The blank, positive, and negative control samples were prepared similarly to the swab method recovery study. This procedure was performed in triplicate as well.

The percentage recovery (R_i,%) of the combination of sampling and microbiological enumeration test methods for each challenge microorganism was calculated by Equation 1:

$$R_i, \% = \frac{CFU_1}{CFU_2} \times 100 \qquad \text{(Eq. 1)}$$

CFU1 is the average number of recovered colonies (recovered amount), and CFU_2 is the average number of inoculated colonies (amount added).

The percentage mean recovery (R,%) was calculated by Equation 2:

$$R, \% = \frac{\sum_i^n R_i}{n} \qquad \text{(Eq. 2)}$$

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Where n is the number of test microorganisms.

3. RESULTS AND DISCUSSION:

Recovery studies were conducted using all five bacterial and fungal test cultures on all three types of material coupons. Swab and rinse test samples were prepared in triplicate, as well as positive control, negative control, and blank samples in duplicate. Average recovery rates (R_i, %) for each challenge microorganism and mean recoveries (R, %) for both sampling methods, as the RSD of the enumerated colonies for each test sample were calculated. An acceptance limit (AL) for the mean recovery (R, %) is ≥35 %, and a recommendation limit for the relative standard deviation (RSD) - ≤15 %. The enumerated colonies obtained with test samples on three types of material coupons are given in Table 1. The calculated values of the R, %, the R_i, and the RSD % for each test microorganism are depicted as charts (Figure 1, 2). No growth was observed in the blank and negative control samples, which shows that the environment and materials used are free from microbiological contamination and confirms that the recovery studies were performed under aseptic conditions, and glassware, solvents, swabs, media, and coupons were sterile. Depending on the type of coupon material, the recovery results of the test microorganisms are different. The decreasing tendency was revealed in the following order: plastic, stainless steel, and glass. This tendency is typical for both sampling methods. The lowest recovery was observed for glass, which is a smooth, non-porous, inert material. In dry conditions, the tendency of viable bacteria to die is observed. However, better recovery results were obtained on the stainless steel surface. It is also a non-porous, smooth, inert material, but it shows increased adherence to microorganisms. All the good recoveries were obtained on plastic material, which is a porous inert material; therefore, the adherence ability is increased, and the death of microorganisms is less. The plastic can absorb the bacteria adherent to the surface and improve the recovery result. The results show that the recovery rate depends on the type and nature of test microorganism, which is caused by the viability of the microorganism, compatibility with the material, and different ability of adherence of the surface. The highest recovery was obtained in the case of *E.coli* for both sampling methods. The recovery rate is higher for the swab sampling method compared to the rinsing method. This difference is small; in particular, it is equal to 60.5 % for the swab sampling method and 46.8 % for the rinsing. The mean recovery is much more than the acceptance limit for both sampling methods, which confirms the validity and appropriateness of the combination of sampling and analytical methods. For the swabbing, the RSD of the numbers of enumerated forming colonies from the test samples is below the recommended limit (≤15 %). However, for the rinsing method, this value exceeds this limit in the case of some microorganisms but does not exceed 20 %, which is explained by the fact that the rinsing method, although characterized by high recovery, has less precision due to its performance technique.

4. CONCLUSIONS:

Hence, swab and rinse sampling methods for microbiological contamination testing on surfaces of pharmaceutical equipment were developed in order to obtain a good recovery. The recovery studies were performed using five bacterial and fungal cultures and three different types of surfaces for both types of sampling methods. The highest recovery was obtained in the case of *E.coli* for both sampling methods. The recovery rate is higher for the swab sampling method (60.5 %) compared to the rinsing method (46.8 %). The combination of the developed sampling and the microbiological enumeration test methods gives a good recovery (>36.17%) with high precision (RSD<19.25%). The proposed methodology can be used to successfully perform cleaning validation.

5. DECLARATIONS

5.1. Open Access

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2. Rubashvili, I. *Per. Tchê Quím.,* **2022,** 19(40), 26.

Table 1. *The results of recovery studies for swab and rinse sampling methods*

Sample/ Coupon material	Swab sampling					Rinse sampling				
	Number of CFU					*Number of CFU*				
	S. aureus	***P. aeruginosa***	***C. albicans***	***E. coli***	***B. subtilis***	***S. aureus***	***P. aeruginosa***	***C. albicans***	***E. coli***	***B. subtilis***
Test sample (n=3)/ Plastic	27	35	21	39	32	20	29	16	31	27
Test sample (n=3)/ Glass	18	28	17	34	23	16	19	12	26	17
Test sample (n=3)/ Stainless steel	25	33	19	36	29	17	25	15	28	25
Positive control sample (n=2)	41	52	32	56	47	41	52	32	56	47
Negative control sample (n=2)	No growth	No growth	No growth	No growth	No growth	No growth	No growth	No growth	No growth	No growth
Blank (n=2)	No growth	No growth	No growth	No growth	No growth	No growth	No growth	No growth	No growth	No growth

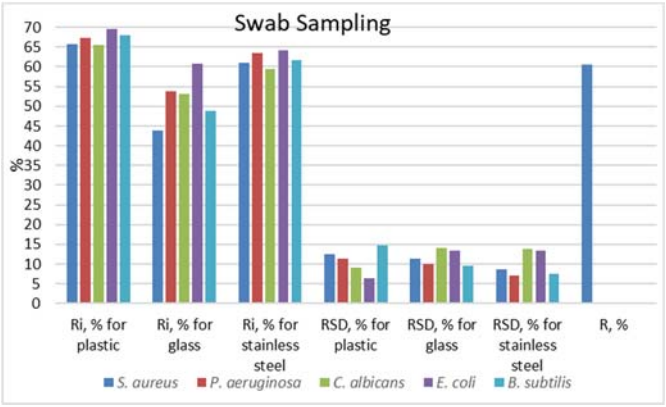


Figure 2. *Chart of calculated values of the mean recovery (R, %), the average recoveries (R_i) and the relative standard deviations (RSD, %) for each test microorganism for the swab sampling method*

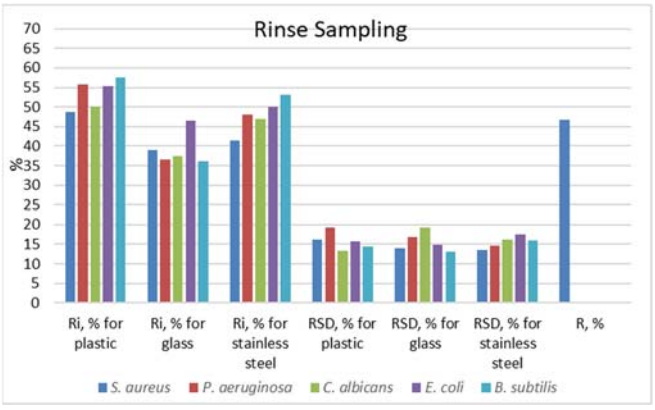


Figure 3. *Chart of calculated values of the mean recovery (R, %), the average recoveries (R_i) and the relative standard deviations (RSD, %) for each test microorganism for the rinse sampling method*

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RECOVERY STUDIES OF MICROBIOLOGICAL SAMPLING METHODS TO SUPPORT CLEANING VALIDATION IN THE PHARMACEUTICAL INDUSTRY

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November/2024

INTRODUCTION

- **Problem Statement:** In the pharmaceutical industry, ensuring the compliance with the GMP requirements of GMP) and the cleanliness of shared manufacturing equipment is essential to prevent contamination of the produced drug products with other active ingredients, cleaning and biocide agents, airborne materials, and microbial bioburden. This contamination risk may pose serious health risks to patients.

- **Reason for the Work:** Cleaning validation plays a crucial role in maintaining drug quality and patient safety. It ensures that no residues from previous manufacturing processes or harmful microorganisms are present in subsequent production batches. Despite the importance of cleaning validation, current guidelines provide insufficient focus on microbiological aspects.

- **Hypotheses/Key Focus:** The focus of this work is to develop a robust cleaning validation process that addresses both chemical and microbiological residues. The focus of the present work is to develop and validate suitable and robust sampling methods in order to perform cleaning validation at an appropriate level in compliance with GMP requirements that effectively assess the cleanliness of equipment, particularly in the context of shared pharmaceutical and confirm that pharmaceutical formulations produced on shared pharmaceutical facilities are free from the risk of microbiological contamination.

- **Essential Background:** Cleaning validation is a GMP requirement and has been established to prevent contamination in pharmaceutical production. Regulatory agencies like the FDA and EMA provide guidelines focused on chemical residues, but there are limited principles on microbiological risks. This research intends to fill this gap by establishing reliable microbiological sampling and validation methods for cleaning procedures.

AIM/OBJETIVE/PURPOSE

Aim:

The aim of this work is to validate direct (swab) and indirect (rinse) sampling methods in combination with microbiological enumeration test methods for bioburden determination on the shared manufacturing equipment surfaces in support of cleaning validation

Objectives:

- Development of swab and rinse sampling techniques including selection of swab and solvent
- Preparation of coupons of different materials
- Preparation of challenge microorganism suspensions, test, negative, blank and positive control samples
- Microbiological enumeration testing of samples
- Calculation of recovery rates

METHODOLOGY

Materials and Equipment:

- Sterile saline solution for moistening swabs
- Sterile 10 cm polyester swabs
- Sterile screw-cap test tubes containing 10 mL of saline solution
- Coupons (10×10 cm, made of plastic, glass, and stainless steel)
- Disinfectant-detergent (0.25% quaternary ammonium salts solution) and 70% isopropanol
- 5 Challenge bacterial and fungal microorganisms:

Staphylococcus aureus ATCC 6538; *Pseudomonas aeruginosa ATCC 9027*; *Candida albicans ATCC 2091*; *Escherichia coli ATCC 8739*; *Bacillus subtilis ATCC 6633*

- UV-Vis spectrophotometer (Shimadzu UV-1800) for bacterial suspension adjustment
- Biosan Den-1 densitometer for fungi suspension adjustment
- Micropipette, vortex mixer, thermostat incubator (Thermo Scientific), and vacuum filtration system for sample processing













METHODOLOGY

Sampling Methods:

Swab Sampling

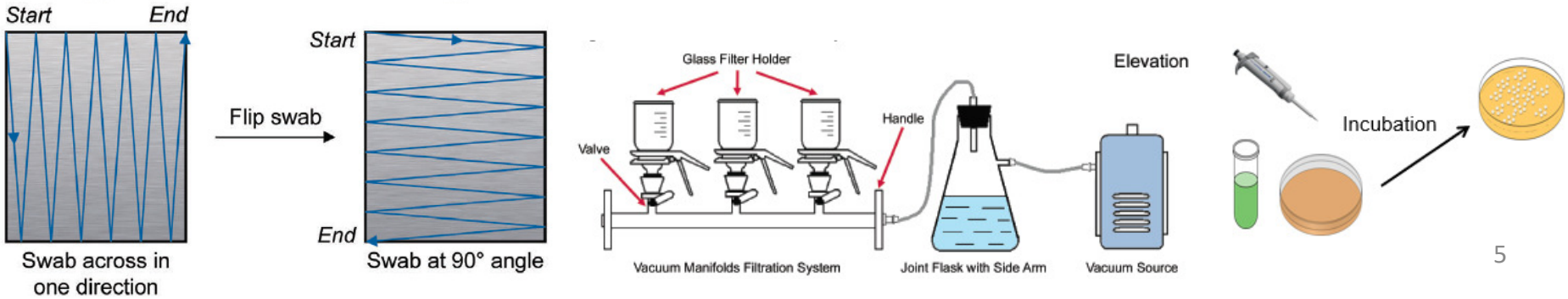
- A sterile swab is moistened with sterile saline and used to sample the surface of a 100 cm^2 coupon
- The swab is passed over the surface in an overlapping zigzag pattern: first vertically (up and down), then horizontally (back and forth) after rotating the swab.
- After sampling, the swab is placed in a sterile screw-cap tube with 10 mL saline solution; The obtained swab sample is vortexed for 1-2 minutes.

Rinse Sampling:

- Rinse sampling is performed with rinsing into a sterile beaker through a fixed volume (100 mL) of water for injection (WFI) from coupon
- Then rinse sample is transferred and diluted to volume with the same diluent to 100 mL in a sterile flask, mixed well.

Microbiological Enumeration Test Methods:

- 100 µL of the swab sample is plated on tryptic soy agar (TSA) for bacteria and sabouraud dextrose agar (SDA) for fungi
- The obtained rinse samples were tested using the membrane filtration method; then filter is plated on tryptic soy agar (TSA) for bacteria and sabouraud dextrose agar (SDA) for fungi
- **Incubation:** Bacterial plates are incubated at 35°C for 3 days; Fungal plates are incubated at 25°C for 5 days.



METHODOLOGY

Sample Preparation for Recovery Studies (1):

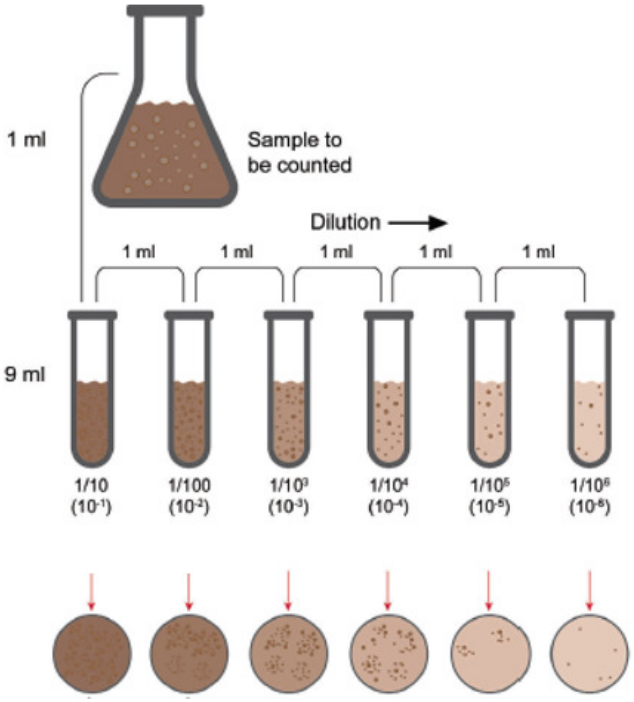
- The bacterial suspensions were adjusted to a value absorption of 0.2 by buffer diluent (0.05 % polysorbate 80 solutions)
- The fungi suspensions were also adjusted to 5.0 McF standard by buffer diluent
- Using a standard serial dilution method, the inoculum solution of each challenge microorganism was prepared in the sterile saline from the suspensions
- **Control Samples**:

➢ **Test samples (n=3)**: Each type of coupon surface is inoculated (spiked) with 100 µL (10^2 CFU for swabbing) and 1 mL (10^3 CFU for rinsing) of the inoculum's solution using a micropipette so as to spread the solution onto the coupon. After drying the surface, the sampling is performed; swab and rinse samples for three plastic, glass and stainless steel coupons

➢ **Negative control sample (n=2)**: A sterile swab placed in 10 mL saline

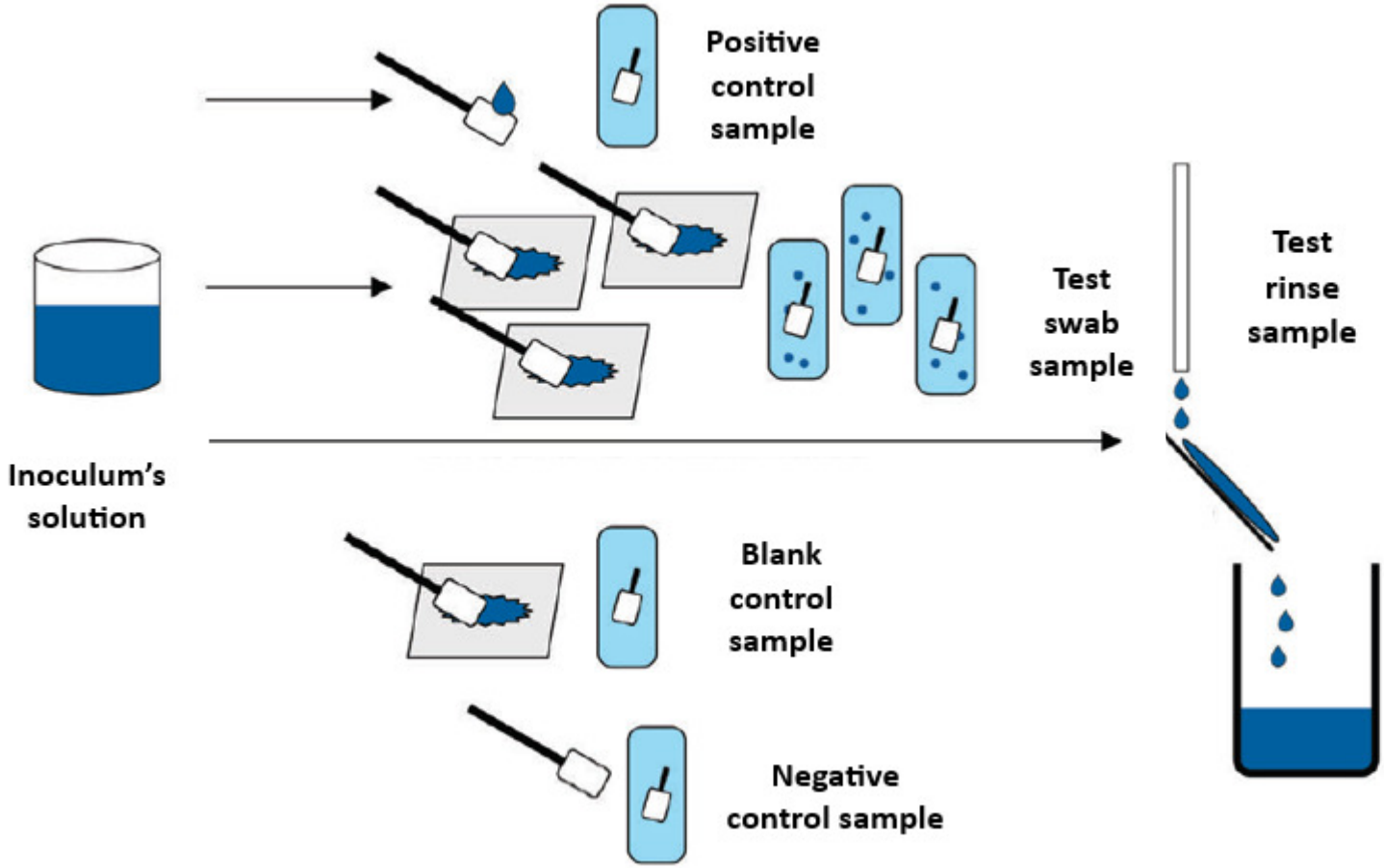
➢ **Positive control sample (n=2)**: A sterile swab inoculated with 100 CFU of each microorganism before being placed in 10 mL saline.

➢ **Blank control sample (n=2)**: Untreated coupon swabbed with a sterile swab moistened with saline.



METHODOLOGY

Sample Preparation for Recovery Studies (2):



METHODOLOGY

Calculation of Recovery:

- The percentage recovery ($\mathbf{R_{i,}\%}$) of the combination of sampling and microbiological enumeration test methods for each challenge microorganism was calculated by Equation:

$$\boldsymbol{R_i}, \% = \frac{\boldsymbol{CFU_1}}{\boldsymbol{CFU_2}} \times \mathbf{100}$$

CFU_1 is the average number of recovered colonies (recovered amount), and **CFU_2** is the average number of inoculated colonies (amount added).

- The percentage mean recovery ($R_{,}\%$) was calculated by Equation:

$$\boldsymbol{R}, \% = \frac{\sum_i^n \boldsymbol{R_i}}{\boldsymbol{n}}$$

Where **n** is the number of test microorganisms.

RESULTS AND DISCUSSION

The Results of Recovery Studies for Swab and Rinse Sampling Methods:

Sample/ Coupon material	Swab sampling					Rinse sampling				
	Number of CFU					Number of CFU				
	S. aureus	P. aeruginosa	C. albicans	E. coli	B. subtilis	S. aureus	P. aeruginosa	C. albicans	E. coli	B. subtilis
Test sample (n=3)/ Plastic	27	35	21	39	32	20	29	16	31	27
Test sample (n=3)/ Glass	18	28	17	34	23	16	19	12	26	17
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Blank (n=2)	No growth	No growth	No growth	No growth	No growth	No growth	No growth	No growth	No growth	No growth

RESULTS AND DISCUSSION

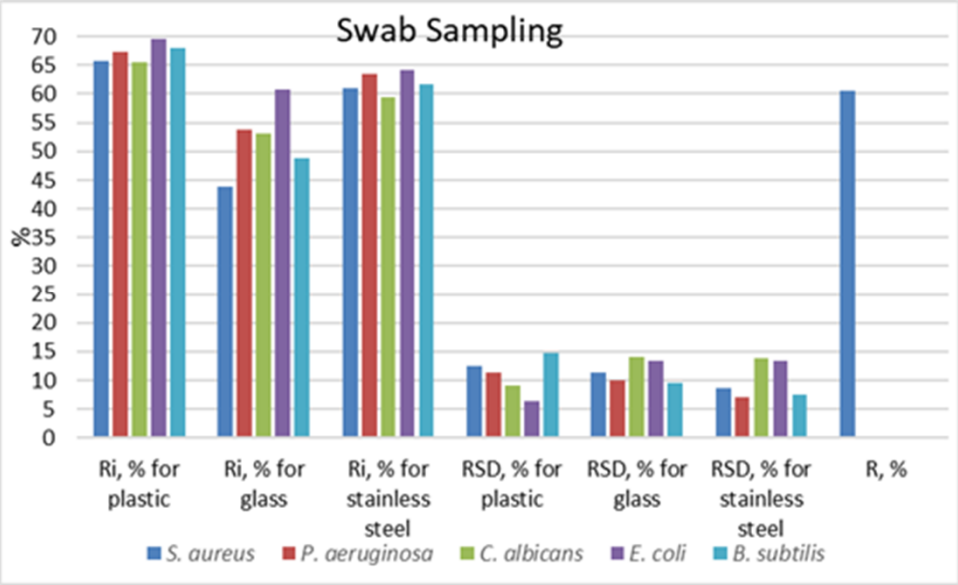


Chart of calculated values of the mean recovery (R, %), the average recoveries (R_i) and the relative standard deviations (RSD, %) for each test microorganism for the swab sampling method

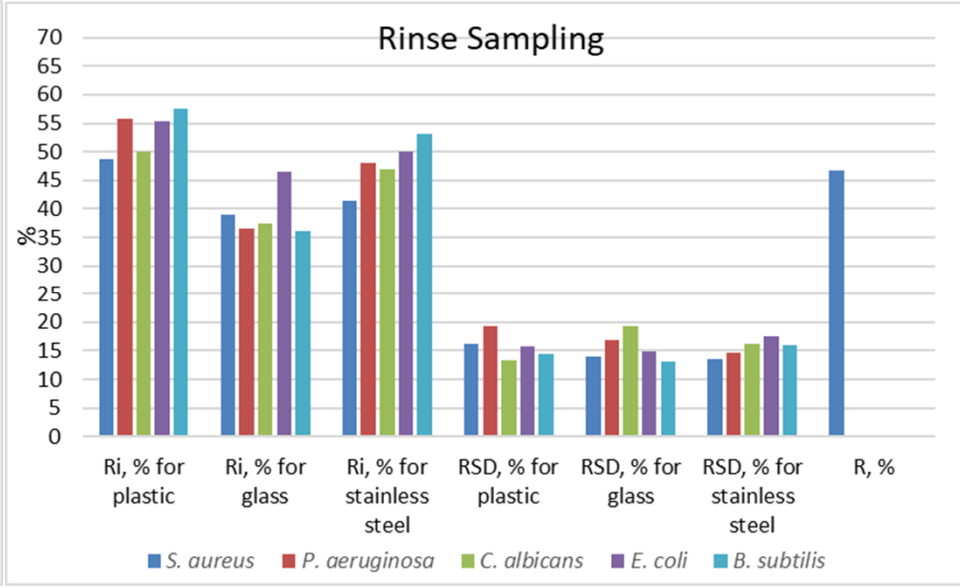


Chart of calculated values of the mean recovery (R, %), the average recoveries (R_i) and the relative standard deviations (RSD, %) for each test microorganism for the rinse sampling method

RESULTS AND DISCUSSION

- No growth was observed in the blank and negative control samples, which shows that the environment and materials used are free from microbiological contamination and confirms that the recovery studies were performed under aseptic conditions, and glassware, solvents, swabs, media, and coupons were sterile

- The decreasing tendency was revealed in the following order: plastic, stainless steel, and glass. The lowest recovery was observed for glass, which is a smooth, non-porous, inert material. In dry conditions, the tendency of viable bacteria to die is observed. However, better recovery results were obtained on the stainless steel surface. It is also a non-porous, smooth, inert material, but it shows increased adherence to microorganisms. All the good recoveries were obtained on plastic material, which is a porous inert material; therefore, the adherence ability is increased, and the death of microorganisms is less. The plastic can absorb the bacteria adherent to the surface and improve the recovery result.

- The highest recovery was obtained in the case of E.coli for both sampling methods. The recovery rate depends on the type and nature of test microorganism, which is caused by the viability of the microorganism, compatibility with the material, and different ability of adherence of the surface

- The recovery rate is higher for the swab sampling method compared to the rinsing method. This difference is small; in particular, it is equal to 60.5 % for the swab sampling method and 46.8 % for the rinsing

- The mean recovery is much more than the acceptance limit for both sampling methods, which confirms the validity and appropriateness of the combination of sampling and analytical methods. For the swabbing, the RSD of the numbers of enumerated forming colonies from the test samples is below the recommended limit (≤15 %). However, for the rinsing method, this value exceeds this limit in the case of some microorganisms but does not exceed 20 %, which is explained by the fact that the rinsing method, although characterized by high recovery, has less precision due to its performance technique

CONCLUSIONS

- Swab and rinse sampling methods were developed for microbiological contamination testing on pharmaceutical equipment surfaces
- Recovery studies involved five bacterial and fungal cultures on three different surface types
- The highest recovery was achieved with ***Escherichia coli*** for both sampling methods
- The swab sampling method showed a higher recovery rate (60.5%) compared to the rinse method (46.8%)
- The combination of sampling and microbiological enumeration methods provided good recovery (>36.17%) with high precision (RSD <19.25%)
- The proposed methodology is suitable for cleaning validation in pharmaceutical environments

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SUSTAINABILITY STRATEGIES IN BASIC EDUCATION: USE OF WASTE COOKING OIL IN BIOFUEL PRODUCTION AS AN INTERDISCIPLINARY TOOL TO PROMOTE ENVIRONMENTAL AWARENESS

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ABSTRACT

This work aims to report on the transformation of waste cooking oil into biodiesel, soap, and bioplastic, which can enable the insertion of science themes from the National Curricular Base content in a transversal and interdisciplinary manner for students and teachers in basic education. In this context, through students and teachers of the Professional Master's in Environmental Sciences at Univassouras, teachers were trained to work practically with Chemistry contents as recommended by the National Curricular Guidelines and Parameters. The professional training was supported by didactic material (follow-up module) and enabled the adoption of practical classes with process innovation where recycling artifacts and equipment, called alternative materials, were developed. Discarded toy car motors were used as an agitation system for the waste oil, and PET bottles were used as decanters for separating glycerin and biofuel, pieces of PVC pipes and wood for supports, and household stoves and burners as heating systems. The results are being evaluated and inserted into a follow-up report and will be part of dissertations by Master's students.

***Keywords**: Environmental Education, Biodiesel, Practical Teaching.*

1. INTRODUCTION

A inquietação crescente com o meio ambiente impulsiona a busca por ações sustentáveis em diversas esferas, especialmente, em como fomentar a conscientização ambiental. Assim, o contexto escolar surge como um terreno próspero para fomentar a conscientização e ação ambiental, através da educação ambiental. Conforme apresentado pela UNESCO (2005, p.44), a educação ambiental (EA) pode ser entendida como "uma disciplina bem estabelecida que enfatiza a relação dos homens com o ambiente natural, as formas de conservá-lo, preservá-lo e de administrar seus recursos adequadamente", contribuindo de forma efetiva para o desenvolvimento sustentável do meio ambiente. Esta educação não se restringe apenas ao ambiente escolar, mas também, se estende para o ambiente familiar.

A dimensão ambiental envolve diversos atores do universo educativo, apresentando uma perspectiva interdisciplinar, uma vez que insere o sistema de conhecimento, a capacitação de profissionais, e a comunidade escolar e acadêmica. Isto denota a necessidade de maior reflexão nas relações entre os diversos saberes (JACOBI, 2003).

Assim, a educação ambiental nas escolas oportuniza o desenvolvimento de intervenções e o aprimoramento de processos de ensino-aprendizagem. Neste cenário, tratando-se de problemas ambientais oriundos da falta de conscientização e informação da sociedade, têm se os resíduos sólidos, provenientes da ação do homem. Dentre estes resíduos, o óleo residual de fritura apresenta como um dos tipos que apresenta grande dano ao meio ambiente, uma vez que em sua maioria o seu descarte acontece de forma inapropriada, em pias de cozinha. Braga (2007) apresenta que um litro de óleo pode contaminar um milhão de litros de água potável, afetando a qualidade da água.

Em conformidade, a Associação Brasileira da Indústria de Óleos Vegetais (Abiove) cerca de

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1 bilhão de litros de óleo é descartado de forma inadequada por ano no Brasil. Embora estes dados apresentam o grande impacto para a saúde do meio ambiente, existem formas que contribuem para mitigar o descarte incorreto, como através do processo de reciclagem, produzindo tinta, sabão ou biocombustível e o biodiesel.

Deste modo, este estudo visa fazer a reciclagem do óleo residual de fritura como ferramenta interdisciplinar para o ensino e a produção do biodiesel. O biodiesel é um tipo de combustível renovável que gera menos danos ao meio ambiente, sendo produzido a partir do óleo vegetal através da transesterificação. Além disso, a partir da produção do biocombustível tem-se outros subprodutos, como a glicerina.

Neste sentido, objetivou-se investigar e avaliar a eficácia das estratégias interdisciplinares, com ênfase na utilização do descarte de óleo de fritura residual como ferramenta educativa, na promoção da conscientização ambiental e na adesão de práticas sustentáveis pela comunidade escolar do Município de Três Rios- RJ e Vassouras- RJ. Este estudo justifica-se a partir da necessidade de promoção da conscientização ambiental, ainda na educação básica, além do impacto na formação educacional e consciência ambiental. Assim, contribui para a educação e políticas públicas, estimulando a independência proativa em relação ao meio ambiente.

Ademais, consegue alcançar alguns dos Objetivos de Desenvolvimento Sustentável (ODS), como: ODS3, ODS4 ODS6 ODS11 ODS15, ODS16, ODS17.

Além disso, com a aplicação da metodologia e avaliação dos resultados produzidos o presente estudo teve como produto final a produção de material didático, Módulo de apoio. O material didático pode auxiliar no processo de ensino aprendizagem, de forma eficaz e eficiente, além de ser um orientador para o avanço do trabalho do professor.

Vale destacar que o Mestrado Profissional em Ciências Ambientais da Univassouras tem arrolado na sua pesquisa o projeto Intitulado em: "PRESTABILIDADE AMBIENTAL, RECICLAGEM, OBTENÇÃO, ESTUDO, OTIMIZAÇÃO E AVALIAÇÃO NO USO DE BIODIESEL DERIVADO DO ÓLEO DE FRITURA EM MOTORES À DIESEL". Este projeto é também cadastrado no diretório de grupos da CNPq como BIOVASSOURAS e tem por objetivo produzir biodiesel, de forma simples, com parâmetros de qualidade segundo a norma da ANP a partir do óleo residual de fritura. Com o subproduto da produção do biocombustível (Glicerina) é possível elaborar bioprodutos e bioplástico de forma sustentável e com o tema reciclagem.

Então, destinou-se capacitar professores da educação básica, por intermédio de alunos da Pós Graduação, com a disseminação de metodologia alternativa de ensino que visa a instrução de ciências de forma prática. Em conclusão, por intermédio de alunos e professores do Mestrado foi possível capacitar professores de ensino básico para trabalhar de forma prática com materiais alternativos do cotidiano do aluno com os conteúdos de Química conforme recomendado pelas Diretrizes e Parâmetros Curriculares Nacionais.

2. MATERIALS AND METHODS

Na capacitação, produz- se biodiesel e sabão a partir do óleo residual de fritura (SATO, 2005), um resíduo muito tóxico e poluente, de forma simples e alternativa. A inovação do processo ocorre pela elaboração de artefatos e equipamentos de reciclagem, como por exemplo o uso de agitação com motor de carros de brinquedos descartados e manta para aquecimentos residênciais.

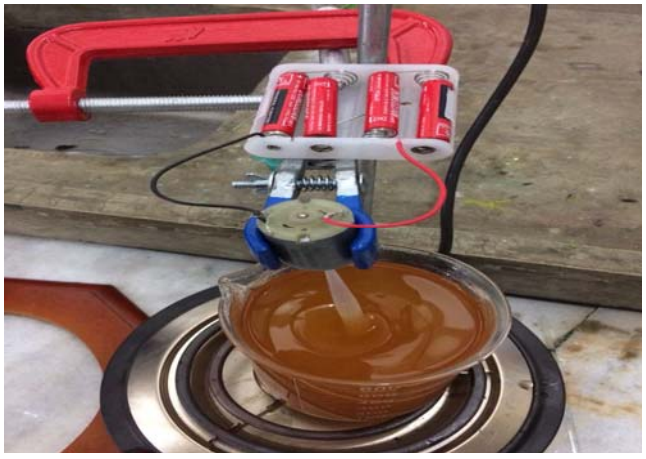


***Figura 1**. Sistema de agitação e aquecimento da produção de biodiesel a partir do óleo de fritura por motor de carrinho reciclado e ponteira de plástico.*

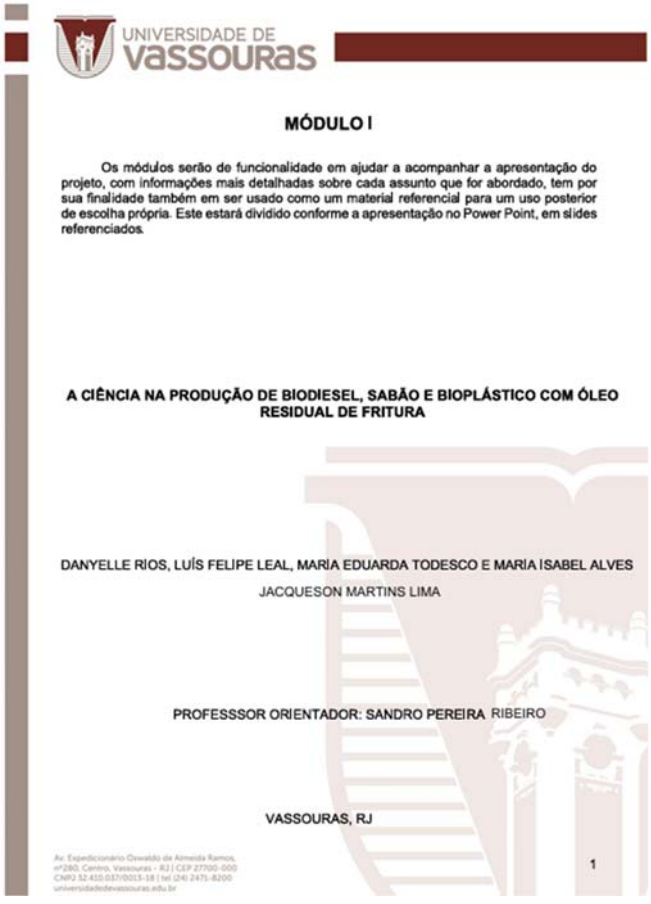
Também foram utilizados utensílios como garrafas PETs utilizadas como decantadores, pedaços de tubos de PVC e madeiras para suportes.

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***Figura 2**. Sistema de decantação da produção de biodiesel a partir do óleo de fritura com uso de garrafas PETs e resíduos de madeira, ferro e plásticos.*

A capacitação ocorre desde 2021 em pelo menos uma vez no ano com a instrução disseminada através de módulos de apoio criado pelos professores e alunos do projeto.



UNIVERSIDADE DE VASSOURAS

MÓDULO I

Os módulos serão de funcionalidade em ajudar a acompanhar a apresentação do projeto, com informações mais detalhadas sobre cada assunto que for abordado, tem por sua finalidade também em ser usado como um material referencial para um uso posterior de escolha própria. Este estará dividido conforme a apresentação no Power Point, em slides referenciados.

A CIÊNCIA NA PRODUÇÃO DE BIODIESEL, SABÃO E BIOPLÁSTICO COM ÓLEO RESIDUAL DE FRITURA

DANYELLE RIOS, LUÍS FELIPE LEAL, MARIA EDUARDA TODESCO E MARIA ISABEL ALVES

JACQUESON MARTINS LIMA

PROFESSSOR ORIENTADOR: SANDRO PEREIRA RIBEIRO

VASSOURAS, RJ

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***Figura 3**. Módulo de apoio a produção de biodiesel a partir do óleo de fritura para professores do ensino básico.*

Diante do *exposto*, *buscou-se* a contribuição e conscientização ambiental, impulsionada pelo desenvolvimento de uma metodologia cientifica baseada na adequação do ensino prático da ciência química do currículo mínimo da SEEDUC-RJ, vizando a preparação para as provas, o Exame Nacional de Ensino Médio- ENEM e a formação de cidadãos conscientes, críticos e envolvidos com as ciências da natureza. Com isso, a obtenção do biodiesel e sabão pode corroborar com o aprendizado e a integração dos alunos de ensino médio com a pesquisa, a prática científica para melhor desempenho em provas, bem como, recrudenciar o professor com uma metodologia que permita preparar de maneira otimizada os alunos para as provas e a garantia das gerações futuras ao desenvolvimento sustentável, a conscientização, o crescimento econômico, à educação de qualidade, a proteção ambiental e o bem-estar social.

3. RESULTS AND DISCUSSION:

O presente estudo aconteceu em algumas etapas. Primeiro foi realizada uma revisão bibliográfica sobre a temática deste trabalho, a fim de dar embasamento teórico, sendo pesquisada as palavras-chave: biocombustíveis, processos de produção, descarte de óleo residual de fritura e educação ambiental. Ademais, foi realizado um levantamento sobre as legislações brasileiras e as diretrizes básicas pertinentes ao tema. Em relação a população de aplicação deste estudo foi com alunos do ensino médio do município de Três Rios/RJ e Vassouras. Foi possível contemplar mais de quatro mil alunos nos três anos da ação. Com a aplicação prática da produção do biocombustível obteve-se o desenvolvimento de uma consciência sustentável e ensino inovador aos estudantes. Fato que promove mudança positiva nas atitudes dos alunos em relação ao descarte de óleo residual de fritura, adotando práticas de reciclagem mais conscientes e incorporando princípios sustentáveis em suas vidas cotidianas. Além disso, proporcionou um maior engajamento às aulas e o melhor aproveitamento nas provas. Também é importante mencionar a contribuição com a disseminação do ensino pelos alunos à comunidade escolar e local em iniciativas de reciclagem de óleo residual de fritura e outras práticas sustentáveis, impactando positivamente o entorno da escola. Assim, os alunos demonstraram uma compreensão aprimorada sobre a produção de biodiesel a partir do óleo de fritura, a reutilização da glicerina como subproduto e a fabricação de sabão artesanal, assim como os princípios gerais de sustentabilidade e conservação ambiental. O desenpenho nas avaliações pode ser comprovada com as notas bimestrais e o rendimento significativo nas provas do ENEM para alunos do terceiro ano. Portanto,

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este trabalho torna-se fundamental devido a seu potencial de impacto sustentável, ao longo de sua execução com as práticas educacionais que contribuem para uma cultura mais sustentável e consciente, impactando positivamente o meio ambiente e a sociedade.

4. CONCLUSIONS

Por fim, com o legado do trabalho científico, as capacitações, valorizando a importância crítica de novas metodologias de ensino para o futuro, foi possível proporcionar cultura, respeito, educação e cuidado através de aulas práticas que propocionam qualidade e enriquecimento no ensino didático o que garente as gerações futuras o desenvolvimento sustentável, a conscientização, o crescimento econômico, à educação, a proteção ambiental e o bem-estar social.

5. DECLARATIONS

5.1. Open Access

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Southern Science Conference, 2024.

ESTRATÉGIAS DE SUSTENTABILIDADE NA EDUCAÇÃO NA EDUCAÇÃO BÁSICA: UTILIZAÇÃO DO ÓLEO RESIDUAL DE FRITURA NA PRODUÇÃO DE BIOCOMBUSTÍVEL COMO FERRAMENTA INTERDISCIPLINAR PARA PROMOVER A CONSCIENTIZAÇÃO AMBIENTAL

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September/2024

INTRODUCTION

A crescente preocupação com o meio ambiente exige ações eficazes para promover a sustentabilidade.

É preciso mobilizar a sociedade e buscar soluções inovadoras para garantir a saúde do planeta.

A educação desempenha um papel fundamental nesse processo de transformação e é um terreno próspero para fomentar a conscientização individual e coletiva.



Poluição ambiental x Ambiente natural
Fonte: https://www.pngwing.com/

INTRODUCTION

O Mestrado Profissional em Ciências Ambientais da Univassouras tem arrolado na sua pesquisa o projeto Intitulado em: "PRESTABILIDADE AMBIENTAL, RECICLAGEM, OBTENÇÃO, ESTUDO, OTIMIZAÇÃO E AVALIAÇÃO NO USO DE BIODIESEL DERIVADO DO ÓLEO DE FRITURA EM MOTORES À DIESEL". Este projeto é também cadastrado no diretório de grupos da CNPq como BIOVASSOURAS e tem por objetivo produzir biodiesel, de forma simples.

Conforme apresentado pela UNESCO (2005, p.44), a educação ambiental (EA) pode ser entendida como "uma disciplina bem estabelecida que enfatiza a relação dos homens com o ambiente natural, as formas de conservá-lo, preservá-lo e de administrar seus recursos adequadamente", contribuindo de forma efetiva para o desenvolvimento sustentável do meio ambiente. Esta educação não se restringe apenas ao ambiente escolar, mas também, se estende para o ambiente familiar.



Sustentabilidade
Fonte: https://www.pngwing.com/

INTRODUCTION

O contexto escolar é um espaço privilegiado para fomentar a consciência ambiental e inspirar ações transformadoras.

É preciso integrar a educação ambiental ao currículo escolar de forma transversal e interdisciplinar.

Aprender fazendo é fundamental para que os alunos se tornem agentes de mudanças e protagonistas de suas aprendizagens.





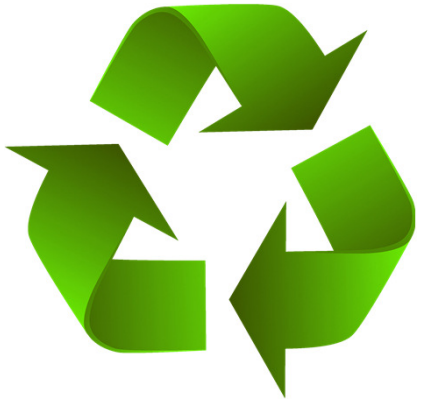
Educação ambiental
Fonte: https://www.pngwing.com/

INTRODUCTION

O descarte inadequado de óleo de fritura causa graves danos ao meio ambiente.

A reciclagem do óleo residual de fritura apresenta-se como uma solução sustentável.

Transformar esse problema em oportunidade de aprendizagem é o desafio!





Óleo de soja e reciclagem
Fonte: https://www.pngwing.com/

OBJETIVE

Investigar e avaliar a eficácia das estratégias interdisciplinares, com ênfase na utilização do descarte de óleo de fritura residual como ferramenta educativa, na promoção da conscientização ambiental e na adesão de práticas sustentáveis pela comunidade escolar do Município de Três Rios- RJ e Vassouras- RJ.

Na capacitação que o trabalho propõe, produz- se biodiesel e sabão a partir do óleo residual de fritura, um resíduo muito tóxico e poluente, de forma simples e alternativa.



Investigação
Fonte: https://www.pngwing.com/

METHODOLOGY

Treinamento prático para transformar óleo residual de fritura em biodiesel e sabão.

Utilização de materiais de apoio a produção de biodiesel a partir do óleo de fritura para professores do ensino básico.

Apresentação de recursos simples e acessíveis para produção de biodiesel e sabão.

A inovação do processo ocorre pela elaboração de artefatos e equipamentos de reciclagem, como por exemplo o uso de agitação com motor de carros de brinquedos descartados e manta para aquecimentos residenciais.



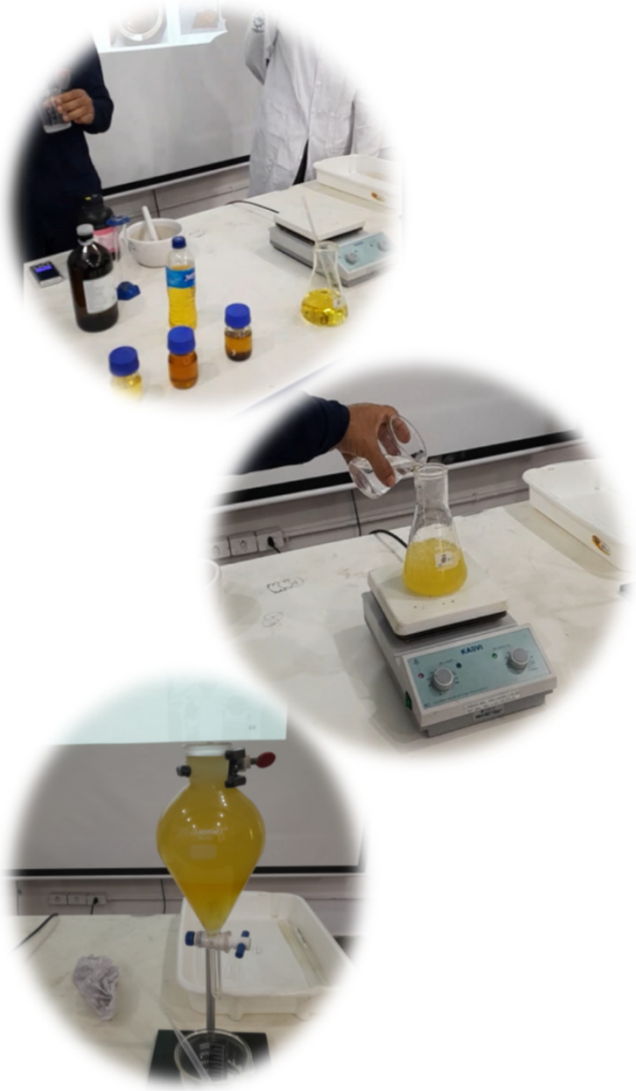
Treinamento sobre produção de biodiesel
Fonte: dos autores

METHODOLOGY

Implementação da metodologia em turmas de ensino médio, adaptando-a à realidade local.

Participação ativa dos alunos na produção de biodiesel e sabão, vivenciando os conceitos na prática.

Incentivo à coleta de óleo residual de fritura nas residências dos alunos, sensibilizando a comunidade escolar.



Treinamento sobre produção de biodiesel
Fonte: dos autores

RESULTS AND DISCUSSION

Observação de melhoras no desempenho escolar dos alunos, na disciplina de Química, e maior interesse pelas disciplinas do bloco de Ciências da Natureza e suas tecnologias.

Compreensão mais profunda sobre a importância da reciclagem e seus benefícios para o meio ambiente.

Desenvolvimento do pensamento crítico, da investigação científica e do trabalho em equipe.



Produção de biodiesel com equipamentos alternativos
Fonte: dos autores

RESULTS AND DISCUSSION

Alunos incorporaram práticas sustentáveis em seu dia a dia, como a coleta seletiva e a redução do consumo.

Disseminação do conhecimento adquirido para familiares e amigos, ampliando o impacto da iniciativa.

Aumento significativo na coleta de
óleo residual de fritura na comunidade escolar.



Coleta de óleo de cozinha
Fonte: https://www.pngwing.com/

RESULTS AND DISCUSSION

Participação dos alunos em feiras de ciências, expondo seus trabalhos para a comunidade.

Desenvolvimento do protagonismo juvenil e do interesse em atuar como agentes de transformação.

Impacto social positivo na comunidade, com a formação de cidadãos mais conscientes e engajados.



Apresentação do projeto do biodiesel na FECTI
Fonte: dos autores

RESULTS AND DISCUSSION

Destacar o entusiasmo e a participação ativa dos alunos durante todo o projeto.

Mostrar a importância do trabalho em equipe e da colaboração entre alunos e professores.

Enfatizar o impacto positivo do projeto
na comunidade escolar e local.

Ademais, o trabalho consegue alcançar alguns dos Objetivos de Desenvolvimento Sustentável (ODS), como: ODS3, ODS4 ODS6 ODS11 ODS15, ODS16, ODS17.



Trabalho em equipe
Fonte: https://www.pngwing.com/

CONCLUSIONS

A utilização do óleo residual de fritura como ferramenta pedagógica é uma estratégia eficaz para a educação ambiental.

O uso de equipamentos e aparatos de reciclagem para processos de produção envolvendo as ciências Ambientais é fundamental para o processo educativo e o meio ambiente.

O projeto estimulou a consciência ambiental, a adoção de práticas sustentáveis e o protagonismo juvenil.

A iniciativa demonstra o potencial da escola na construção de um futuro mais sustentável.

O desenpenho nas avaliações pode ser comprovada com as notas bimestrais e o rendimento significativo nas provas do ENEM para alunos do terceiro ano.

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FAST PYROLYSIS OF COCOA BEAN SHELL

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ABSTRACT

The increasing demand for sustainable waste utilization has led to growing interest in cocoa shells as a valuable biomass resource. This study investigates the pyrolysis of cocoa shells, both untreated and acid-treated, at temperatures of 300, 400, and 500°C to extract valuable compounds with potential commercial applications. Pyrolysis, a thermochemical decomposition process in the absence of oxygen, was carried out using nitrogen as the pyrolysis atmosphere to ensure optimal reaction conditions. The aim was to optimize the production of bio-oils enriched with value-added compounds, such as fatty acids (FA) and anhydrosugars. These pyrolytic oils were analyzed using gas chromatography-mass spectrometry (GC-MS), revealing significant amounts of fatty acids, including palmitic acid, cis-vaccenic acid, and stearic acid. Notably, acid-washed cocoa shells exhibited higher bio-oil yields compared to untreated samples, with 500°C being the optimal temperature, yielding the highest amount of bio-oil. Furthermore, this temperature favored the formation of specific compounds, enhancing the overall value of the pyrolytic products. Additionally, the pyrolysis of acid-treated biomass resulted in a high concentration of levoglucosan, a valuable anhydrosugar, which accounted for over 50% at 500°C. These findings suggest that the pyrolysis of cocoa shells, especially when pretreated with acid, not only provides an efficient method of waste valorization but also generates bio-oil and biochar with potential properties for health, energy production, and environmental applications. This research highlights the importance of exploring agricultural residues, such as cocoa shells, for sustainable bioresource development, contributing to a circular economy and reducing the environmental impact of agro-industrial waste.

Keywords: *waste valorization; acid treatment; bio-oil analysis; fatty acids; levoglucosan.*

1. INTRODUCTION

The depletion of crude oil reserves and the effect of greenhouse gases on global warming call for the substitution of petrochemical processes with biomass-based processes for chemical production. Biomass, as a renewable resource, stands out as the sole raw material capable of supporting the sustainable production of chemicals. In recent years, a pivotal shift has occurred toward using waste biomass, driven by its significantly lower cost in comparison to virgin biomass (Mansur D. *et al.*, 2014). This transition is of critical relevance, especially for industries that produce large quantities of by-products, transforming waste into a valuable resource for chemical production. One such industry is cocoa production. Cocoa beans (*Theobroma cacao L.*) are widely used in the food, pharmaceutical, and cosmetic sectors. It is estimated that the world's production of cocoa beans reached approximately 4 million tons in 2010 (FAO), yet only a fraction of this production is fully exploited. Substantial amounts of cocoa pod husk, bean shell, and mucilage are often considered waste, presenting an opportunity to incorporate these by-products into biomass-based processes (Pagliari *et al.*, 2022). By leveraging these waste materials, industries can contribute to sustainable chemical production while addressing the challenges of waste management and resource depletion.

Pyrolysis can be used to degrade organic compounds from biomass to produce various products such as liquid smoke, biochar, tar, and gas. Compared to the combustion process, pyrolysis requires low temperatures and results in

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low air pollution emissions (Putri *et al.* 2019). A key fraction obtained from pyrolysis is bio-oil, which contains a variety of compounds with significant commercial potential. Notably, fatty acids and methylxanthines are present in biomass, and ways to extract or separate them could be explored to enhance the value of this renewable resource. (Wijaya, *et al* 2019).

This study explores the pyrolysis of raw and acid-treated cocoa bean shell waste, aiming to unlock its full potential. The primary objectives are to maximize the yield of liquid smoke during the pyrolysis process, identify the key chemical components of the resulting bio-oils, and thoroughly evaluate the properties of these pyrolyzates. By doing so, this research seeks to reveal new possibilities for transforming agricultural waste into valuable products.

2. MATERIALS AND METHODS

2.1. Cocoa bean shell sample

The cocoa shell used was donated by local dietitians in the city of Córdoba and was used directly (CS) for the standard assays. Additionally, a portion of the cocoa shell was washed with hydrochloric acid (5%v/v) as a pretreatment to compare both treatments and optimize yields (CS-A).

2.2. Fast pyrolysis experiments

Fast pyrolysis experiments were conducted in a quartz tube reactor under a nitrogen atmosphere. The reactor, externally heated by a tube furnace, had its temperature controlled by a thermocouple and a controller. With a length of 25 cm and an inner diameter of 2.5 cm, the reactor was connected to a vacuum line maintained by a vacuum pump, achieving pressures of approximately 1-5 Torr. A continuous flow of nitrogen at a rate of 0.1 mL/s was introduced during and after the pyrolysis to prevent the presence of oxygen. At the end of the hot zone, a condensation trap cooled with liquid nitrogen collected the condensable volatile products. Biomass (3-3,5 g) was placed in a quartz boat within the reactor's cold zone. A reaction was initiated once the vacuum line achieved the target pressure and temperature. The reaction time was monitored from when the material was positioned in the center of the hot zone. After each pyrolysis, the solid residue in the boat was recovered and weighed, and the bio-oil was extracted from the trap with acetone, evaporated, weighed, and analyzed using gas chromatography coupled to mass spectrometry (GC-MS). The weight difference between the initial mass of the cocoa shell and the solid and liquid fractions determined the gaseous fraction. Each pyrolysis experiment lasted 20 minutes, with temperatures set at 300, 400, and 500 °C.

2.3. Bio-oil characterization

A fraction of bio-oil was dissolved in acetone, and the mixture was homogenized. The samples were filtered with filter paper (cellulose) and transferred to 1.5 mL vials. Finally, 0.5 µL of supernatant was analyzed by GC-MS using a QP-2020 ULTRA Shimadzu spectrometer. The injector temperature was 250 ºC, and the separation was performed using a Mega 5-ms capillary column. Helium was used as a carrier gas with a split injection mode, pressure as a flow control mode (65.2 kPa), and a total flow rate of 7.5 mL/min. The oven temperature was programmed from 80 ºC (3 min) to 280 ºC (7 min) with a heating rate of 10 ºC/min. The temperature of the GC-MS interface was held at 280 ºC, and the mass spectrometer was operated at 70 eV under electron ionization. The area corresponding to each compound is proportional to the amount of that compound in the pyrolytic bio-oil sample. Consequently, the peak area percentage of a compound was used to compare the change in the relative amount in the different bio-oils. Different databases available in the GC-MS software solution, such as Wiley and NIST, were used to identify the compounds from the chromatographic peaks (> 85 % match).

3. RESULTS AND DISCUSSION

3.1. Cocoa bean shell (CS) characterization

The raw biomass was characterized by assessing the ash content, fixed carbon, and volatile matter. Additionally, an elemental analysis was conducted to determine the contents of carbon (C), hydrogen (H), and nitrogen (N), with oxygen (O) calculated as the difference. These results were consistent with those reported by Patnaik and Goldfarb (2015). A biomass

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composition analysis was also conducted to determine the contents of cellulose, hemicellulose, lignin, and extractives.

3.2. Fast pyrolysis experiments of CS and CS-A

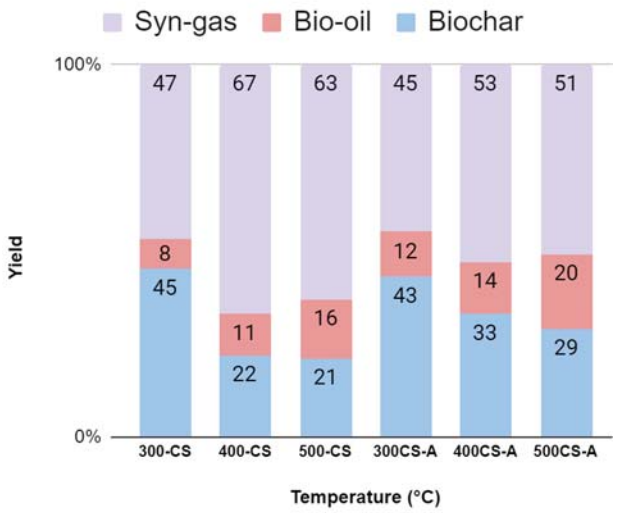


Figure 1. *Distribution of products in pyrolysis reactions of cocoa shells at different temperatures.*

The variations in the fractions obtained: liquid (bio-oil), solid (biochar), and gaseous (syn-gas) are presented in Figure 1. The results of the untreated cocoa shell (CS) reactions at different temperatures are presented for 300-CS, 400-CS, and 500-CS. The reactions conducted with acid-pretreated cocoa shells (CS-A) are labeled as 300-CSA, 400CS-A, and 500CS-A. Biochar formation was particularly significant, especially in reactions conducted at lower temperatures. Regardless of the initial biomass used, the gaseous fraction was the predominant product, comprising between 47 % and 68 % w/w. The yields of bio-oil ranged from 8 to 20 % w/w, values consistent with those reported in other pyrolysis studies (M. Wijaya and M. Wiharto, 2020). Regarding the results, a slight increase in bio-oil yield was observed when experiments were performed using acid-washed cocoa shells. The maximum production of pyrolytic oil from both biomasses was achieved at 500 °C.

3.3. CS and CS-A bio-oils characterization

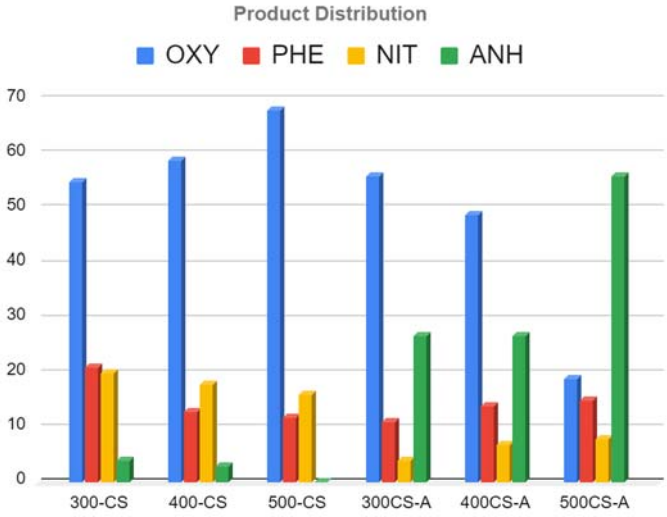


Figure 2. *Composition of the bio-oils obtained by fast pyrolysis of CS and CS-A*

The composition of bio-oils from the pyrolysis of CS and CS-A was analyzed using GC–MS. According to the ion chromatograms and the main families of compounds in each bio-oil, the following groups could be distinguished: OXY: oxygenated, PHE: phenolic compounds, NIT: nitrogenated compounds, and ANH: anhydrosugars. The variation in these types of compounds according to the temperature process is shown in Figure 2.

Oxygenated compounds were present in all pyrolysis reactions, but they were predominant in non-acid-washed bio-oil, with the highest proportion achieved at 500 °C. Among the oxygenated compounds, the main ones were fatty acids, such as palmitic acid, *cis*-vaccenic acid, stearic acid, and glycidyl palmitate, among others. Palmitic acid is the main compound obtained in all CS reactions, representing 20-25% of the oxygenated compounds. Some of these compounds have also been reported in the literature, but not in very significant quantities (M. Wijaya and M. Wiharto, 2020).

Phenolic compounds were present in small amounts across all experiments. These findings are consistent with previous studies and match results observed in other similar lignocellulosic biomass, like cocoa pods (Ogunjobi J. *et al.,* 2015). Within the main derivatives, phenol, cresols, and catechols, among others, were found. It has been reported that phenol derivatives are products derived primarily from the fractionation of lignin polymer present in the biomass.

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The formation of nitrogen-containing compounds was more prominent in reactions involving raw CS, with caffeine and theobromine emerging as the main components. It is well-established that methylxanthines are present in cocoa bean shells (Pagliari S. *et al.*, 2022), and our findings suggested that these valuable compounds can be efficiently extracted through thermal processes.

The sugar fraction was especially prominent in the oils derived from CS-A. Although oxygenated compounds (especially fatty acids) are still present in the CS-A reactions at 300°C and 400°C, it is observed that anhydrosugars begin to gain importance in these reactions, becoming predominant at 500°C. In the pyrolysis of CS-A, the highest yield was obtained at 500 °C, making up about 55 % of the total area. As observed with other lignocellulosic biomasses studied previously, the acid treatment had a significant impact on sugar production (Téllez J. F *et al.*, 2021). The main component of this fraction was levoglucosan (LG), which represented approximately 20% of the total area in CS300-A and CS400-A and 50% in CS500-A, Levoglucosan is an organic compound that forms when cellulose undergoes pyrolysis, a thermal decomposition process, typically in the absence of oxygen. It is commonly used as a molecular marker to trace biomass burning, especially in atmospheric studies, since it is a major product released when wood and other plant materials are burned. Other anhydrosugars, such as 1,4:3,6-dianhydro-α-D-glucopyranose (DGP) and 1,6-anhydro-D-glucofuranose (AGP), were also identified in smaller amounts. Additionally, levoglucosenone (1,6-anhydro-3,4-dideoxyhex-3-enopyran-2-ulose) was detected in experiments conducted at 300°C.

4. CONCLUSIONS

This study explored the fast pyrolysis of cocoa shells (CS) and acid-treated cocoa shells (CS-A) at temperatures ranging from 300 to 500 °C. The acid treatment of the biomass enhanced bio-oil yields, achieving up to a 20% increase at 500 °C. In terms of valuable products, untreated CS primarily produced fatty acids, especially at 500 °C. In contrast, pyrolysis of CS-A resulted in bio-oils rich in sugars, with levoglucosan (LG) as the main component, particularly at 500 °C. These findings demonstrate that the same biomass can be tailored to yield different high-value compounds depending on the treatment applied. This highlights the potential of cocoa shells, a common waste product, to be efficiently transformed into valuable resources. Future research should focus on optimizing extraction methods to better isolate these compounds, enhancing their recovery, and expanding their applications.

5. DECLARATIONS

5.1. Acknowledgments

This work was supported by the National Research Council of Argentina (CONICET) and the Secretary of Science and Technology from the National University of Cordoba (Projects SECyT-Consolidar 2024-2027).

5.2. Open Access

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Southern Science Conference, 2024.

FAST PYROLYSIS OF COCOA BEAN SHELL

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October/2024

INTRODUCTION

- The depletion of crude oil reserves and the impact of greenhouse gases on global warming necessitate the substitution of petrochemical processes with biomass-based processes.
- Biomass is a renewable resource and the only raw material capable of supporting the sustainable production of chemicals.
- The use of waste biomass has gained importance due to its significantly lower cost compared to virgin biomass.
- Cocoa production generates large amounts of by-products, such as pod husks and bean shells, which are considered waste, presenting an opportunity for their use in biomass-based processes.
- The pyrolysis of these cocoa waste materials can produce bio-oil and other useful products, contributing to sustainable chemical production and waste management.

Mansur, D. *et al.*, 2014. Pagliari *et al.*, 2022. Putri, *et al* 2019. Wijaya, *et al* 2019.

OBJECTIVE

This study explores the pyrolysis of raw and acid-treated cocoa bean shell waste, aiming to unlock its full potential. The primary objectives are to maximize the yield of liquid smoke during the pyrolysis process, identify the key chemical components of the resulting bio-oils, and thoroughly evaluate the properties of these pyrolyzates. By doing so, this research seeks to reveal new possibilities for transforming agricultural waste into valuable products.

METHODOLOGY

- **Cocoa bean shell sample.** The cocoa shell used was donated by local dietitians in the city of Córdoba and was used directly (CS) for the standard assays. Additionally, a portion of the cocoa shell was washed with hydrochloric acid (5%v/v) as a pretreatment to compare both treatments and optimize yields (CS-A).
- **Fast pyrolysis experiments** were conducted in a quartz tube reactor under a nitrogen atmosphere. The reactor, was connected to a vacuum line. A continuous flow of nitrogen at 0.1 mL/s was introduced to prevent oxygen presence. Liquid products were collected in a condensation trap cooled with liquid nitrogen. Biomass was placed in the reactor's cold zone, and the reaction was initiated once the target pressure and temperature were reached. After each pyrolysis, the solid residue was recovered, and the bio-oil was extracted with acetone, evaporated, weighed, and analyzed using GC-MS. The gaseous fraction was determined by the weight difference between the initial mass of the cocoa shell and the solid and liquid fractions. Each pyrolysis experiment lasted 20 minutes, with temperatures set at 300, 400, and 500 °C.
- **Bio-oils characterization.** A fraction of bio-oil dissolved in acetone and the mixture was homogenized. The samples were filtered, transferred to 1.5 mL vials, and was analyzed by GC-MS using a Shimadzu QP-2020 ULTRA spectrometer. The mass spectrometer operated at 70 eV under electron ionization. Peak area percentages of compounds were used to compare relative amounts in the bio-oils, with compound identification aided by databases like Wiley and NIST (> 85% match).

RESULTS AND DISCUSSION

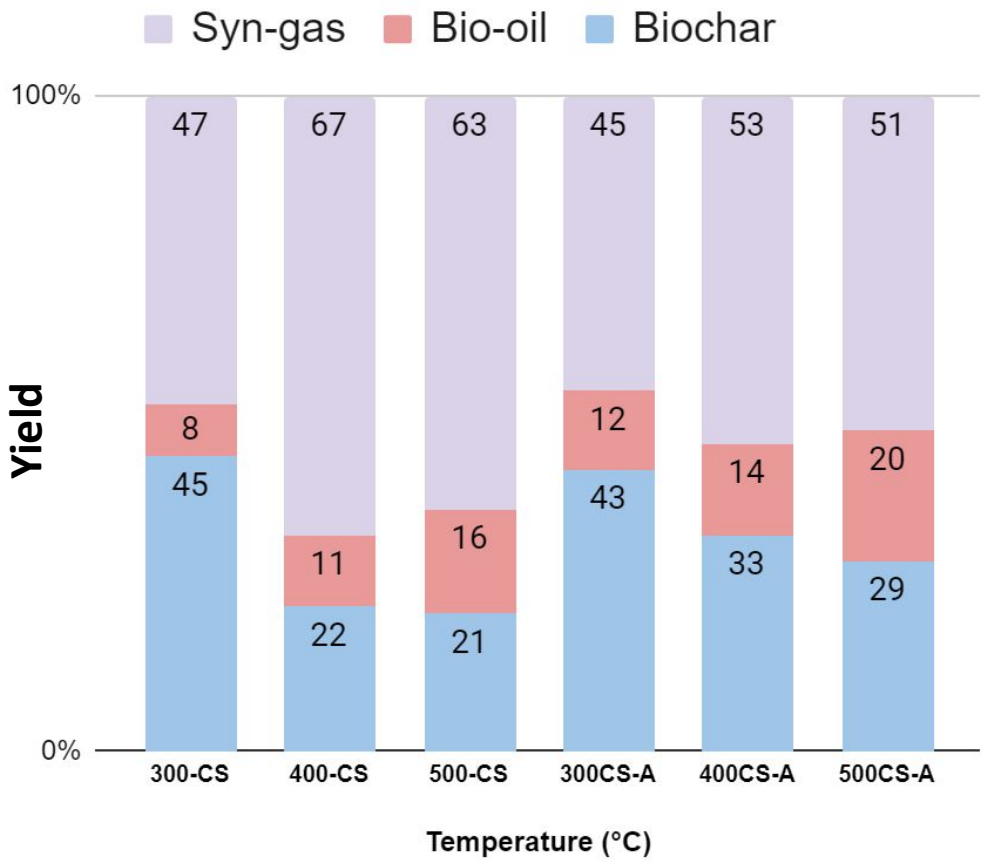


Figure 1.

The variations in the fractions obtained (liquid bio-oil, solid biochar, and gaseous syn-gas) are shown in **Figure 1.**

- Results for untreated cocoa shells (CS) are labeled as 300-CS, 400-CS, and 500-CS, while those for acid-pretreated cocoa shells (CS-A) are labeled as 300CS-A, 400CS-A, and 500CS-A.
- Biochar formation was notably significant, especially at lower temperatures.
- The gaseous fraction was the predominant product, accounting for 47% to 68% w/w, regardless of the biomass used.
- Bio-oil yields ranged from 8% to 20% w/w, aligning with values reported in other pyrolysis studies.
- A slight increase in bio-oil yield was observed when using acid-washed cocoa shells, with maximum pyrolytic oil production achieved at 500 °C for both types of biomass.

RESULTS AND DISCUSSION

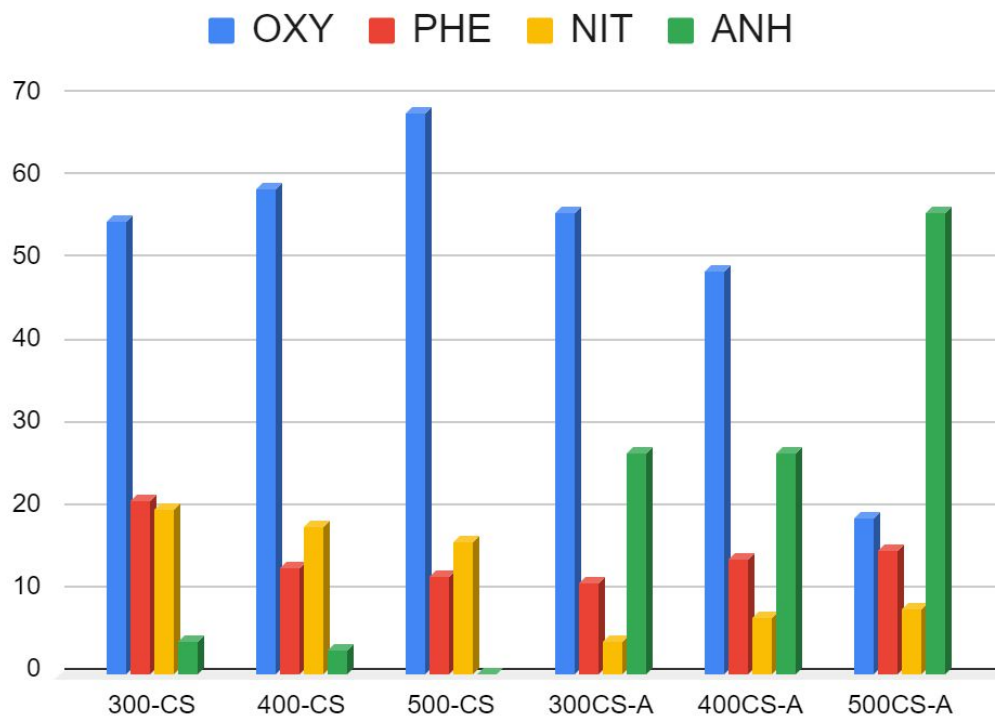


Figure 2. The composition of bio-oils from the pyrolysis of CS and CS-A was analyzed using GC–MS.

The following groups could be distinguished: OXY: oxygenated, PHE: phenolic compounds, NIT: nitrogenated compounds and ANH: anhydrosugars.

- Phenolic compounds were found in small amounts. These findings are consistent with previous studies and match results observed in another similar lignocellulosic biomass, like cocoa pods (Ogunjobi, J. et al 2015). Within the main derivatives, phenol, cresols, catechols, among others were found. It has been reported that phenol derivatives are products derived primarily from the fractionation of lignin polymer present in the biomass
- Nitrogen-containing compounds were more prominent in reactions involving raw cocoa shells, with caffeine and theobromine identified as the main components. It is well-established that methylxanthines are present in cocoa bean shell (Pagliari, S. *et al*, 2022), and our findings suggested that these valuable compounds can be efficiently extracted through thermal processes.

RESULTS AND DISCUSSION

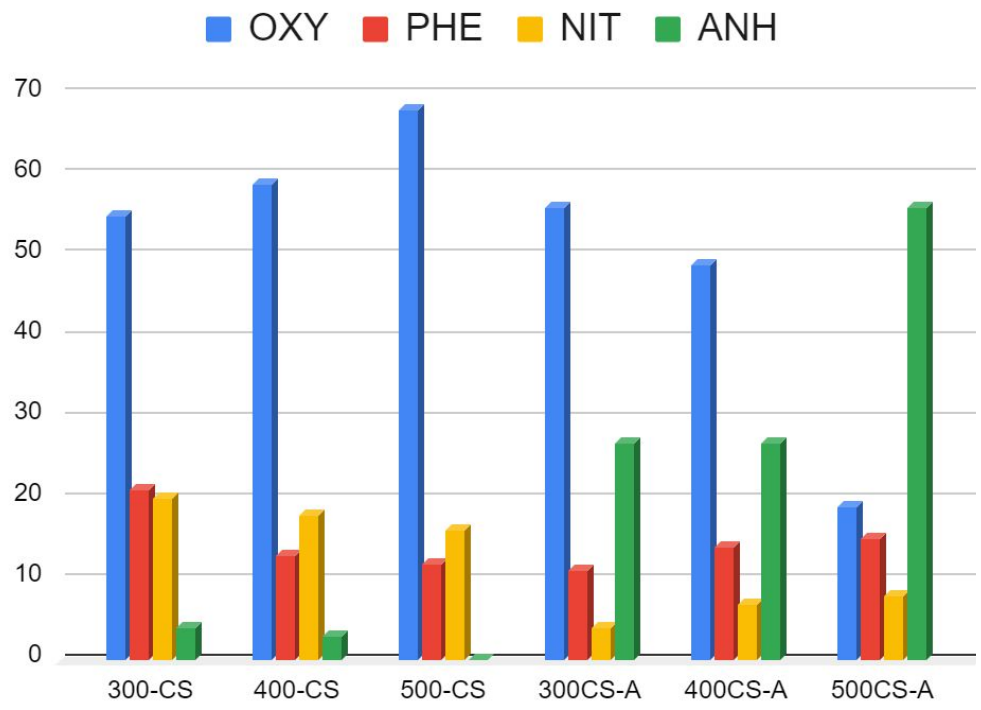


Figure 2.

- Oxygenated compounds were present in all pyrolysis reactions, predominantly in non-acid-washed bio-oil at 500 °C. The main compounds identified included fatty acids such as palmitic acid, cis-vaccenic acid, stearic acid, and glycidyl palmitate. **Palmitic acid** is the main compound obtained in all CS reactions, representing 20-25% of the oxygenated compounds. Some of these compounds have also been reported in literature, but not in very significant quantities (M. Wijaya and M. Wiharto, 2020).

- The sugar fraction was particularly prominent in the oils derived from CS-A. Anhydrosugars became increasingly significant, dominating at 500 °C, where the highest yield in pyrolysis of CS-A was achieved, constituting about 55% of the total area. Acid treatment notably influenced sugar production, as seen in previous studies of other lignocellulosic biomasses (Téllez, J. F, *et al*, 2021). The key component of the sugar fraction was **levoglucosan**, which represented approximately 20% of the total area in 300CS-A and 400CS-A, increasing to 50% in 500CS-A.

CONCLUSIONS

•The study investigated fast pyrolysis of cocoa shell (CS) and acid-treated cocoa shell (CS-A) at temperatures between 300 and 500°C.

•Acid treatment enhanced bio-oil yields by up to 20% at 500 °C.

•Untreated CS primarily produced fatty acids, especially at 500 °C.

•Pyrolysis of CS-A resulted in bio-oils rich in sugars, with levoglucosan (LG) as the main component at 500 °C.

•The findings indicate that the same biomass can be tailored to produce different high-value compounds based on the treatment applied.

•Cocoa shell, a common waste product, has significant potential for transformation into valuable resources.

•Future research should focus on optimizing extraction methods to better isolate and recover these compounds for expanded applications.

ACKNOWLEDGEMENTS

- This work was supported by National Research Council of Argentina (CONICET) and Secretary of Science and Technology from National University of Cordoba (Projects SECyT-Consolidar 2024-2027).

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STATISTICAL ANALYSIS OF DENGUE CASES IN THE MÉDIO PARAÍBA DO SUL REGION, RJ

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ABSTRACT

Dengue is an arbovirus transmitted to humans through the bite of the female Aedes aegypti mosquito. The clinical presentation ranges from a nonspecific and benign viral syndrome to a severe and fatal condition. The objective of this study was to analyze data on dengue cases from 2019 and 2022 in the Médio Paraíba do Sul Region using Minitab® software. Statistical analysis revealed a difference in the average number of cases, with a higher concentration in 2019, attributed to factors such as the Covid-19 pandemic, which may have contributed to underreporting in 2022 due to the restructuring of epidemiological surveillance actions. The research concludes that new public policies and investigations are necessary for the effective control of dengue, a reemerging disease with high morbidity and mortality, reinforcing the importance of accurate case reporting to support health policies.

Keywords: *Arboviruses, Statistics, Public Health.*

1. INTRODUÇÃO

A dengue é uma doença viral reemergente, considerada um dos principais problemas de saúde pública global. Transmitida pelo mosquito *Aedes aegypti*, que se prolifera em regiões tropicais e subtropicais, o mosquito também é responsável pela transmissão de chikungunya e zika, doenças que contribuem para altas taxas de morbidade e mortalidade (Klempner, 2007).

Atualmente, a forma mais eficaz de prevenir a dengue é a eliminação dos mosquitos vetores, já que a vacina disponível possui diversas contraindicações (Aguiar *et a*l., 2016), e ainda não está disponível no sistema único de saúde (SUS) (Domingues; Garcia, 2020). No momento, outra vacina contra a dengue está sendo desenvolvida pelo Instituto Butantan. Em fase de testes, ela é considerada potencialmente eficaz (Instituto Butantan, 2020).

Para combater as arboviroses, é essencial focar na promoção da saúde e na educação ambiental, abordando comportamentos inadequados e a falta de saneamento. Ações sustentáveis e contínuas de controle vetorial são necessárias para reduzir a proliferação do mosquito.

Assim, objetiva-se com este artigo analisar os dados dos casos de dengue dos anos de 2019 e 2022 na Região do Médio Paraíba do Sul, através do aplicativo *Minitab*®. Dessa maneira, será possível identificar a média de casos de dengue na região.

2. MATERIAIS E MÉTODOS

A área de estudo do presente trabalho compreende a Região do Médio Paraíba do Sul, estado do Rio de Janeiro, com uma extensão de 6.203.4 km², é composta por 12 municípios: Barra do Piraí, Barra Mansa, Itatiaia, Pinheiral, Piraí, Porto Real, Quatis, Resende, Rio Claro, Rio das Flores, Valença e Volta Redonda conforme na figura 1.

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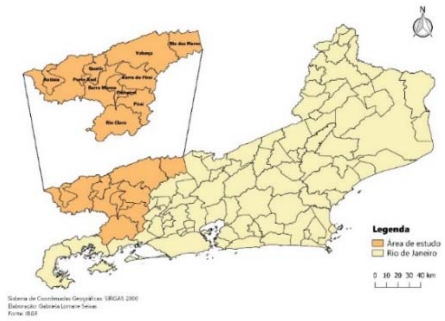


Figura 1. *Localização da Região do Médio Paraíba do Sul, estado do Rio de Janeiro - Fonte: IBGE*

Os dados referentes aos casos de dengue na Região do Médio Paraíba do Sul, Estado do Rio de Janeiro, foram coletados na plataforma do SINAN (Sistema Nacional de Agravos de Notificação), disponibilizados pelo Ministério da Saúde através do Departamento de Informática do Sistema Único de Saúde (DATASUS, 2024).

Os dados estatísticos foram tratados e aplicados ao *Software Minitab*® para comprovação do nível de significância dos casos de dengue na Região do Médio Paraíba do Sul.

3. RESULTADOS E DISCUSSÃO:

O total de casos de dengue, nos municípios da Região do Médio Paraíba do Sul, notificados no SINAN, durante os anos de 2019 e 2022 foram 8.553 casos (Tabela 1). A dengue é uma doença compulsória. Com a estratificação dos dados, constataram-se os seguintes resultados. Conforme a figura 2, é possível identificar uma diferença entre as médias anuais.

Tabela 1. *Casos de dengue, anos de 2019 e 2022*

Município	2019	2022
Barra do Piraí	928	28
Barra Mansa	603	86
Itatiaia	147	184
Pinheiral	224	5
Piraí	305	76
Porto Real	67	87
Quatis	109	177
Resende	1010	936
Rio Claro	19	6
Rio das Flores	38	2
Valença	191	147
Volta Redonda	3146	33

Fonte: Ministério da Saúde, DATASUS.

Variável	Ano	N	N*	Média	EP Média	DesvPad	Mínimo	Q1	Mediana	Q3	Máximo
Casos Dengue	2019	12	0	565,583	254,104	880,241	19	77,5	207,5	846,75	3146
	2022	12	0	147,25	74,1302	256,795	2	11,5	81	169,5	936

Figura 2. *Estatística Descritiva – Fonte: A autora (2024).*

Essa diferença pode ser visualizada no gráfico 1, em que, para o ano de 2019, a variação dos valores dos casos de dengue está mais concentrada, isto é, mais próximos da média, enquanto isto não se verifica para o ano de 2022. Segue-se os testes estatísticos para verificar se essa diferença é significativa.

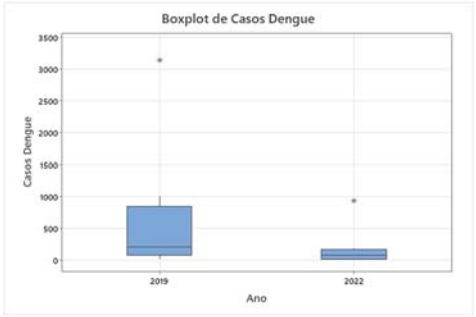


Gráfico 1. *Boxplot dos Casos*

Para atestar a diferença entre as médias, primeiro se verifica a normalidade dos dados, para se saber qual tipo de teste de hipótese será empregado. Considerando que são menos de trinta amostras, o teste utilizado é o de Shapiro-Wilk, que remeteu um *p-value* de menos de 0,010, muito inferior ao 0,05 convencional na literatura, de modo que os dados não são normais. Desnecessário verificar a igualdade de variância, neste caso segue para o teste de hipótese.

Teste de Normalidade

HO: Dados possuem distribuição normal

H1: Dados não possuem distribuição normal (Gráfico 2)

Significância = 5%

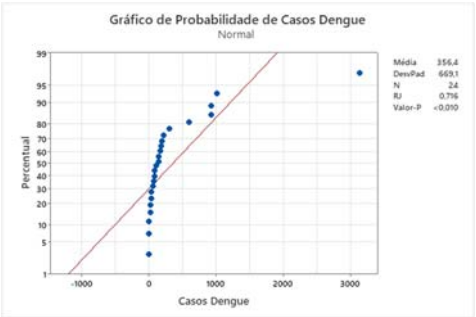


Gráfico 2. *Teste de Normalidade*

Considerando as amostras não normais, a opção é o uso de testes não paramétricos. Tendo em vista que são um fator, casos, dividido em dois grupos, os anos em questão, o teste mais adequado é o de Mann-Whitney, cujo resultado está ilustrado na figura 3.

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Hipótese nula	H_0: $\eta_1 - \eta_2 = 0$
Hipótese alternativa	H_1: $\eta_1 - \eta_2 \neq 0$

Método	Valor W	Valor-p
Não ajustado para empates	186,50	0,038
Ajustado para empates	186,50	0,038

Figura 3. *Teste de Hipótese – Fonte: Autora (2024).*

Pelo teste de Mann-Whitney, como *p-value* = 0,038, é inferior ao nível de significância estabelecido de 5% (= 0,05), então aceita-se a hipótese alternativa de que houve diferença significativa entre as amostras.

Há hipóteses que podem ser levantadas para justificá-lo: no Brasil, devido à mobilização nacional para o enfrentamento da pandemia da Covid-19, as equipes de vigilância epidemiológica estaduais e municipais tiveram que concentrar os seus esforços na identificação dos casos, corroborando com a hipótese de subnotificações das arboviroses durante esse período pandêmico (Mascarenhas *et al.,* 2020).

Algumas das medidas tomadas pelo Ministério da Saúde com o intuito de diminuir a transmissão do novo Coronavírus na população brasileira podem ter interferido para subnotificação das arboviroses. Durante a pandemia, recomendou-se que os Agentes de Combate às Endemias (ACE), evitassem entrar em residências para inspeções, alterando a rotina habitual. Além disso, houve a suspensão temporária das fiscalizações para eliminação dos criadouros do *Aedes aegypti* em alguns domicílios, e o afastamento dos profissionais com sintomas gripais. São fatores que poderiam ter dificultado as ações efetivas ao combate do vetor (Brasil, 2020).

Outro estudo também incluiu a subnotificação de dengue em 2020, observando uma mudança no comportamento dos dados epidemiológicos da doença. Houve uma queda significativa nas notificações, indicando a possibilidade de subnotificação dos casos de arboviroses (Leandro *et al.,* 2020). De acordo com Mascarenhas e colaboradores (2020), no estado do Piauí, outro estudo detectou a hipótese de subnotificação nos casos de dengue, observando apenas os coeficientes de incidência.

Vale ressaltar que a subnotificação de arboviroses distorce a realidade dos casos no país, reduzindo a percepção da gravidade da situação. É essencial que os casos sejam notificados corretamente para que os órgãos competentes utilizem esses dados de forma precisa e implementem medidas mais eficazes de promoção, proteção e controle em saúde, fortalecendo a ação multiprofissional.

4. CONCLUSÃO:

Após análise estatística dos dados em questão, chega-se à conclusão que a dengue é uma arbovirose reemergente e que constitui, hoje, a mais importante doença viral humana transmitida por mosquitos. E que a variação significativa dos casos de dengue na Região do Médio Paraíba do Sul nos anos de 2019 e 2022 reforça a necessidade de novas pesquisas e políticas públicas mais eficazes para o controle de doenças.

5. AGRADECIMENTOS:

Gostaria de agradecer à minha orientadora, pelo apoio e orientação, à Universidade de Vassouras (UNIVASSOURAS), especialmente ao Curso de Mestrado Profissional em Ciências Ambientais, e ao Centro Universitário de Barra Mansa (UBM). Agradeço também ao comitê organizador da *Southern Science Conference* por esta oportunidade de compartilhar o estudo.

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Southern Science Conference, 2024.

ANÁLISE ESTATÍSTICA DOS CASOS DE DENGUE NA REGIÃO DO MÉDIO PARAÍBA DO SUL, RJ

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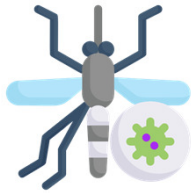
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November/2024

INTRODUÇÃO



A dengue é uma doença febril aguda de origem viral e reemergente que se destaca atualmente como um dos principais problemas de saúde pública.



O seu principal vetor de transmissão é o mosquito *Aedes aegypti.*



Atualmente, a forma mais eficaz de prevenir a dengue é a eliminação dos mosquitos vetores, uma vez que a vacina ainda não está disponível no Sistema Único de Saúde (SUS).



Para enfrentar as arboviroses, é crucial investir em promoção de saúde e prevenção, com ênfase na educação ambiental.

OBJETIVO

Assim, objetiva-se com este artigo analisar os dados dos casos de dengue dos anos de 2019 e 2022 na Região do Médio Paraíba do Sul, através do aplicativo *Minitab®*. Dessa maneira, será possível identificar a média de casos de dengue na região.

METODOLOGIA

A área de estudo compreende a Região do Médio Paraíba do Sul, estado do Rio de Janeiro, com uma extensão de 6.203.4 km², é composta por 12 municípios.

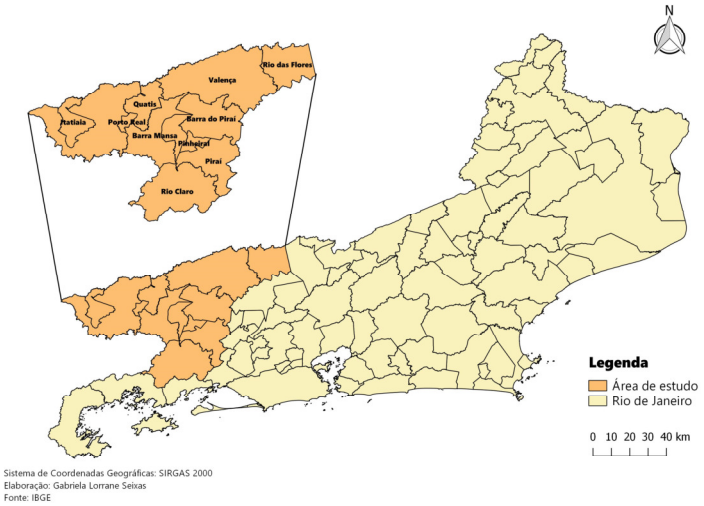


Figura 1: Localização da Região do Médio Paraíba do Sul, estado do Rio de Janeiro - Fonte: IBGE



SINAN
(Sistema Nacional de Agravos de Notificação)

DATASUS
Departamento de Informática do Sistema Único de Saúde

Os dados estatísticos foram tratados e aplicados ao *Software Minitab®* para comprovação do nível de significância dos casos de dengue na Região do Médio Paraíba do Sul.

RESULTADOS E DISCUSSÕES

Tabela 1: Casos de dengue, anos de 2019 e 2022

Município	2019	2022
Barra do Piraí	928	28
Barra Mansa	603	86
Itatiaia	147	184
Pinheiral	224	5
Piraí	305	76
Porto Real	67	87
Quatis	109	177
Resende	1010	936
Rio Claro	19	6
Rio das Flores	38	2
Valença	191	147
Volta Redonda	3146	33

Fonte: Ministério da Saúde, DATASUS.

Variável	Ano	N	N*	Média	EP Média	DesvPad	Mínimo	Q1	Mediana	Q3	Máximo
Casos Dengue	2019	12	0	565,583	254,104	880,241	19	77,5	207,5	846,75	3146
	2022	12	0	147,25	74,1302	256,795	2	11,5	81	169,5	936

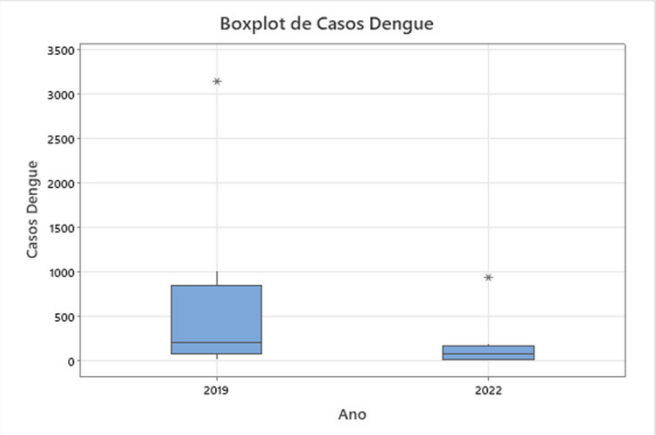
Figura 2: Estatística Descritiva – Fonte: A autora (2024).

Para o ano de 2019, a variação dos valores dos casos de dengue está mais concentrada;

Enquanto isto não se verifica para o ano de 2022.

Segue-se os testes estatísticos para verificar se essa diferença é significativa.

Gráfico 1: Boxplot dos casos



RESULTADOS E DISCUSSÕES



O teste utilizado é o de Shapiro-Wilk, que remeteu um *p-value* de menos de 0,010, muito inferior ao 0,05 convencional na literatura, de modo que os dados não são normais.

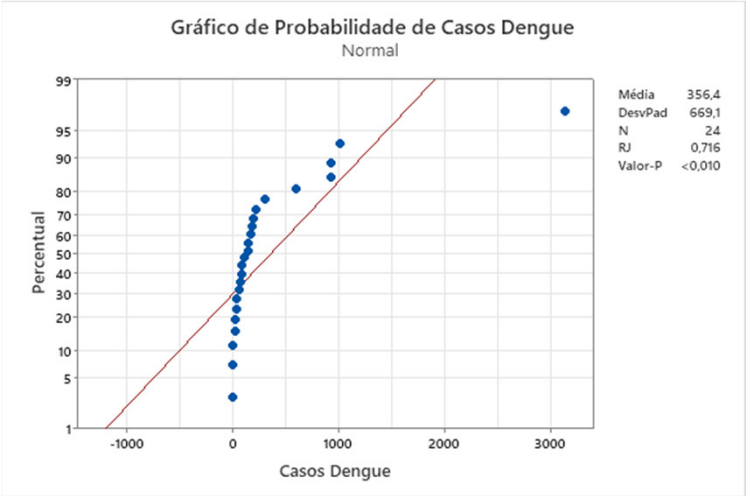


Desnecessário verificar a igualdade de variância, neste caso segue para o teste de hipótese.



Teste de Normalidade
HO: Dados possuem distribuição normal
H1: Dados não possuem distribuição normal (Gráfico 2)
Significância = 5%

Gráfico 2: Teste de Normalidade



RESULTADOS E DISCUSSÕES

Hipótese nula	$H_0: \eta_1 - \eta_2 = 0$
Hipótese alternativa	$H_1: \eta_1 - \eta_2 \neq 0$

Método	Valor W	Valor-p
Não ajustado para empates	186,50	0,038
Ajustado para empates	186,50	0,038

Figura 3. Teste de Hipótese – Fonte: Autora (2024).



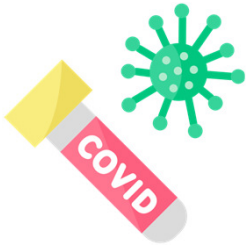
Pelo teste de Mann-Whitney, como ***p-value* = 0,038**, é inferior ao nível de significância estabelecido de 5% (= 0,05), então aceita-se a hipótese alternativa de que houve diferença significativa entre as amostras.



Mascarenhas *et al*. (2020)
Hipótese de subnotificações das arboviroses durante o período pandêmico.



Brasil (2020)
Suspensão temporária das fiscalizações para eliminação dos criadouros do *Aedes aegypti* em domicílios. São fatores que poderiam ter dificultado as ações efetivas ao combate do vetor.



Leandro *et al.* (2020).
Outro estudo incluiu a subnotificação de dengue em 2020, observando uma mudança no comportamento dos dados epidemiológicos da doença. Houve uma queda significativa nas notificações, indicando a possibilidade de subnotificação dos casos de arboviroses

CONCLUSÃO

• Após análise estatística dos dados em questão, chega-se à conclusão que a dengue é uma arbovirose reemergente e que constitui, hoje, a mais importante doença viral humana transmitida por mosquitos.

• E a variação significativa dos casos de dengue na Região do Médio Paraíba do Sul nos anos de 2019 e 2022 reforça a necessidade de novas pesquisas e políticas públicas mais eficazes para o controle de doenças.

AGRADECIMENTOS

Gostaria de agradecer à minha orientadora, pelo apoio e orientação, à Universidade de Vassouras (UNIVASSOURAS), especialmente ao Curso de Mestrado Profissional em Ciências Ambientais, e ao Centro Universitário de Barra Mansa (UBM). Agradeço também ao comitê organizador da *Southern Science Conference* por esta oportunidade de compartilhar o estudo.

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GAS-PHASE REACTIVITY OF SUBNANOMETRIC BARIUM CLUSTERS WITH METHANOL UNDER THERMALIZATION CONDITIONS

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ABSTRACT

Basic oxides play a crucial role in various industrial catalytic processes due to their ability to activate the O-H, C-H, and C-O bonds of simple alcohols on the M^{2+}-O^{2-} catalytic center, which consists of a Lewis acid and a Brønsted base. This study investigated the mechanisms at the molecular level of gas-phase reactions between methanol and cationic subnanometric barium-containing clusters, namely, $Ba^{\bullet+}$, $Ba(OH)^+$, and $Ba(H_2O)^{\bullet+}$, which are used as model systems for the active sites of heterogeneous basic oxide catalysts. The experiments were performed under thermalization conditions at 291.5 K on a new experimental setup based on a Smalley cluster source coupled to a fast flow reactor, which is enclosed in a molecular beam apparatus with time-of-flight mass spectrometry detection. Complementary theoretical calculations at the density functional theory level were carried out on the various relevant reactions to aid in the interpretation of the experiments. The joint experimental and theoretical results suggest that the adsorptive behavior of basic oxides like BaO towards methanol and water molecules can already be evidenced in these small clusters, reinforcing their role as potential active sites in heterogeneous basic catalysts.

Keywords: *subnanometric barium-containing clusters, methanol, gas-phase reactions, thermalization conditions, fast flow reactor.*

1. INTRODUCTION

The gas-phase research on subnanometric metallic clusters has deepened the understanding of processes relevant to heterogeneous catalysis,[1] as these clusters can be conceived as models of active sites in macroscopic-scale catalysts.[2] These reactive systems are relatively small, making their theoretical investigation feasible through *ab initio* methods. Theoretical results can be directly compared with experimental gas-phase studies, affording a complete mechanistic picture for catalytically relevant reactions. This work presents a newly developed experimental methodology based on a fast flow reactor, which, in combination with molecular beam techniques and mass spectrometry, allowed for the first study of the mechanistic aspects of reactions between barium-containing cationic clusters and methanol at the molecular level, under thermalization conditions near room temperature (291.5 K).

Amongst various types of catalysts used in the chemical industry, basic oxides like BaO stand out as relevant in several chemical processes, including dehydration, decarboxylation, transesterification, and hydrocarbon reforming. Their minimum active center is a M^{2+}-O^{2-} pair, where the M^{2+} and the O^{2-} sites act as a Lewis acid and a Brønsted base, respectively, which are capable of accepting an electron pair and an H^+. This endows basic oxides with the capability to adsorb acidic species from the environment (CO, CO_2, H_2O, O_2), which in the case of water is industrially relevant because its adsorption leads to catalyst passivation. Pretreatment to desorb H_2O is thus mandatory for such basic catalysts.[2]

At the M^{2+}-O^{2-} catalytic center, water can either adsorb or dissociate (dissociative adsorption) into OH^- and H^+. In the last case, OH^-

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and H^+ are adsorbed onto the M^{2+} and O^{2-} sites, respectively,[1] thereby inhibiting them. For this reason, this work addressed the study of the reactions of $Ba^{\bullet+}$, $Ba(OH)^+$, and $Ba(H_2O)^{\bullet+}$, used as models for the active sites of solid BaO. The $Ba^{\bullet+}$ species represents an extreme case of low coordination, where a barium atom is highly exposed. The $Ba(H_2O)^{\bullet+}$ and $Ba(OH)^+$ species could result from the ability of BaO(s) to adsorb and react with ambient moisture. The present combined experimental and theoretical results allow us to infer the potential of these systems to promote the dissociative adsorption of methanol.

2. MATERIALS AND METHODS

The experiments were performed under high vacuum conditions in a molecular beam instrument coupled to a time-of-flight mass spectrometer (TOF-MS) (Figure 1). It encloses a lab-made laser desorption/supersonic expansion (Smalley type) cluster source coupled to a fast flow reactor (FFR).[1] In the Smalley source, a barium disk (10 mm diam) was vaporized by the focussed 532 nm output of a Nd:YAG laser and the vapor was entrained into a He flow arising from a pulsed valve (backing pressure: 2 bar), the relative delays being chosen to maximize production of the desired species. Hydrated clusters were produced by the presence of ambient humidity in the carrier gas. Barium-containing clusters were formed in the inner channel (diam: 2.0 mm) of the Smalley source and expanded into the FFR (inner diam: 6 mm; length: 60 mm),[1,3] where the reactant CH_3OH gas (seeded in He; backing pressure: 1 bar) was injected by a second pulsed valve. This is admitted into the FFR 30 mm downstream from the exit of the cluster source. The time delay between the two valve openings was adjusted to maximize the reaction of the relevant clusters with methanol. The total pressure and the temperature in the FFR are estimated at ~ 5.7 torr and 291.5 K, respectively, in the presence of a reactant gas pulse.[3] The latter is close to ambient temperature (298 K) due to the large number of collisions between the clusters and the He bath in the FFR.

Barium clusters exiting the Smalley source are expected to be rotationally cold (T_{rot} ~ 70 K) and vibrationally hot (T_{vib} ~ 500 K).[3] The number of collisions that a $Ba(OH)^+$ cluster (radius: 0.31 nm) experiences with the He bath (radius = 0.05 nm; T: 291.5 K; P: 5.7 Torr) in the FFR is about 65 per 1 mm of forward motion. This corresponds to a collision rate of 10^7 s^{-1} for an approaching velocity of 697.7 m/s. Considering that the reactor length (60 mm) is much longer than 1 mm, the intracluster vibrations are likely equilibrated to the He bath temperature before reacting with the diluted (0.05-0.2%) CH_3OH gas. The reactant and product ionic species in the cluster beam were detected by the TOF-MS running in pulsed mode.

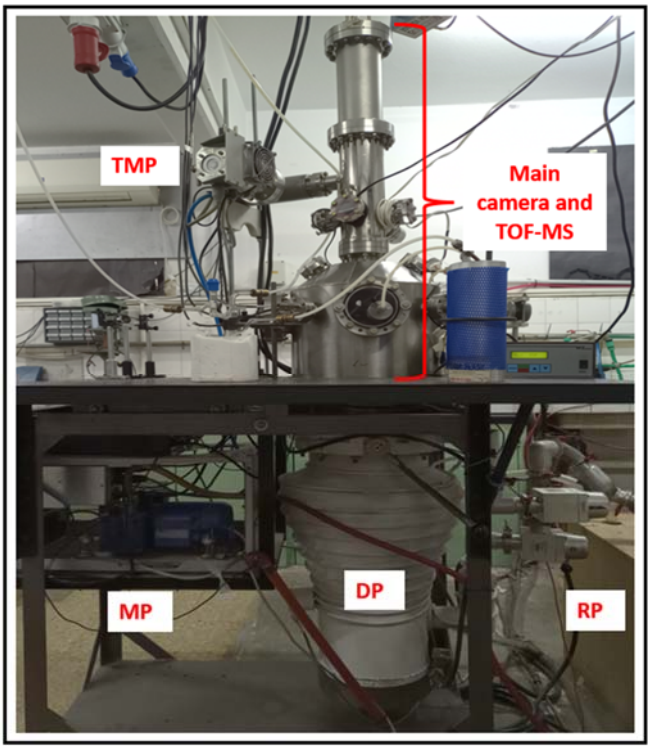


Figure 1. *Experimental setup. TMP: turbomolecular pump; MP: mechanical pump; DP: Diffusion pump; RP: rotary pump.*

Density functional theory (DFT) calculations using the GAUSSIAN 16 software were employed to study reactions of $Ba^{\bullet+}$, $Ba(OH)^+$, and $Ba(H_2O)^{\bullet+}$ with CH_3OH. This involved geometry optimization of stable species, reaction intermediates, and transition states. For the latter, either the Berny algorithm or the synchronous transit-guided quasi-Newton (STQN) method were used. Harmonic vibrational frequency calculations were performed to identify stable species/reaction intermediates (all positive frequencies) and transition states (one imaginary frequency). The hybrid B3LYP exchange-correlation functional was used, along with the standard TZVP basis set for the C, O, and H atoms and the SDD pseudo-potential for Ba atoms. The Gibbs free energies at 291.5 K ($\Delta G^{\circ}_{291.5\ K}$) are reported in this study.

3. RESULTS AND DISCUSSION:

The Smalley source produced supersonic beams of barium-containing clusters with low internal energies, ensuring that the generated

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species populated their lowest roe-vibronic levels. Such clusters passed through the FFR and were collimated before entering the detection chamber of the TOF-MS. The reactivity experiments were conducted in two stages. First, a mass spectrum of the clusters with He (buffer) gas inside the FFR and in the absence of reactants were recorded to obtain accurate distributions of the size and composition of the reactants. Second, methanol seeded in He was introduced in the FFR, leading to the formation of van der Waals complexes with the barium clusters and their subsequent reaction, and the record of another mass spectrum allowed to identify the various reaction products.

Figure 2 shows the overlaid spectra corresponding to both reactive experiments of $Ba^{\bullet+}$, $Ba(OH)^+$, and $Ba(H_2O)^{\bullet+}$ with CH_3OH. $Ba^{\bullet+}$ is predominantly observed, along with $Ba(OH)^+$ and $Ba(H_2O)^{\bullet+}$, in the spectrum corresponding to He within the FFR (blue line). In the methanol spectrum (red line), the intensity of $Ba^{\bullet+}$ decreases compared to that in the He spectrum, alike the peaks corresponding to $Ba(OH)^+$ and $Ba(H_2O)^{\bullet+}$, indicating that all three species react with CH_3OH. As well it is observed the appearance of mass peaks at 169 and 170 amu, corresponding to the $Ba(OCH_3)^+$ and $Ba(CH_3OH)^{\bullet+}$ reaction products, respectively. These products are consistent with the reaction of $Ba^{\bullet+}$ with methanol and were previously identified in experiments carried out under single-collision conditions.[4] Mass peaks at 187 and 188 amu also appear, corresponding to the $Ba(OH)(CH_3OH)^+$ and $Ba(H_2O)(CH_3OH)^{\bullet+}$ association products of $Ba(OH)^+$ and $Ba(H_2O)^{\bullet+}$ with CH_3OH, respectively.

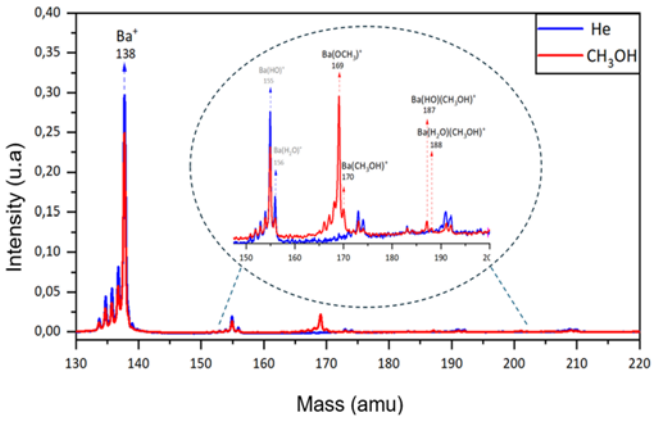


Figure 2. *Superimposed mass spectra of the experiments with He and with CH_3OH:He in the FFR.*

On this basis, a preliminary reaction mechanism is proposed to explain the observations, starting with collisions between $Ba^{\bullet+}$ and CH_3OH:

$$Ba^{\bullet+} + CH_3OH \rightarrow Ba(CH_3OH)^{\bullet+} \quad \text{(Eq. 1)}$$

$$Ba(CH_3OH)^{\bullet+} \rightarrow Ba(OH)^+ + CH_3^{\bullet} \quad \text{(Eq. 2)}$$

$$Ba(CH_3OH)^{\bullet+} \rightarrow Ba(OCH_3)^+ + H^{\bullet} \quad \text{(Eq. 3)}$$

For collisions between $Ba(OH)^+$ and $Ba(H_2O)^{\bullet+}$ with CH_3OH:

$$Ba(OH)^+ + CH_3OH \rightarrow Ba(OH)(CH_3OH)^+ \quad \text{(Eq. 4)}$$

$$Ba(H_2O)^{\bullet+} + CH_3OH \rightarrow Ba(H_2O)(CH_3OH)^{\bullet+} \quad \text{(Eq. 5)}$$

To corroborate the proposed reaction mechanism, the differences in the integrated intensities of the reactant and product species (considering only the ^{138}Ba isotope) were derived from the two mass spectra. By comparing the drop in the $Ba^{\bullet+}$ intensity, of -0.00909 ± 0.00006, with the total intensity increase for its products (mass peaks 169, 170 amu), of 0.0094 ± 0.0001, it is found that they do not match within the experimental error. The amount of product is greater than expected, indicating that some of these products are formed through an additional reaction pathway. Similarly, the drop in $Ba(OH)^+$ intensity, of -0.00103 ± 0.00006, and the increase in $Ba(OH)(CH_3OH)^+$ intensity, of 0.00066 ± 0.00003, do not match as well. In this case, less product than expected is produced, suggesting that $Ba(OH)^+$ might participate in an additional reaction channel, apart from that leading to $Ba(OH)(CH_3OH)^+$. A different situation is found when comparing the drop in $Ba(H_2O)^{\bullet+}$ intensity, of -0.00029 ± 0.00006, with the increase in $Ba(H_2O)(CH_3OH)^{\bullet+}$ intensity, of 0.00029 ± 0.00003, i.e., the values do match within experimental error. Altogether, it is apparent that the proposed mechanism is incomplete, and an additional condensation reaction between $Ba(OH)^+$ and methanol is proposed to complete the mechanism:

$$Ba(OH)(CH_3OH)^+ \rightarrow Ba(OCH_3)^+ + H_2O \quad \text{(Eq. 6)}$$

Equation 6 describes a dehydration channel for the $Ba(OH)^+ + CH_3OH$ reaction (Eq. 4), yielding the 169 amu product, which is the same as the hydrogen loss product (Eq. 3) of the $Ba^{\bullet+} + CH_3OH$ reaction. It allows to reconcile the observation of a greater product intensity for the $Ba^{\bullet+}$ reaction and a smaller intensity for the $Ba(OH)^+$ association product. This is evident by

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comparing the total intensity drop for the $Ba^{\bullet+}$ and $Ba(OH)^+$ reactants, of -0.0101 ± 0.0001, with the total intensity increase for the products from Eqs. 1-4 and 6, of 0.0100 ± 0.0003, which confirms the success of the full reaction mechanism to explain the observations.

The experimental results were complemented by DFT theoretical calculations exploring the reactivity of methanol towards any metal cluster due to the activation of one of its three different types of bonds.

For $Ba^{\bullet+}$, it was found that only two bonds are susceptible to activation: The O-H and C-O bonds. These lead to the $Ba(OCH_3)^+ + H^\bullet$ and the $BaOH^+ + CH_3^\bullet$ exit channels with $\Delta G^o_{291.5\,K}$ values of -0.25 and -1.78 eV, respectively. Both reaction pathways have barriers below the Gibbs energy for the entrance channel. The activation of the C-H bond has a barrier above the entrance channel for 0.44 eV and a $\Delta G^o_{291.5\ K}$ of 1.34 eV for the $Ba(HOCH_2)^+ + H^\bullet$ exit channel.

For $Ba(OH)^+$, the activation of the O-H, C-H, and C-O bonds leads to the $Ba(OH)(OCH_3)^+ + H^\bullet$, $Ba(OH)(HOCH_2)^+ + H^\bullet$ and $Ba(OH)_2^+ + CH_3^\bullet$ exit channels featuring $\Delta G^o_{291.5\,K}$ values of 3.60 eV, 3.50 eV, and 2.49 eV, respectively. The full reaction channel for Eqs. 4 and 6 is energetically favoured with $\Delta G^o_{291.5\,K}$ = -0.06 eV.

For $Ba(H_2O)^{\bullet+}$, it was found that the activation of the O-H, C-H, and C-O bonds are energetically disallowed. In the case of the C-H and O-H bond activations, lead to the $Ba(H_2O)(HOCH_2)^+ + H^\bullet$ and $Ba(H_2O)(OCH_3)^+ + H^\bullet$ exit channels have $\Delta G^o_{291.5\,K}$ values of 2.00 eV and 0.40 eV, respectively. Instead, $Ba(H_2O)(OH)^+ + CH_3^\bullet$ exit channel for C-O bond activation has a $\Delta G^o_{291.5\ K}$ value of -1.18 eV, yet its Gibbs energy barrier is 0.19 eV, thus preventing the process.

In summary, theoretical calculations support the experimentally observed products. The products with masses 170, 187, and 188 amu correspond to methanol association complexes with $Ba^{\bullet+}$, $Ba(OH)^+$, and $Ba(H_2O)^{\bullet+}$, which are energetically allowed. The 169 amu product arises from two different reaction pathways, i.e., with $Ba^{\bullet+}$ and $Ba(OH)^+$. Finally, the $Ba(H_2O)^{\bullet+}$ cluster does not present any reactive pathways.

4. CONCLUSIONS:

In this study, the gas-phase reactivity of subnanometric barium-containing clusters, which model the active sites of solid BaO was investigated. The joint experimental and theoretical results suggest that the adsorptive behavior of such basic oxide towards methanol can already be evidenced in these small clusters.

The $Ba^{\bullet+}$, $Ba(OH)^+$, and $Ba(H_2O)^{\bullet+}$ species exhibit stable association complexes with methanol, as expected for heterogeneous basic catalysts featuring favorable adsorption sites for methanol.[2] Furthermore, the $Ba^{\bullet+}$ and $Ba(OH)^+$ species show a tendency to activate the O-H bond of CH_3OH leading to the product of dissociative adsorption, $Ba(OCH_3)^+$. This is the initial intermediate species in the reaction mechanisms proposed for processes requiring methanol activation.[2] In contrast, the observation of only the association product for the $Ba(H_2O)^{\bullet+}$ cluster is compatible with the evidence for active site inhibition by adsorbed water in heterogeneous basic catalysts.

5. DECLARATIONS

5.1. Open Access

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GAS-PHASE REACTIVITY OF SUBNANOMETRIC BARIUM CLUSTERS WITH METHANOL UNDER THERMALIZATION CONDITIONS

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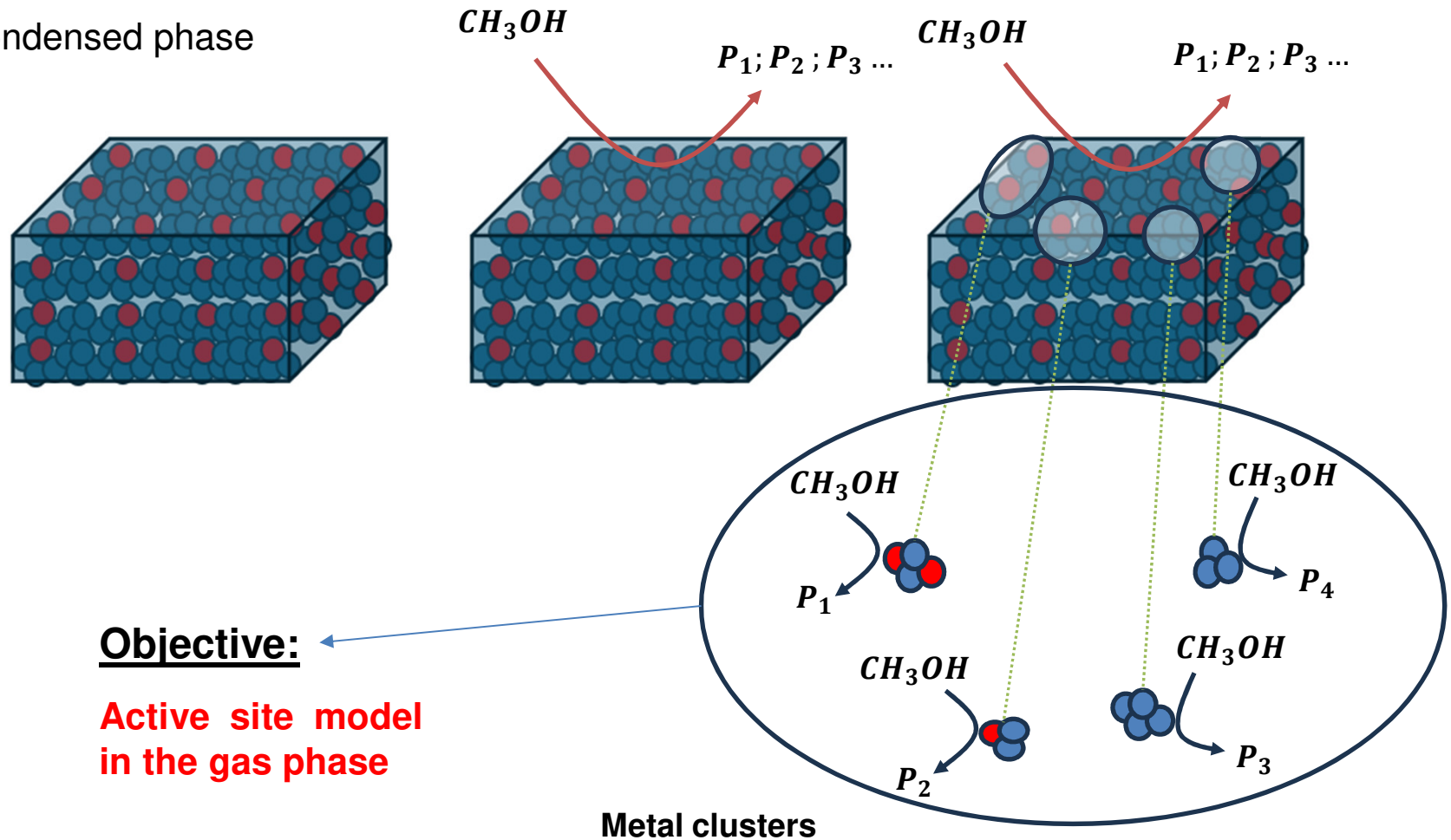
Centro Láser de Ciencias Moleculares, Universidad Nacional de Córdoba, X5000HUA, Córdoba, Argentina.

November /2024

INTRODUCTION

Basic heterogeneous catalysts

Condensed phase



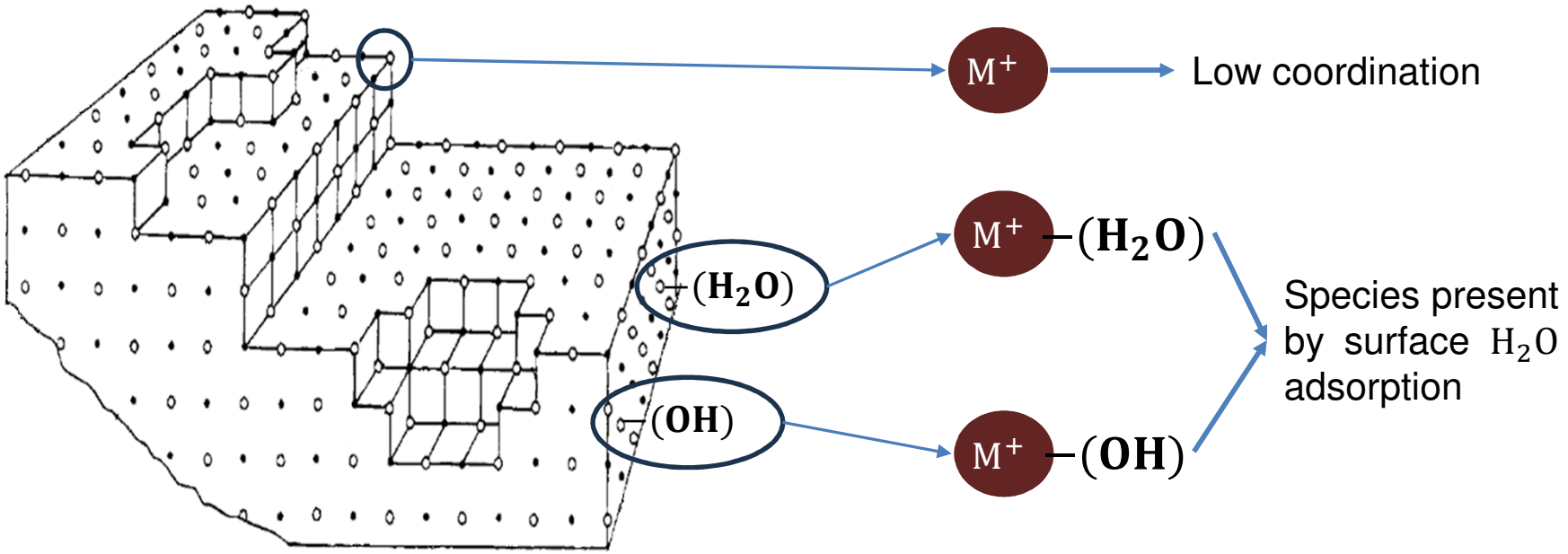
Objective:

Active site model in the gas phase

INTRODUCTION

Barium oxide

Barium containing clusters



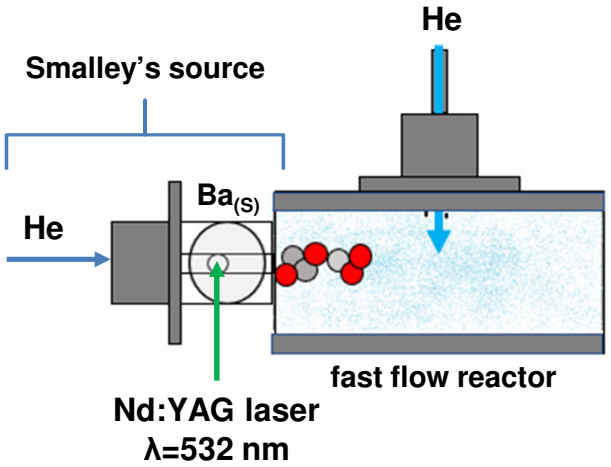
Representation of the different surface defects on BaO. Spheres: Black: O^{2-}; White: Ba^{2+}.

Active site models

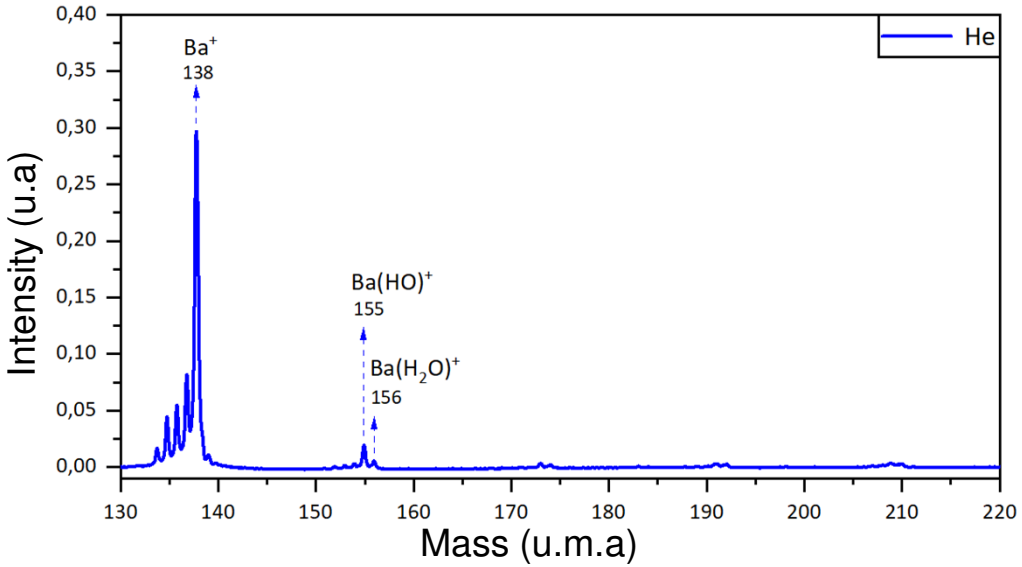
Macroscopic

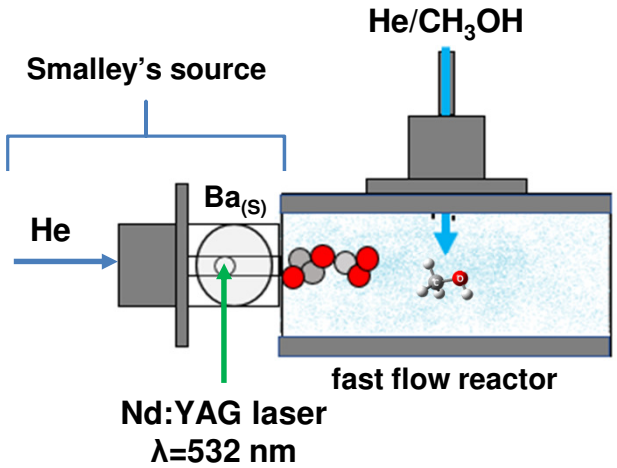
Subnanometric

RESULTS AND DISCUSSION

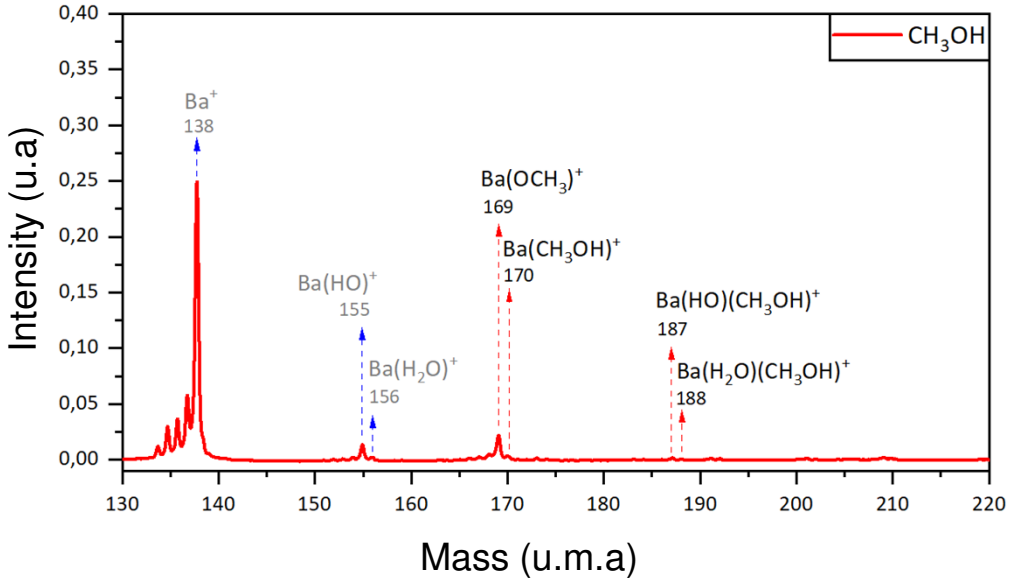


High vacuum:1x10-5 mbar



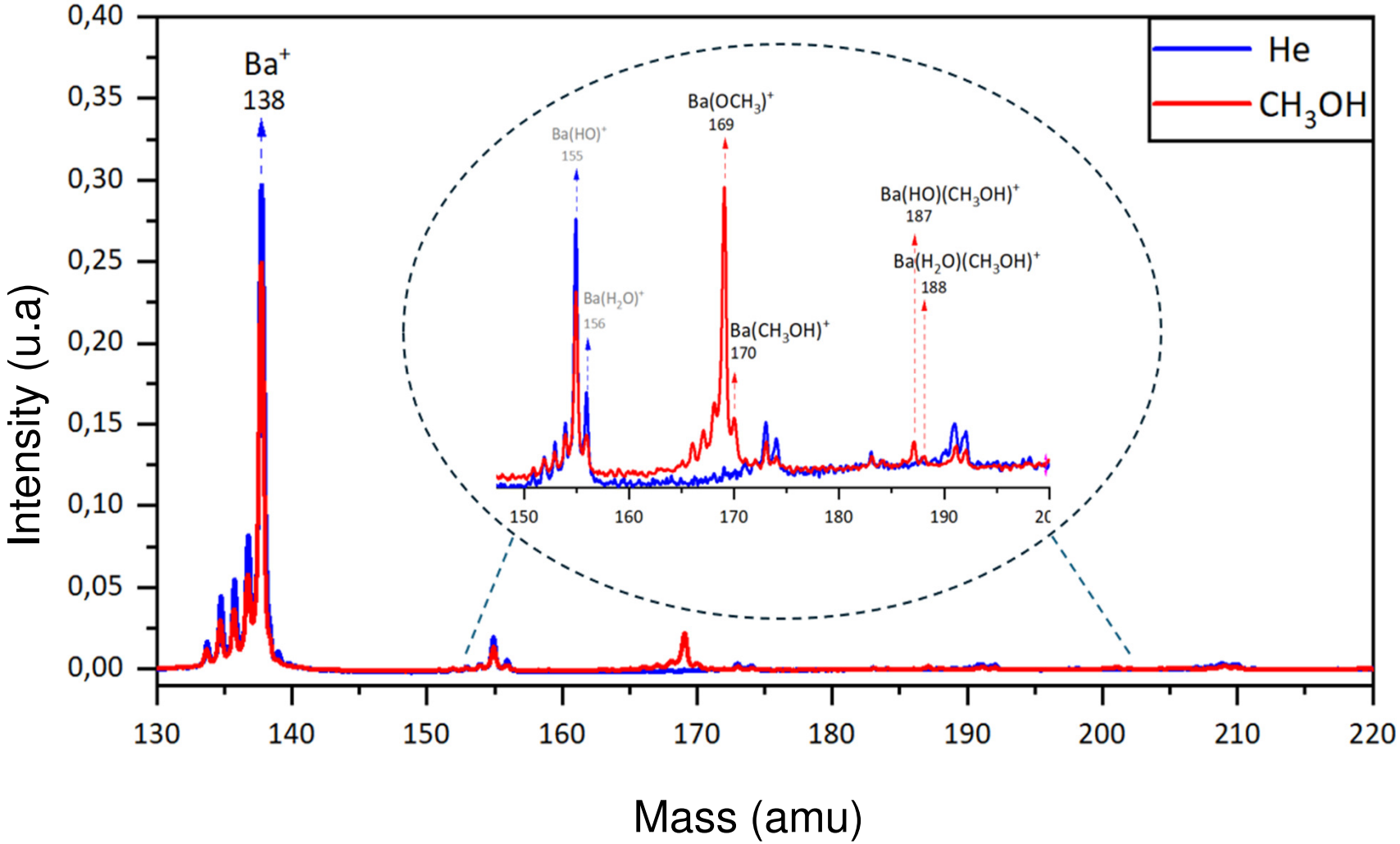


High vacuum:1x10-5 mbar



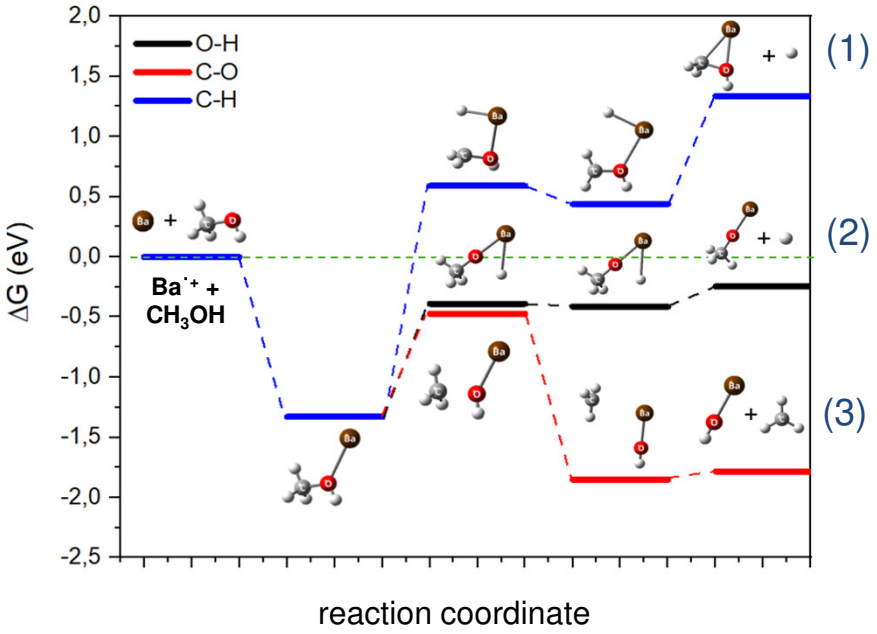
RESULTS AND DISCUSSION

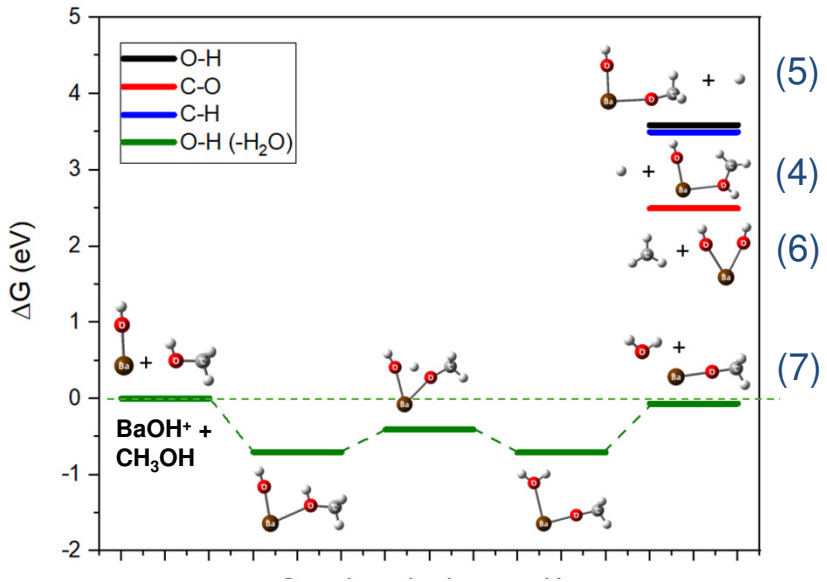
Analysis of the overlapping mass spectra

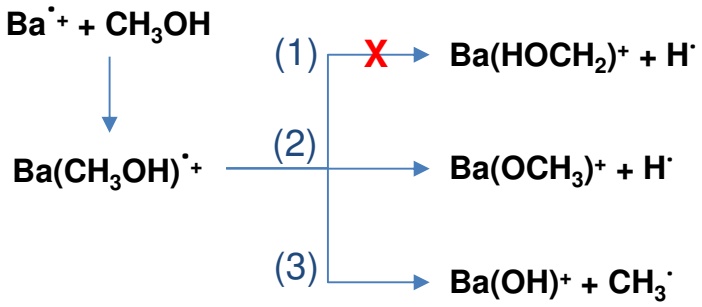


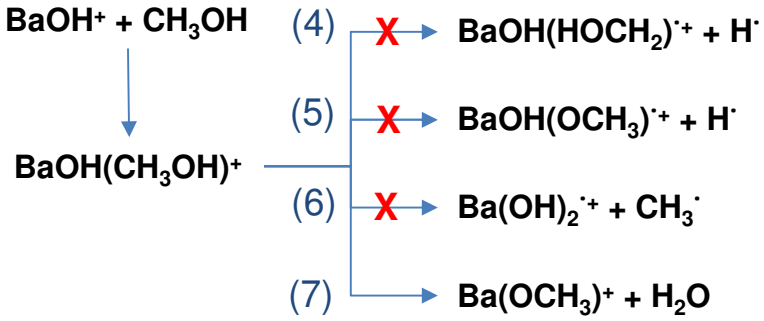
RESULTS AND DISCUSSION

Theoretical calculations at the DFT level:
B3LYP functional and the TZVP basis set (for C, H, and O) and LSS pseudopotential (for Ba).





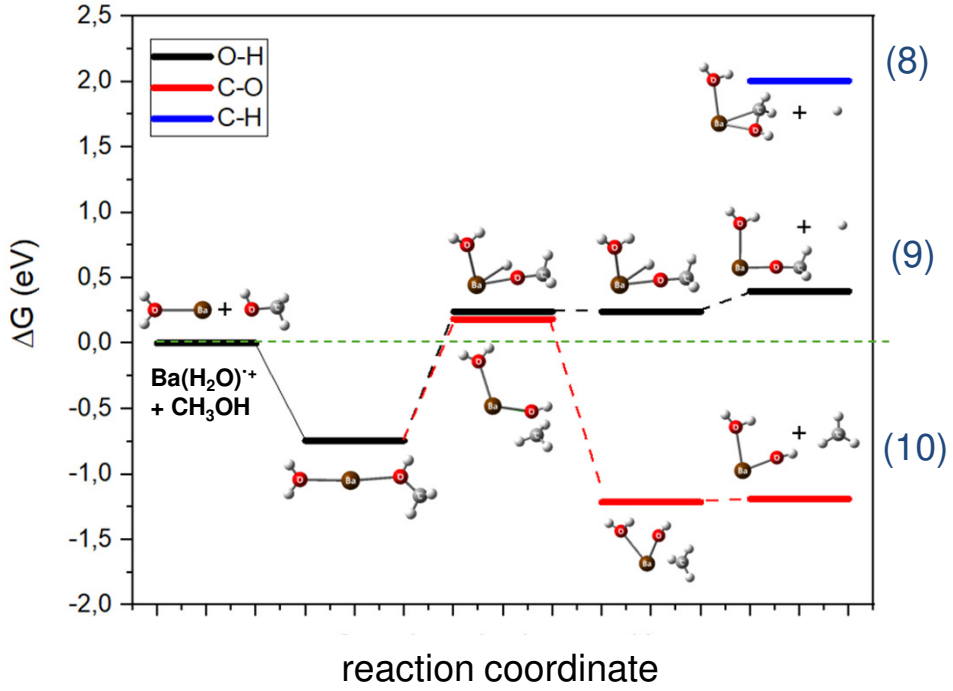


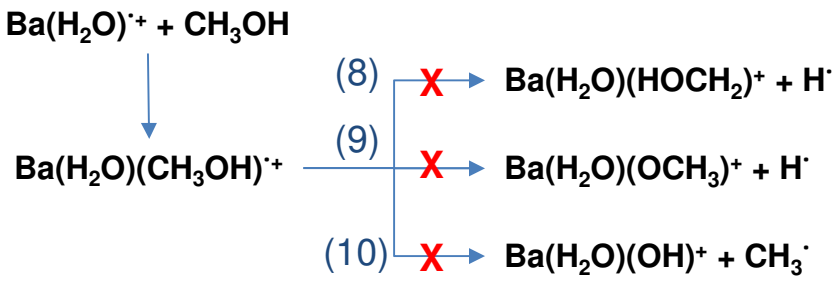


RESULTS AND DISCUSSION

Theoretical calculations at the DFT level:

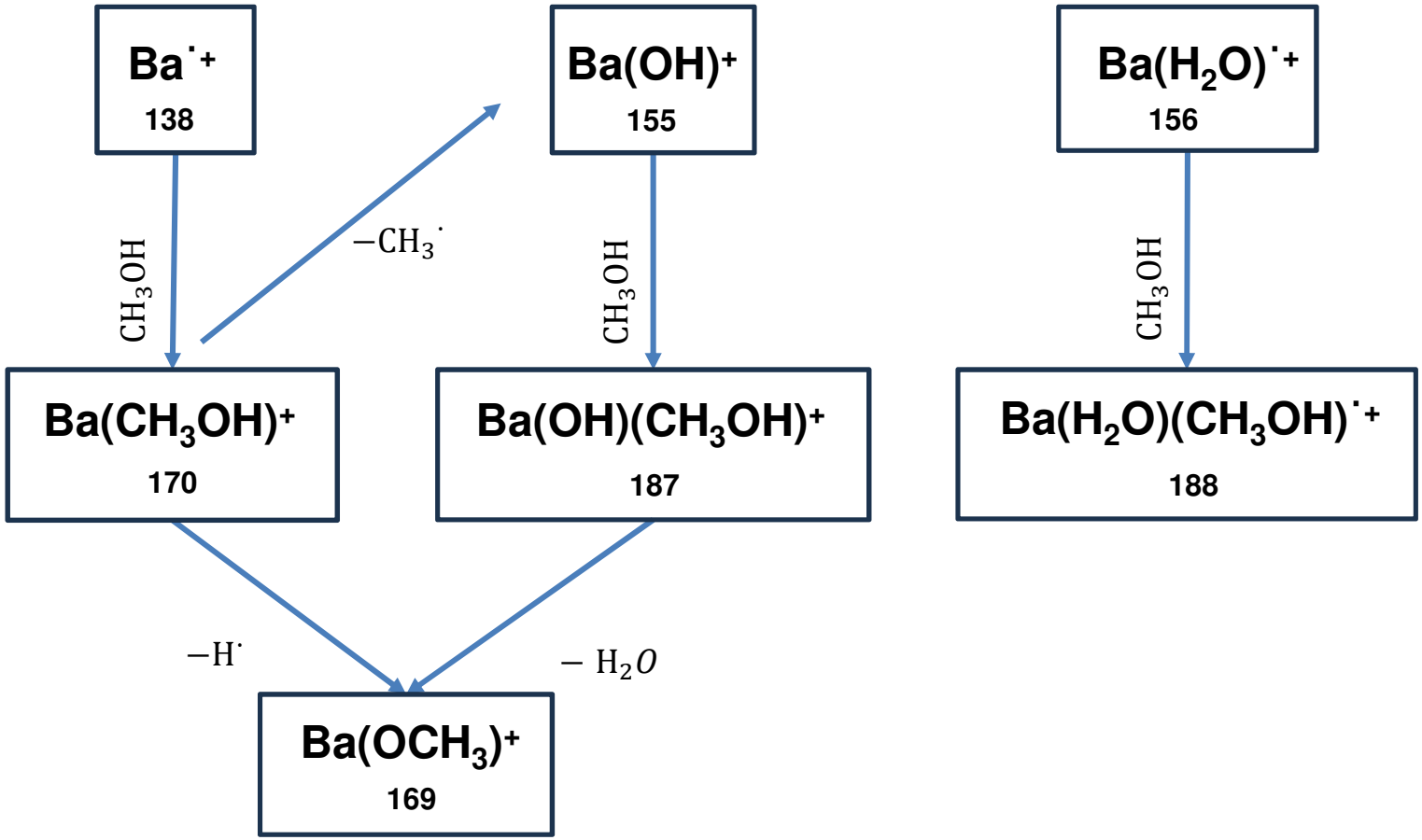
B3LYP functional and the TZVP basis set (for C, H, and O) and LSS pseudopotential (for Ba).





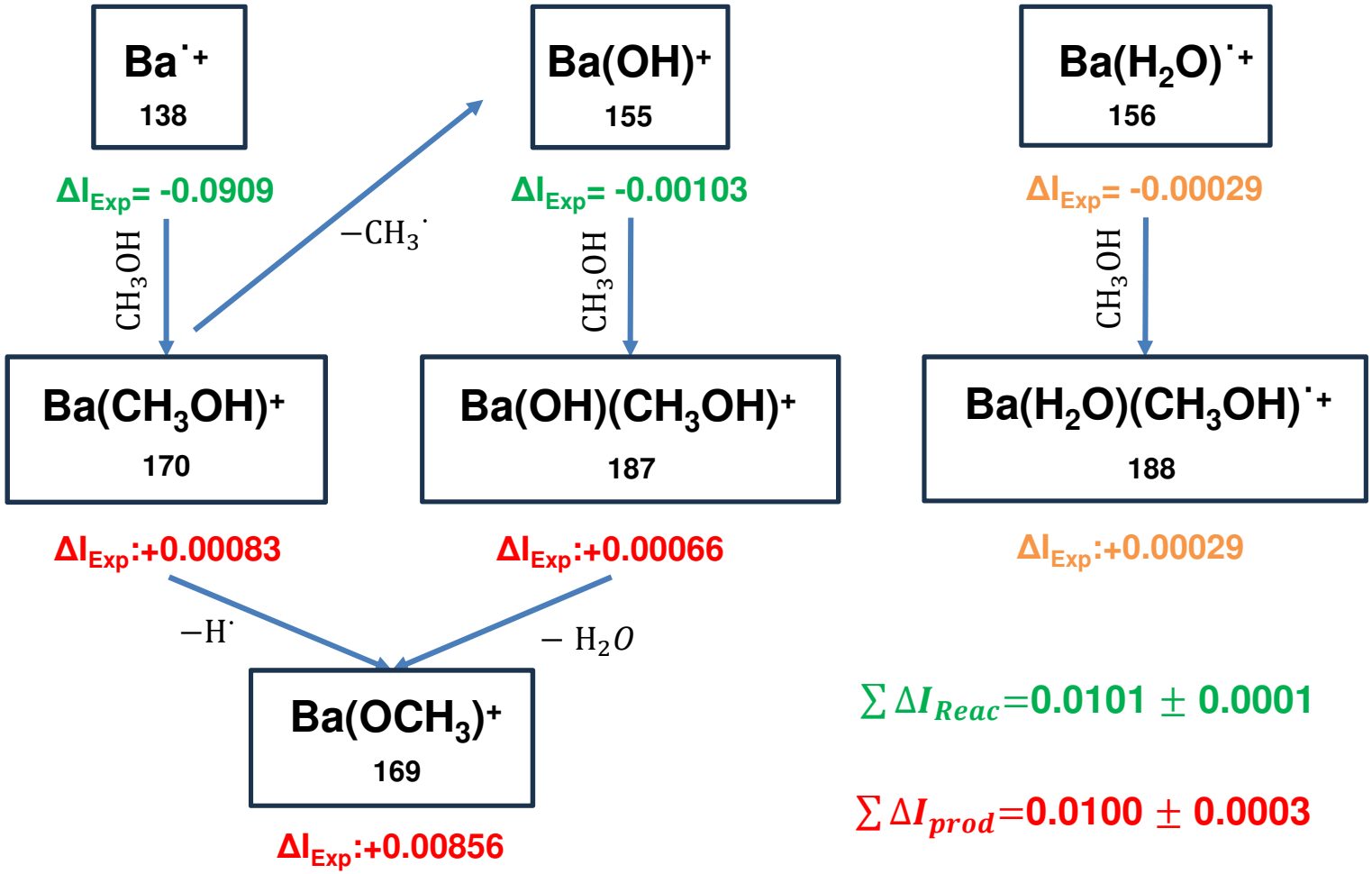
RESULTS AND DISCUSSION

Summary of experimental and theoretical results



RESULTS AND DISCUSSION

Summary of experimental and theoretical results



$\sum \Delta I_{Reac}$=0.0101 ± 0.0001

$\sum \Delta I_{prod}$=0.0100 ± 0.0003

ΔI_{Exp}: Intensity difference between helium and methanol experiments in RFR

CONCLUSIONS

- An experimental **methodology** was developed and optimized using a **fast-flow reactor** coupled with a **Smalley source**, enabling the study of reaction **mechanisms at the atomic-molecular scale** for **sub-nanometric clusters** in catalytically relevant processes.

- The **Ba species** exhibit a tendency to form stable **association complexes**, consistent with observations in basic catalysts, which feature different adsorption sites for methanol. (*Hereijgers, Bart PC; Weckhuysen, Bert M. Chem.Sus.Chem, 2009, vol. 2, no 8, p. 743-748.).*

- The **Ba^+ and $Ba(OH)^+$ species** are capable to **activate the O-H bond** in CH_3OH (dissociative adsorption).

- The **$Ba(H_2O)^+$** cluster shows that adsorbed water inhibits the **active site (Ba^+)**, which is in line with known behavior for several basic heterogeneous catalysts (*Hattori, Hideshi.Applied Catalysis A, 2015, vol. 504, p. 103-109*).

ACKNOWLEDGEMENTS

Laser Chemistry and Non-Covalent Interactions



UNC Universidad Nacional de Córdoba

DFQ Departamento de Fisicoquímica

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SILICA NANOPARTICLES: EXPLORING A GREENER ONE-POT SYNTHESIS

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ABSTRACT

In this work, we report a facile one-pot synthesis of silica nanoparticles (SiO_2NPs) than the classical Stöber method, involving sodium metasilicate as a cheaper Si source than TEOS and shorter reaction times under neutral reaction conditions at room temperature. A multi-technical characterization of the SiO_2NPs (XRD, FTIR, UV-vis DR,TEM, Z-potential, and N_2 adsorption-desorption isotherms at 77 K) evidenced the formation of spherical NPs, with a polydisperse nature, negatively charged surface, and porous structure. A metric to assess the "greenness" of the proposed SiO_2NPs synthesis allows to indicate that is a more environmentally friendly process than other chemical procedures, which was performed under mild conditions, such as room temperature and ambient pressure, without a derivatization process, using only water as solvent, and generating innocuous waste.

Keywords: *SiO_2 nanoparticles; Eco-friendly synthesis; Mild conditions; Green star analysis*

1. INTRODUCTION

There are three distinct strategies available for the synthesis of silica nanoparticles (SiO_2NPs): biological, physical, and chemical. The former has been introduced as a novel methodology to synthesize nanoparticles easily and cheaply. In this sense, the SiO_2NPs synthesis using plant extracts, fungi, algae, and microbes has taken a lot of interest due to its numerous advantages, especially for biomedical applications. In contrast, physical techniques often require sophisticated and expensive equipment, operating under harsh pressure and temperature conditions. In the case of chemical procedures, the sol-gel method is the best known and most widely used (Paul *et al.*, 2019). It consists of the hydrolysis and subsequent condensation of metal alkoxides such as TEOS and TMOS, or inorganic salts like sodium silicate, in the presence of an acidic or basic catalyst (Akhter *et al.*, 2022). Typically, acid-catalyzed systems produce a gel-like structure, while base-catalyzed ones as the classical Stöber method, give monodisperse silica particles (Tabisz *et al.*, 2020).

In this work, we provide a facile and eco-friendly one-pot sol-gel method as a promising alternative for the chemical synthesis of silica nanoparticles. The synthesized SiO_2NPs were characterized by XRD, FTIR, UV-vis DR,TEM, Z-potential, and N_2 adsorption-desorption isotherms at 77 K, being the most important techniques discussed. Although most chemical syntheses are neither economical nor environmentally friendly, we have found a methodology that requires a cheaper Si source and greener synthesis conditions than the conventional method, and short reaction times.

2. MATERIALS AND METHODS

2.1. Materials

Sodium metasilicate pentahydrate ($Na_2SiO_3.5H_2O$, Aldrich > 95%), hydrochloric acid (HCl, Alkemit 37%), nitric acid (HNO_3, Cicarelli ≥ 96%), glacial acetic acid (CH_3COOH, Anedra 99.7%), and phosphoric acid (H_3PO_4, Cicarelli 85%).

2.2. Synthesis of SiO_2NPs

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DOI: 10.48141/SSCON_12_2024.pdf

Under optimized synthesis conditions, an aqueous Na_2SiO_3 solution (0.30 M, initial pH = 14) at pH = 7 adjusted drop by drop with 4.0 M CH_3COOH, was stirred vigorously for 4 h at room temperature. The gel was separated by vacuum filtration and washed with Milli-Q water repeatedly. Finally, it was dried in an oven at 200 °C for 5 h. Different variables, such as synthesis temperature, pH, drying temperature, and time, were previously explored until the optimal conditions were reached.

2.3. Characterization

X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR) allowed to analyze the structure and the functional groups of the SiO_2NPs, respectively. Their formation was confimed by UV-vis diffuse reflectance spectroscopy (UV-vis DR) and their surface morphology was studied by transmission electron microscopy (TEM). Z-potential measurements were performed to determine the surface charge of SiO_2NPs. The surface morphology of the nanoparticles was studied by transmission electron microscopy (TEM) and their textural properties by N_2 adsorption-desorption isotherms at 77 K using a Micromeritics instrument.

2.4. 'Green Star' analysis

Green Star (GS) is a semi-quantitative metric designed to evaluate the greenness of a chemical procedure implementing the principles of green chemistry as cornerstones. The star is constructed with 10 corners corresponding to the green principles that apply to the study. For each principle a score from 1 to 3 is assigned (being 3 the maximum greenness value), considering the predefined criteria reported by Ribero *et al.* (2010). The GS of our synthesis procedure of SiO_2NPs was compared with previous ones of similar nature, which helped to choose the most environmentally friendly protocol.

3. RESULTS AND DISCUSSION

One-pot synthesis of SiO_2NPs involves two reaction steps: first, the acidic hydrolysis of Na_2SiO_3 leads to the formation of silanol groups of silicic acid, and subsequently, the condensation reaction takes place. Experimentally, these steps were evidenced by a change in the consistency of the solution as it gelled, while a mild drying process allowed to obtain the SiO_2NPs as a white solid. To improve the yield and efficiency of this synthesis, the following parameters were modified: reaction temperature, pH, acid catalyst, and drying conditions (temperature and time). All synthesized materials were evaluated for their Methylene Blue (MB) adsorption capacity (Table 1, see last page). Comparison of the results for Entry 1 and Entry 2 shows that an increase in the reaction temperature does not significantly improve the adsorption efficiency. On the other hand, a decrease in the drying time (Entries 3 and 4) and an increase in the drying temperature from 200 °C to 500 °C (Entry 5) and are unfavorable changes since all materials produced exhibit a considerable drop in their adsorption capacity. In this sense, it appears that low drying times are not favorable for the SiO_2NPs formation from the gel and that higher drying temperatures result in a material with a lower surface area due to the agglomeration of SiO_2NPs. On the contrary, a change in the catalyst used during synthesis (HNO_3, H_3PO_4, and CH_3COOH) led to a more adsorbent material, improving efficiency by 10 to 20 percent (Entries 6 to 8). In order to achieve the most sustainable synthesis conditions, it was decided to continue working with acetic acid, the greenest acid used, which also allowed a less exhaustive washing stage as this acid generated significantly less impurities in the final gel. Lastly, the synthesis pH was varied taking into account that the gelation process occurs in the pH range between 6 and 8 (Entries 8 to 10). From the results obtained, a neutral pH of 7 was selected as the optimal pH considering that it is the most eco-friendly condition and the adsorption efficiency did not differ significantly from those obtained in the other entries. In summary, a simple and optimized synthesis protocol allowed the production of SiO_2NPs using an aqueous Na_2SiO_3 solution adjusted to pH = 7 with CH_3COOH and stirred for 4 h at room temperature and then filtered and dried for 5 h at 200 °C.

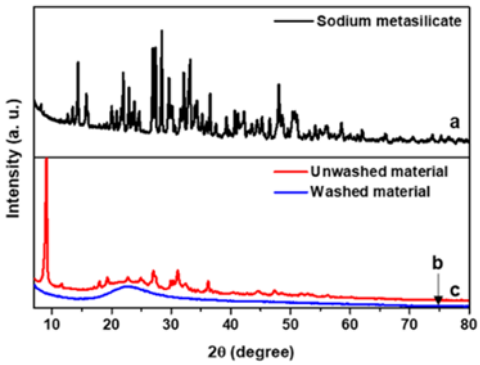


Figure 1. *XRD patterns of sodium metasilicate* ***(a)****, washed SiO_2NPs (pure)* ***(b),*** *and unwashed SiO_2NPs (impure)* ***(c)****.*

The most relevant physicochemical techniques (XRD, TEM, and N_2 adsorption-

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desorption isotherms at 77 K) are presented as follows. Figure 1 shows the X-ray diffraction patterns of sodium metasilicate and SiO_2NPs before and after washing. Unlike pattern (a), patterns (b) and (c) exhibit a broad signal around 23° that denotes nanoparticle formation with amorphous nature. In pattern (c), very sharp XRD peaks at 9.1°, 17.9°, 27.0°, and 36.2°, indicate the presence of sodium acetate as an impurity, therefore justifying the need to include a washing step during synthesis.

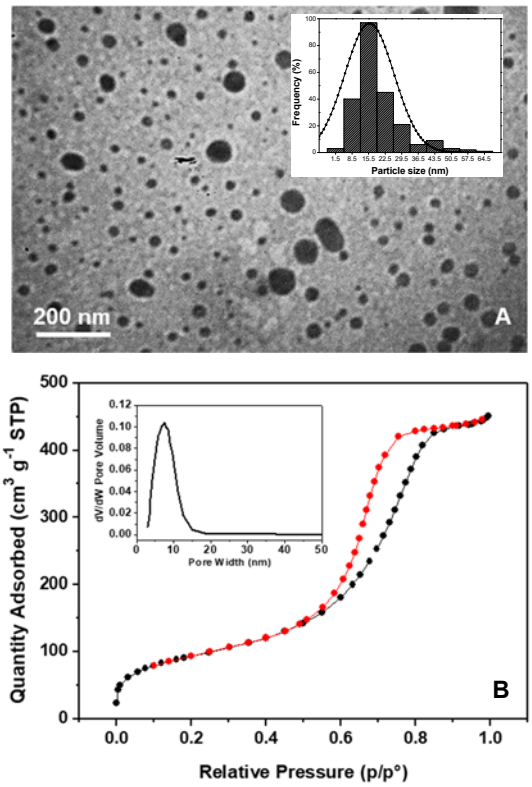


Figure 2. *TEM image at high magnification with its size histogram inset (A) and N_2 adsorption-desorption isotherms at 77 K and pore size distribution (inset) (B) of SiO_2NPs.*

Figure 2A displays the TEM image of SiO_2NPs. Here it can be observed that nanoparticles have a mostly spherical shape exhibiting low aggregation. They are polydisperse and according to the histogram in the same figure, their size follows a normal distribution where the main value is 15.5 nm. The SiO_2NPs N_2 adsorption-desorption isotherms is presented in Figure 2B. The isotherm profile is type IV according to the IUPAC classification, typical of mesoporous materials. The hysteresis could be attributed to a disorder solid where an interconnected network of large cavities is surrounded by slightly smaller openings (ink-bottle pore system). The corresponding pore size distribution (PSD) is shown as an inset in Figure 2B. It covers a range between 5 nm to 15 nm, presenting a maximum at approximately 7 nm. All these observations are then likely to be consistent with a secondary mesoporous system (textural mesoporosity) generated from the interstitial space between assembled SiO_2NPs during solvent evaporation.

Finally, an assessment of the "greenness" of the SiO_2NPs synthesis was performed by applying the principles of green chemistry together with the GS metric. For this analysis it was necessary to examine the synthesis protocol, the substances involved in the reaction (reagents, catalyst, solvents), and the wastes, considering the identification of hazards for each of them (risks to human health, to the environment, and of chemical accidents). Our optimal synthesis process for SiO_2NPs was compared with the Stöber procedure since it is the classical method used to obtain this type of nanoparticles. Stöber method involves the use of TEOS as a silicon source, ammonium hydroxide (NH_4OH) as a catalyst, and ethanol (EtOH) as a solvent under stirring at 22 °C for 72 h (Stöber et al., 1968; Tabisz et al., 2020). Additionally, a representative synthetic route using rice husk (RH) as a silicon source was also analyzed for comparative purposes. This process employs acid leaching and calcination of raw RH and NaOH and HCl with heating steps for silica synthesis (Song, 2018).

Table 2: *Green chemistry principles and corresponding scores to construct the GS analysis.*

Principles	GS1	GS2	GS3
1- Prevention	1	1	3
2- Atom economy	2	2	2
3- Less hazardous chemical synthesis	1	1	1
5- Safer solvents and auxiliary substances	1	2	3
6- Increase energy efficiency	3	1	3
7- Use of renewable feedstocks	1	3	1
8- Reduce derivatives	3	2	3
9- Catalysts	1	2	2
10- Design for degradation	1	1	1
12- Safer chemistry for accident prevention	1	1	2
GS Area Index (GSAI)	**25**	**30**	**55**

Table 2 shows the scores assigned to each principle according to the GS metric criteria for

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each synthesis: GS1 corresponds to the Stöber method, GS2 to the synthesis from rice husk, and GS3 to the present work.Initially, it can be observed that both the Stöber method and the one proposed here share the highest score in the P6 and P8 principles because the syntheses were performed under mild conditions, such as room temperature and ambient pressure, and were carried out without a derivatization process. On the other hand, none of the synthesis methods complies with the P3 and P10 principles. According to this metric, the lowest value is assigned to these principles since each synthesis involves chemicals with acute hazard to human health and, in none of the methods, all substances are degradable or break down to harmless products. Finally, the green star for the synthesis proposed in this work presents a higher green area (GS3 score = 55) indicating that it is a more environmentally friendly process, reaching a higher total score by generating innocuous waste (P1) and using only water as solvent (P5).

4. CONCLUSIONS

In this study, silica nanoparticles (SiO_2NPs) were successfully synthesized using an environmentally friendly sol-gel method, employing sodium metasilicate as a cheap Si source and short reaction times under neutral reaction conditions at room temperature. In addition, they were characterized by multiple physicochemical techniques that confirmed the production of nanostructured silica with negatively charged surface and porous structure and also, the efficiency of the proposed synthesis methodology. It should be noted that the objective of developing a more eco-friendly synthesis procedure, considering the principles of green chemistry, was achieved. Furthermore, the successful adsorption of the cationic MB dye on our nanoadsorbent opens the doors to future applications such as the removal of emerging pollutants in wastewater.

5. DECLARATIONS

5.1. Acknowledgments

The authors thank ANPCyT, CONICET, and SCTyP-UTN for the financial support.

5.2. Open Access

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Table 1. *Parameters evaluated in the optimization of SiO_2NPs synthesis.*

Entry	$T_{reaction}$	Acid	$t_{reaction}$ (h)	pH	T_{dry} (°C)	t_{dry} (h)	Adsorption capacity[#] (%)
1	RT	HCl	4	8	200	5	41
2	60 °C	HCl	4	8	200	5	47
3	RT	HCl	4	8	200	3	19
4	RT	HCl	4	8	200	1	19
5	RT	HCl	4	8	500	5	31
6	RT	HNO_3	4	8	200	5	55
7	RT	H_3PO_4	4	8	200	5	61
8	RT	CH_3COOH	4	8	200	5	59
9	RT	CH_3COOH	4	7	200	5	65
10	RT	CH_3COOH	4	6	200	5	68

RT: room temperature.

[#] $[(C_0 - C_t) / C_0] * 100$

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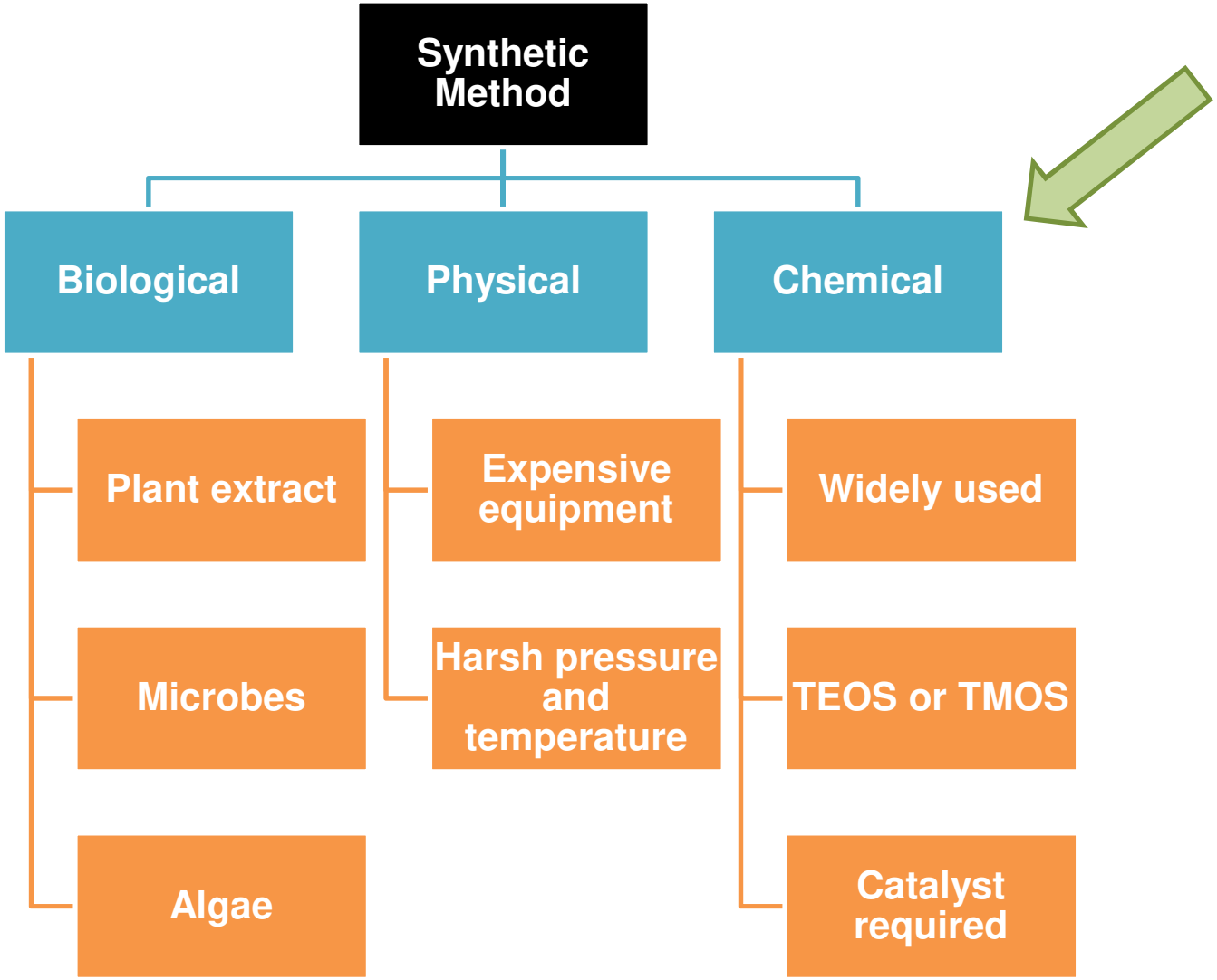
SILICA NANOPARTICLES: EXPLORING A GREENER ONE-POT SYNTHESIS

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CIQA, CONICET, UTN, Facultad Regional Córdoba, Departamento de Ingeniería Química, Argentina

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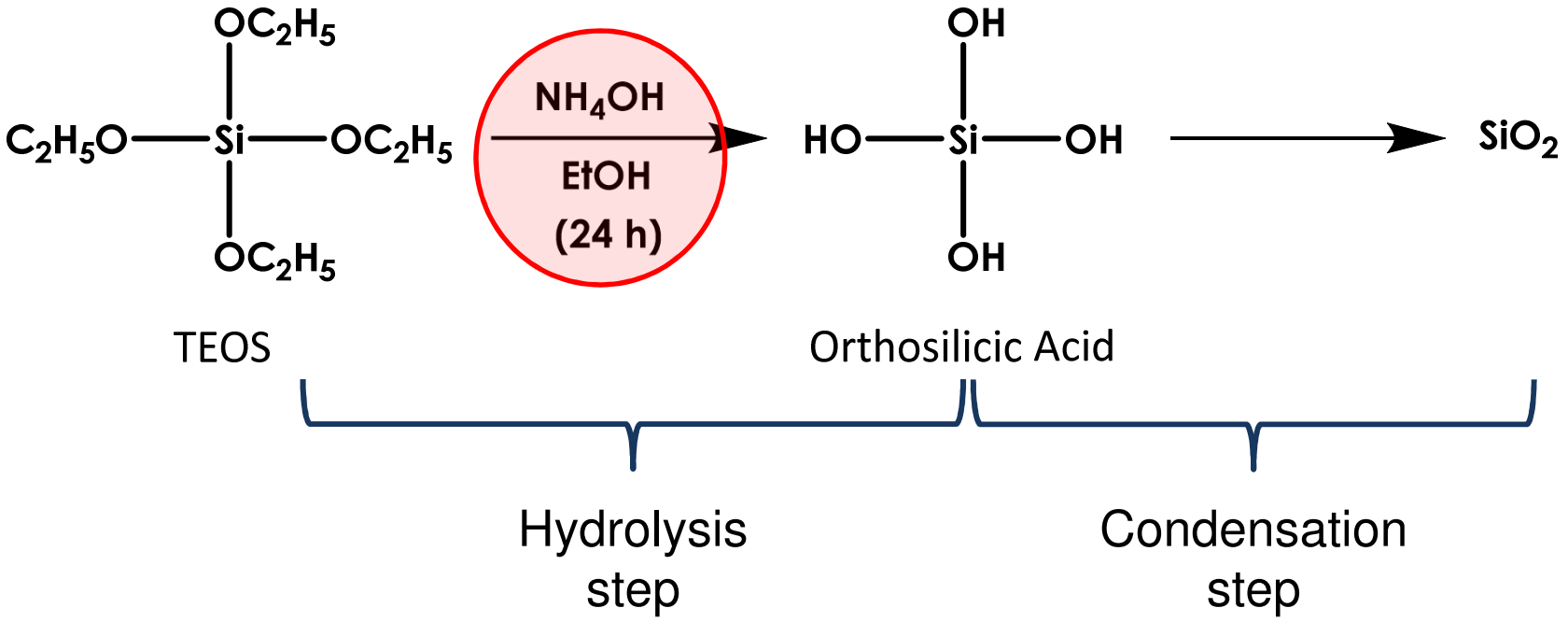
INTRODUCTION

There are three distinct strategies available for the synthesis of SiO_2NPs:



BACKGROUND

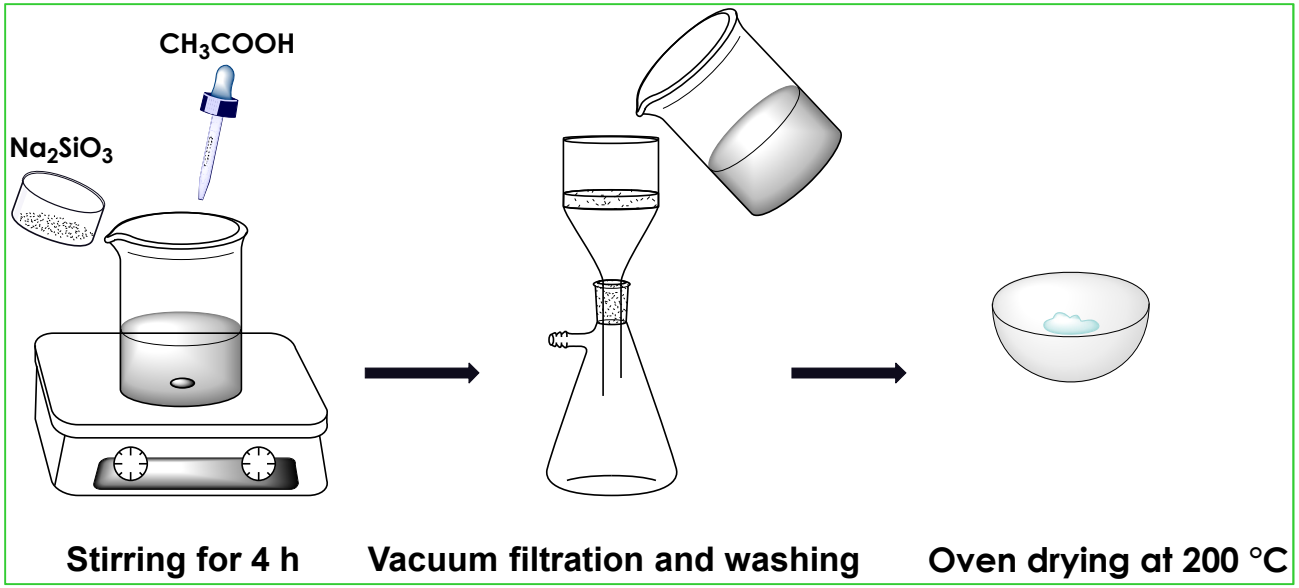
Stöber sol-gel method is the best known and most widely used



AIM

METHODOLOGY

An aqueous Na_2SiO_3 solution (0.30 M, initial pH = 14) at pH = 7 adjusted drop by drop with 4.0 M CH_3COOH, was stirred vigorously for 4 h at room temperature. The gel was separated by vacuum filtration and washed with Milli-Q water repeatedly. Finally, it was dried at 200 °C for 5 h.



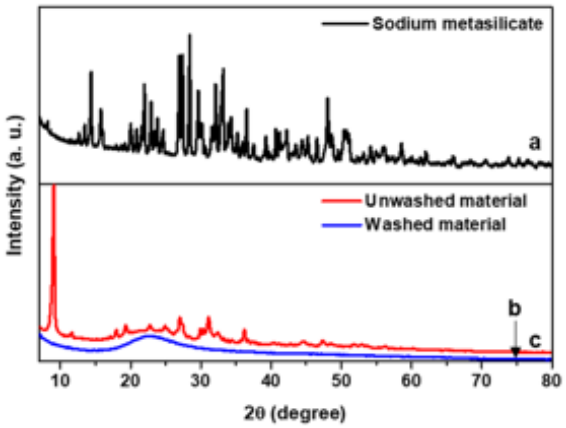
Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), UV-vis diffuse reflectance spectroscopy (UV-vis DR), Dynamic light scattering (DLS), Z-potential, Transmission electron microscopy (TEM), and N_2 adsorption-desorption isotherms at 77 K were used as characterisation techniques.

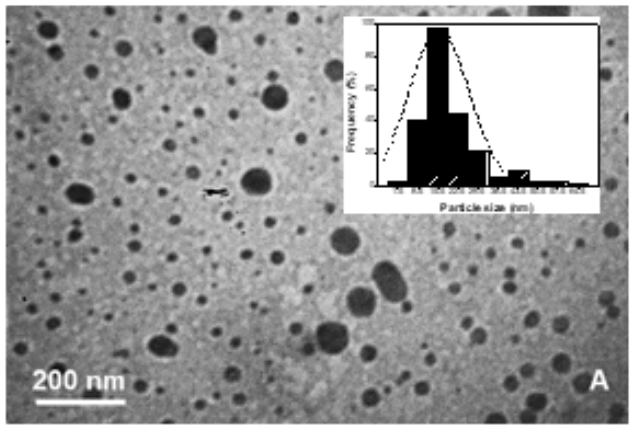
RESULTS AND DISCUSSION

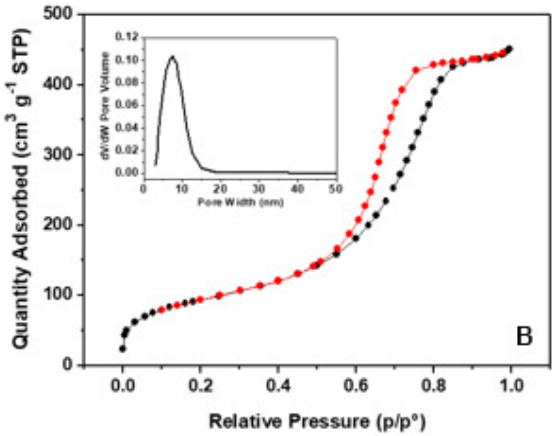
Table 1. *Parameters evaluated in the optimization of SiO_2NPs synthesis*

Entry	$T_{reaction}$	Acid	$t_{reaction}$ (h)	pH	T_{dry} (°C)	t_{dry} (h)	Adsorption capacity# (%)
1	RT	HCl	4	8	200	5	41
2	60 °C	HCl	4	8	200	5	47
3	RT	HCl	4	8	200	3	19
4	RT	HCl	4	8	200	1	19
5	RT	HCl	4	8	500	5	31
6	RT	HNO_3	4	8	200	5	55
7	RT	H_3PO_4	4	8	200	5	61
8	RT	CH_3COOH	4	8	200	5	59
9	RT	CH_3COOH	4	7	200	5	65
10	RT	CH_3COOH	4	6	200	5	68

← **Optimum condition**





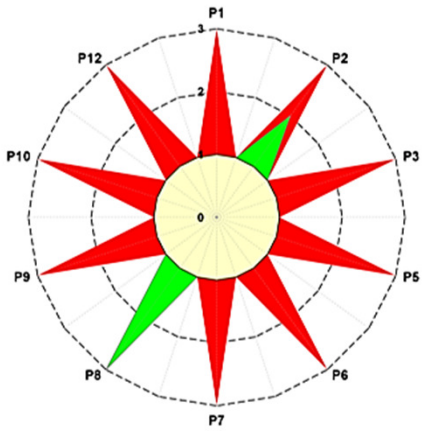


RESULTS AND DISCUSSION

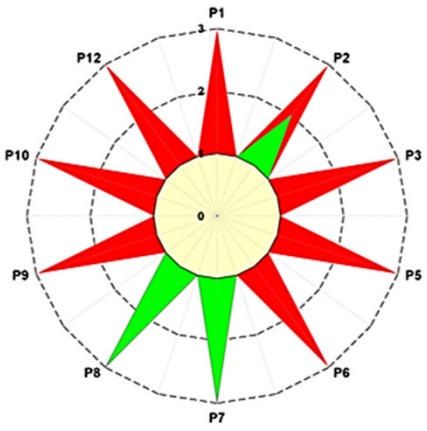
'Green chemistry' analysis

Principles	**GS1**	**GS2**	**GS3**
1- Prevention	1	1	3
2- Atom economy	2	2	2
3- Less hazardous chemical synthesis	1	1	1
5- Safer solvents and auxiliary substances	1	2	3
6- Increase energy efficiency	3	1	3
7- Use of renewable feedstocks	1	3	1
8- Reduce derivatives	3	2	3
9- Catalysts	1	2	2
10- Design for degradation	1	1	1
12- Safer chemistry for accident prevention	1	1	2
GS Area Index (GSAI)	**25**	**30**	**55**

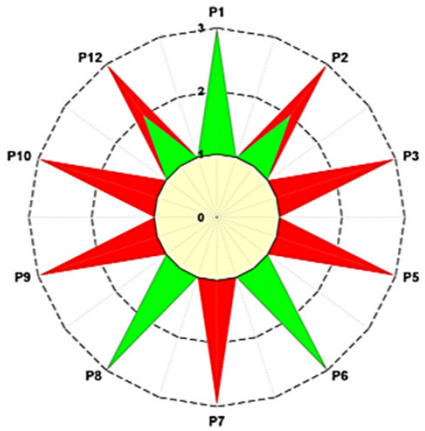
The synthesis proposed in this work presents a higher green area (GS3 score = 55) indicating that it is a more environmentally friendly process, reaching a higher total score by generating innocuous waste (P1) and using only water as solvent (P5).



GS1



GS2



GS3

CONCLUSIONS

- SiO_2NPs were successfully synthesized using an environmentally friendly sol-gel method, employing sodium metasilicate with short reaction times at room temperature;
- SiO_2NPs were characterised by different techniques such as FTIR, XRD, TEM, etc;
- The objective of developing a more eco-friendly synthesis procedure, with respect to the principles of green chemistry, was achieved.

ACKNOWLEDGEMENTS

For their financial and institutional support, the authors are grateful to:

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- **CONICET;**
- **SCTyP-UTN**

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EFFECT OF CONFINEMENT STRESS ON PLASMA LEVELS OF PROTEINS, GLUCOSE AND HEMATOLOGICAL INDEXES IN NILE TILAPIA (*OREOCHROMIS NILOTICUS*)

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ABSTRACT

The present study investigated the effects of confinement on secondary biochemical and physiological stress responses in Nile tilapia (*Oreochromis niloticus*). Stress is a central issue in physiology due to its impact on animal health and life. In this study, 36 juvenile tilapia (n = 12/group) were divided into three groups: control (CT), confinement stress (EC), and confinement plus "aggression" stress (CA). The CT group was free from manipulation, while the EC group was confined for 30 minutes in a space representing 10% of the original tank volume. The CA group was confined under the same conditions and then subjected to the "mirror test" paradigm. This test is a stressor for the animal, as it simulates the presence of another fish through its reflection in the mirror, generally inducing stress by triggering aggressive-like behavior. After the experiments, blood was collected, and the following parameters were evaluated: ventilatory frequency (VF), blood glucose, hemoglobin, hematocrit, erythrocytes, hematimetric indices (VCM, HCM, and CHCM), and plasma proteins. Our results showed that only confinement combined with stress from the "mirror test" (CA group) significantly elevated FV and glucose levels compared to the CT group and hemoglobin and plasma protein levels compared to the CT and EC groups ($p < 0.05$). These results suggest that confinement alone (for 30 minutes) is not sufficient to alter the biochemical and physiological parameters evaluated. Additionally, confinement in a restricted space may trigger an exaggerated biochemical and physiological response when the animal is subjected to another type of stressor. The study highlights the importance of strategies to mitigate the effects of stress, as it can cause various disorders that directly impact the animal's life.

Keywords: *stress, confinement, blood glucose, aggressiveness*

1. INTRODUCTION

According to Selye (1950), stress can be characterized as a series of adaptive responses. These physiological changes are known as the general adaptation syndrome and occur in three stages: the first stage involves the activation of brain centers, resulting in the massive release of catecholamines and corticosteroids; the second stage is usually defined as the channeling of the actions and immediate effects of these hormones into the blood and other tissues, including an increase in heart rate and oxygen uptake, along with the mobilization of energy substrates and disruption of hydromineral balance. Finally, the third stage manifests at the population level, resulting in inhibited growth, reproduction, and immune response. When prolonged, stress leads to physiological disorders, including excessive cortisol release, increased glucose levels, and immune suppression, which affect animal performance, especially in fish (Wendelaar Bonga, 1997). The Nile tilapia is a widely farmed species but is sensitive to confinement stress, which can be exacerbated by agonistic interactions, as observed in studies on aggressive-like behavior (Camargo-dos-Santos *et al*., 2021). In this study, we aim to evaluate how confinement in a restricted environment affects the secondary physiological and biochemical stress parameters in juvenile tilapia.

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2. MATERIALS AND METHODS

Initially, all animals were acclimated for 20 days in a water recirculation system in 250 L tanks with continuous aeration, a biological filter, and constant monitoring of water quality parameters until the experimental trials (pH: 6.8–7.2, DO: > 5ppm, Temperature: 25–30°C, toxic ammonia < 0.05 ppm, and nitrite < 0.5 ppm). Prior to the tests, the fish were fasted and isolated for 24 hours. Afterward, 36 juvenile Nile tilapia (n=12/group) were randomized into three experimental groups: control (CT), confinement (EC), and confinement followed by the "aggression" test (CA). The EC group was subjected to confinement for 30 minutes, restricted to 10% of the original tank volume (Fig. 1 exemplifies this type of confinement restricted to a space 10% of its original size). The CA group, in addition to being confined under the same conditions, was exposed to the "mirror test" simulating the presence of another fish to induce aggressive-like behavior (Fig. 2 exemplifies the paradigm that induces the fish to relate its own image with that of an intruder).

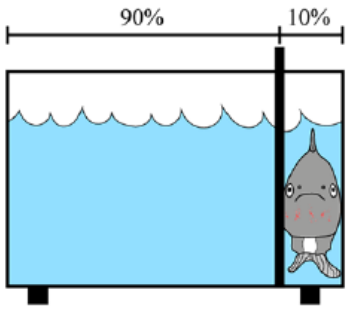


Figure 1: Representative image of the experimental apparatus used as a model for stress induction by confinement (modified from Camargo-dos-Santos *et al*., 2022).

After these experiments, blood was collected from the caudal vessels, and the following parameters were analyzed: ventilatory frequency (FV), blood glucose (mg/dL), hemoglobin (g/dL), hematocrit (%), erythrocytes ($x10^6$ μL^{-1}), VCM (fL), HCM (pg), CHCM (g/dL), and plasma proteins (g/dL). After data normalization, one-way ANOVA was used to compare means, followed by Tukey's post-hoc test with a significance level of 5%. In the case of the FV variable, the non-parametric Kruskal–Wallis test was used, followed by Dunn's multiple comparisons test (significance level of 5%).

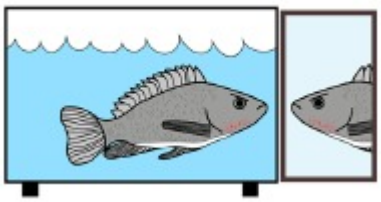


Figure 2: Representative image of the "mirror test," which induces "aggressive-type" behavior in Nile tilapia (modified from Camargo-dos-Santos et al., 2022).

3. RESULTS AND DISCUSSION

The results showed that the CA group had a significant increase in blood glucose levels compared to the CT group ($t = 5.04$; $p = 0.0035$), plasma proteins compared to the EC group ($t = 3.96$; $p = 0.0247$), and hemoglobin levels compared to both CT and EC groups ($t = 4.56$; $p = 0.0082$ and $t = 3.66$; $p = 0.0381$, respectively), as shown in Table 1. These findings suggest that confinement alone was not sufficient to trigger significant biochemical responses, but the combination with the induction of "aggressive-like" behavior exacerbated the negative effects. Confinement in a restricted environment, combined with an additional stressor, triggers an exaggerated physiological response, characterized by increases in glucose, hemoglobin, and plasma proteins, typical of a secondary stress response. Hyperglycemia in fish is a relatively common alteration often observed in stress studies under laboratory and field conditions (Hattingh, 1976). The increase in glucose is an indicator of some need for energy adjustment in response to the stressful conditions of the fish being exposed to the mirror, seeing its own reflection. The increased synthesis of plasma proteins may be related to the upregulation of chaperone proteins, which are responsible for repairing damaged cells (Himmelfarb & Ellen, 2001) and are elevated in situations of stress or metabolic challenges (Meyer and Silva, 1999). Our results also showed that ventilatory frequency (FV) was significantly higher in the CA group compared to the CT group ($z = 3.25$; $p = 0.0034$) (Fig. 3).

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Table 1: Hematological variables (mean ± SE) of Nile tilapia subjected to confinement stress. CT, control group; EC, confinement group; CA, group subjected to confinement and the "aggressive-like" behavior test. *P<0.05, statistically different from CT; #P<0.05, statistically different from EC.

Parameters	Treatments		
	CT	EC	CA
Glucose (mg/dL)	42,60 ± 2,57	52,27 ± 4,81	65,17 ± 5,75*
Hematocrit (%)	19,94 ± 3,73	27,55 ± 2,13	29,29 ± 3,24
Hemoglobin (g/dL)	4,16 ± 0,58	4,86 ± 0,32	6,24 ± 0,27*#
Erythrocytes (x10^6 μL^{-1})	1,20 ± 0,17	1,56 ± 0,17	1,64 ± 0,07
Proteins (g/dL)	2,28 ± 0,18	2,18 ± 0,23	3,03 ± 0,23
VCM (fL)	159,72 ± 22,31	202,55 ± 25,55	176,94 ± 15,8(
HCM (pg)	36,14 ± 3,96	35,00 ± 4,81	38,83 ± 2,55
CHCM (g/dL)	26,04 ± 4,09	18,45 ± 1,63	23,66 ± 2,18

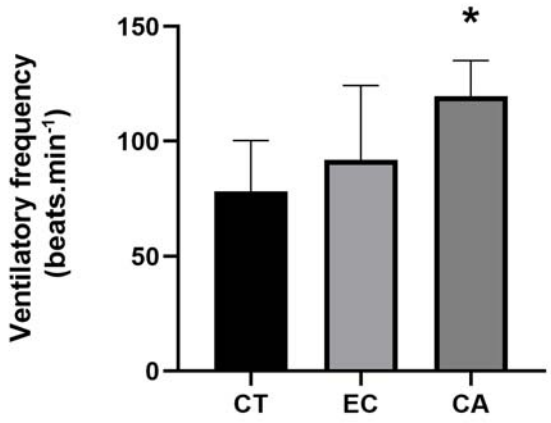


Fig. 3. Effect of confinement and the aggression test on ventilatory frequency (beats.min^{-1}). CT, control group; EC, confinement group; CA, group subjected to confinement and the "aggressive-like" behavior test. *P<0.05, statistically different from CT fish.

The increase in FV indicates a higher energy demand and respiratory effort, possibly due to the increased metabolic rate needed to cope with the stress of the behavior in front of the mirror. These results corroborate previous studies that associate chronic stress with behavioral and physiological changes in fish (Ellis et al., 2002). Management strategies that minimize confinement and aggression are essential to improve the welfare of fish in intensive aquaculture systems.

4. CONCLUSIONS

The study demonstrates that subjecting the animal to restricted confinement for 30 minutes, where it cannot explore its surrounding environment, was not able to alter the secondary stress responses. This finding leads us to conclude that tilapia is a species of fish that is more resistant to acute stressors, an important result for aquaculture, since it is one of the most cultivated fish in Brazil and around the world. On the other hand, when this restriction was combined with another type of stress, specifically the induction of "aggressive-like" behavior, there was a significant impact on the biochemical and physiological responses of the fish. It is necessary to include other durations of confinement induction and evaluate the animal's behavior (aggressiveness levels) when subjected to the mirror test. Because if animal behavior is actually more aggressive, we can associate the biochemical and physiological changes with the behavior itself and not with stress directly. The study highlights the importance of strategies that can mitigate the effects of stress, as it can lead to various disorders that directly impact the animal's well-being.

5. DECLARATIONS

5.1. Acknowledgments

We would like to thank the Laboratory of Aquaculture of Tropical Species – LAET for the technical and logistical support of this research and the Federal Institute of Education, Science, and Technology of Pará – IFPA Castanhal campus for all the encouragement. We also thank our colleagues and collaborators who contributed to the development of this project. A special thanks to the advisor of this work, Dr. Caroline Azevedo Rosa, and to collaborators Ma. Brenda Maria Pereira Alho da Costa and Dr. Marcelo Ferreira Torres for their valuable discussions and support during the experimental stages.

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EFEITO DO ESTRESSE DE CONFINAMENTO SOBRE OS NÍVEIS PLASMÁTICOS DE PROTEÍNAS, GLICEMIA E DOS ÍNDICES HEMATOLÓGICOS EM TILÁPIAS DO NILO (*OREOCHROMIS NILOTICUS*)

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November/2024

INTRODUCTION

Estresse em Peixes:

- O estresse é central na fisiologia animal, impactando sua saúde e desempenho.
- Tilápias-do-Nilo são suscetíveis ao estresse de confinamento.

Estudo Focado no Estresse de Confinamento:

- Avaliar respostas bioquímicas e fisiológicas.
- Analisar efeitos combinados de confinamento e estresse comportamental.



Tilápia do Nilo (*Oreochromis niloticus)*

AIM/OBJETIVE/PURPOSE

Objetivo Geral:

- Investigar os efeitos do confinamento sobre respostas bioquímicas e fisiológicas secundárias ao estresse em Tilápias-do-Nilo juvenis.

Objetivos Específicos:

- Analisar parâmetros como frequência ventilatória (FV), glicemia, hemoglobina, hematócrito, eritrócitos, índices hematimétricos e proteínas plasmáticas.

- Comparar os efeitos do confinamento isolado e associado ao estresse do comportamento “tipo-agressivo”.

METHODOLOGY

Divisão dos Grupos Experimentais:

- 36 tilápias juvenis, divididas em 3 grupos (n = 12/grupo):
- Controle (CT) – sem manipulação
- Estresse de Confinamento (EC) – confinamento por 30 minutos
- Confinamento + Agressividade (CA) – confinamento + “teste do espelho”

Procedimentos:

- Grupo EC confinado em espaço reduzido (10% do volume do aquário).
- Grupo CA submetido ao "teste do espelho" após o confinamento.
- Coleta de sangue para análise de parâmetros bioquímicos e fisiológicos.

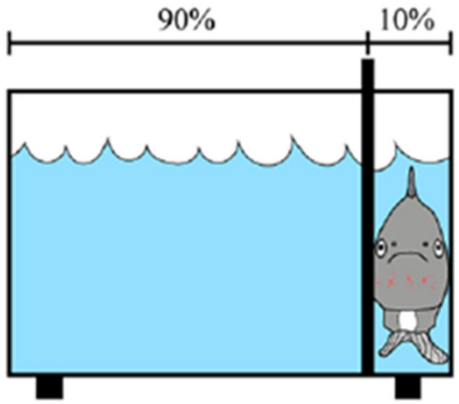


Imagem 1: representativa do aparato experimental utilizado como modelo de indução de estresse por confinamento (modificado de Camargo-dos-Santos et al., 2022).

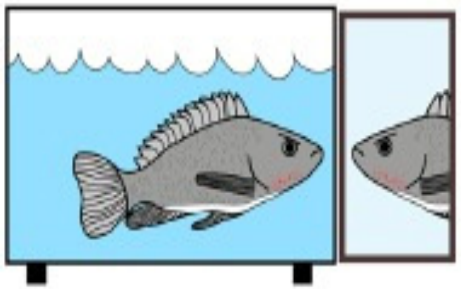


Imagem 2: representativa do aparato experimental utilizado como modelo de indução de estresse por confinamento (modificado de Camargo-dos-Santos et al., 2022).

RESULTS AND DISCUSSION

Glicemia:

- Aumento significativo no grupo CA em comparação ao grupo CT ($p < 0,05$).

Hemoglobina e Proteínas Plasmáticas:

- Níveis elevados no grupo CA em comparação aos grupos CT e EC ($p < 0,05$).

Hematócrito e Índices Hematimétricos:

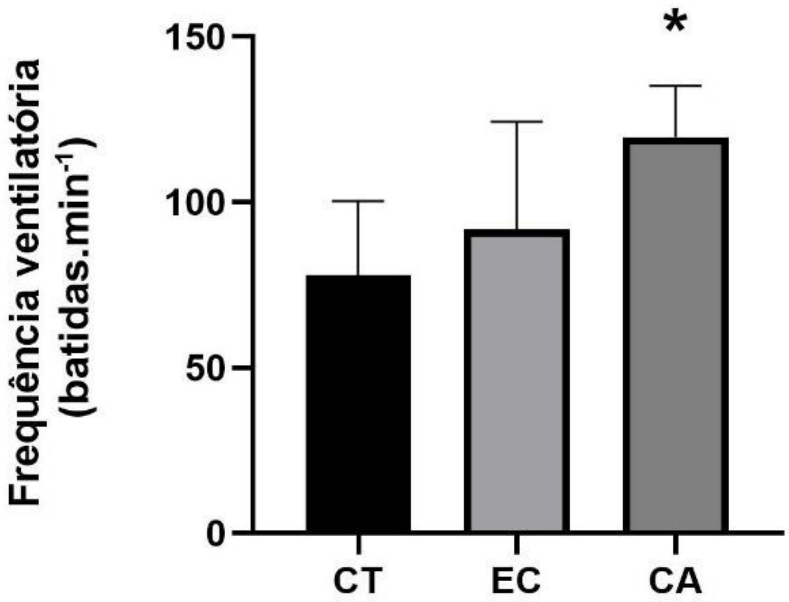
- Não houve diferenças significativas entre os grupos.

Parâmetros	Tratamentos		
	CT	EC	CA
Glicose (mg/dL)	42,60 ± 2,57	52,27 ± 4,81	65,17 ± 5,75*
Hematócrito (%)	19,94 ± 3,73	27,55 ± 2,13	29,29 ± 3,24
Hemoglobina (g/dL)	4,16 ± 0,58	4,86 ± 0,32	6,24 ± 0,27*#
Eritrócitos ($x10^6$ μL^{-1})	1,20 ± 0,17	1,56 ± 0,17	1,64 ± 0,07
Proteinas (g/dL)	2,28 ± 0,18	2,18 ± 0,23	3,03 ± 0,23#
VCM (fL)	159,72 ± 22,31	202,55 ± 25,55	176,94 ± 15,80
HCM (pg)	36,14 ± 3,96	35,00 ± 4,81	38,83 ± 2,55
CHCM (g/dL)	26,04 ± 4,09	18,45 ± 1,63	23,66 ± 2,18

RESULTS AND DISCUSSION

Frequência ventilatória

- Aumento significativo no grupo CA em comparação ao grupo CT ($p < 0,05$).



RESULTS AND DISCUSSION

O aumento da glicose é um indicador de alguma necessidade de ajuste energético, frente às condições estressantes da exposição do peixe ao espelho, vendo a imagem de si mesmo.

A síntese aumentada de proteínas plasmáticas pode estar relacionada ao aumento da expressão das proteínas do tipo chaperonas, que são responsáveis pela reconstrução de células danificadas (Himmelfarb & Ellen, 2001) e estão elevadas em situações de estresse ou algum desafio metabólico (Meyer e Silva, 1999).

O aumento da FV indica maior demanda energética e esforço respiratório, possivelmente devido ao aumento da taxa metabólica para lidar com o estresse do comportamento frente ao espelho.

RESULTS AND DISCUSSION

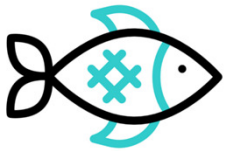
Confinamento Isolado (EC):

- Não foi suficiente para alterar significativamente os parâmetros bioquímicos e fisiológicos.

Confinamento com Estresse do comportamento tipo-agressivo (CA):

- Elevou algumas respostas bioquímicas e fisiológicas, sugerindo uma interação negativa entre confinamento e o “teste do espelho”.

Implicações: O estresse comportamental associado ao confinamento exacerba a resposta ao estresse, evidenciando a necessidade de mitigar esses efeitos.



CONCLUSIONS

- O confinamento isolado por 30 minutos não altera os parâmetros bioquímicos e fisiológicos.
- A combinação de confinamento e o “teste do espelho” desencadeia uma resposta exagerada ao estresse.
- Estratégias de manejo são necessárias para reduzir o estresse em sistemas de cultivo de tilápias, visando melhorar o bem-estar e o desempenho.



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II SOUTHERN SCIENCE CONFERENCE
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RE-APPRAISAL OF THE PROCEDURE OF QUALITATIVE INDUCED POLARISATION VALIDATION OF GROUNDWATER PROSPECTS AT THE SOUTHERN PHASE II DEVELOPMENT, GIDAN KWANO CAMPUS, MINNA, NIGERIA

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ABSTRACT

It is a desired situation if complementary geophysical data is available to aid deductions made based on analysis of a body of core data, like a corpus of vertical electrical soundings, say. At the southern Phase II Development of the Gidan Kwano Campus, Federal University of Technology, Minna, complementary induced polarisation data was acquired in tandem with vertical electrical sounding data in a dedicated survey program. The approach of the initial qualitative induced polarisation validation of the groundwater-resource deductions based on the interpretation of the sounding data fixed the number of groundwater prospects at 57 out of a total of *circa* 309 stations surveyed. This study concerns adopting a different course of qualitative induced polarisation validation that was de-emphasized in the earlier study and observing if there are disparities in the deductive outcomes regarding assured groundwater locations at the study area; this approach emphasizes strong bearings on “zero-weighted” induced polarisation values in the correlation regime. Thus, the number of groundwater prospects is now fixed at 47 post-induced polarisation validation from a list of soundings tagged as 89 prospect locations out of a total of *circa* 309 stations surveyed. There are *circa* 19 points that are tagged as coincident points in the earlier study and in the one herein. In order to solve the vexing groundwater problem plaguing the developed tranche of the Gidan Kwano Campus, it is recommended that the University adopts the idea of a multi-well single-output water scheme whence the survey locations flagged herein for their characteristic and comparatively deep-seated fractures should be exploited for their groundwater resource. Any planned drilling regime based on the recommendation herein must be guided by the full-length paper that is the work herein so as to pinpoint those locations where induced polarisation-data regimes actually point to very dependable groundwater exploitable potentials.

Keywords: *Geophysical; correlation; zero-weighted; fracture; groundwater*

1. INTRODUCTION

This text discusses the use of vertical electrical sounding (VES) and induced polarization (IP) data to analyze groundwater potential in the Phase II Development of the Gidan Kwano Campus, Federal University of Technology, Minna.

The approach relied on two key principles: negative IP values indicating lower resistivity in deeper layers (ABEM, 1999) and significant IP anomalies suggesting water-filled shear zones (Kearey and Brooks, 1984). However, the author questions whether these criteria are sufficient for pinpointing groundwater locations with high certainty, particularly in the context of the Nigerian Basement Complex where deep-seated groundwater-filled fractures in fresh basement rock are desired.

The text emphasizes the importance of continually exploring supplementary interpretation techniques to improve the accuracy of groundwater location identification. It describes a study by Jonah and Olasehinde (2015) that used IP data as a quality control measure for a 2 km² VES study, which was part of a larger 4 km² survey. This approach allowed for refinement of previous VES interpretations, with some locations previously identified as "strongly aquiferous" being upgraded to "very strongly aquiferous."

Jonah and Olasehinde's 2017 study focused on a 4 km² area of the Gidan Kwano Campus Phase II, using closely spaced VES data at 100 m intervals. The survey employed the Schlumberger array in an east-west direction with

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south-north profiling. The interpretation considered log-log plots, geoelectric cross-sections, iso-resistivity signatures, and pseudosections. IP data was again used qualitatively for quality control.

The 2017 study identified potential "geological fault-sources" near the southeast and "geological fault-sinks" near the southwest of the study area. The authors concluded that these fault sinks, located on the slope of the landform, were the most promising aquifer locations due to their position on the low slope of subsurface fault lines.

2. METHOD

The re-evaluation endeavor herein concerns the effort of the Jonah and Olasehinde (2017) work, whence only 57 groundwater prospect locations were tagged as “hydro-centric” after imposition of the IP validation route mentioned in Sec.1.0. Of the planned 441 dual VES-IP survey schedule of the Jonah and Olasehinde (2017) work, only *circa* 307 locations were occupied because of reasons bordering on barriers to surveys arising from a myriad of obstructions like wet-stream paths at coincident points of a planned survey, rock outcrops at coincident points of a planned survey, thick bush-thickets at coincident points of a planned survey, built-up hostels at coincident points of planned survey, recreation, gym, and clinic facilities at coincident points of planned survey, as well as the worst of them, risk of encountering raw sewage wastes emanating from human bowels and non-existent drainage and processing facilities in the perimeters of the students’ hostels buildings. Information on the nature of the prevailing geology of the local study area (mainly three-layer geological units of topsoil, weathered basement, and fresh basement) provides a convenient rule-of-thumb to make a reasonable conclusion on groundwater prospects at the study area. Analyses indicating multiple layers at any survey point can be approximated to a three-layer sequence with an eye on the range of the apparent resistivity values at the fractured basement showings corresponding to the last layer or just below the layers indicating fresh basement materials. This is a convenient course indeed, albeit at the empirical level.

3. RESULTS AND DISCUSSION

3.1 Results

3.1.1 WinResist® Log-Log Plots

According to Jonah and Olasehinde (2017), the computed apparent resistivity values at the 307 stations were initially subjected to the log-log plot routine of the Windows-compatible WinResist® software, whence corresponding field curves for all the stations occupied were produced. Each of the WinResist® log-log plots provides information on the number of layers, the average resistivity values of these layers, and their approximate thicknesses.

3.1.2 Hydro-centric Designations of Survey stations from information Gleaned in Sec. 3.1.1

In this respect, then, along with Profile 1, P1-3, P1-4, P1-5, P1-6, P1-13, and P1-14 are flagged as hydro-centric. Along Profile 2, P2-1, P2-3, P2-10, and P2-13 are flagged as hydro-centric. Along Profile 3, P3-1, P3-3, and P3-9 are flagged as hydro-centric. Along Profile 4, P4-1, P4-5, and P4-9 are flagged as hydro-centric. Along Profile 5, P5-2 and P5-12 are flagged as hydro-centric. Along Profile 6, P6-2, P6-3, P6-4, P6-5, P6-9, P6-11, P6-13, P6-16, P6-19 and P6-20 are flagged as hydro-centric. Along Profile 7, P7-3, P7-4, P7-6, P7-7, P7-8, and P7-16 are flagged as hydro-centric. Along Profile 8, P8-1, P8-2, P8-4, P8-5, P8-6, P8-7, P8-9, P8-18 and P8-21 are flagged as hydro-centric. Along Profile 9, P9-1, P9-3, P9-4, P9-6, P9-8, P9-12, and P9-13 are flagged as hydro-centric. Along Profile 10, P10-1, P10-5, and P10-7 are flagged as hydro-centric. Along Profile 12, P12-5, P12-6, P12-8, P12-9, and P12-11 are flagged as hydro-centric. Along Profile 13, P13-6, P13-8, and P13-10 are flagged as hydro-centric. Along Profile 14, no survey point was flagged as hydro-centric. Along Profile 15, P15-2, P15-4, and P15-12 are flagged as hydro-centric. Along Profile 16, P16-5 and P16-9 are flagged as hydro-centric. Along Profile 17, P17-8, P17-13, P17-14, and P17-15 are flagged as hydro-centric. Along Profile 18, P18-6, P18-8, P18-9, and P18-15 are flagged as hydro-centric. Along Profile 19, P19-2, P19-5, P19-7, P19-8, P19-9, P19-12, and P19-15 are flagged as hydro-centric. Along Profile 20, P20-2 and P20-15 are flagged as hydro-centric. Along Profile 21, P21-7, P21-8, P21-9, P21-11, P21-12, and P21-13 are flagged as hydro-centric. It is observed that there are 89 points flagged as hydro-centric locations in the first instance without the imposition of a stricter geophysical validation constraint to the VES interpretation. For the Jonah and Olasehinde (2017) study, there were 57 points flagged as hydro-centric locations in the second instance after applying IP validation constraint based on information gleaned from ABEM (1999) and Kearey and Brooks (1984).

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3.1.3 Concomitantly-Acquired Induced Polarisation Data for the Inferred 89 Hydro-centric Locations

The concomitantly-acquired induced polarisation data for the inferred 89 hydro-centric locations were extracted from the archive. It is instructive to point out that interest also centers on the 40-m depth-mark and greater depth-marks, as qualitative analyses go [especially for the works of Jonah and Olasehnde (2015) and Jonah and Olasehnde (2017)], "examination of each of the separate IP set of values was fixed for a benchmark depth of 40 m because this 40 m-window restriction was due to the fact that, in the larger basement complex region of which the present study area is but a small constituent, the thicknesses of the different phases of overburden materials never exceed 35 m." This desirability being reasonable or not, if there is observed continuous low-resistivity regime from shallower depths through the 40-m depth-mark onward to greater depths that implies groundwater prospects, then the IP validation scheme is a required procedure indeed for correlation could be carried out for groundwater presence at depths as well as the nature of the rock materials at those corresponding depths. Bearing these facts in mind, several chargeability values were also highlighted in the IP body of data.

3.2 Discussions

For the P1-3 groundwater prospect, it is observed that the desired fractured basement segment begins from the 6.5-m depth downwards to the maximum surveyed depth point of 100 m. Highlighted at the 8-m depth point is the IP designator corresponding to a chargeability value of -0.031 ms. It has been mentioned that according to ABEM (1999), negative IP values can only mean that the resistivity of the current layer is less than that of the layer just above it. However, since it is now known that the study area of the Jonah and Olasehinde (2017) work is actually located on the vestigial route of the Kazaure-Karaukarau-Kushaka-Ilesha Schist Lineament trending in a northeast-southwest direction and this lineament being bounded at the east-central local area of the Gidan Kwano Campus by a continuous body of granitic mass, interest is also focused on those charge-ability values that are pointers to either schist-rock material or to granite-rock material. Thus, the chargeability values at the 30 m depth point, the 40 m depth point, the 60 m depth point, the 70 m depth point, and the 100 m depth point have been heightened too. Incidentally, all the chargeability values posted negative signs.

For the P1-4 groundwater prospect, it is observed that the desired fractured basement segment begins from the 4.3-m depth downwards to the maximum surveyed depth point of 100 m. Highlighted at the 5-m depth point is the IP designator corresponding to a chargeability value of 0.46 ms. The charge ability values at the local-basement threshold depth point of 40 m (which corresponds to a VES "repeat-point") are highlighted, as well as that at the 80-m depth point.

For the P1-5 groundwater prospect, it is observed that the desired fractured basement segment begins from the 35-m depth downwards to the maximum surveyed depth point of 100 m. Highlighted at the 40-m depth point is the IP designator corresponding to a chargeability value of -0.57 ms. The chargeability values at the greater than 40 m depth points of 70 m, 90 m, and 100 m have also been highlighted.

For the P1-6 groundwater prospect, it is observed that the desired fractured basement segment begins from the 50-m depth downwards to the maximum surveyed depth point of 90 m. Highlighted at the 50-m depth point is the IP designator corresponding to a chargeability value of -0.75 ms. At the 70-m depth point is the IP designator, which corresponds to a chargeability value of -0.88 ms, and this is highlighted, too. The 100-m depth point was not occupied for data collection because the equipment battery was down and exhausted.

For the P1-13 groundwater prospect, it is observed that the desired fractured basement segment begins from the 73.1-m depth downwards to the maximum surveyed depth point of 80 m. Highlighted at the 80-m depth point is the IP designator, corresponding to a chargeability value of 5.56 ms. Wet-stream and thicket barriers at planned survey stations of 90 m and 100 m were the reasons data-collection was not taken through to the specified maximum survey depth of 100 m at P1-13 for the real-time survey exercise.

For the P1-14 groundwater prospect, it is observed that the indication for a desired fractured basement segment begins from the 2.8-m depth downwards to the maximum surveyed depth point of 20 m. From the 30-m depth point to the planned maximum surveyed depth of 100 m, data collection at planned survey stations was inhibited by the wet-stream barrier.

More in a pedagogical sense, the format of the foregoing arguments provides the basis for

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analyzing the other IP data sequences that are germane to each survey location.

4. CONCLUSIONS

There are 47 survey points tagged as "deep-seated low-resistivity hydro-centric" showings from the 89 survey points flagged as a result of the re-appraisal analysis carried out herein whereas for the Jonah and Olasehinde (2017) work there are 57 survey points tagged as "hydro-centric" as a result of IP qualitative validation analysis of the same format adopted herein, albeit of a different base-perspective. Ultimately, both studies strengthen the other and no identified point either of the suite of 47 hydro-centric locations or of the suite of 57 hydro-centric locations should be de-emphasised in favour of the other. Actually, there are *circa* 19 points that are tagged as coincident points in both studies.
In order to solve the vexing groundwater problem plaguing the developed tranche of the Gidan Kwano Campus, it recommended that the University adopts the idea of multi-well single-output water scheme whence the following survey locations flagged for their characteristic and comparatively deep-seated fractures should be exploited for their groundwater resource, videlicet: P1-4; P1-5; P1-6; P2-10; P3-1; P3-9; P5-2; P5-12; P6-4; P6-9; P6-11; P6-13; P6-16; P6-19; P6-20; P7-4; P7-6; P7-8; P7-16; P8-4; P8-5; P8-6; P8-9; P9-6; P9-8; P9-12; P9-13; P10-1; P12-8; P12-11; P13-10; P15-2; P15-4; P15-12; P16-9; P17-8; P17-13; P18-6; P18-8; P19-7; P19-8; P19-9; P20-15; P21-7; P21-9; P21-12; P21-13.

Any planned drilling regime based on the recommendation herein must be guided by the full-length paper that is the work herein so as to pinpoint those locations where IP-data regimes actually points to very dependable groundwater exploitable potentials (especially those with "shallow-prospect" tags) in relation to locations that also flagged "hydro-centric," implying those characterised by relatively deep-seated fractures. It must not be assumed that the groundwater prospects flagged in the Jonah and Olasehinde (2017) work which are not correspondingly tagged herein are not viable prospects. Actually, the Jonah and Olasehinde (2017) work and the study herein complements and reinforces each other. This is a case of different perspectives reinforcing the overall picture.

5. DECLARATIONS

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RE-APPRAISAL OF THE PROCEDURE OF QUALITATIVE INDUCED POLARISATION VALIDATION OF GROUNDWATER PROSPECTS AT THE SOUTHERN PHASE II DEVELOPMENT, GIDAN KWANO CAMPUS, MINNA, NIGERIA

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November/2024

INTRODUCTION

- **Information 1;** Combination of strictly "textbook" procedures (ABEM,1999; Kearey and Brooks,1984) to apply IP data in qualitative mode to validate the results of VES interpretation insufficient to provide desired results
- **Information 2;** This "insufficiency" is lack of focus on deep-seated groundwater-filled fractures in the fresh basement rock here at the local Minna Area tranche of the greater Nigerian Basement Complex
- **Information 3;** Thus, this study was undertaken to adopt a complementary validation approach that focuses mainly on deep-seated groundwater-filled fractures as principal target of investigation based on imposition of very strict conditions on deductions made regarding hydro-centric locations in the Jonah and Olasehnde (2017) work
- **Information 4;** Jonah and Olasehinde (2015) examined qualitative induced polarisation validation of the results of a 2 km^2 vertical electrical sounding study completed at the Gidan Kwano Campus Phase II Development. The authors reported that the 2 km^2 VES study under consideration here was Jonah *et al.* (2015) for which no tandem and coincident-point IP data-set was collected in the course of that survey completed in 2013.

AIM

In the quest to answer the question of groundwater-location availability to a great degree of fidelity at the Phase II Development, it is fitting and proper to continuously explore supplementary interpretation techniques in complementary modes to the rich archive of geoelectrical database that has been built for this purpose.

METHODOLOGY

- Originally, 307 locations occupied from the planned 441 dual VES-IP survey schedule
- The VES-IP survey schedule was sounding in Schlumberger array mode
- Information gleaned from correspondingly-generated summary tables germane to initial interpretation pre-IP validation
- Information to be extracted from reference table of resistivity values of rock types in the basement complex of Nigeria provides a convenient rule-of-thumb to make reasonable conclusion on groundwater prospects at the study area
- Interpretation hinges on information on the nature of the prevailing geology of the local study area (mainly three-layer geological units of topsoil, weathered basement, and fresh basement)
- Analyses indicating multiple layers at any survey point can be approximated to a three-layer sequence with an eye on the range of the apparent resistivity values at the fractured basement showings corresponding to the last layer or just below the layers indicating fresh basement materials
- New qualitative validation approaches hinges on specifically-defined “zero-weighting” evaluation of IP signatures

RESULTS AND DISCUSSION

- **Results**

- **WinResist® Log-Log Plots Summary Tables:** The computed apparent resistivity values at the 307 stations were initially subjected to the log-log plot routine of the Windows-compatible WinResist® software whence corresponding field curves for all the stations occupied were produced. Each of the WinResist® log-log plot provides information on the numbers of layers, the average resistivity values of these layers, and their approximate thicknesses.
- **Hydro-centric Designations of Survey Stations from WinResist® Log-Log Plots Summary Tables:** Range of apparent resistivity values at the fractured basement showings aided compilation of plausible hydro-centric locations
- **Concomitantly-Acquired Induced Polarisation Tables for Inferred Hydro-centric Locations:** The concomitantly-acquired induced polarisation tables for the inferred 89 hydro-centric locations were extracted from the archive

- **Discussion**

- Fracture signatures in fresh basement material were tracked in the interpretation sequences
- Corresponding depths where “zero-weighted” IP values were observed were noted
- “Zero-weighted” IP values occuring less that 40-m depth not of significant interest
- “Zero-weighted” IP values occuring more that 40-m depth of significant interest
- Format of foregoing arguments provides basis for analysing other tables that are germane to each survey location

CONCLUSIONS

- **Conclusion 1;** There are 47 survey points tagged as “deep-seated low-resistivity hydro-centric” showings from the 89 survey points flagged as a result of the re-appraisal analysis carried out herein
- **Conclusion 2;** Whereas for the Jonah and Olasehinde (2017) work there are 57 survey points tagged as “hydro-centric” as a result of IP qualitative validation analysis of the same format adopted herein, albeit without the “zeroth-weighting constraint”
- **Conclusion 3;** Ultimately, both studies strengthen the other and no identified point either of the suite of 47 hydro-centric locations or of the suite of 57 hydro-centric locations should be de-emphasised in favour of the other.
- **Conclusion 4;** There are *circa* 19 points that are tagged as coincident points in both studies
- **Conclusion 5;** In order to solve the vexing groundwater problem plaguing the developed tranche of the Gidan Kwano Campus, it recommended that the University adopts the idea of multi-well single-output water scheme whence the 47 survey points tagged as “deep-seated low-resistivity hydro-centric” showings should be exploited for their groundwater resource

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ANÁLISE DOS INVENTÁRIOS DE EMISSÕES DE GASES DE EFEITO ESTUFA PUBLICADOS VOLUNTARIAMENTE NO PROGRAMA BRASILEIRO GHG PROTOCOL

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ABSTRACT

The increase in greenhouse gas (GHG) emissions is a global concern due to its impact on climate change. To address this challenge, the development of corporate GHG inventories is crucial, enabling organizations to understand and mitigate their emissions. This study aims to statistically analyze whether there was a significant increase in GHG emissions over a 10-year period by organizations from various sectors of the economy that voluntarily published their inventories in the Brazilian GHG Protocol Program. Data were obtained from the inventories of 66 organizations that published at 2013 and 2022 in the Brazilian GHG Protocol Program. The data was processed and analyzed using Minitab software to determine the significance level of the increase in GHG emissions. A total increase of 159,264,734.26 tCO_2e in GHG emissions was observed from 2013 to 2022, with 29 organizations reporting higher emissions and 37 showing reductions. However, statistical analysis demonstrated that there was no significant increase in GHG emissions over the study period. The results highlight the importance of organizations conducting their GHG inventories to enhance transparency and make strategic decisions aimed at mitigating their emissions. Publishing inventories allows for monitoring progress and identifying priority areas for effective interventions. No significant increase in GHG emissions was observed over the 10-year period; therefore, this study reinforces the importance of preparing GHG inventories by organizations. The findings can impact public policies on climate change, supporting the introduction of regulations that mandate the development of inventories and the setting of emission reduction and offsetting targets.

Keywords: *Global Warming, Climate Change, Mitigation, Statistics*

1. INTRODUÇÃO

O aumento das emissões de gases de efeito estufa (GEE) é uma preocupação global devido ao impacto nas mudanças climáticas. Desde a Revolução Industrial, a concentração desses gases aumentou, principalmente pelo uso de combustíveis fósseis. Esses gases retêm calor solar, elevando a temperatura global e gerando consequências ambientais, sociais e econômicas (IPCC, 2023).

Para enfrentar esse desafio, a Convenção-Quadro das Nações Unidas sobre Mudança do Clima (UNFCCC) foi criada em 1992 para reduzir as emissões de GEE. Desde então, iniciativas como o Protocolo de Quioto, o Acordo de Paris e as Conferências das Partes (COPs) estabeleceram metas para mitigar mudanças climáticas (UNFCCC, 2021).

Inventários corporativos de emissões de GEE são ferramentas fundamentais para as organizações compreenderem e mitigarem suas emissões (WRI, 2024). Esses inventários permitem quantificar e classificar emissões e estabelecer metas de redução (Gomes et al., 2021). Uma metodologia bastante utilizada no mundo é o Greenhouse Gas Protocol (GHG Protocol), desenvolvido pelo World Resources Institute (WRI) em parceria com o World Business Council for Sustainable Development (WBCSD).

No Brasil, o GHG Protocol foi implementado em 2008 com o Programa Brasileiro GHG Protocol, adaptado ao contexto nacional. Esse programa é promovido pelo Centro de Estudos em Sustentabilidade da FGV e pelo WRI, em parceria com o Ministério do Meio Ambiente (MMA), o Conselho Empresarial Brasileiro para o Desenvolvimento Sustentável

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(CEBDS) e o WBCSD (FGV, 2008).

Estudos recentes destacam a importância dos inventários de GEE pelas organizações. Santos (2016) observou o aumento da adesão ao Programa Brasileiro GHG Protocol, impulsionado pela melhoria da imagem corporativa. Cordeiro et al. (2017) ressaltaram que a divulgação voluntária dos inventários amplia a compreensão sobre o impacto dos recursos organizacionais na adesão.

Este estudo tem como objetivo analisar estatisticamente se houve aumento significativo nas emissões de GEE, em 10 anos, por organizações de diversos setores que publicaram voluntariamente seus inventários no Programa Brasileiro GHG Protocol.

2. MATERIAIS E MÉTODOS

2.1. Materiais

- Plataforma do Programa Brasileiro GHG Protocol, desenvolvida pela Fundação Getúlio Vargas, para obtenção dos dados dos inventários de emissões de GEE publicados pelas organizações de diversos setores da economia nos anos de 2013 e 2022;
- Microsoft Excel 365 versão 2409 para organização e tabulação dos dados;
- Minitab Statistical Software versão 21 on-line (disponível em maio/2024) para análise estatística dos dados obtidos;
- Base de dados do Google Acadêmico para a revisão sistemática da literatura, buscando artigos publicados em idioma português relacionados ao tema da pesquisa.

2.2. Métodos

A pesquisa foi realizada em duas etapas principais: a coleta e análise de dados dos inventários de emissões de GEE e a revisão sistemática da literatura.

Na primeira etapa, foram obtidos dados dos inventários de 66 organizações que publicaram seus inventários de emissões de GEE nos anos de 2013 e 2022 na plataforma do Programa Brasileiro. Os dados foram organizados e tabulados no Microsoft Excel, somando-se as emissões dos escopos 1, 2 e 3 para obter o total de emissões em tCO_2e, toneladas de dióxido de carbono equivalentes, por organização e por ano (Marconi & Lakatos, 2017).

Em seguida, os dados foram analisados estatisticamente utilizando o software Minitab. Foram realizadas estatísticas descritivas, teste de normalidade de Kolmogorov-Smirnov e o teste não-paramétrico de Mann-Whitney para verificar se houve diferença significativa entre as emissões de GEE nos anos de 2013 e 2022 (Marconi & Lakatos, 2017).

Na segunda etapa, foi realizada uma revisão sistemática da literatura na base de dados do Google Acadêmico, buscando artigos em português relacionados ao tema da pesquisa. Utilizou-se a seguinte string de busca: estatística AND mitigação AND ("inventário de emissão" OR "inventário de emissões OR inventário) AND (GEE OR "gases efeito estufa") AND (setores OR segmentos) AND economia. Dos 79 resultados iniciais, foram selecionados 18 artigos pelos títulos, dos quais 10 tiveram seus resumos lidos e, por fim, 4 artigos foram selecionados para contribuir com o assunto após a leitura completa (Marconi & Lakatos, 2017).

3. RESULTADOS E DISCUSSÕES

Inicialmente na análise estatística, utilizando o software Minitab, foram obtidas as estatísticas descritivas, Quadro 1, para os conjuntos de dados referentes às emissões de GEE em tCO_2e das 66 organizações nos anos de 2013 e 2022. Foram calculadas as médias, medianas e desvios-padrão para cada ano.

Quadro 01. *Estatísticas Descritivas*

Ano	Média	DesvPad	Mediana
2013	1256561	3198197	118054
2022	3669663	12269840	121276

Fonte: Minitab Statistical Software

Em seguida, foi elaborado um gráfico de BoxPlot, Figura 1, para visualizar a distribuição dos dados, identificar possíveis outliers e comparar os valores máximos, mínimos e medianas entre os dois anos.

Para determinar se os dados seguiam uma distribuição normal, foi aplicado o teste de normalidade de Kolmogorov-Smirnov, uma vez que a amostra possuía mais de 50 elementos.

As hipóteses testadas foram:
- H0: Os dados apresentam distribuição normal
- H1: Os dados não apresentam distribuição normal

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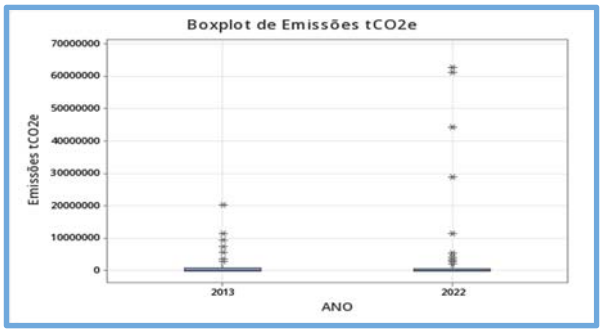


Figura 1. *Boxplot de Emissões tCO_2e*

O nível de significância adotado foi de 5% (α = 0,05). O resultado do teste de Kolmogorov-Smirnov indicou um p-value < 0,010, inferior ao nível de significância estabelecido, Figura 2. Portanto, a hipótese nula (H0) foi rejeitada, aceitando-se a hipótese alternativa (H1) de que os dados não possuem distribuição normal.

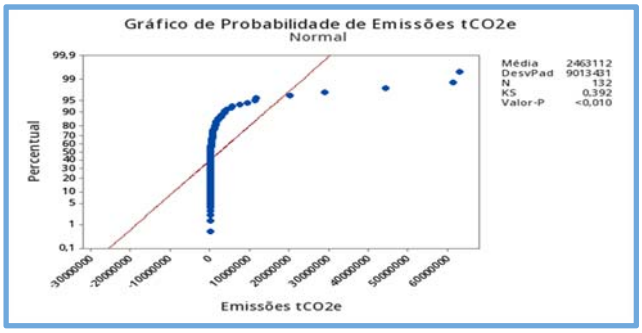


Figura 2. *Probabilidade de Emissões tCO_2e*

Como os dados não apresentaram distribuição normal, aplicou-se o teste não-paramétrico de Mann-Whitney para comparar as amostras dos anos de 2013 e 2022. As hipóteses testadas foram:
- H0: As amostras possuem medianas iguais
- H1: As amostras não possuem medianas iguais

O nível de significância adotado foi de 5% (α = 0,05). O resultado do teste de Mann-Whitney indicou um p-value = 0,984, superior ao nível de significância estabelecido. Assim, a hipótese nula (H0) foi aceita, indicando que não existe diferença significativa entre as medianas das amostras dos anos de 2013 e 2022.

Considerando os 66 inventários de emissões de GEE publicados no Programa Brasileiro, constatou-se um acréscimo total nas emissões de GEE de 159.264.734,26 tCO2e de 2013 para 2022. Das organizações analisadas, 29 apresentaram acréscimos nas emissões, enquanto 37 tiveram diminuição.

Com base nos resultados da análise estatística, concluiu-se que não houve acréscimo significativo (superior a 5%) nas emissões de gases de efeito estufa do ano de 2013 para o ano de 2022, considerando as organizações que publicaram seus inventários no Programa Brasileiro GHG Protocol, aumento de 2,7%, de acordo com dados da mediana. No entanto, a análise estatística fornece insights valiosos sobre o comportamento das emissões de GEE no período analisado e destaca a importância da elaboração e publicação dos inventários de emissões pelas organizações.

Esses resultados corroboram com o estudo de Cordeiro (2017) que destaca a divulgação voluntária dos inventários de GEE em diferentes contextos geográficos amplia a compreensão de como os recursos técnicos, humanos e financeiros impactam na adesão das organizações às divulgações de GEE. Isso possibilita a implementação de técnicas mais eficientes de controle ambiental.

Santos (2016), não encontrou uma relação positiva entre a adoção de inventários de emissões de GEE e os desempenhos operacional e financeiro das empresas. No entanto, o autor ressalta a necessidade de mais investigações sobre o impacto das ações ambientais no desempenho das organizações.

Vasconcelos (2020) indica que um maior percentual de ações nas mãos de investidores institucionais favorece a redução de emissões de GEE. Porém, os resultados do estudo não apontaram uma redução significativa nas emissões, sugerindo que outros fatores, como a estrutura regulatória e a maturidade das empresas, também podem influenciar na priorização da redução de emissões.

Segundo Silva (2023), a participação das organizações em programas de compensação de carbono também é recomendada, quando a redução direta não for possível, a compensação através de plantios anuais de árvores, aquisição de créditos de carbono e projetos de arborização e reflorestamento são essenciais.

4. CONCLUSÕES

O estudo comparou as emissões de GEE de diversas organizações nos anos de 2013 e 2022 e, com base em métodos estatísticos concluiu que não houve variação significativa nas medianas das emissões ao longo desse período. Embora não tenha sido observado um aumento relevante, o trabalho destaca a importância das organizações realizarem inventários de GEE, prática que melhora a transparência e facilita

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decisões estratégicas para mitigar emissões e otimizar resultados futuros.

A divulgação desses inventários permite que as empresas monitorem seu progresso e identifiquem áreas prioritárias para intervenções mais eficazes. Além disso, os resultados indicam que políticas públicas poderiam estabelecer a obrigatoriedade de inventários de GEE em diversos setores da economia, com metas claras para a redução e compensação de emissões não evitáveis. Essas medidas contribuiriam para mitigar os impactos das mudanças climáticas e promover um desenvolvimento mais sustentável.

5. DECLARAÇÕES E AGRADECIMENTOS

5. DECLARAÇÕES

5.1. Agradecimentos

Este estudo apresenta limitações. A amostra de 66 organizações que publicaram inventários de GEE em 2013 e 2022 no Programa Brasileiro, embora representativa, não abrange todas as que realizam inventários no Brasil. O período de 10 anos, apesar de relevante, pode não captar tendências de longo prazo, sugerindo que pesquisas futuras considerem intervalos maiores. Outra limitação é o uso de dados voluntários, que, mesmo seguindo as diretrizes do GHG Protocol, podem apresentar variações em metodologia e qualidade.

Os autores expressam sua gratidão à Fundação Getúlio Vargas e ao Programa Brasileiro GHG Protocol por disponibilizarem os dados dos inventários de emissões de GEE.

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Southern Science Conference, 2024.

ANALYSIS OF GREENHOUSE GAS EMISSIONS INVENTORIES VOLUNTARILY PUBLISHED IN THE BRAZILIAN GHG PROTOCOL PROGRAM

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October/2024

INTRODUCTION

- Increases in greenhouse gas (GHG) emissions and their impact on climate change;

- Initiatives such as UNFCCC, the Paris Agreement, and COPs aim to mitigate this issue;

- Corporate GHG emission inventories are essential for monitoring and reducing emissions;

- In Brazil, the Brazilian GHG Protocol Program, initiated in 2008, is a reference.

AIM

To statistically analyze whether there was a significant increase in GHG emissions after 10 years by organizations from different sectors of the economy that voluntarily published their GHG inventories in the Brazilian GHG Protocol Program.







METHODOLOGY

1st Step:

- Data from 66 organizations that published their GHG emissions inventories in 2013 and 2022 on the Brazilian GHG Protocol Program platform were obtained.



- The data were organized and tabulated in Microsoft Excel, adding emissions from Scopes 1, 2, and 3 to obtain the total emissions in tCO_2e (tons of carbon dioxide equivalents) per organization and year.

- The data were statistically analyzed using Minitab to verify if there was a significant difference in GHG emissions between 2013 and 2022.

METHODOLOGY

2nd Step:

- Systematic literature review using the Google Scholar database, searching for articles in Portuguese related to the research topic.

- The following search string was used: statistics AND mitigation AND ("emission inventory" OR "emission inventories OR inventory") AND (GHG OR "greenhouse gases") AND (sectors OR segments) AND economy.

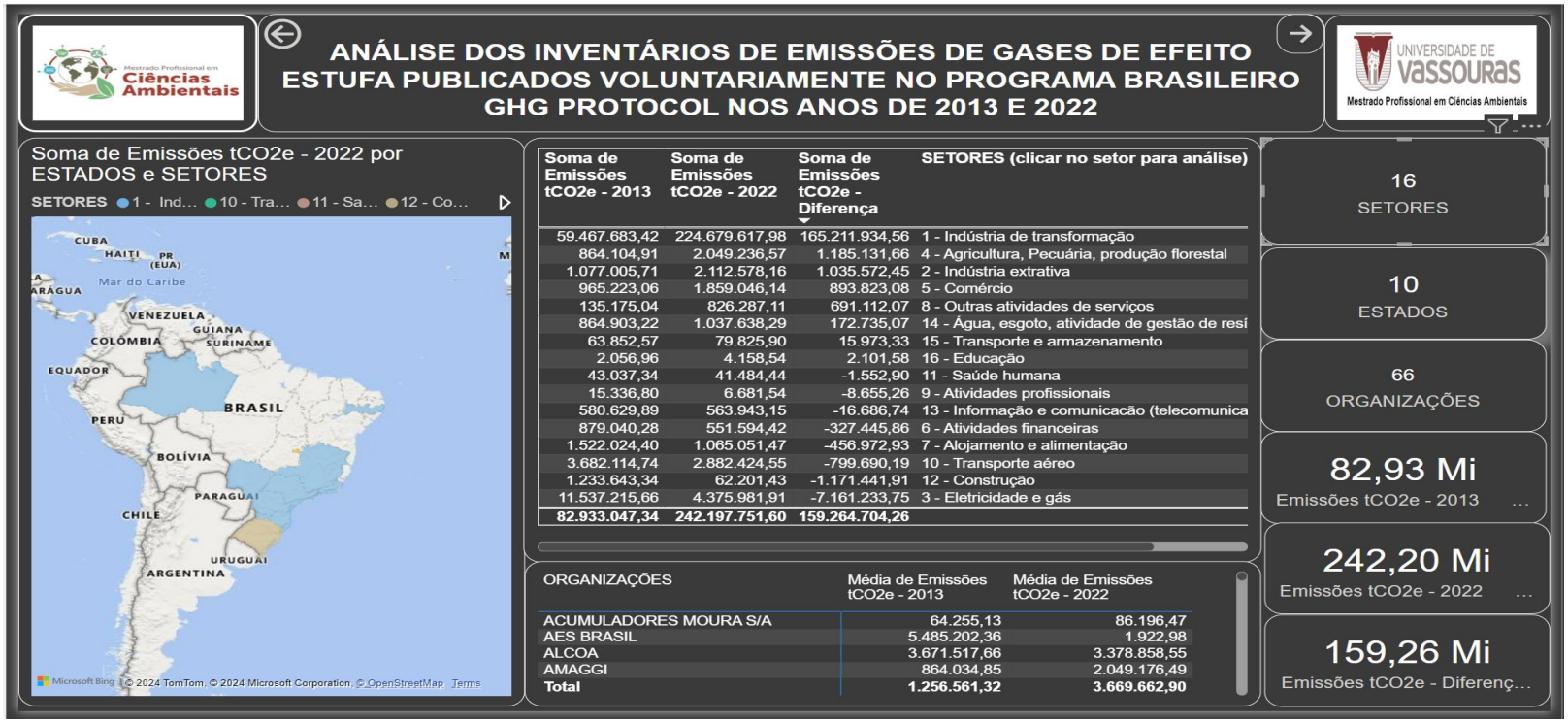
Steps	**Works**	Amount
1ª Phase	Initial search	79
2ª Phase	Selected by title	18
3ª Phase	Selected by summary	10
4ª Phase	Selected by article	04

RESULTS AND DISCUSSION

RESULTS AND DISCUSSION

Of the 66 analyzed GHG emission inventories published in the Brazilian GHG Protocol Program:

- Increase in greenhouse gas emissions by 159,264,734.26 tCO2e (tons of carbon dioxide equivalents) from 2013 to 2022;
- Of the organizations analyzed, 29 showed increases in emissions, while 37 showed decreases.



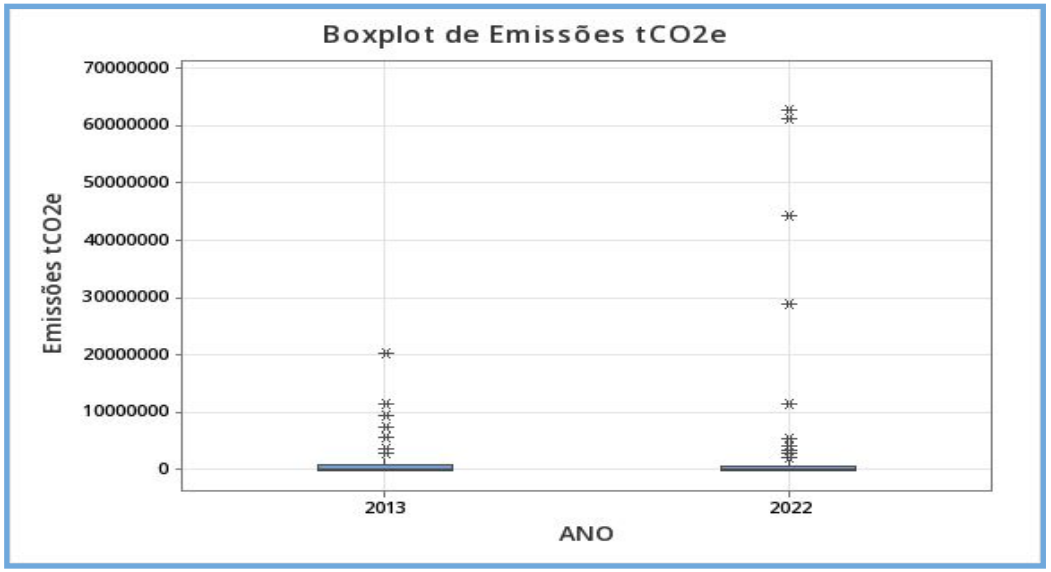
RESULTS AND DISCUSSION

Statistical Results

- Means, medians, and standard deviations for 2013 and 2022 were calculated.
- A BoxPlot was used to visualize the data distribution, identify potential outliers, and compare maximum, minimum, and median values between the two years.

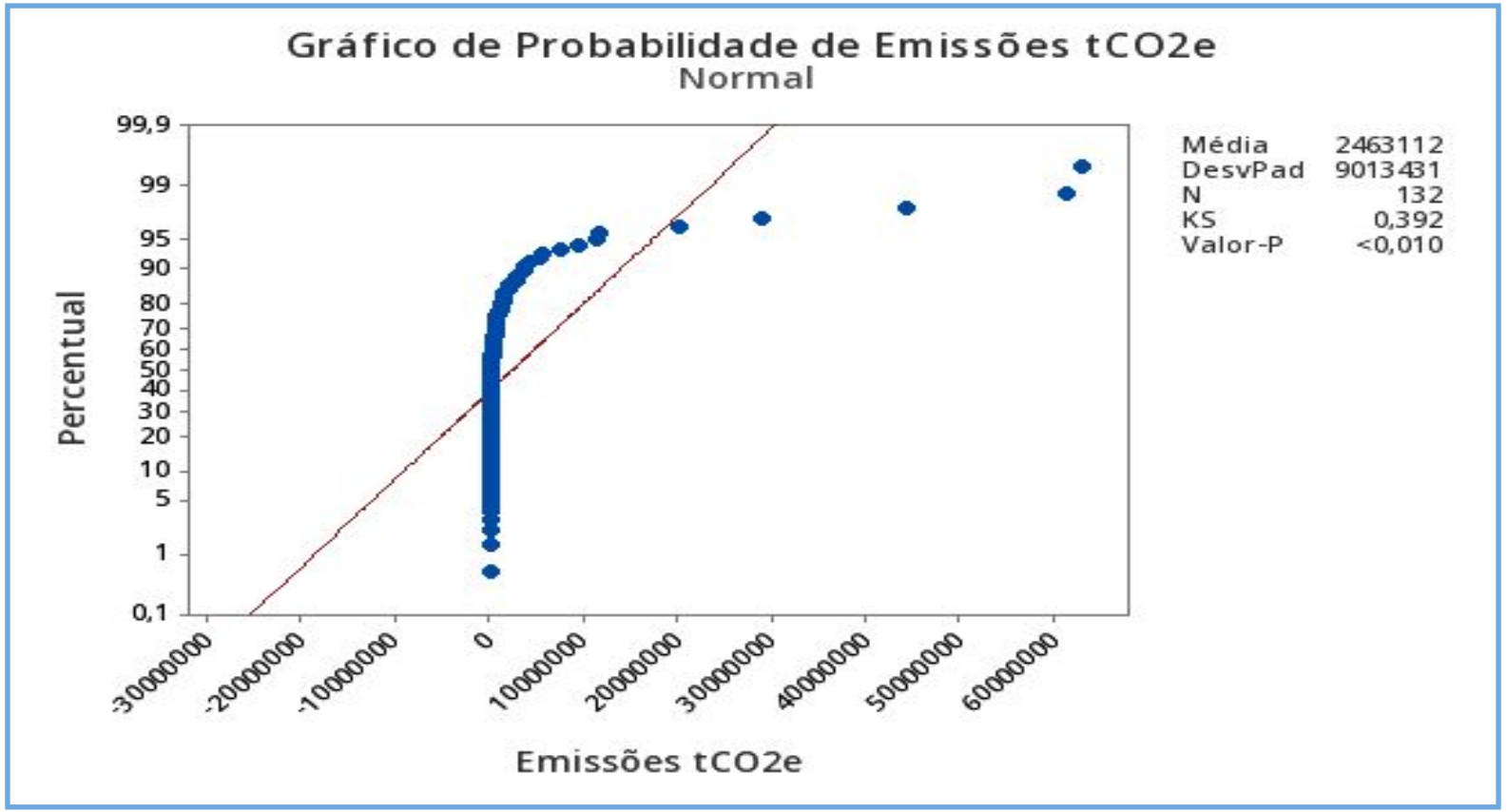
Variável	ANO	N	N*	Média	EP Média	DesvPad	Mínimo	Q1	Mediana	Q3	Máximo
Emissões tCO2e	2013	66	0	1256561	393671	3198197	32,18	16485,7	118054	864252	20182737
	2022	66	0	3669663	1510313	12269840	60,08	8686,94	121276	708366	62768571

- Box plot graph, to visualize data distribution, identify potential outliers, and compare maximum, minimum, and median values between the two years



RESULTS AND DISCUSSION

- The Kolmogorov-Smirnov normality test (as the sample had more than 50 elements) was applied to determine if the data followed a normal distribution.



- The data did not follow a normal distribution

RESULTS AND DISCUSSION

- The data did not follow a normal distribution, so the non-parametric Mann-Whitney test was applied. Hypotheses tested:
  H0: The samples have equal medians
  H1: The samples do not have equal medians
  A significance level of 5% (α = 0.05) was adopted.

Teste

Hipótese nula	$H_0: \eta_1 - \eta_2 = 0$
Hipótese alternativa	$H_1: \eta_1 - \eta_2 \neq 0$

Valor W	Valor-p
4394,00	0,984

- The Mann-Whitney test result showed a p-value = 0.984, higher than the significance level.

- The null hypothesis (H0) was accepted, indicating no significant increase in greenhouse gas emissions from 2013 to 2022.

- ❑ Important insights into GHG emission behavior
- ❑ Valuable insights into the behavior of GHG emissions and the importance of the preparation and publication of emission inventories by organizations.

RESULTS AND DISCUSSION

- **Santos (2016):**

❑ Found no positive correlation between the adoption of GHG emission inventories and the operational and financial performance of companies.
❑ The study highlights the need for further research on the impact of environmental actions on organizational performance.

- **Cordeiro (2017) highlights:**

❑ The understanding of how technical, human, and financial resources impact the adherence of organizations to GHG disclosures.
❑ It enables the implementation of more efficient environmental control techniques in the most critical areas.

RESULTS AND DISCUSSION

- **Vasconcelos (2020):**

- ❑ Indicates that a higher percentage of shares held by institutional investors favors the reduction of GHG emissions.
- ❑ Regulatory frameworks and company maturity can influence the prioritization of emission reductions

- **According to Silva (2023):**

- ❑ The participation of organizations in carbon offset programs is recommended when direct reduction is not possible.
- ❑ Offsetting through annual tree planting, carbon credit acquisition, afforestation projects, and reforestation are essential

CONCLUSIONS

- Statistical methods indicate no significant difference in GHG emissions from 2013 to 2022.

- The results suggest the implementation of regulations that require organizations to inventory GHG emissions.

- By conducting and publishing inventories, organizations:

❑ Identify and quantify their emissions
❑ Increase transparency
❑ Empower themselves to make strategic decisions for mitigating GHG emissions
❑ Publicize their progress.

- **The results of this study may influence public policies related to climate change.**

DECLARATIONS AND ACKNOWLEDGEMENTS

- The study presents limitations:

- ❑ The sample does not cover all organizations conducting inventories in Brazil
- ❑ The focus on a 10-year period may not reflect long-term trends
- ❑ The use of voluntarily reported data may vary in methodology and quality.

- **Gratitude to Fundação Getúlio Vargas and the Brazilian GHG Protocol Program for providing the GHG emission inventory data.**

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PROTEIN RECOVERY FROM WHEY BY COACERVATION USING CARBOXYMETHYLCELLULOSE: SCALING FROM LABORATORY TO PILOT

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ABSTRACT

Whey is the liquid by-product from cheese production. It contains a set of proteins, along with water, lactose, lipids, and mineral salts. It is an effluent from the cheese industry that is difficult and costly to treat, and efforts to revalorize. The objective of the work is the recovery of whey proteins by coacervation and its scaling. Coacervation is a technique to recover proteins with ionizable polysaccharides. The results show that it is possible to scale the process from 1 to 250 liters with a protein recovery close to 90 %. Despite increasing variability in some assays and incorporating minor modifications, the coacervation system proved to be scalable without significantly compromising protein recovery efficiency. The viability of the method and its scaling are confirmed, offering an economical alternative compared to membrane technology

Keywords: *whey protein recovery, coacervation, carboxymethylcellulose, scale-up process, sustainable dairy processing, protein precipitation, cheese byproducts, industrial biotechnology*

1. INTRODUCTION

Whey (W) is the liquid by-product of cheese production. It contains a set of proteins, along with water, lactose, lipids, and mineral salts. It is an effluent from the cheese industry that is difficult and costly to treat. For decades, efforts have been made to recover its value with variable results, and it is often used as animal feed (Gonzalez Siso, 1996).

Argentina produces around 11 million liters of whey per day, representing a large amount of quality protein that remains unused. Whey processing as a food ingredient using ultrafiltration methods is profitable at large scales of between 50,000 and 250,000 liters of processed milk per day. 81% of Argentine dairy companies are SMEs, which process less than 25,000 liters of milk daily and lack the appropriate technology for whey treatment (INTI, 2023).

Whey contains several proteins of high nutritional value, with the two main ones being: β-lactoglobulin, and α-lactalbumin. Other proteins include: Immunoglobulins, Serum proteins, Lactoferrin, and Glycomacropeptide. (Doultani and others, 2004).

Coacervation is a technique used in laboratories to recover proteins from various sources, employing ionizable polysaccharides. These polymers dissolve in water and acquire an electrical charge on their monomers, allowing them to electrostatically interact with oppositely charged protein molecules. The main forces driving the interaction between proteins and polysaccharides include electrostatic forces, hydrogen bonds, Van der Waals interactions, and hydrophobic effects (Spelzini and others, 2018). As these oppositely charged molecules interact, macromolecular complexes of proteins and polysaccharides are formed. These complexes tend to remain soluble, but under certain

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conditions, large aggregates form, separating from the rest of the solution as a new concentrated phase of proteins and polysaccharides, called coacervate. This protein- and polysaccharide-rich phase separates from the aqueous solvent, forming droplets or a denser suspended phase. This precipitate allows for the simple separation of these proteins from the rest of the solution (Koupantsis and Kiosseoglou, 2008).

Carboxymethyl cellulose (CMC) is a polysaccharide derived from cellulose, chemically modified by the addition of carboxymethyl groups (-CH_2-COOH) to its structure. It is water-soluble and forms viscous solutions, making it a widely used additive in the food industry due to its versatility and functional properties (Ingrassia and others, 2022).

2. MATERIALS AND METHODS:

1.1 Whey: obtained from the processing of 1000 L of Holando Argentino milk for the production of Pategrás cheese**.**

1.2 Reagents: citric acid monohydrate for pH regulation and sodium carboxymethyl cellulose (CMC) as an additive.

1.3 Measuring equipment: Ohaus analytical balance, Krenz commercial scale. pH measurements were taken with a Hanna device. Absorbance was measured with a Hach DR6000 spectrophotometer**.**

1.4 Mixing equipment: IKA T50 disperser, Trevi disperser with Cowles propeller. Armando Equipos mixer with Cowles propeller and a ¾ HP pump that provides axial flow to aid mixing**.**

1.5 Coacervation: the process involved mixing one-tenth of the whey with CMC, then homogenizing it with the rest of the whey, and adjusting the pH to 3 using citric acid. The mixture was stabilized at 24°C for 30 minutes and then refrigerated for 24 hours, resulting in a precipitate. Protein quantification was performed using the Bradford method at 595 nm (Kruger, 1994)**.**

1.6The results are reported as the percentage yield of recovery (RY):

$$RY = 100 \times (PT - PS)/PT \quad \text{(Eq. 1)}$$

Where PT represents the protein concentration in the whey before the coacervation process begins, and PS is the final concentration measured in the supernatant at pH 3.

3. RESULTS AND DISCUSSION

Our working strategy involves optimizing the coacervation technique with CMC for whey proteins at the laboratory scale (one liter). This includes measuring the protein concentration in whey with and without CMC, as well as how this amount varies with pH changes caused by the addition of citric acid. After determining the optimal pH values, the process will be scaled up to the pilot plant level.

3.1 Determination of the optimal pH for coacervate formation at the laboratory scale

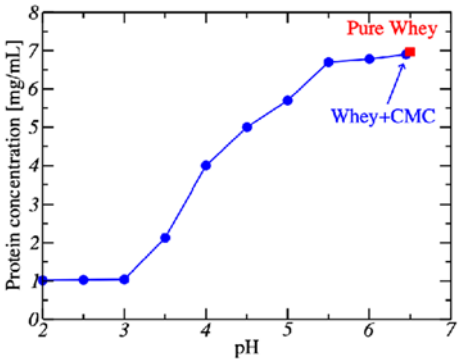


Figure 1. *Effect of pH on the concentration of proteins in the supernatant.*

Figure 1 shows the values of protein concentration as a function of the pH of the solution. The untreated whey is shown at the red point in Figure 1. We can observe that the untreated whey has a natural pH of around 6.5. Additionally, the average protein value is 6.97 mg/mL. This value aligns with the range of values reported in the literature for whey from different bibliographic sources (Kosikowski and Mistry 1997). The addition of 2 g of CMC to the whey does not substantially modify the pH and protein concentration values, as observed in the first point of the blue curve marked (Whey+CMC). As previously mentioned, each point on the curve corresponds to an independent experiment. In each experiment, except for the red point, 2 g of CMC was added to a 1-liter sample of whey, and the pH was subsequently adjusted by adding precise amounts of citric acid to achieve a specific final pH value in each case. The proteins present in each sample were then quantified using the Bradford method. It is observed that the reduction of pH to a value of 5.5 does not significantly alter the protein concentration in the whey, suggesting that there is no appreciable interaction between the proteins and the CMC in this range. However, as the pH decreases below 5.5, a notable reduction in protein concentration is detected. This reduction shows a linear trend with the pH until reaching a value of 3, from which the protein concentration remains practically constant. The final protein concentration is approximately 1 mg/mL.

As previously mentioned, citric acid was

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added to lower the pH of the mixture. The relationship between the amount of added acid and the resulting pH provides valuable information about the process, which is presented below.

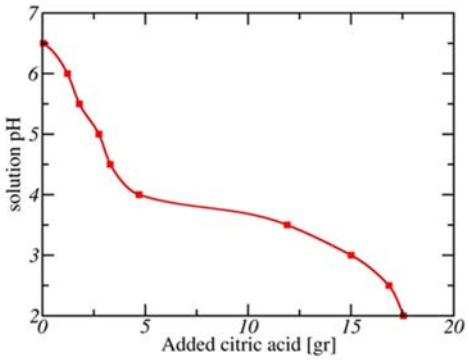


Figure 2. *Relation between the final solution pH and the citric acid added to the solution.*

Without the addition of citric acid, the initial pH of the whey protein and CMC mixture is approximately 6.5. As citric acid is incrementally added (measured in grams), the pH of the solution decreases almost linearly. The pH continues to drop until it reaches around 4, after which a greater amount of acid is required to further lower the pH. This effect is particularly evident in the plateau observed between pH 4 and 3. Beyond this range, the pH decreases more easily. This behavior indicates that the solution acts as a buffer system.

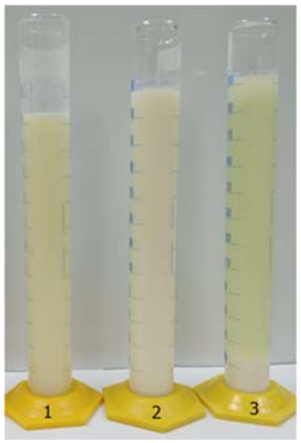


Figure 3. *Phase states of the whey and CMC mixture at different pH values.*
1) pH = 6.5; 2) pH = 4; and 3) pH = 3.

The phases and appearances of the whey-CMC mixture are shown in Figure 3 at three distinct points of the process, each characterized by a specific pH value. In test tube 1, we observe that the mixture at the initial working pH of 6.5 resembles pure whey. In fact, under these conditions, the measured protein concentration is very similar to the reference value for pure whey, as seen in Figure 1.

With acidification to pH 4 (test tube 2), the solution appears whiter or clearer, and there is a significant reduction in the amount of protein present in the solution, as shown in Figure 1.

Finally, at pH 3 (test tube 3), we can clearly observe a phase separation between a translucent solution and a precipitate at the bottom of the test tube. This point is critical, as it allows us to separate a precipitated phase rich in proteins, CMC, and fats. Moreover, the amount of protein in the solution is drastically reduced.

3.2 Scaling Up the Whey Protein Coacervation Process

We will now proceed to scale up the process to the pilot plant level. Essentially, we will increase the volume of whey and treat it with proportionate amounts of CMC and citric acid based on the values used for processing one liter of whey. Our initial plan was to treat 100 liters of whey. However, we were able to handle up to 250 liters of material. The equipment used for this purpose is shown in Figure 4.

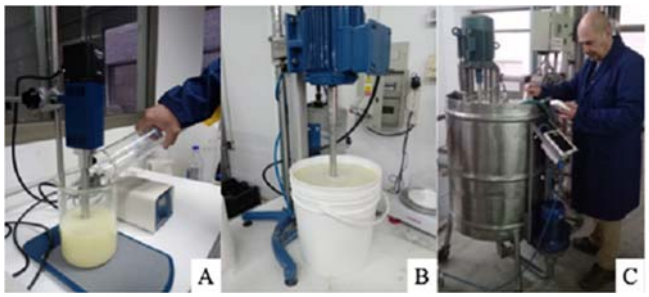


Figure 4. *Devices used to carry out the coacervation of whey using CMC at different scales: A) 1 L; B) 10 L; and C) 100 and 250 L.*

3.3 Percentage yield of recovery (RY):

Table 1. Recovery values (in percentage) of whey proteins depending on the volume of work.

Vol (L)	RY (%)
1	89 ± 1
10	87 ± 1
100	90 ± 3
250	90 ± 3

Note that at working volumes of 1 and 10 liters (see Figure 4A and 4B, respectively), the recovery values

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are around 90 % of the total. For working volumes of 100 and 250 liters, the recovery values are significantly higher, around 90%. However, in these cases, the device used (Panel C of Figure 3) is equipped with a powerful stirrer and a pump, which causes foaming on the surface of the liquid. A considerable proportion of the protein can end up in this foam.

Despite the increase in variability in the 100 liter trial, the coacervation system proved to be scalable without significantly compromising efficiency. The overall yield across the four scales averaged 88.83%, with an average standard deviation of 1.35%. These results suggest that the coacervation technique is suitable for implementation in larger volumes, with the axial flow pump optimizing the protein recovery process. (Eq. 1).

4. CONCLUSIONS

Considering the small amounts of CMC (2 grams) and citric acid (15 grams) used per 1 liter of SL, and the linear scalability for larger volumes, as well as the simplicity and accessibility of the materials, the protein concentration quantified in the supernatant after 24 hours of coacervation is highly promising. This represents a positive and encouraging result for the future implementation of coacervation in small to medium-sized enterprises (SMEs). Analysis of the averages from the four experiments demonstrates that the coacervation process is scalable from 1 liter to 250 liters without significantly compromising the efficiency of the method. As the volume increases, the protein recovery percentage remains high and consistent, reaching values close to 90% at 250 liters, thanks to equipment improvements aimed at achieving better reagent distribution (Table1). The process is repeatable and reliable across all scales. This success in scaling the process suggests that, with proper adjustments, such as using an axial flow pump to improve homogeneity, the coacervation method can be efficiently implemented in larger volumes without losing effectiveness in whey protein recovery. These favorable protein yields open the door to the successful transfer of this low-cost technology, especially when compared to membrane technology, from the laboratory to cheese production plants. These results support the potential to utilize large volumes of whey, which are often discarded or used in animal feed, to obtain a protein enriched phase of high quality. This could have a positive impact on the future formulation and production of food products.

5. DECLARATIONS

5.1. Acknowledgments

This work is part of the Doctoral Thesis of Martín Moyano, as part of the Doctorate in Engineering of Products and Processes in Industry. The authors wish to express their gratitude to Vilma Morata, Carolina Martin, Valentín Lavastrou, Daniela Mauceri, Silvana Martinez, and Luisa Tapia for their contribution in this work.

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Southern Science Conference, 2024.

PROTEIN RECOVERY FROM WHEY BY COACERVATION USING CARBOXYMETHYLCELLULOSE: SCALING FROM LABORATORY TO PILOT

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November/2024

INTRODUCTION

- Whey is the liquid by-product of cheese production. (Gonzalez Siso, 1996)
- Contains a set of proteins, along with water, lactose, lipids, and minerals salts.
- Argentina produces around 11 million liters of whey per day (INTI, 2023).
- Whey contains several proteins of high nutritional value. (Doultani and others, 2004).
- Coacervation is a technique to recover proteins with ionizable polysaccharides (CMC). (Koupantsis and Kiosseoglou, 2008).
- The results show that it is possible to scale the process from 1 to 250 liters with a protein recovery close to 90 %.

AIM

- Perform the coacervation technique at the laboratory scale, using an initial volume of 1 liter, to determine the optimal conditions for the formation of the coacervate complex.

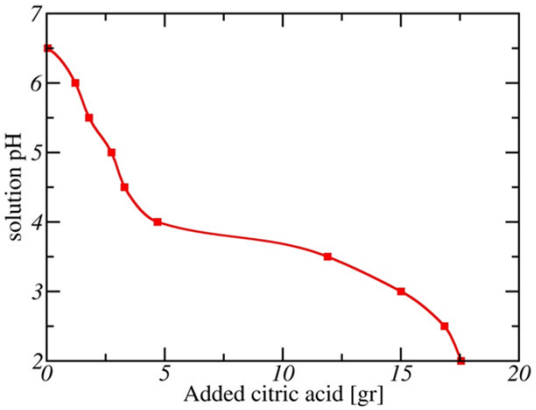
- Quantify the protein content present in the whey available in the San Rafael area, using this value as the maximum recovery reference.

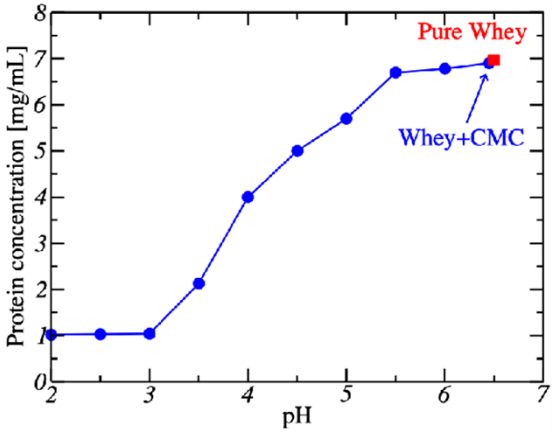
- Assess the feasibility of the optimized laboratory process through successive scale-ups, applying the conditions to pilot volumes of 10 and 100 liters.

METHODOLOGY

- **Coacervation Process:** A defined volume of 0.1L of whey (SL) is mixed with 2g of CMC per liter, stirring until a creamy consistency is achieved. Then, 90% of the remaining SL is added and homogenized at 500 RPM. The pH is adjusted to 3 with citric acid over 40 minutes, keeping the temperature below 24 °C. After stabilization for 30 minutes, the mixture is refrigerated at 4 °C for 24 hours, leading to the formation of a whitish precipitate.
- **Yield Quantification:** The protein concentration in a refrigerated SL sample is measured using the Bradford method at 595 nm, with a 1/50 dilution considered the maximum recoverable protein. The same analysis is performed on the supernatant without dilution, and the precipitated protein is determined as the difference between the SL and the supernatant.
- **Optimal pH Determination:** Ten coacervation experiments are conducted at different pH levels (ranging from 2.00 to 6.50) to evaluate the coacervation efficiency relative to the isoelectric points of α-lactalbumin and β-lactoglobulin. A sample of the SL without additives is included for comparison in a graph.
- **Citric Acid Consumption:** The amount of citric acid needed to adjust the pH is quantified, using graphs to show the relationship between citric acid consumption and the pH of the solution, considering the initial pH values of the SL with and without CMC.
- **Scaling Up:** The process starts with 1L and scales up to 10 and 100 liters, maintaining the proportion of CMC and the conditions for mixing, stabilization, and temperature. Replicates are controlled, with 3 for each trial and 2 for the 100L due to supply limitations. The consumption of citric acid is related to the initial pH of the SL.

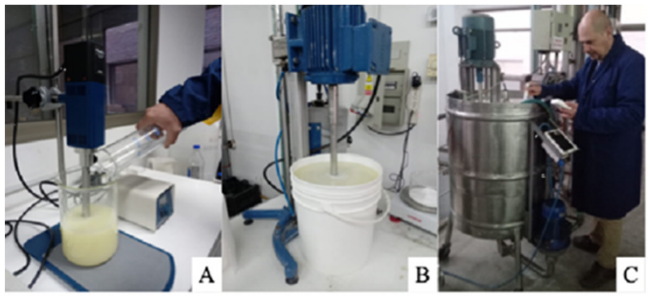
RESULTS AND DISCUSSION





Determination of the optimal pH for coacervate formation at the laboratory scale

Beyond this range, the pH decreases more easily. This behavior indicates that the solution acts as a buffer system.



Vol (L)	RY (%)
1	89 ± 1
10	87 ± 1
100	90 ± 3
250	90 ± 3

Scaling Up the Whey Protein Coacervation Process and RY

Our initial plan was to treat 100 liters of whey. However, we were able to handle up to 250 liters

CONCLUSIONS

- This work represents a positive and encouraging result for the future implementation of coacervation in small and medium-sized enterprises (SMEs).

- The analysis demonstrates that the coacervation process is scalable from 1 liter to 250 liters without significantly compromising the efficiency of the method.

- As volume increases, protein recovery percentage remains high and constant.

- This success in scaling up the process suggests that, with appropriate adjustments, the coacervation method can be efficiently implemented in large volumes.

- Favorable protein yields open the door to the successful transfer of this low-cost technology to cheese production plants.

- The whey from the area have protein content values that agree with those provided by the specialized literature.

ACKNOWLEDGEMENTS

- Acknowledgement 1This work is part of the Doctoral Thesis of Martín Moyano, as part of the Doctorate in Engineering of Products and Processes in Industry.

- The authors wish to express their gratitude to Vilma Morata, Carolina Martin, Valentín Lavastrou, Daniela Mauceri, Silvana Martinez, and Luisa Tapia for their contribution in this work.

- C.F.N. acknowledges the financial support from AGENCIA I + D + i (FONCyT), PICT-2021-GRFTI-00090 and from Universidad Tecnologica Nacional (PIDs PATCASR0008459 and PATCASR0008463).

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MOTIVATION TOWARDS SCIENCE OF SPANISH SECONDARY STUDENTS

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ABSTRACT

This study explores the motivation toward science of 185 Spanish secondary school students pertaining to two educational centers in Valencia. Five different dimensions of motivation toward science (self-efficacy, self-determination, intrinsic motivation, career, and grade motivation) were measured using the Science Motivation Questionnaire II (SMQ-II). Results show a general decrease in motivation in older students, with statistically significant differences between first graders and third and fourth graders, which may imply the pursuit of scientific careers.

Keywords: *motivation, secondary education, level.*

1. INTRODUCTION

The issue of student motivation towards learning subjects in the science area is an important concern for Spanish teachers. They confirm a lack of interest in students towards these subjects and a greater academic failure in scientific disciplines compared to other disciplines. On their part, students blame their lack of interest to decontextualized science teaching along with other factors, such as teaching methods (Furió, 2006).

The educational world has been changing in the last decades, moving on from traditional methodologies based on the mere transmission and presentation of content by teachers that are not enough for students to have meaningful learning. In general, students present some difficulties in understanding the content to be studied, but these difficulties are greater in subjects related to science. Flores-Caballero (2019) points out the lack of motivation as one of the causes of those difficulties. On the other hand, the misconceptions about science and scientific activity, which are explicitly or implicitly transmitted by the media and textbooks as well as by some teachers, contribute to the lack of motivation, giving rise to distorted visions of science. That also distorts the interests and realities of the students and makes them conceive a person dedicated to science as a “genius” or “crazy” (Vergara, 2012).

Teachers, therefore, must opt for pedagogical techniques that not only improve conceptual understanding but also motivate students to participate and be an active part of the teaching and learning process. Cabling and Magday (2022) investigated the students' level of motivation in science when using the concept mapping technique in teaching. After analyzing the results, they encourage teachers to consider this technique as a strategy for providing instruction in the science classroom because it provides a positive outcome and can motivate students.

Among the motivational predictors, self-concept and self-efficacy are among the most important in terms of educational results. In the research of Jansen *et al.* (2015), it was shown that practical activities in science provide opportunities for students to acquire mastery experiences that are essential for the development of self-efficacy. On the other hand, Teig and Nilsen (2022) mention that teacher self-efficacy in science teaching is a good indicator of teaching competence and that it is positively associated with the quality of instruction and student results.

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Teacher motivation towards STEM fields is also important, both in terms of carrying out STEM activities in classes and motivating students in these fields. The research carried out by Dökme *et al.* (2022) showed that the motivations of female science education university students towards STEM fields differed according to different variables: "father's education level", "having received STEM education", "having participated in STEM activities", and “having a role model working in a STEM field”. On the other hand, the research findings of Hiğde and Aktamış (2022) suggested that STEM activities can be implemented to improve students' scientific process skills, STEM career interests and motivation, as well as opinions about education in this field.

Science self-efficacy is an important driver of interest in science, STEM career choice, and persistence toward those career goals. Specifically, female students have significantly lower self-efficacy than male students in STEM fields, and this self-efficacy gap contributes in part to the underrepresentation of women in science and engineering fields. Female students may even assume that they have to make extra efforts to succeed and experience additional stress. When girls succeed, they attribute their success to luck, and boys attribute it to their own inner ability, while when they fail, girls attribute failure to lack of ability and boys to lack of effort. Because of this, even girls who do well in school subjects do not develop the kind of self-confidence that men have (Marshman *et al.*, 2018).

2. MATERIALS AND METHODS

The sample was composed of 185 students belonging to two educational centers in Valencia (Spain). They pertained to all levels of compulsory Secondary Education (first to fourth grade), with 53,5% being female and 46,5% male.

To measure motivation toward science, the “Science Motivation Questionnaire II (SMQ-II)” by Glynn *et al.* (2011) was used with the translation to Spanish provided by Ardura et al. (2018). This questionnaire includes five scales, each one with 5 items: intrinsic motivation, self-determination, self-efficacy, professional motivation, and degree motivation. Each item is answered on a temporal frequency rating scale: never (0), rarely (1), sometimes (2), frequently (3), or always (4), with a maximum score on each of the five scales of 20 points. The total student motivation towards science is calculated as the sum of the five motivation scales.

Descriptive and inferential statistical analyses were carried out with SPSS v26 software. First, mean and standard deviations were calculated for each scale and the total score. Next, the Kolmogorov-Smirnov test was performed to determine the normality of the distributions. Since all of them were non-normally distributed, non-parametric tests were used to assess the differences between levels (Kruskall-Wallis test) and genders (Mann-Whitney U). The level of statistical significance was 0.05 in all cases.

3. RESULTS AND DISCUSSION:

The results of motivation towards science, in the five scales, are presented in Table 1. It is apparent that the students have scored higher on the five scales during the first two years of secondary education, with the exception of the degree motivation scale. Regarding the third and fourth grades of secondary education, the results indicate that fourth-year students presented greater intrinsic motivation and self-determination than third-year students, while the latter presented greater self-efficacy, professional motivation, and degree motivation when compared to fourth graders. However, it should be noted that, in general, the results obtained are not too different when compared to the courses of the same cycle. However, a greater difference is observed when comparing the results of the first and last course, reaching 4 points of difference in the professional motivation scale and 3 points in the rest of the scales. It is worth mentioning that these results are measured on a scale from 0 to 20, so the motivation experienced by the students is not very high in any case. Furthermore, the total motivation score shows a clear trend: first-year students are the ones with the highest score, which decreases as the grade increases.

These results are in accordance with those of Ardura and Pérez-Bitrián (2018), Salta and Koulougliotis (2015), and Schumm and Bogner (2016), where the students had also a higher score on the scale of degree motivation. However, it should be noted that, in the present work, intrinsic motivation is the second scale with the highest score, while in the three aforementioned investigations, this second place was occupied by self-efficacy.

In order to establish the possible existence of significant differences depending on the grade, the non-parametric Kruskall-Wallis test was applied. The results show that there are

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statistically significant differences ($p < 0.05$) between the courses in almost all dimensions of motivation, with the exception of self-efficacy. In order to assess between which courses lay those statistically significant differences, the Bonferroni post hoc test was carried out. The results show that there were statistically significant differences between the first and fourth graders in four of the five scales of motivation (with the exception of self-determination) and in total motivation scores. Furthermore, the differences between the first and third graders are significant in two of the five scales (intrinsic motivation and self-determination) and in total motivation. In the research by Salta and Koulougliotis (2015), which carried out a study between lower secondary school (14-15 years old) and upper secondary school (16-17 years old), no statistically significant differences were obtained between the two groups in any of the scales, except for grade motivation. Furthermore, there are studies such as that of Gentry *et al.* (2002) or Gottfried *et al.* (2001), among others, who mention that as the years go by in school, students experience progressive deterioration in motivation.

Overall, these results have several implications for science education. First, they suggest a need for early intervention to sustain motivation from the start of secondary education, where enthusiasm for science is highest. This could include providing more engaging and hands-on learning opportunities early on, which could sustain motivation throughout secondary school. Although the general trend shows a decline, certain dimensions of motivation (intrinsic motivation and self-determination) are higher among fourth-year students compared to third-year students. This suggests that, although overall motivation decreases, students may still experience deeper internal forms of motivation as they approach the final years of secondary education. This could reflect a growing sense of autonomy and a more intrinsic connection to science for those students who remain engaged. Such findings emphasize the importance of supporting students' self-determination in science learning by promoting activities that align with their personal interests and goals. Educators could, for example, design curricula that offer more autonomy and choice in learning activities for older students, potentially counteracting the general motivational decline.

4. CONCLUSIONS:

Motivation is a key factor for effective learning, as it acts as the driving force that encourages students to actively engage in the educational process, facilitating the understanding and assimilation of new knowledge. Specifically, motivation towards science is of utmost importance at this school stage since Allows them to develop critical thinking, experimentation, and problem-solving skills.

The results show that the motivation towards the science of Spanish compulsory secondary students is average and that this motivation decreases with time as the students advance in the educational system. The students with the highest motivation are those in the first year, with this score decreasing steadily. These results call for a reflection on the attention to scientific subjects in secondary education and the teaching methodologies used. It is very important to take into account that the motivation towards science in this educational stage significantly influences students' interest in pursuing scientific or technological careers.

5. DECLARATIONS

5.2. Open Access

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Table 1. *Results of the five scales of student motivation towards science and total score according to level.*

Grade	Intrinsic Motivation	Self-determination	Self-efficacy	Career motivation	Grade motivation	Total motivation
1st grade	14,79 ± 4,19	13,24 ± 4,14	12,14 ± 4,29	13,64 ± 3,96	15,79 ± 3,18	69,90 ± 15,91
2nd grade	12,98 ± 4,02	12,05 ± 5,94	11,29 ± 4,32	12,24 ± 4,59	13,34 ± 5,15	61,90 ± 19,30
3rd grade	11,59 ± 4,73	9,98 ± 5,18	11,04 ± 3,90	10,98 ± 5,09	14,20 ± 4,10	57,78 ± 18,83
4th grade	12,02 ± 4,55	10,57 ± 5,95	9,61 ± 4,53	9,92 ± 4,58	13,06 ± 4,71	55,18 ± 20,33

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Southern Science Conference, 2024.

MOTIVATION TOWARDS SCIENCE OF SPANISH SECONDARY STUDENTS

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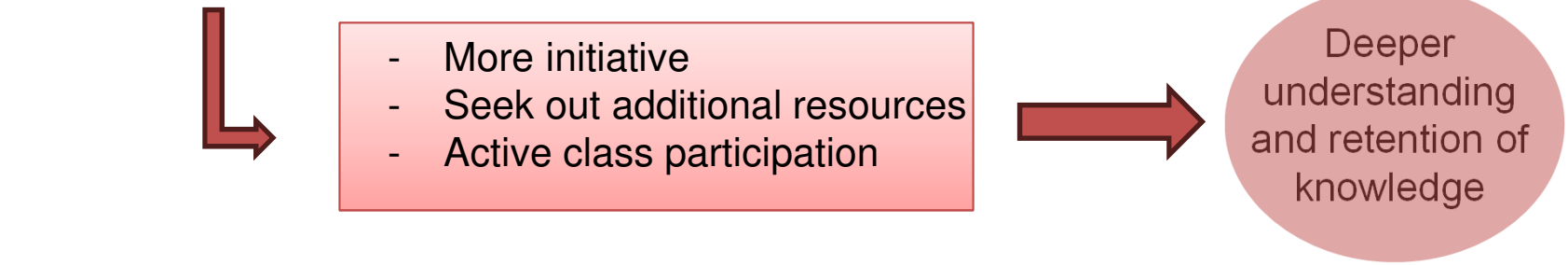
Yolanda Echegoyen Sanz
Universitat de València, Facultat de Magisteri - España

November/2024

INTRODUCTION



MOTIVATED STUDENT



In **Science**… motivation helps:

- better understand complex concepts
- to develop critical thinking, experimentation, and problem-solving skills.

BACKGROUND

Teaching a decontextualized and less useful science and the use of traditional methodologies drives to a **lack of student interest in science** (Furió, 2006).

Students present some **difficulties in understanding** the content they study, especially when it comes to science, and one of the causes is the **lack of motivation** (Flores-Caballero, 2019), to which contributes the transmission of **misconceptions** about science and scientific activity transmitted by the media, books, and even teachers. That also distance the interests and realities of the students and make them conceive a person dedicated to science as a "genius" or "crazy" (Vergara, 2012).

Teachers must opt for **pedagogical techniques** that not only improve conceptual understanding, but also motivate students to **participate and be an active part** of the teaching and learning process (Cabiling and Magday, 2022).

AIM/OBJETIVE/PURPOSE

- Study the motivation towards science presented by secondary education students. Analyze whether this is low, medium or high and see how it varies throughout the secondary stage

METHODOLOGY

SAMPLE: 185 students belonging to two educational centers in Valencia (Spain) and pertained to all levels of secondary education (1st to 4th grade) with 53,5% being female and 46,5% male.

HOW TO MESURE MOTIVATION TOWARDS SCIENCE?

Science Motivation Questionnaire II (SMQ-II) (Glynn et al., 2011) with the translation to Spanish provided by Ardura et al. (2018)

5 scales each one with 5 items: intrinsic motivation, self-determination, self-efficacy, professional motivation and degree motivation.

Answered on a **temporal frequency rating scale**: never (0), rarely (1), sometimes (2), frequently (3) or always (4) with a **maximum score** on each of the five scales of **20 points**. Total motivation is calculated as the sum of the five motivation scales.

Mean and standard desviation were calculated for each scale and the total score. Since all the distributions were non-normally distributed (Kolmogorov-Smirnov), non-parametric tests were used to assess the differences between levels (Kruskall-Wallis test) and genders (Mann-Whitney U). The level of statistical significance was 0.05 in all cases.

RESULTS AND DISCUSSION

	Intrinsic motivation	Self-determination	Self-efficacy	Career motivation	Degree motivation	Total motivation
1st grade	14,79 ± 4,19	13,24 ± 4,14	12,14 ± 4,29	13,64 ± 3,96	15,79 ± 3,18	69,90 ± 15,91
2nd grade	12,98 ± 4,02	12,05 ± 5,94	11,29 ± 4,32	12,24 ± 4,59	13,34 ± 5,15	61,90 ± 19,30
3rd grade	11,59 ± 4,73	9,98 ± 5,18	11,04 ± 3,90	10,98 ± 5,09	14,20 ± 4,10	57,78 ± 18,83
4th grade	12,02 ± 4,55	10,57 ± 5,95	9,61 ± 4,53	9,92 ± 4,58	13,06 ± 4,71	55,18 ± 20,33
TOTAL	12,74 ± 4,54	11,34 ± 5,48	10,95 ± 4,33	11,57 ± 4,79	14,05 ± 4,44	60,66 ± 19,37

- 1st grade students present the highest motivation score and 4th grade students the smallest one.

- Students of the first stage of secondary education show higher score in the five scales of motivation, except for degree motivation.

- Degree motivation is the scale with the highest score. This is in accordance with the results obtained by Ardura and Pérez-Bitrián (2018), Salta and Koulougliotis (2015), and Schumm and Bogner (2016).

RESULTS AND DISCUSSION

- There are significant differences in almost all motivation scales except for self-efficacy.

- Significant differences are established between the 1st and 4th grades in four of the five scales of motivation, with the exception of self-determination, and in total motivation.

- The differences between the 1st and 3rd courses are significant in two of the five scales (intrinsic motivation and self-determination) and in total motivation .

Other studies such as that of Gentry et al. (2002) or Gottfried et al. (2001) talks about the progressive deterioration as the years go by in school.

		1º--2º	1º--3º	1º--4º	2º--3º	2º--4º	3º--4º
Motivación intrínseca	p	0,120	0,001*	0,007*	1,000	1,000	1,000
Autodeterminación	p	1,000	0,030*	0,187	0,058	1,000	1,000
Autoeficacia	p	1,000	1,000	0,039*	1,000	0,504	0,746
Motivación profesional	p	1,000	0,062	0,001*	1,000	0,133	1,000
Motivación de grado	p	0,203	0,515	0,027*	1,000	1,000	1,000
Motivación total	p	0,512	0,019	0,003	1,000	0,607	1,000

CONCLUSIONS

- The motivation towards science of Spanish compulsory secondary students is average.

- The students with the highest motivation are those in the 1st grade, with this score decreasing steadily. The motivation decreases with time as the students advance in the educational system.

- Call for a reflection on the attention to scientific subjects in secondary education and the teaching methodologies used. Motivation towards science influences student's interest in pursuing scientific or technological careers.

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ATMOSPHERIC DEGRADATION OF METHYL GLYCOLATE

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ABSTRACT

This study presents the atmospheric degradation of methyl glycolate, a semivolatile compound used in the industry. Its rate coefficient with Cl atoms and hydroxyl radicals, photooxidation products, and reaction mechanism were determined. Atmospheric implications of its emissions are presented.

Keywords: Atmosphere, Kinetics, Mechanism reaction, Photooxidation, Infrared spectroscopy.

1. INTRODUCTION

Methyl glycolate (MG, $HOCH_2C(O)OCH_3$) is a semivolatile compound widely used in industry, so it is possible that it could be emitted into the atmosphere. A priori, as with similar organic compounds, can be degraded in several ways: photochemical rupture, reaction with hydroxyl radicals (HO(), chlorine atoms (Cl), or nitrate radicals. The relative importance of these processes was needed to determine its atmospheric lifetime. To assess the potential environmental impact of its emissions, it was also required to determine which products are formed as a result of its atmospheric degradation.

In the present study, the gas-phase rate coefficient of the reaction between MG and Cl atoms was determined, and the corresponding one with the $HO^{\bullet}$ radical was estimated (Eqs. 1 and 2, respectively) in order to determine the influence of both reactions on the atmospheric lifetime:

$HOCH_2C(O)OCH_3 + Cl \rightarrow$ Products (Eq. 1)

$HOCH_2C(O)OCH_3 + HO^{\bullet} \rightarrow$ Products (Eq. 2)

The gas-phase photooxidation of MG in the absence and presence of NO_2 was also studied to determine its reaction products and reaction mechanism. Finally, the potential environmental impact of its emissions to the atmosphere was discussed.

2. MATERIALS AND METHODS

The gas mixtures were manipulated using a high vacuum system. The kinetic determinations, as well as the identification and quantification of the reaction products, were performed using a Fourier Transform Infrared Spectrophotometer (FTIR) with a resolution of 2 cm^{-1} and an infrared gas cell.

The rate coefficient of the reaction between MG and Cl atoms ($k_{Cl,exp}$) was determined using a relative method by comparing the temporal variation of the MG concentration with the corresponding to a reference compound (acetone), $k_{Ace} = (2.1 \pm 0.3) \times 10^{-12}$ cm^3 $molec^{-1}$ s^{-1} (Calvert et al., 2011). The value of $k_{Cl,exp}$ was then compared with that estimated by the SAR method, $k_{Cl,\ SAR}$. This allows us to estimate the rate coefficient of a compound from its structure, considering the abstraction of a hydrogen atom from the $-CH_3$, $-CH_2-$ and -CH< groups that form the molecule and taking into account the substituent groups (Kwok et al., 1995).

Gas mixtures for kinetic experiments were

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prepared in the reaction cell, using 0.96 mbar MG (or acetone), 1.35 mbar Cl_2, and 1000 mbar N_2. For photooxidation, nitrogen was replaced by O_2, and 0.50 mbar NO_2 was added when it was required. The mixtures were irradiated with black lamps (which provide radiation longer than 360 nm) to produce the rupture of the Cl_2 molecule and the consequent formation of Cl atoms.

The identification and quantification of the reaction products were performed using reference infrared spectra. From these products and the kinetic analysis, the photooxidation mechanism was proposed.

The rate coefficients of the reactions of organic compounds with hydroxyl radicals (k_{HO}) generally have lower values than those of their reactions with Cl atoms (k_{Cl}), which sometimes leads to difficulties in their experimental determination. An estimate of the value of k_{HO} for a given compound can be obtained by making a linear correlation between the values of -log(k_{HO}) and -log(k_{Cl}) for compounds whose rate coefficient has been determined experimentally (*e.g.,* Vila et al., 2025). The value of the MG rate coefficient with HO• radicals was determined from compounds with similar structures.

Finally, the lifetime of the MG was determined from the rate coefficients measured in this work and the concentrations of Cl atoms and HO• radicals present in the atmosphere, using Eqs. 3 and 4:

$$\tau_{Cl} = \frac{1}{k_{MG}\,[Cl]} \qquad \text{(Eq. 3)}$$

$$\tau_{HO} = \frac{1}{k_{MG}\,[HO]} \qquad \text{(Eq. 4)}$$

where [Cl] and [HO•] correspond to the average concentrations of Cl atoms and HO• radicals in the atmosphere: 3.3 x 10^4 atoms cm^{-3} (Wingenter et al., 1996) y 2 x 10^6 radicals cm^{-3} (Hein et al., 1997), respectively.

3. RESULTS AND DISCUSSION

3.1. Determination of the rate coefficient of MG with Cl atoms

The value of the rate coefficient $k_{Cl,exp}$ was determined using Eq. 5:

$\ln([MG]_0/[MG]_t) = k_{MG}/k_{Ace}\ln([Ace]_0/[Ace]_t)$ (Eq. 5)

where $[MG]_0$ and $[MG]_t$ represent the MG concentration at initial and *t* time, respectively, and $[Ace]_0$ and $[Ace]_t$ correspond to the acetone concentrations at the times mentioned above. After plotting $\ln([MG]_0/[MG]_t)$ *vs.* $\ln([Ace]_0/[Ace]_t)$, Figure 1, the value of the slope was obtained, and subsequently $k_{Cl,exp}$ = (4.7 ± 0.8) x 10^{-12} cm^3 $molec^{-1}$ s^{-1}.

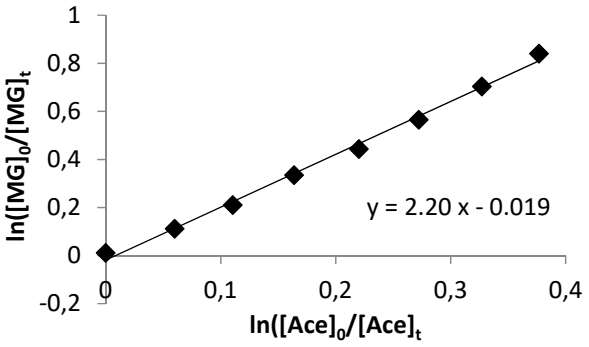


Figure 1. *Determination of the rate coefficient of MG with Cl atoms using acetone as reference.*

The value of $k_{Cl,exp}$ was compared with that determined by the SAR method, $k_{MG,\,SAR}$. The rate coefficient was obtained by Eq. 5, using the values of the parameters informed in bibliography: k(-CH_3) = 3.32 x 10^{-11} cm^3 $molec^{-1}$ s^{-1}, k(-CH_2-) = 8.34 x 10^{-11} cm^3 $molec^{-1}$ s^{-1} (Aschmann et al., 1995); F(-OH) = 1.18 (Calvert et al., 2011); F(-C(O)O) = 0.04, F(-OC(O)) = 0.05 (Notario et al., 1998).

$$k_{MG,SAR} = k_{-CH2-}\,x\,F(-OH)\,x\,F(-C(O)O) + k_{-CH3}\,x\,F\big(-OC(O)\big) \qquad \text{(Eq. 5)}$$

$$k_{MG,SAR} = 5{,}6\,x10^{-12}\ cm^3\ molec^{-1}\ s^{-1}$$

The value of $k_{MG,SAR}$ is consistent with $k_{Cl,exp}$, taking into account that the former is an estimation, and the latter has an experimental associated error.

On the other hand, $k_{Cl,exp}$ is substantially lower than the corresponding to ethyl glycolate ($CH_3C(O)OCH_2CH_3$), (6.4 ± 0.7) x 10^{-11} cm^3 $molecule^{-1}$ s^{-1} (Straccia et al., 2023), as a consequence of the fact that MG has one less -CH_2- group. The comparison of the rate coefficient of MG with Cl atoms and the one corresponding to the reaction of methyl acetate ($CH_3C(O)OCH_3$) (2.55 x 10^{-12} cm^3 $molecule^{-1}$ s^{-1}; Calvert et al., 2011) shows the activation produced by the -OH group in the MG molecule.

3.2. Estimation of the rate coefficient of MG with HO• radical

Figure 2 shows the plot -log(k_{OH}) *vs.* -log(k_{Cl}) obtained from the rate coefficient of the selected compounds: methyl acetate, ethyl

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acetate, propyl acetate, n-butyl acetate, hydroxyacetone, ethyl glycolate, methyl propionate, and methyl formate. From the slope of the plot, a value of k_{HO} = 4.4 x 10^{-13} cm^3 $molecule^{-1}$ s^{-1} was determined.

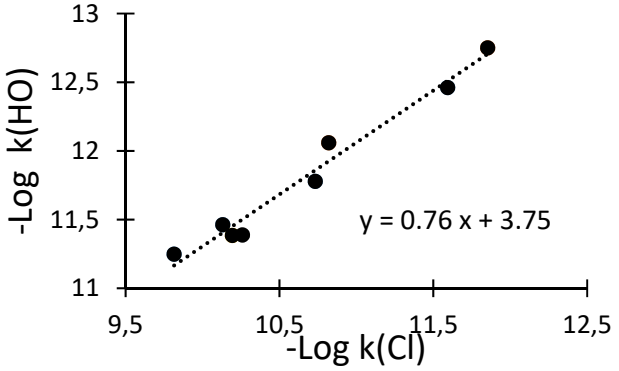


Figure 2. *Determination of kOH from* -log(k_{OH}) vs -log(k_{Cl})

3.3. Identification of the photooxidation products of MG. Determination of the reaction mechanism

The analysis of the infrared spectra obtained in the photooxidation in the absence of NO_2 reveals the formation of formic acid (peaks at: 637, 1105, and 1775 cm^{-1}), methyl glyoxylate (1754, 1741, 1289, 1225, and 1024 cm^{-1}) and CO_2 (667 and 2340-2360 cm^{-1}). The spectra obtained when photooxidation is carried out in the NO_2 presence show the formation of $CH_3OC(O)OONO_2$ (796, 930, 1197, 1237, 1302, 1448, 1748 and 1834 cm^{-1}) and formic acid.

On the basis of these results, the reaction mechanism shown in Figure 3 is proposed. As can be seen, the Cl atom can react with the -CH_3 and -CH_2- groups (*vias* 1 and 2, respectively). The attack on the hydrogen of the hydroxyl group (*via* 3) is negligible (Cavalli, 2000).

The $HOCH_2C(O)OCH_2^{\bullet}$ radicals formed in via 1 react with O_2 and subsequently with Cl atoms or other peroxide radicals ($ROO^{\bullet}$) to form $HOCH_2C(O)OCH_2O^{\bullet}$ radical. This is similar to $CH_3C(O)OCH_2O^{\bullet}$ or $CH_3CH_2C(O)OCH_2O^{\bullet}$, which is reached mainly by rearrangement α-ester (via 1.a) and reaction with O_2 (via 1.b) (Christensen et al., 2000). When photolysis takes place in the presence of NO_2, an additional pathway is opened to form $HOCH_2C(O)OCH_2ONO_2$, which was not observed. The expected products of the subsequent reactions are glycolic acid ($HOCH_2C(O)OH$), CO, $HOCH_2C(O)OC(O)H$. The formation of glycolic acid was not observed, probably because it is solid at room temperature and should be deposited on the walls of the reaction cell. The percentage of CO formation accounts for a 5 % disappearance of MG. On the other hand, $HOCH_2C(O)OC(O)H$ was not observed as a reaction product due to heterogeneous decomposition to formic acid. The percentage of this acid when the photooxidation is carried out in the absence of NO_2 is 30 %. Considering that CO is formed from via 1.a and HC(O)OH arises from via 1.b, the reaction of the $HOCH_2C(O)OCH_2O^{\bullet}$ radical with O_2 is favoured. The results are in agreement with those obtained for the $CH_3C(O)OCH_2O^{\bullet}$ radical, by Christensen et al. (2000), who determined that this reaction is favoured at high O_2 pressures, as the used in our experimental set-up.

The $HOCH^{\bullet}C(O)OCH_3$ radical formed from *via* 2, can react with O_2 to lead to the formation of methyl glyoxylate ($HC(O)C(O)OCH_3$), *via* 2.a, or the peroxide radical $HOCHOO^{\bullet}C(O)OCH_3$ (*via* 2. b), which from subsequent reactions finally leads to the formation of formic acid, carbon dioxide and formaldehyde. Orlando et al. (2020) studied the relative importance of both *vias* and determined that 95 % of the reaction occurs *via* 2.a. This is consistent with the low percentage of carbon dioxide formed when photolysis is performed in the absence of NO_2 and the non formation of CH_2O.

When photooxidation is carried out in the presence of NO_2, the formation of formic acid (50 %) and $CH_3OC(O)OONO_2$ (39 %) was observed. The quantification of peroxynitrate is indicative of the reactivity of the hydrogen atoms corresponding to the -CH_2- group of the MG molecule. The formation of methyl glyoxylate is not observed, and a fraction of NO_2 is photolyzed to form NO, which favours the occurrence of *via* 2.b (Orlando et al., 2020).

4. CONCLUSIONS

The atmospheric lifetime was determined using equations (3) and (4). The values obtained, τ_{Cl} = 75 days and τ_{HO} = 13 days, indicate that the lifetime of MG is mainly controlled by its reaction with the $HO^{\bullet}$ radical.

The degradation in NO_2-polluted environments leads mostly to the formation of $CH_3OC(O)OONO_2$ and formic acid. The former is relatively stable and can be transported from its formation site to higher altitudes or remote locations where its thermal decomposition can inject peroxy radicals and NO_2 (Kirchner et al, 1997). Formic acid could have an impact on the acidity of clouds and raindrops (Franco et al.,

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2021), and the nucleation rate of cloud droplets by facilitating their formation (Yu, 2000). Therefore, MG degradation could have some impact on such processes on a regional scale.

5. DECLARATIONS

5.1. Acknowledgments

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5.2. Open Access

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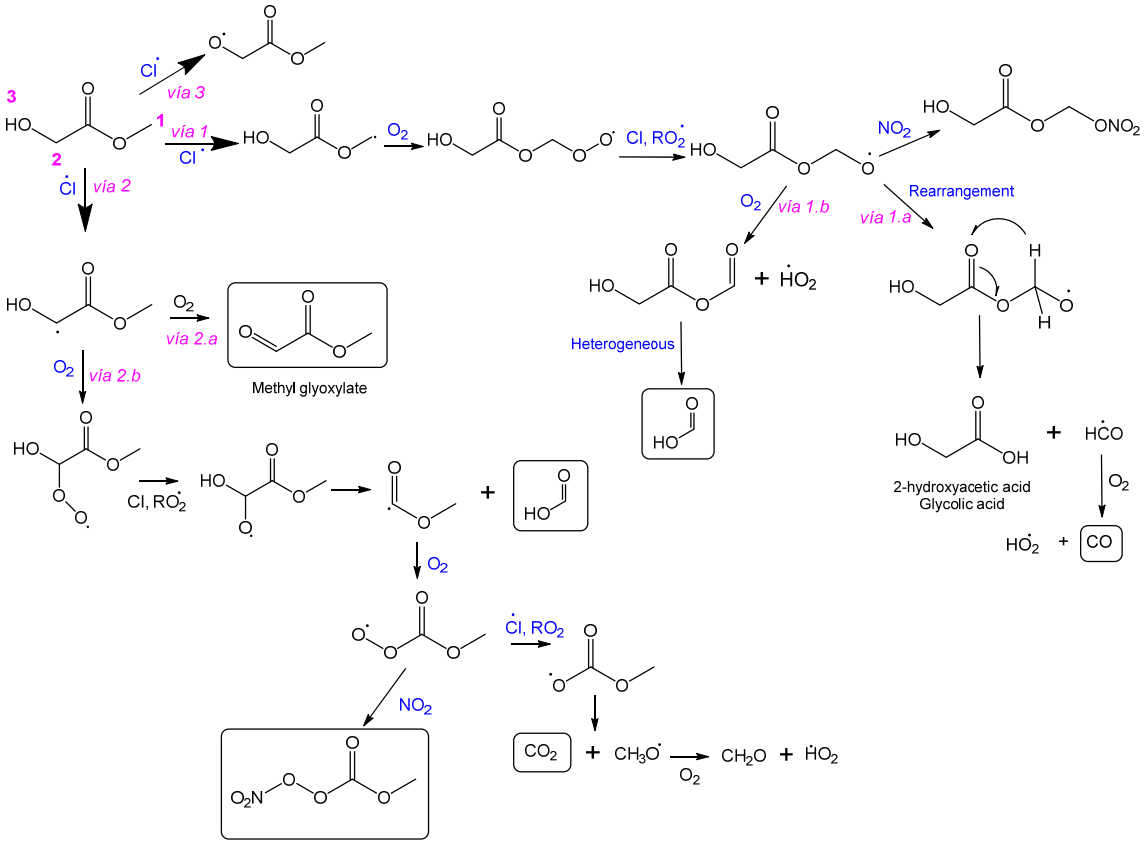


Figure 3. *Photooxidation mechanism of MG*

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Atmospheric degradation of methyl glycolate

FASSANELLI GIULIANA G., MALANCA FABIO E.

Química teórica-experimental de moléculas de interés ambiental

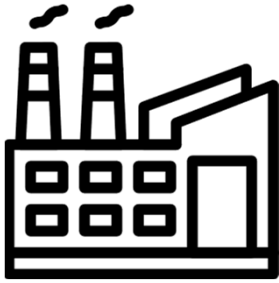
FCQ Facultad de Ciencias Químicas

CONICET UNC Universidad Nacional de Córdoba

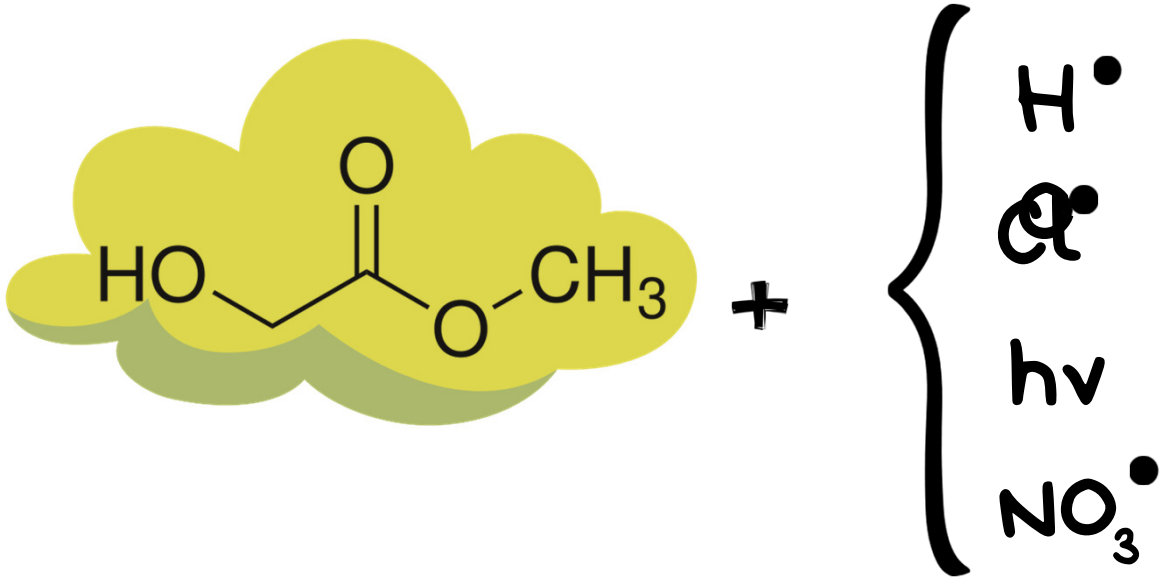
INFIQC

Why methyl glycolate?

Methyl glycolate is a semi-volatile compound widely used in industry.



Its degradation could occur from several ways.



The relative importance of these processes was needed to determine its atmospheric lifetime.

What we study?

Determination of the rate coefficient





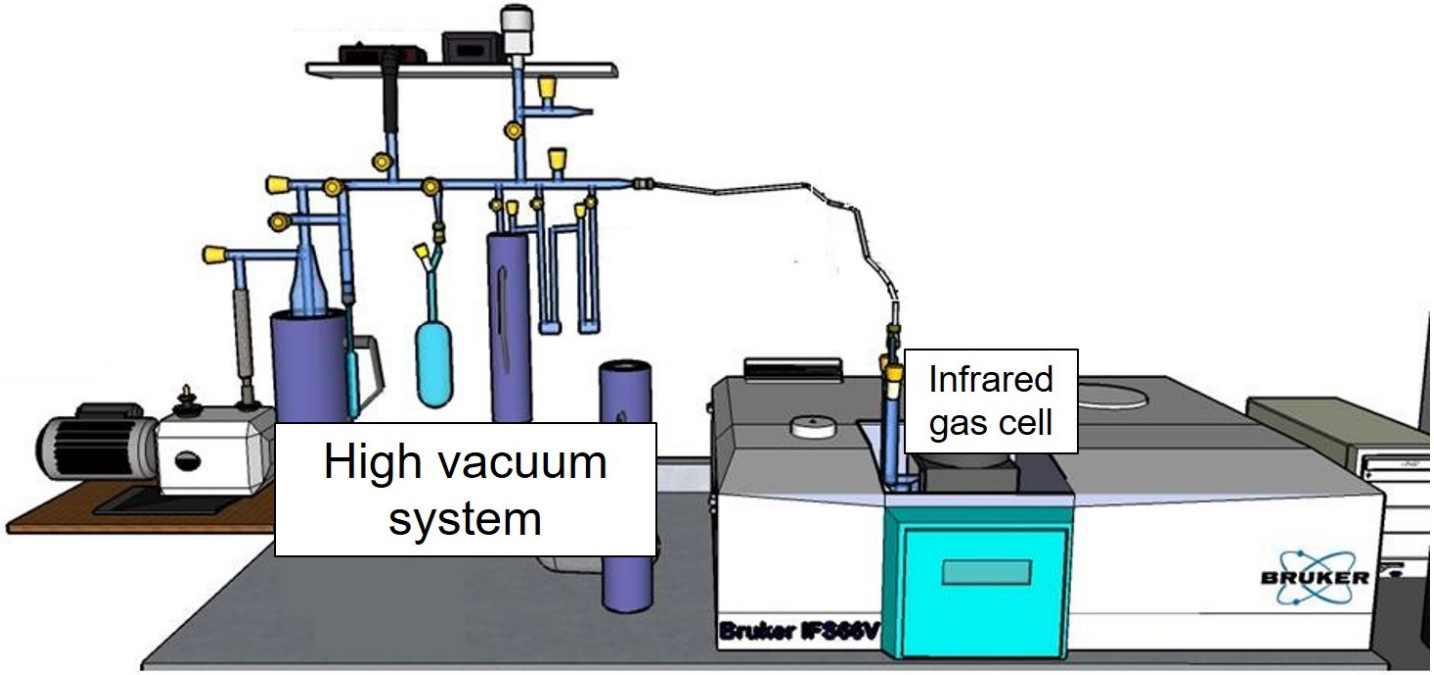
Relative method

Photooxidation

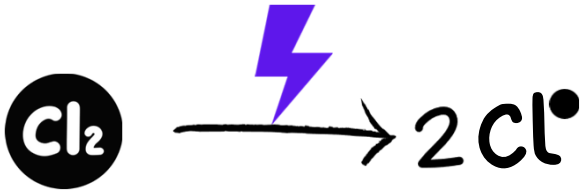
In the absence and presence of NO_2

- Identification of reaction products
- Determination of reaction mechanism

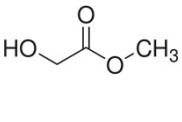
How was it studied?



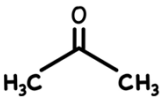
Fourier Transform Infrared Spectrophotometer (FTIR)



Kinetic measurements



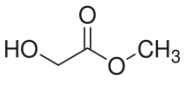
Cl2 + N2



Cl2 + N2

} Gas Mixtures

Photooxidation



Cl2 + O2

$NO_2^{\cdot}$

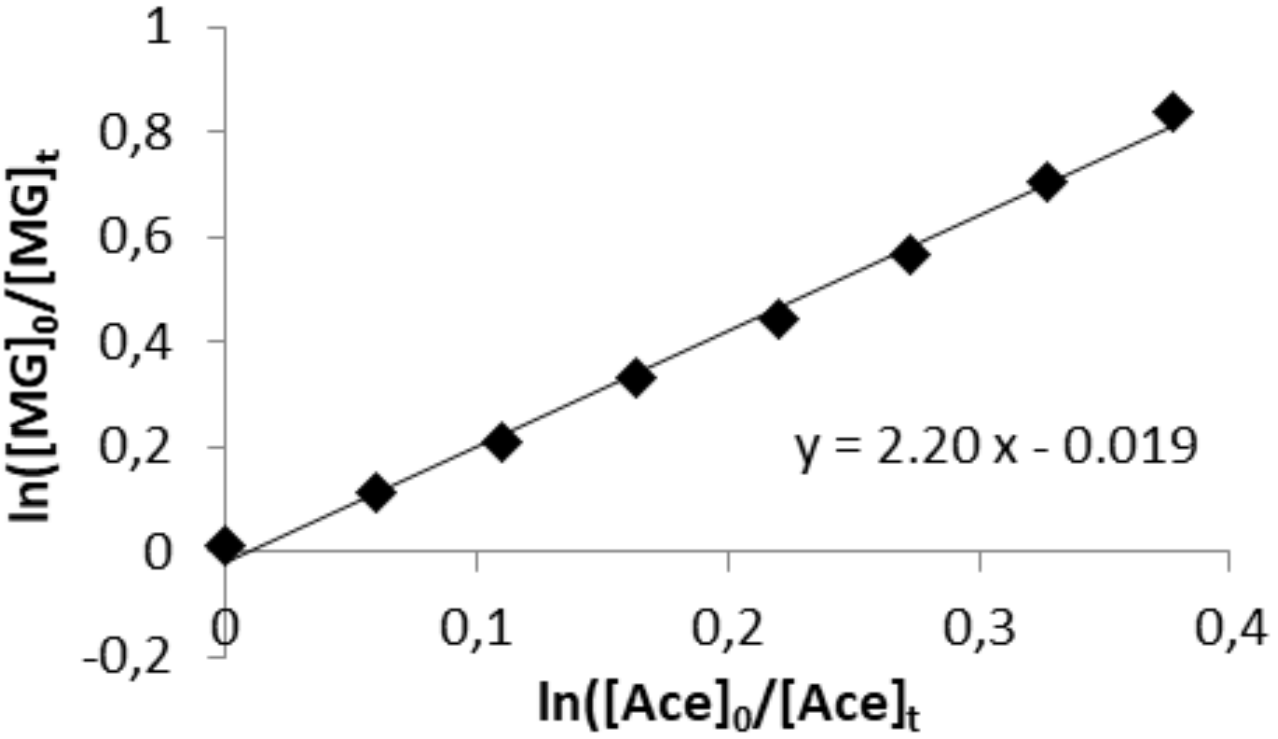
} Gas Mixtures

Determination of the rate coefficient of MG with Cl atoms

$$\ln([MG]_0/[MG]_t) = kMG/kAce \ln([Ace]_0/[Ace]_t)$$

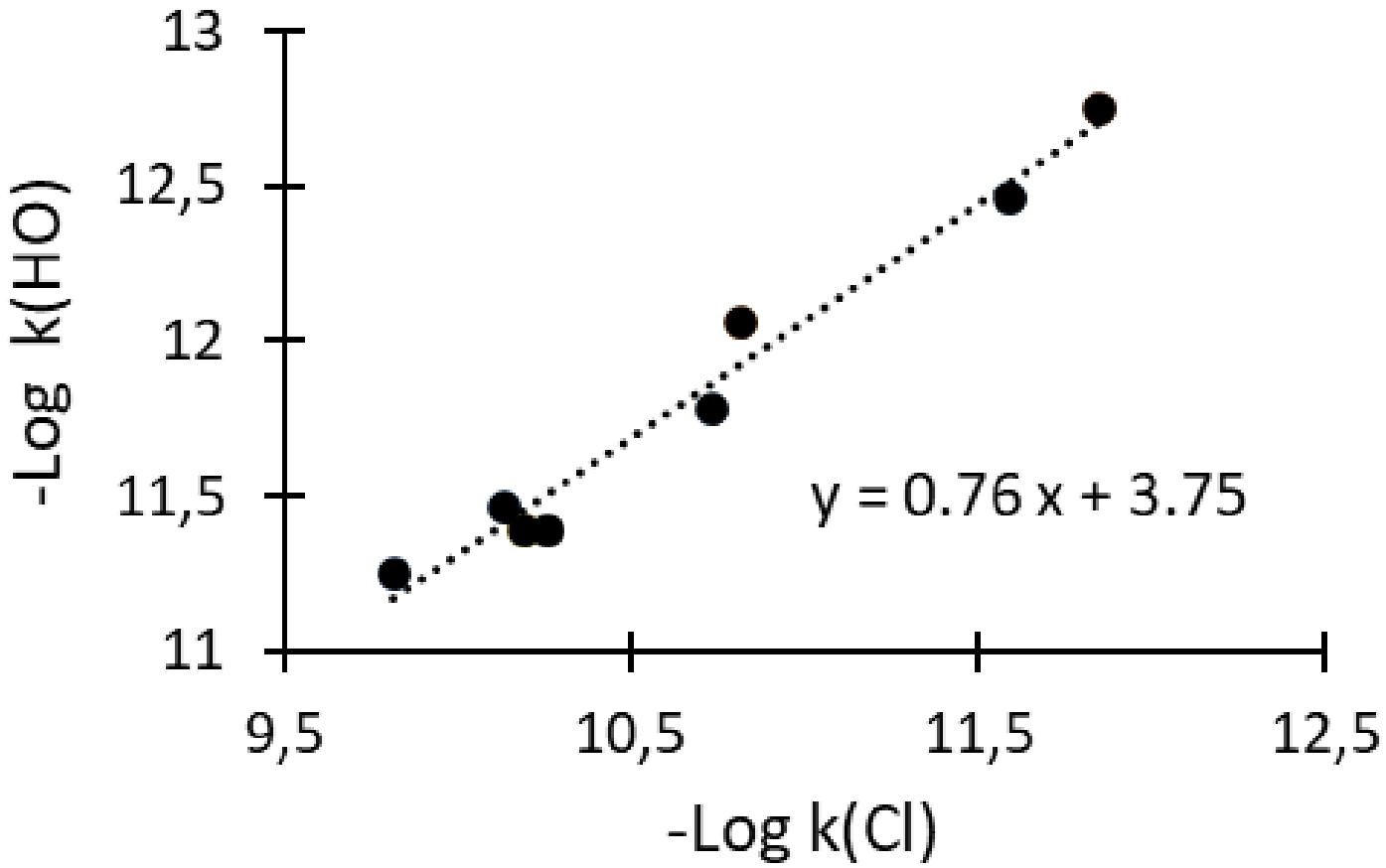
$kCl_{exp} = (4.7 \pm 0.8) \times 10^{-12}$ cm^{3}molec^{-1} s^{-1}

- $[MG]_0$ and $[MG]_t$ represent the MG concentration at initial and t time, respectively;
- $[Ace]_0$ and $[Ace]_t$ correspond to the acetone concentrations at the times mentioned above.

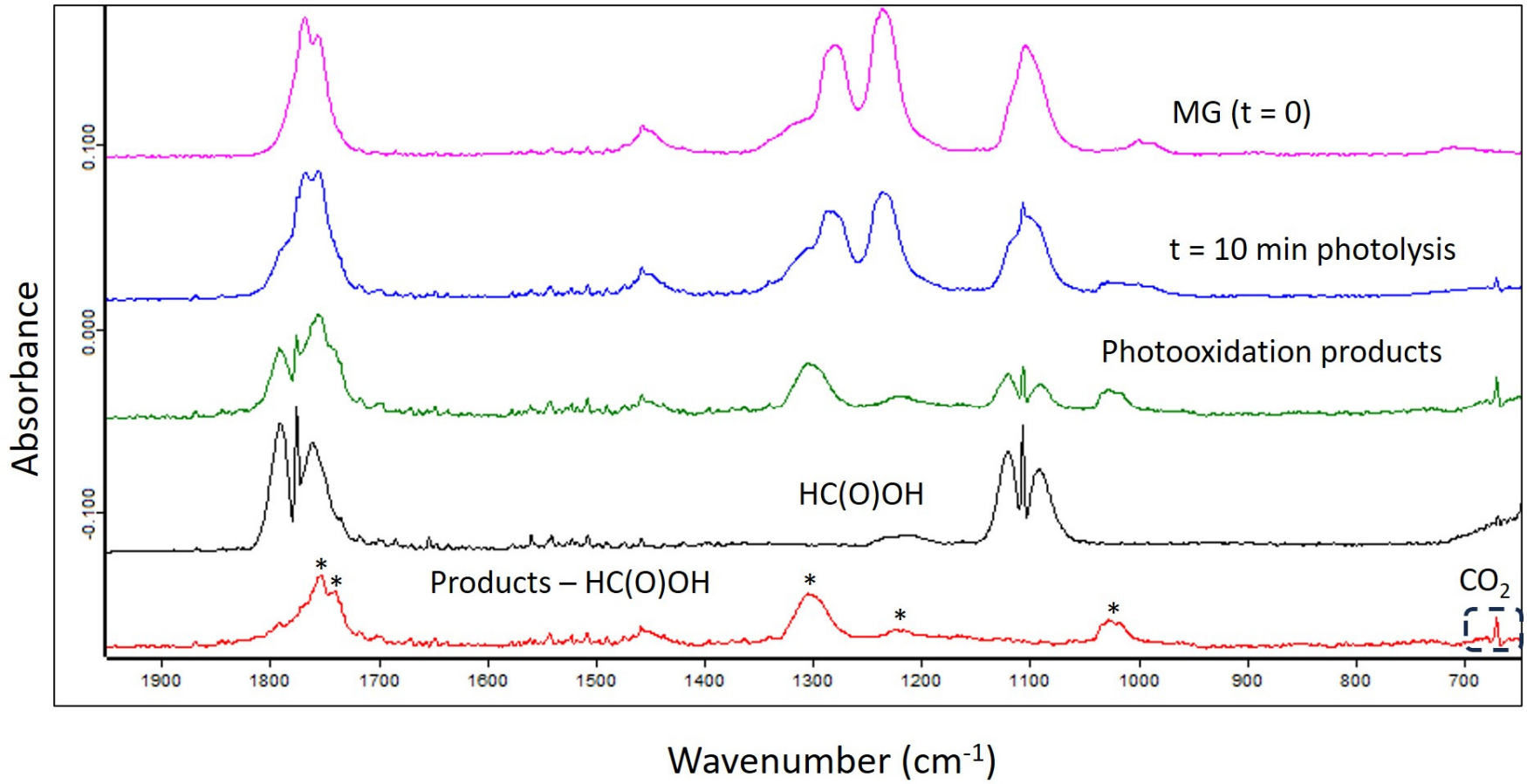


Estimation of the rate coefficient of MG with HO• radical

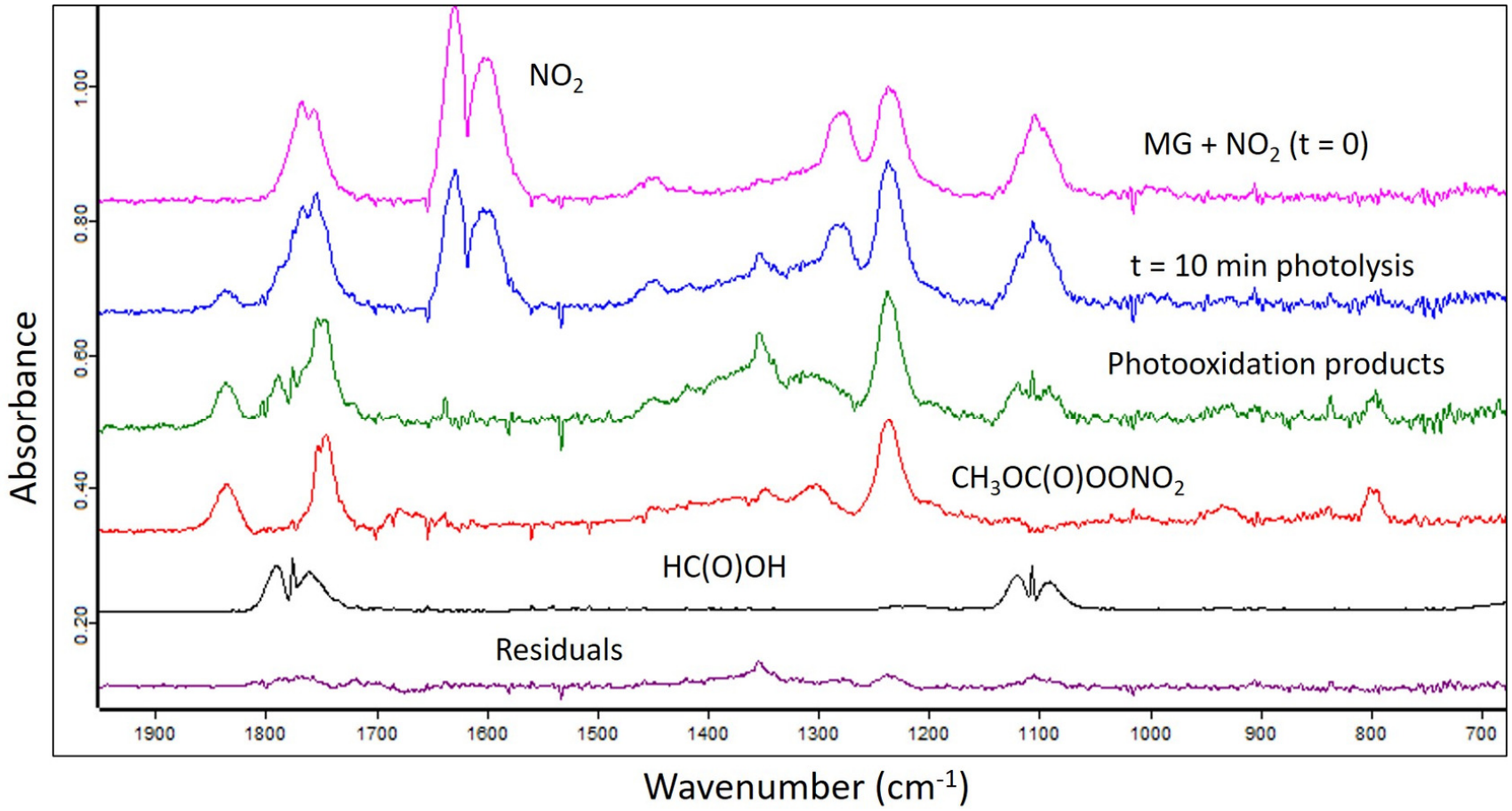
$k_{HO} = 4.4 \times 10^{-13}\ cm^3\ molec^{-1}\ s^{-1}$



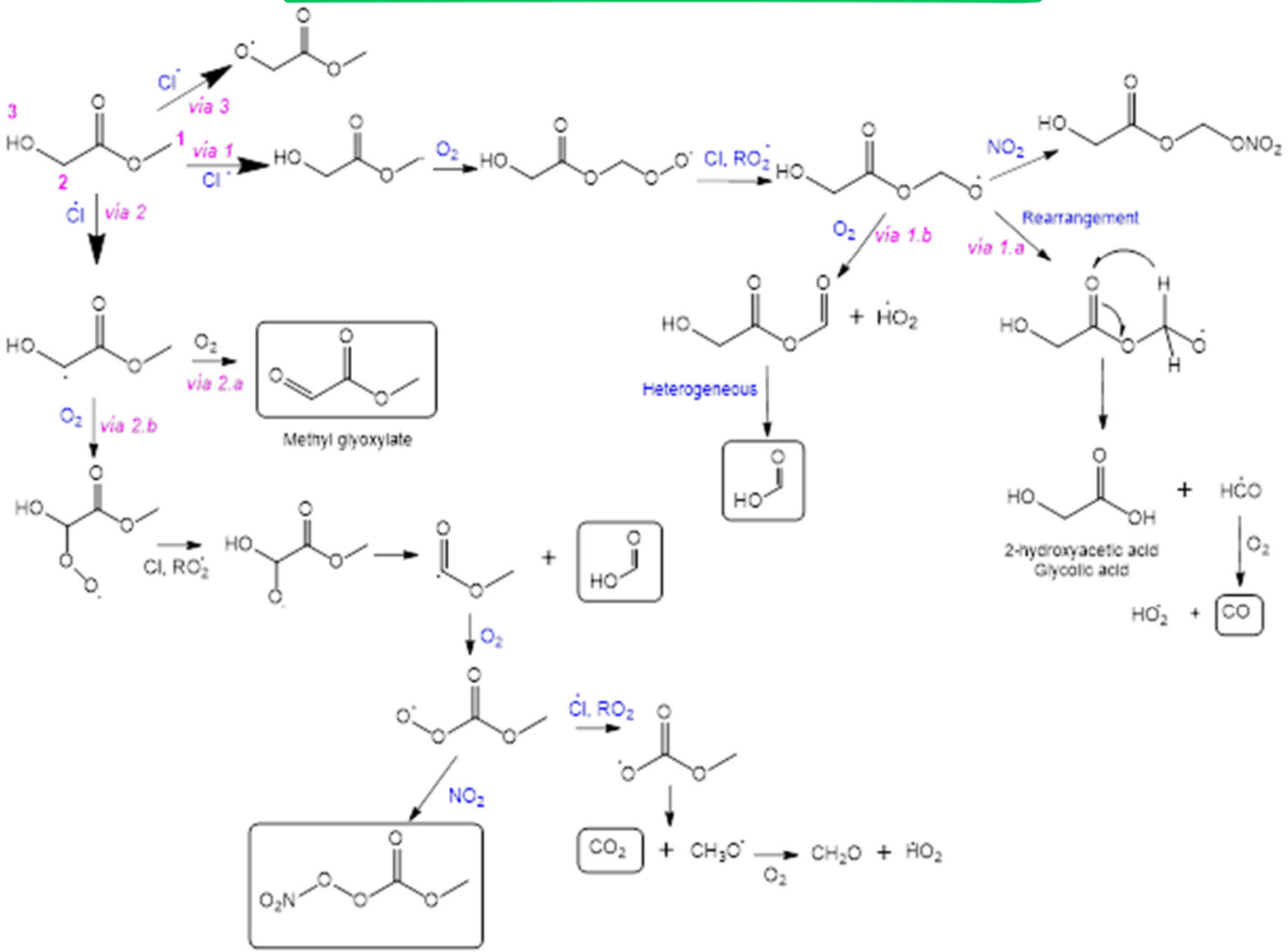
Photooxidation. Identification of reaction products in absence of NO_2



Photooxidation. Identification of reaction products in the presence of NO_2



Reaction mechanism



Atmospheric implications



τ_{Cl} = 75 days

τ_{HO} = 13 days

Lifetime is mainly controlled by its reaction with the HO• radical.



The degradation in NO_2 polluted environments leads to the formation of formic acid and $CH3OC(O)OONO_2$



Formic acid could have an impact on the acidity of the clouds and raindrops, and the nucleation rate of cloud droplets.

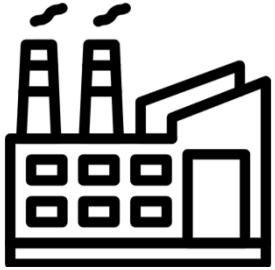
$ROONO_2$

$CH3OC(O)OONO_2$ can be transported to higher altitudes or remote locations where can inject peroxy radicals and NO_2





Thanks!





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THE IMPORTANCE OF PHOTOVOLTAIC ENERGY IN THE TRANSITION TO RENEWABLE SOURCES

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RESUMO

The Brazilian energy matrix is predominantly from renewable sources, with hydropower being the most prominent, which comes from water resources. In this context, among renewable energy sources, photovoltaic energy has shown considerable expansion in the Brazilian energy matrix. Thus, this article aims to analyze the energy transition and investments made in the Northeast and Southeast regions of Brazil. To this end, the methodology used was a literature review. The results demonstrate that the Northeast region has presented various state incentives for the installation of solar panels, as these states have the highest solar potential in the country. However, the greatest potential for solar energy installation is in the Brazilian Southeast region, with states such as São Paulo and Minas Gerais standing out in the national ranking.

Palavras-chave: *Solar Energy. Energy Matrix. Clean Energy. Sustainability*.

1. INTRODUÇÃO:

Atualmente, várias ONGs e Institutos não governamentais fazem pesquisas com o tema energia renováveis, a partir dos impactos gerados com a produção de energia não renovável como nuclear, petróleo, carvão mineral e gás natural. Os estudos têm investigado novos tipos de geração de energia com os menores impactos possíveis ao meio ambiente.

A literatura classifica a energia conforme a sua fonte de produção. Sendo, a energia não renovável obtida através de fontes não renováveis que são consideradas finitas, como por exemplo as que possuem como base o carvão, gás natural ou o petróleo (RODRIGUES, et al, 2018).

Em relação as fontes renováveis de energia, estas são entendidas como infinitas, como exemplo tem-se a energia oriunda do sol, vento e da água (RODRIGUES, et al, 2018). A geração hídrica, aquela proveniente da água, é a principal fonte de produção de energia elétrica no Brasil (EPE, 2022).

Dentro desse contexto, tem-se a energia solar, denominada como fotovoltaica, que é uma fonte de energia renovável e limpa que utiliza a radiação solar para gerar eletricidade. Baseia-se no denominado efeito fotoelétrico, através do qual determinados materiais são capazes de absorver fótons (partículas luminosas) e liberar elétrons, gerando corrente elétrica.

Capeletto (2010) indica que a previsão de demanda de energia para os períodos de até 2030 aumentará 196,25%, já que o consumo de energia crescerá a uma taxa de 2,6% ao ano, passando de 202,9 milhões de tep para 398,2 milhões de tep em 2030. Consoante a isto, quanto maior for o consumo de energia maior será os riscos e incertezas em relação a degradação do meio ambiente torna-se um ponto de discussão relevante e um grande desafio para o crescimento econômico sustentável. Assim, nas últimas décadas, tendências no uso de energia renovável e mais limpa foram introduzidas no país (MONTOYA; PASQUAL, 2015).

Deste modo, o Brasil tem incentivado e fomentado formas de implementação de energia renovável, especialmente a energia fotovoltaica. Na região nordeste do país tem o Financiamento de Energia Solar (FNE Sol) um programa do Banco do Nordeste (BNB), que tem como objetivo

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"financiar projetos de micro e mini geração distribuída de energia por fontes renováveis, inclusive de forma isolada, para consumo próprio do ou destinados à locação, reduzindo os custos com energia elétrica de forma sustentável para o planeta". Além disso, bancos como Santander, Bradesco, Banco Nacional de Desenvolvimento (BNDES) possuem financiamentos próprios para a instalação das placas solares, tais bancos atendem todas as regiões do país.

Portanto, este artigo tem como objetivo analisar a transição energética e os investimentos dados nas regiões Nordeste e Sudeste do Brasil. Deste modo, objetiva-se entender os impactos destes incentivos para a expansão da energia solar no país. Para alcançar o objetivo proposto optou-se por utilizar como metodologia a pesquisa bibliográfica.

2. MATERIAIS E METODOS

Este estudo consiste numa pesquisa qualitativa, descritiva. No primeiro momento foi realizada uma revisão de literatura que tem como objetivo conhecer o pano de fundo da literatura das energias não renováveis e as renováveis. No entanto, o foco deste artigo está em compreender os incentivos financeiros e fiscais das regiões Nordeste e Sudeste do Brasil para a expansão da instalação de energia fotovoltaica.

Para realização deste artigo foi feita uma pesquisa no Google Acadêmico para conhecer a literatura sobre o tema "energia fotovoltaica". A *STRING* de pesquisa utilizada foi *("*energia fotovoltaica*" OR "photovoltaic energy") AND* sustentabilidade *AND* Brasil *AND* nordeste *AND* sudeste*)*. O período de referência foi entre 2010 e 2024.

3. RESULTADOS E DISCUSSÃO

Esta seção destina-se a analisar e discutir o fomento concedido a instalação de energia solar nos estados do Rio de Janeiro e da Bahia, realizando um comparativo entre eles.

Segundo relatório do Balanço Energético Nacional (BEN) publicado em 2022, a geração elétrica a partir de fontes não renováveis representou 22,6% do total nacional, contra 16,8% em 2020. O Gráfico 1 mostra a geração de energia elétrica por fontes não renováveis do período de 2000 a 2021. Destaca-se o aumento significativo do gás natural que ao longo dos últimos anos ao deslocar o óleo combustível e o diesel, contribuiu para minimizar as emissões provenientes da geração de eletricidade a partir de fontes não renováveis (EPE, 2022).

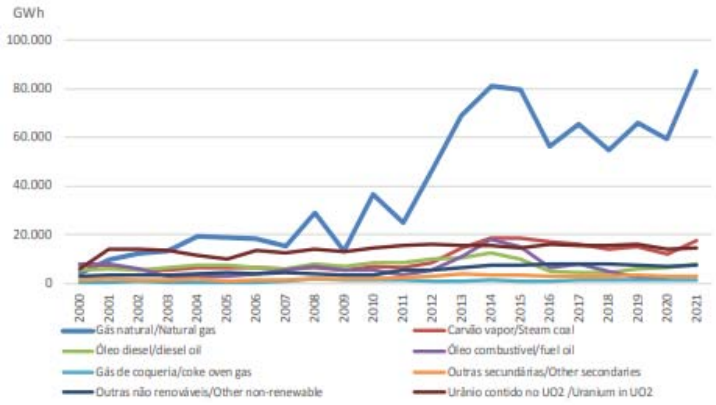


***Gráfico 1**. Geração de energia elétrica: fontes não renováveis*

Dados do relatório do BEN (2022) apontam que o Brasil dispõe de uma matriz elétrica de origem predominantemente renovável, com destaque para a fonte hídrica que responde por 53,4% da oferta interna, conforme o Gráfico 2 abaixo. As fontes renováveis representam 78,1% da oferta interna de eletricidade no Brasil, que é a resultante da soma dos montantes referentes à produção nacional mais as importações, que são essencialmente de origem renovável (EPE, 2022).

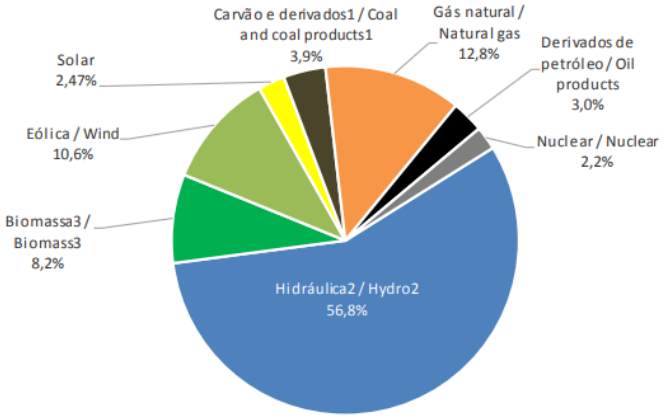


***Gráfico 2**. Oferta interna de energia elétrica por fonte*

A revisão de literatura permitiu compreender que a energia fotovoltaica é uma importante fonte de energia renovável, na qual o Brasil tem procurado expandir a sua instalação através dos incentivos dados pelo próprio governo

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do país. Isso, não se dá apenas pelos inúmeros benefícios deste tipo de energia renovável, mas também devido ao potencial solar do país.

Na Figura 1 abaixo apresenta dados de um estudo realizado pela Associação Brasileira de Energia Solar Fotovoltaica (ABOVE) em 2024 apresenta o *ranking* estadual da geração fotovoltaica no Brasil. Destaca-se os estados Nordestinos como Bahia, Ceará, Pernambuco, Rio Grande do Norte, ocupando as seguintes posições no ranking, 9º, 12º, 13º, 15º, respectivamente.



Figura 1. *Ranking Estadual Brasileiro*

A Associação Brasileira de Energia Solar Fotovoltaica (ABSOLAR, 2020) apresenta diversos pontos para a expansão da energia solar no Brasil, como: considerar uma matriz de menor custo global, valoração dos benefícios determinados por fonte e pelo portfólio conjunto, busca de uniformidade no licenciamento ambiental entre estados.

Na região Nordeste do Brasil possui como fonte de energia principal a energia elétrica hídrica sendo o seu principal provedor o rio São Francisco. A partir de 2013 ganhou-se destaque para a energia eólica, gerada pelos ventos, isso se deu em razão da baixa pluviometria e do aumento da capacidade instalada de geração eólica na região (BEZERRA, 2018).

Embora a região Nordeste apresente vários incentivos dos governos localizados na região a utilização da energia solar é insignificante, mas tem crescido por causa da entrada em operação de projetos vencedores de leilões promovidos pela Aneel (BEZERRA, 2018). Dessa forma, entende-se que existe uma tendência a expansão da energia de fonte solar na matriz elétrica da região nordestina.

Em relação a região Sudeste, a sua matriz energética predominantes são aquelas oriundas de fontes não renováveis e grande participação das hidroelétricas, porém a participação de energias renováveis como a solar e eólica é bem baixa na região. Segundo Portal Solar, a região Sudeste detém de 45% dos sistemas de geração existente no Brasil.

4. CONCLUSÕES

A preocupação universal que tem tomado conta dos debates é a degradação ambiental. Neste contexto, temas relevantes são levantados como formas de diminuir os impactos no meio ambiente, como a redução de emissão de gases poluentes. Para isso, tem se o estímulo da utilização de fontes renováveis de energia.

O Brasil apresenta um país com forte potencial para a utilização de energia de fontes renováveis, destacando a energia solar. Isso se dá devido ao clima brasileiro ser predominantemente equatorial, semiárido e tropical, contribuindo para a emissão de raios solares. Assim, nota-se que o país tem grande potencial de aproveitamento para o uso de energia solar, porém a sua utilização está muito aquém do seu potencial.

Portanto, conclui-se este artigo ressalta-se a importância de existirem mais estímulos fiscais e financeiro a fim de contribuir para a expansão da energia solar no país. Além disso, é preciso investir em publicidade e divulgação para que a população tome conhecimentos de tais incentivos. Assim, acredita-se que com os estímulos aumentar a utilização de energia solar na matriz energética brasileira que permitirá trazer diversos benefícios para o meio ambienta e sociedade.

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Ademais, este estudo tem algumas implicações para as pesquisas futuras. As questões incluem pesquisas sobre a eficácia e o impacto das políticas e subsídios fiscais existentes sobre a implementação da energia solar. Mais pesquisas sobre as inovações de materiais e tecnologias que poderiam desempenhar um papel na melhoria da eficiência e redução dos custo dos sistemas. Pesquisa sobre energia fotovoltaica, a fim de facilitar sua integração na rede existente de uma maneira que corresponda à demanda e armazenamento de energia. A virada na investigação também servirá para entender melhor a dinâmica do mercado que influencia a adoção do sol. A pesquisa comparativa ilustrará a maneira pela qual a fosfato foi adotada em países e certos erros que podem ser evitados no Brasil. Isso contribuirá para assegurar uma larga difusão e eficácia energia fotovoltaica.

5. DECLARAÇÕES

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Southern Science Conference, 2024.

A IMPORTÂNCIA DA ENERGIA FOTOVOLTAICA NA TRANSIÇÃO PARA FONTES RENOVÁVEIS

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INTRODUÇÃO

Atualmente, várias ONGs e Institutos não governamentais fazem pesquisas com o tema energia renováveis, a partir dos impactos gerados com a produção de energia não renovável como nuclear, petróleo, carvão mineral e gás natural. Os estudos têm investigado novos tipos de geração de energia com os menores impactos possíveis ao meio ambiente.

A literatura classifica a energia conforme a sua fonte de produção.

Energia não renovável obtida através de fontes não renováveis, por exemplo o carvão, gás, etc.

Energia renovável, estas são entendidas como infinitas, como por exemplo a energia oriunda do sol, vento e da água.

OBJETIVO

Analisar a transição energética e os investimentos dados nas regiões Nordeste e Sudeste do Brasil.

MATERIAL E MÉTODOS

Pesquisa qualitativa, descritiva.

No primeiro momento foi realizada uma revisão de literatura que tem como objetivo conhecer o pano de fundo da literatura das energias não renováveis e as renováveis. No entanto, o foco deste artigo está em compreender os incentivos financeiros e fiscais das regiões Nordeste e Sudeste do Brasil para a expansão da instalação de energia fotovoltaica.

STRING de pesquisa utilizada foi *(“*energia fotovoltaica*” OR “photovoltaic energy”) AND* sustentabilidade *AND* Brasil *AND* nordeste *AND* sudeste.

RESULTADOS E DISCUSSÃO

A energia fotovoltaica é uma importante fonte de energia renovável, na qual o Brasil tem procurado expandir a sua instalação através dos incentivos dados pelo próprio governo do país;

A Associação Brasileira de Energia Solar Fotovoltaica (ABSOLAR, 2020) apresenta diversos pontos para a expansão da energia solar no Brasil, como: considerar uma matriz de menor custo global, valoração dos benefícios determinados por fonte e pelo portfólio conjunto, busca de uniformidade no licenciamento ambiental entre estados.

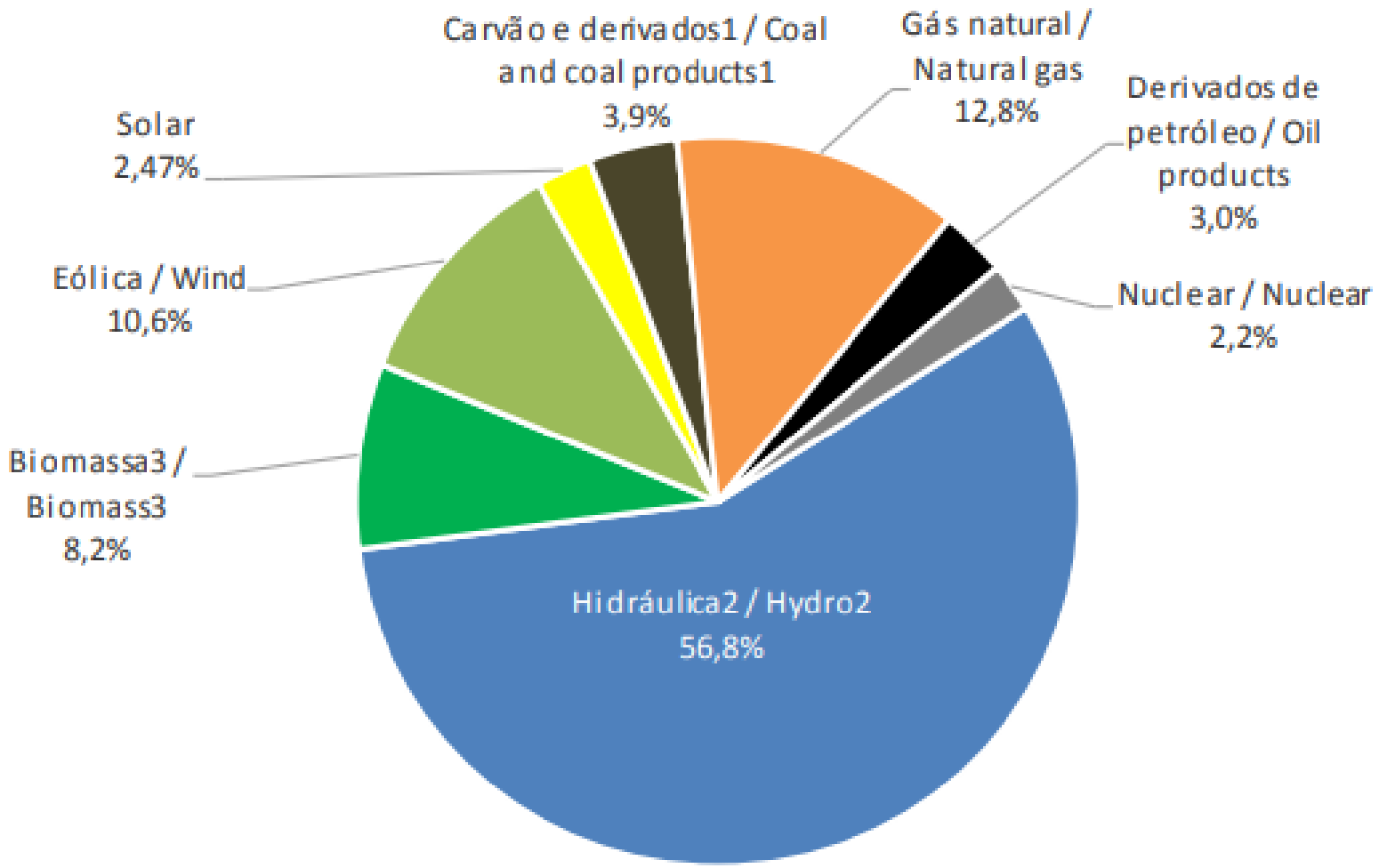
RESULTADOS E DISCUSSÃO

Ranking estadual do Brasil



RESULTADOS E DISCUSSÃO

Gráfico 2. Oferta interna de energia elétrica por fonte



CONCLUSÃO

O Brasil apresenta um país com forte potencial para a utilização de energia de fontes renováveis, destacando a energia solar. Isso se dá devido ao clima brasileiro ser predominantemente equatorial, semiárido e tropical, contribuindo para a emissão de raios solares.

Ressalta-se a importância de existirem mais estímulos fiscais e financeiro a fim de contribuir para a expansão da energia solar no país. Além disso, é preciso investir em publicidade e divulgação para que a população tome conhecimentos de tais incentivos.

Assim, acredita-se que com os estímulos aumentar a utilização de energia solar na matriz energética brasileira que permitirá trazer diversos benefícios para o meio ambiental e sociedade.

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OBTAINING A SCAFFOLD BASED ON POLYSACCHARIDE EXTRACTED FROM THE FIBROUS RESIDUE OF *ANACARDIUM OCCIDENTALE* L. FOR DRUG DELIVERY

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ABSTRACT

Anacardium occidentale, known as the cashew tree, is a plant native to Brazil, particularly abundant in the Northeast, which is responsible for 98% of the species' production. Cashew cultivation yields two main products: the nut, used for oil extraction and edible kernels, and the pseudofruit, which can be consumed directly or processed into various foods. After the pseudofruit is pulped, the remaining bagasse accounts for 15% of the mass and is a still underutilized residue, despite its rich composition, which includes tannins, carotenoids, cellulose, and pectin, as well as antioxidant properties. Due to global sustainability trends, cashew bagasse has gained prominence as a source of valuable compounds, especially polysaccharides. These biomaterials show promise in the pharmaceutical field, where they can be used as vectors for controlled drug release, given their biocompatibility and biodegradability. Such systems offer benefits such as the precise delivery of active substances, reduced doses and side effects, as well as potential for cell regeneration and the transport of growth factors.

Keywords*: Anacardium occidentale, Polysaccharide, Extraction, Characterization.*

1. INTRODUÇÃO:

O *Anacardiumoccidentale*da família Anacardiaceae é uma planta nativa do Brasil e presente na América do Sul. Também conhecida como cajueiro, essa espécie apresenta grande diversidade na região nordeste do Brasil, configurando uma das maiores atividades econômicas dessa região, sendo responsável por 98% da produção (BORGES, 2021). Nesse contexto, a cajucultura produz duas matérias-primas, a castanha, de onde é extraído a amêndoa comestível e o óleo/líquido amplamente usado na indústria, e o pseudofruto, que pode ser consumido *in natura*, e usado para produção de suco, doce, licor e diversos produtos alimentícios (COSTA *et al*., 2020).

O pseudofruto do cajueiro representa a maior parte do fruto, após o seu despolpamento o bagaço ainda representa 15 porcento da massa, sendo um dos principais resíduos dessa cultura. Devido sua baixa estabilidade pós-colheita sua utilização ainda é limitada, embora apresente composição rica (PADILHA *et al*., 2020). Nessa perspectiva, é valido ressaltar que as tendências globais influenciam o reaproveitamento e melhor manejo dos recursos naturais, tornando esses resíduos potenciais matérias-primas para extração de compostos de valor agregado e atividade biológica (SERPA *et al*., 2020).

O bagaço de caju possui uma composição rica e diversificada. Reina et al. (2022) caracterizouseuscomponentes e identificou a presença de taninos, carotenoides, celulose, lignina, proteínas e pectina. Além disso, o autor observou atividade antioxidante no material vegetal analisado. Este resíduo apresenta grande potencial para a extração de polissacarídeos, os quais têm sido explorados como biomateriais para a entrega de fármacos, principalmente

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devido às suas propriedades biodegradáveis e biocompatíveis (Prajapati et al., 2019).

Sistemas de liberação de fármacos utilizando polímeros naturais têm sido amplamente estudados devido à sua biocompatibilidade. Esses sistemas permitem a entrega direcionada de substâncias ativas, reduzindo a dose necessária e minimizando os efeitos adversos, além de controlar o nível plasmático da droga.Essas formulações podem ser desenvolvidas para atingir sítios de ação com difícil acesso, podem ainda ser somados a outros benefícios como a regeneração celular, carreado células ou fatores de crescimento, permite o acúmulo e retenção da droga no local, tornando as investigações por novos polímeros naturais, de extrema importância (YI*et al*., 2023; ZHANG *et al*., 2017). Nesse contexto, o objetivo deste estudo é a extração e caracterização de polissacarídeos de Anacardium occidentale L. como reaproveitamento do resíduo industrial.
ambiente de ar atmosférico e gás hélio, utilizando o modo Omnian.

2. MATERIAIS E MÉTODOS

No planejamento fatorial realizado, optou-se por oito experimentos com o intuito de definir as condições de extração mais favoráveis para esse resíduo, visando assim obter um melhor rendimento. Para a extração do polissacarídeo de *Anacardium occidentale*, empregou-se o resíduo fibroso do pedúnculo proveniente de uma cooperativa de produção de cajuína sediada em Teresina, Piauí. Utilizou-se um planejamento fatorial com o objetivo de otimizar o processo de extração, analisando as variáveis tempo, temperatura e proporção (%) em seus níveis máximos (tempo: 10 h, temperatura: 90 °C, proporção: 5%) e mínimos (tempo: 2 h, temperatura: 50 °C, proporção: 1%), a fim de determinar sua influência na resposta desejada.

Para a extração do polissacarídeo, o bagaço da fruta foi misturado em água destilada em concentrações de 1% e 5% (p/v) e submetido à agitação magnética, mantendo-se a temperatura em 50% e 90°C, sem ferver, por 2 e 10 horas, respectivamente. Após esse período, a mistura foi centrifugada para obtenção do líquido sobrenadante, que foi então precipitado com álcool etílico PA na proporção de 1:4 (líquido extraído/etanol). Essa solução foi armazenada sob refrigeração por 72 horas para a completa precipitação do polissacarídeo. Posteriormente, o material foi submetido a uma segunda centrifugação, e o sobrenadante foi descartado, obtendo-se o polissacarídeo precipitado, que foi seco em estufa a 40°C por 24 horas. Em seguida, o polissacarídeo foi pesado, e rendimento calculado utilizando a Equação 1.

$$Rendimento\ \% = \frac{peso\ de\ polissacarídeo}{peso\ do\ resíuo} \times 100 \quad (1)$$

Para a caracterização do polissacarídeo, foi utilizada a técnica de Fluorescência de Raio - X (FRX). A FRX foi conduzida no equipamento Epsilon3-XL da PANalytical, equipado com tubo de ródio e filtro de prata. A análise ocorreu sob voltagem de 50 kV e corrente de 30 μA, em um

3. RESULTADO E DISCUSSÃO

No planejamento fatorial realizado, optou-se por oito experimentos com o intuito de definir as condições de extração mais favoráveis para esse resíduo, visando assim obter um melhor rendimento. Foram realizados oito experimentos de extração, conforme apresentado na Tabela 1.

Tabela 1 – Rendimento para cada Extração.

N	Tempo	Temperatura (°C)	Razão %	Rendimento (%)
1	2	50	1,0	0,83
2	10	50	1,0	1,6
3	2	90	1,0	0,92
4	10	90	1,0	1,02
5	2	50	5,0	2,17
6	10	50	5,0	1,00
7	2	90	5,0	1,13
8	10	90	5,0	4,32

Fonte: Elaborada pelo autor.

O experimento 1, com tempo de 2 h, temperatura de 50 °C e proporção de 1,0, resultou em um rendimento de 0,83%. No experimento 2, com tempo de 10 h, temperatura de 50 °C e proporção de 1,0, o rendimento foi de 1,6%. O experimento 3, com tempo de 2 h, temperatura de 90 °C e proporção de 1,0, teve um rendimento de 0,92%. O experimento 4, com tempo de 10 h, temperatura de 90 °C e proporção de 1,0, obteve rendimento de 1,05%. O experimento 5, com tempo de 2 h, temperatura de 50 °C e proporção de 5,0, resultou em um rendimento de 2,17%. No experimento 6, com tempo de 10 h, temperatura de 50 °C e proporção de 5,0, o rendimento foi de 1,00%. O experimento 7, com tempo de 2 h, temperatura de 90 °C e proporção de 5,0, obteve rendimento de 1,13%. Por fim, o experimento 8, com tempo de 10 h, temperatura de 90 °C e proporção de 5,0, alcançou o maior rendimento, de 4,32%.

Nesse contexto, observa-se que essas

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variáveis têm influência direta na eficiência da extração, conforme os rendimentos obtidos em cada experimento. O tempo de extração mostrou ser uma variável de grande impacto no rendimento. Ao comparar os experimentos com tempos de 2 horas com os experimentos de número (N), (N1, N3, N5, N7) e 10 horas (N2, N4, N6, N8), nota-se que, de forma geral, o aumento no tempo resulta em incrementos nos rendimentos. Na extração realizada a 50 °C e com uma proporção de 1%, o rendimento aumentou de 0,83% em 2 horas (N1) para 1,6% em 10 horas (N2). Da mesma forma, quando a proporção de extração foi aumentada para 5%, o rendimento subiu de 2,17% (N5) para 4,32% (N8) com a extensão do tempo de extração para 10 horas. Esses resultados indicam que um tempo de extração mais prolongado favorece o rendimento, provavelmente devido à maior exposição do material fibroso ao solvente, facilitando a liberação dos compostos desejados.

A temperatura também desempenha um papel relevante no processo, embora seu efeito seja menos linear do que o observado para o tempo. Ao comparar as extrações realizadas a 50 °C e 90 °C, verifica-se que, em algumas condições, o aumento da temperatura resulta em um maior rendimento. Para um tempo de 2 horas e uma proporção de 1%, o rendimento aumentou de 0,83% a 50 °C (N1) para 0,92% a 90 °C (N3). No entanto, quando a proporção de extração foi elevada para 5%, o efeito da temperatura não foi tão evidente, como demonstrado pela pequena variação de 2,17% a 50 °C (N5) para 1,13% a 90 °C (N7). Essa variação sugere que o impacto da temperatura pode estar condicionado a outras variáveis do processo, como o tempo de extração e a concentração do solvente, indicando uma interação mais complexa entre esses fatores.

Por outro lado, a proporção de extração mostrou-se uma variável determinante para o aumento do rendimento. Ao comparar os resultados para as proporções de 1% e 5%, observa-se um aumento significativo na eficiência de extração com o incremento na concentração de solvente. Em condições de alta temperatura (90 °C) e longo tempo de extração (10 horas), o rendimento aumentou de 1,05% com uma proporção de 1% (N4) para 4,32% com uma proporção de 5% (N8).

Esse aumento expressivo sugere que a elevação da quantidade de solvente favorece a solubilização e extração dos polissacarídeos, especialmente quando combinada com um tempo de extração prolongado.

Nesse contexto, os resultados obtidos evidenciam que tanto o aumento do tempo de extração quanto o incremento na proporção de extração exercem uma influência positiva sobre o rendimento da extração de polissacarídeos de *Anacardium occidentale*. Embora a temperatura também tenha impacto relevante, observa-se que sua eficácia está mais diretamente relacionada a outras variáveis do processo, como o tempo de extração e a concentração do solvente, sugerindo que seu efeito é condicionado pela interação entre esses fatores.

Dessa forma, o experimento número 8, realizado dentro do planejamento fatorial, foi identificado como a condição mais favorável para maximizar o rendimento da extração de polissacarídeos, sendo definido como a melhor metodologia para esse processo. A partir desse experimento, foi possível proceder com a caracterização do polissacarídeo extraído, utilizando a técnica de Fluorescência de Raios-X (FRX). Os elementos presentes em cada amostra foram determinados qualitativa e quantitativamente. Essa técnica oferece alta especificidade e seletividade, pois cada elemento absorve energia em um comprimento de onda específico, e cada energia de transição eletrônica é única para cada elemento. Como cada elemento químico possui níveis de energia distintos, isso resulta em diferentes padrões de absorção ou emissão de energia, permitindo a identificação individual dos elementos (Skoog, Holler, Nieman, 2022).

Por meio da técnica de FRX, foram obtidas linhas espectrais de cada elemento, caracterizadas por comprimentos de onda específicos, sobrepostas a um fundo contínuo de baixa intensidade. Esses resultados apresentaram diferentes padrões de absorção e emissão para cada elemento químico presente no polissacarídeo extraído, conforme apresentado na Tabela 2.

Tabela 2 – Resultados de FRX para o polissacarídeo

Elemento químio	Concentração	Óxido correspondente	Concentração
K(%)	56,137	K_2O(%)	46,886
Ca(%)	22,947	CaO(%)	20,116
P(%)	6,279	P_2O_5(%)	11,546
Si(%)	4,089	SiO_2(%)	7,207
S(%)	3,441	SO_3(%)	6,684
Mg(%)	3,102	MgO(%)	4,359
Ni(%)	494,9	NiO(ppm)	379,8
Cr(%)	0,113	Cr_2O_3(%)	0,101
Mn(%)	0,684	MnO(%)	0,535

Fonte: Elaborado pelo autor.

A análise de fluorescência de raios X

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(FRX) revelou que os elementos predominantes na amostra de polissacarídeo são potássio (K), cálcio (Ca) e fósforo (P), com menores concentrações de silício (Si), enxofre (S) e magnésio (Mg), todos essenciais para o organismo. Além disso, níquel (Ni), cromo (Cr) e manganês (Mn) foram detectados como elementos traço. Resultados semelhantes foram observados por Mathavan et al. (2024) em sua análise de microfluorescência de raios X, utilizando a goma de *Anacardium occidentale* (AO), que apresentou concentrações mais elevadas de cálcio, potássio, magnésio e manganês. Embora o polissacarídeo estudado por Mathavan et al. tenha sido extraído da casca do AO, as semelhanças na composição sugerem uma relação química entre as diferentes partes da planta.

4. CONCLUSÃO

Dessa forma, conclui-se que o planejamento fatorial é uma ferramenta essencial para definir as condições ideais e mais favoráveis à extração de polissacarídeos, visando maximizar o rendimento. Essa abordagem permite avaliar todos os fatores que influenciam o resultado final do processo de extração, possibilitando a escolha da melhor metodologia para otimizar as condições do processo. Os experimentos realizados do 1º ao 8º no planejamento fatorial demonstraram que as variáveis de temperatura e tempo exercem impacto significativo sobre a obtenção e rendimento do polissacarídeo, especialmente com o aumento dessas variáveis. A variação nas condições de temperatura e tempo entre os testes permitiu identificar o experimento número 8 como aquele que apresentou os melhores parâmetros para a extração e rendimento do polissacarídeo. Além disso, a caracterização do polissacarídeo extraído do bagaço de caju, utilizando a técnica de FRX, revelou uma rica composição química, evidenciando que esses biomateriais são biodegradáveis.

5. DECLARAÇÕES

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Southern Science Conference, 2024.

OBTENÇÃO DE SCAFFOLD A BASE DE POLISSACARÍDEO EXTRAÍDO DO RESÍDUO FIBROSO DO ANACARDIUM OCCIDENTALE L. PARA LIBERAÇÃO DE FÁRMACOS

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Outubro/2024

Resumo

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INTRODUÇÃO

Brasil possui uma vasta riqueza em seu patrimônio botânico, contando com uma ampla variedade de plantas que apresentam diversas propriedades terapêuticas.

- O Caju (Anacardium Occidetale), uma planta originária do Nordeste do país, possui propriedades eficaz e terapêutica no tratamento de feridas.
- Esta planta se destaca por sua ação antibacteriana, anti-inflamatória e cicatrizanate, graças aos ácidos anacárdicos que contém.

- Reaproveitamento do resídeo industrial.
- Matérias – primas com atividade biológica.
- Biomatériais para a entrega de fármacos.

OBJETIVO

Extração e caracterização de polissacarídeos de Anacardium occidentale L. como reaproveitamento do resíduo industrial.

METODOLOGIA

- Elaboração de um planejamento fatorial para otimização de processos.
- Extração do polissacarídeo.
- Precipitação do polissacarídeo.
- Centrifugação.
- Obtenção dos rendimento e escolha do experimento padrão.
- Caracterização do polissacarídeo.
- Técnica Fluorescência de Raio - X (FRX).

METODOLOGIA

Tabela – Planejamento Fatorial

N	Tempo (h)	Temperatura (°C)	Razão (%)	Rendimento (%)
1	2	50	1,0	
2	10	50	1,0	
3	2	90	1,0	
4	10	90	1,0	
5	2	50	5,0	
6	10	50	5,0	
7	2	90	5,0	
8	10	90	5,0	

Fonte: Autoria própria.

RESULTADOS E DISCUSSÃO

Tabela 2 - Rendimento para cada experimento realizado

N	Tempo (h)	Temperatura (°C)	Razão (%)	Rendimento (%)
1	2	50	1,0	0,83
2	10	50	1,0	1,6
3	2	90	1,0	0,92
4	10	90	1,0	1,05
5	2	50	5,0	2,17
6	10	50	5,0	1,00
7	2	90	5,0	1,13
8	10	90	5,0	4,32

Fonte: Autoria própria.

RESULTADOS E DISCUSSÃO

- Técnica Fluorescência de Raio - X (FRX).

Tabela 3 – Resultados de FRX para o polissacarídeo do resíduo fibroso de Anacardium occidentale

Elementoquímico	Concentração	Óxido correspondente	Concentração
Mg(%)	3,102	MgO (%)	4,359
Al (ppm)	0	Al_2O_3 (%)	0
Si(%)	4,089	SiO_2(%)	7,207
P(%)	6,279	P_2O_5(%)	11,546
S(%)	3,441	SO_3 (%)	6,684
Cl(%)	1,51	Cl(%)	1,127
K(%)	56,137	K_2O (%)	46,886
Ca(%)	22,947	CaO (%)	20,116
Ti(%)	0,207	TiO_2(%)	0,21
Cr(%)	0,113	Cr_2O_3 (%)	0,101
Mn(%)	0,684	MnO (%)	0,535
Fe(%)	0,949	Fe_2O_3 (%)	0,821
Ni(%)	494,9	NiO(ppm)	379,8
Cu(%)	0,14	CuO (%)	0,106
Zn(%)	0,353	ZnO (%)	0,264

Fonte: Elaborada pelo autor.

CONCLUSÃO

- Utilização do planejamento factorial.
  - Escolha do experimento 8.
- Variáveis: Tempo; Tempetatura; Razão.
  - Influênciam no rendimento.
- Polissacarídeo.
  - Rica composição química.

AGRADECIMENTOS

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ANALYSIS OF THE THERAPEUTIC POTENTIAL OF *ANACARDIUM OCCIDENTALE* L. FOR THE DEVELOPMENT OF PHYTOTHERAPEUTICS

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ABSTRACT

The present study carried out a systematic review with the objective of evaluating the therapeutic potential of *Anacardium occidentale* L. (cashew tree), focusing on the use of the bark extract in the treatment of gastroenteropathies. The research was conducted on the SciELO, PubMed, Web of Science, and Virtual Health Library (VHL) platforms, using descriptors such as "*Anacardium occidentale*", "cajueiro", "dysentery", "ethanolic extract," and "bark", combined with Boolean operators "AND" and "OR". Articles published in English, Portuguese, and Spanish between 2019 and 2024 were included. In addition, technological prospecting was carried out in international patent databases such as the European Patent Office (EPO), World Intellectual Property Organization (WIPO), and United States Patent and Trademark Office (USPTO), in addition to the national base of the National Intellectual Property Institute (INPI). The results revealed innovations focused on the use of cashew bark, with therapeutic potential for the treatment of dysentery and diarrhea, reinforcing the scientific and technological impact of this species in the field of phytotherapy. This study contributes to the valorization of *Anacardium occidentale* in the management of gastrointestinal diseases and highlights the importance of promoting policies that encourage the development of herbal medicines in Brazil.

Keywords: *Diarrheal Diseases, Phytotherapy, Patents, Ethanol Extract.*

1. INTRODUCTION

Gastroenteropathies encompass several diseases that affect the gastrointestinal tract, causing inflammation, damage to the mucosa, and disturbances in the absorption of nutrients. Conditions such as gastritis, colitis, and irritable bowel syndrome are prevalent, particularly in regions with limited access to adequate medical treatments (WHO, 2022). In conventional treatment, anti-inflammatories, antibiotics, and probiotics are used, which can have adverse effects and high costs (Sharma *et al*., 2021).

In this scenario, the use of herbal medicines has shown promise, offering alternatives with fewer side effects (Sampaio *et al*., 2018). Anacardium occidentale L. (cashew tree) is a plant native to Tropical America that is traditionally used in medicine. Cashew tree bark is rich in bioactive compounds with anti-inflammatory, antimicrobial, and antioxidant properties (Silva *et al*., 2020), being promising for the treatment of gastroenteropathies (Mota *et al*., 2019).

However, it is important to recognize the limitations of using cashew bark extracts. Variation in extract composition, lack of standardization in herbal preparations, and scarcity of robust clinical trials may limit their large-scale applicability. Furthermore, the possible interaction with other medications and the need for further studies on its safety in humans are aspects to be considered.

2. MATERIALS AND METHODS

The review was carried out in two stages. Firstly, articles were collected on the use of Anacardium occidentale L. bark in the treatment of acute diarrhea in databases such as SciELO,

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PubMed, Web of Science, and VHL. Descriptors such as "Anacardium occidentale", "cashew tree", "dysentery", "ethanol extract," and "bark" were used, combined with Boolean operators. Articles published between 2019 and 2024 in English, Portuguese, and Spanish that investigated the efficacy of the extract in animal or human models were considered, excluding studies without concrete results.

The selected articles were imported into the Rayyan platform, where two researchers carried out independent and blind screening, resolving disagreements by consensus. The inclusion criteria prioritized experimental studies with comparative methods and quantitative data.

In the second stage, technological prospecting was carried out to identify innovations related to cashew tree bark in the treatment of gastroenteropathy. The search for patents occurred in the EPO, WIPO, USPTO, and INPI databases, using descriptors such as "*Anacardium occidentale* AND peel" and "*Anacardium occidentale* AND dysentery", focusing on the A61K category, which covers the agricultural asset base.

After screening, duplicate or irrelevant patents were discarded, consolidating data from both stages to provide a comprehensive view of the literature and technological innovations on the therapeutic potential for gastroenteropathies.

3. RESULTS AND DISCUSSION:

3.1 Scientific prospecting

201 studies were identified, of which, after exclusions and filtering, there remained studies focused on the effectiveness of *Anacardium occidentale* extract in the treatment of diarrhea. Different aspects were analyzed, such as antimicrobial and antioxidant activity and effects on intestinal motility, as described in Table 1.

Recent studies, such as that by Encarnação *et al.* (2020), demonstrated that the cashew tree has strong antioxidant activity, inhibiting enzymes related to glucose metabolism and reducing oxidative stress, favoring tissue regeneration. The work of Silva *et al.* (2021) highlighted its antimicrobial action against bacteria such as Escherichia coli and Shigella, suggesting its potential as an alternative to antibiotics.

Table 1 – Scientific studies on the effectiveness of *Anacardium occidentale* bark in gastroenteropathy.

Author	Year	Objective and Outcome
Encarnação *et al.* (2020)	2020	Compare the antioxidant efficacy and inhibition of α- and β-glucosidases of *Anacardium occidentale* bark preparations. Both presented antioxidant and inhibitory properties, suggesting applications in gastrointestinal disorders.
Silva *et al.* (2021) e Rodríguez *et al.* (2021)	2021	To evaluate the antimicrobial activity of cashew tree shell extract against diarrhea-causing bacteria. The extract showed strong activity against *E. coli, Shigella* and resistant strains such as *Clostridium difficile.*
Gomez *et al.* (2019) e Oliveira *et al.* (2023)	2019 e 2023	Compare cashew tree extract with conventional herbal medicines in the treatment of acute and chronic diarrhea. The extract showed comparable efficacy and greater efficiency in reducing symptoms compared to conventional treatments.
Santos *et al.* (2022) e Martins *et al.* (2023)	2022, 2023	Investigate the effects of the extract on intestinal motility and recovery in children with acute diarrhea. The extract showed anti-diarrheal properties and positive recovery results compared to standard treatments.
Ferraz *et al.* (2020) e Pineda *et al.* (2019)	2020, 2019	To evaluate the toxicity and efficacy of the extract in preventing diarrhea induced by chemotherapy drugs and in identifying phenolic compounds. The extract demonstrated safety and efficacy, with anti-diarrheal effects comparable to ciprofloxacin.
Nascimento *et al.* (2024)	2024	Investigate the use of the extract as an adjuvant in the treatment of chronic inflammatory diarrhea. The extract reduced inflammatory markers and improved patients' quality of life.

Gomez *et al.* (2019) compared cashew tree extract to other herbal medicines, demonstrating its superiority in reducing diarrheal symptoms. Other studies, such as that by Santos *et al.* (2022), showed that the extract improves liquid absorption and reduces intestinal motility, comparable to loperamide but without side effects.

In clinical models, Martins *et al.* (2023) revealed that the use of cashew tree extract, combined with oral rehydration serum, accelerated the recovery of children with diarrhea. Rodríguez *et al.* (2023) pointed out that the extract helps restore the intestinal microbiota in cases of antibiotic-induced diarrhea.

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Studies such as those by Ferraz *et al.* (2021) and Pineda *et al.* (2022) explored the antiparasitic and antiviral effect of the extract, while Nascimento *et al.* (2024) highlighted its effectiveness combined with prebiotics, offering an innovative solution to restore intestinal health after antibiotic use.

Table 1 consolidates these studies, highlighting the range of applications of *Anacardium occidentale* bark extract, both in the control of gastrointestinal infections and in the regulation of motility and intestinal protection, which justifies its potential as an alternative treatment in different clinical scenarios.

3.2 Technological prospecting

Technological prospecting anticipates trends, allowing strategic decisions in areas such as *Anacardium occidentale* research for the treatment of gastroenteropathies. The patent analysis (INPI, EPO, USPTO, WIPO) focused on the classification of medicinal preparations (IPC A61K), revealing 33 patents at INPI and 178 in other bases, with 12 related to *Anacardium occidentale*. Figure 1 highlights the countries with active patent filings that address the topic and the classification.

Figure 1 - Countries with active patent filings.



Source: MapChart, 2024.

The United States stands out, accounting for 33.3% of these patents, due to its strong culture of innovation and incentives for pharmaceutical research. France and Spain also have an interest, reflected in their two patents each, focused on the valorization of natural products and biodiversity. Countries such as Norway, Sweden, and Italy, with one patent each, show growing interest in sustainable technologies.

Brazil, although rich in biodiversity, faces obstacles such as a lack of investment and bureaucracy, which makes it difficult to register patents. To stand out globally, the country would need greater incentives for innovation and simplification of patenting processes.

Although studies on *Anacardium occidentale* indicate its potential in the treatment of diarrhea, there are limitation s, such as heterogeneity in methodologies, variability in formulations, and the diversity of experimental models, which may affect the comparability of results.

Future research should focus on multicenter clinical trials with different populations and investigate interactions of the extract with other medications. Partnerships between researchers, industries, and government institutions can boost innovation and patent registration, ensuring the full exploitation of the cashew tree's potential for public health.

4. CONCLUSION:

This study confirms the therapeutic potential of *Anacardium occidentale* L. in the treatment of diarrheal diseases. Bark extracts show consistent antidiarrheal, anti-inflammatory, and antimicrobial properties, which are superior in some cases to conventional treatments. Multicenter clinical trials are recommended to validate these effects observed in laboratory studies and animal models.

From a public policy point of view, Brazil should invest more in the development of herbal medicines based on native plants. The lack of patents reflects barriers that limit innovation in the country. It is essential to strengthen cooperation between academia, industry, and government, creating a regulatory environment that is favorable to the registration of herbal medicines.

In summary, this study reinforces the importance of including medicinal plants such as cashew trees in public health protocols, especially in tropical regions. Training professionals in the use of herbal medicines and their integration into the SUS can expand the benefits to public health, valuing traditional knowledge and promoting sustainability.

5. DECLARATIONS

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Federal University of Vale do São Francisco – UNIVASF.

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ANALYSIS OF THE THERAPEUTIC POTENTIAL OF *ANACARDIUM* BARK *OCCIDENTALE* L. FOR THE DEVELOPMENT OF PHYTOTHERAPEUTICS

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Novembro/2024

INTRODUCTION

- **Gastroenteropathies:** Affect the gastrointestinal tract, with inflammation and absorption disorders (WHO, 2022).
- **Current treatments:** Anti-inflammatories, antibiotics, probiotics – adverse effects and high costs (Sharma *et al*., 2021).
- **Phytotherapeutics:** Promising alternative with fewer side effects (Sampaio et al., 2018).
- ***Anacardium occidentale* L.:** Bark rich in anti-inflammatory, antimicrobial and antioxidant compounds (Silva *et al*., 2020).
- **Limitations:** Variation in extracts, lack of standardization and need for more clinical trials (Mota *et al*., 2019).

OBJETIVE

Evaluate the therapeutic potential of *Anacardium occidentale* L. (cashew tree) in the treatment of gastroenteropathies.

METHODOLOGY

Search strategy

Applied descriptors

- Anacardium occidentale;
- cajueiro;
- dysentery;
- ethanolic extract;
- bark.

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Descritores em Ciências da Saúde

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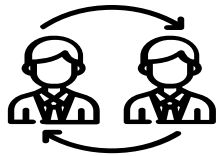
Study selection











Grouping of studies in the *software*

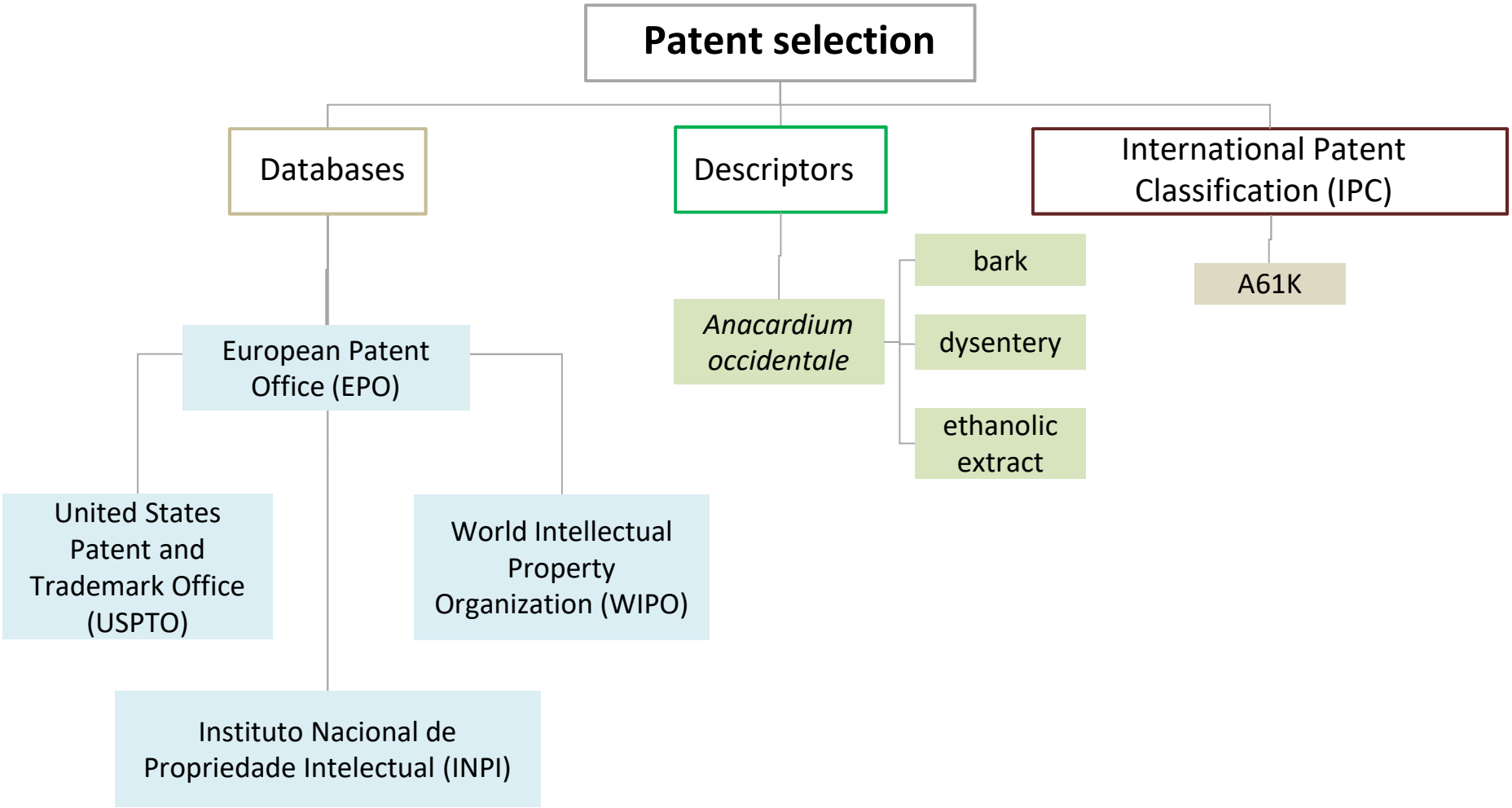
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METHODOLOGY



RESULTS AND DISCUSSION

Scientific Prospecting

Antimicrobial, **antioxidant** activity and effects on **intestinal motility**.

Gomes *et al*. (2019) and **Oliveira *et al*.** (2023): Comparison with conventional herbal medicines, with superior efficacy.



Total: **201 studies**, with an emphasis on the effectiveness of *Anacardium occidentale* extract for the treatment of gastroenteritis.

Silva *et al*. (2021): Antimicrobial activity against *E. coli*, *Shigella*, and *Clostridium difficile*.

Martins *et al*. (2023): Faster recovery of children with acute diarrhea, similar to conventional treatments.

RESULTS AND DISCUSSION

Technological Prospecting

Patent analysis

- Focus on the **A61K** category (medicinal preparations based on natural active ingredients).
- 33 patents at INPI (Brazil);
- 178 on international bases (EPO, WIPO, USPTO).

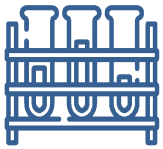
Global Distribution of Active Patents

- USA: **33.3%** of patents, driven by a strong culture of innovation.
- France and Spain: Interest in **natural products** with two patents each.
- Norway, Sweden, Italy: One record each, showing growing interest in **sustainable technologies**.

Brazil

- Challenges in patent registration due to **bureaucracy and lack of investment**.
- Need to encourage innovation to better explore the phytotherapeutic potential of the cashew tree.

CONCLUSIONS



Therapeutic Potential

Demonstrated efficacy in the treatment of gastroenteritis with results superior to conventional treatment.



Final Recommendations

Multicenter clinical trials are needed to validate the effects.



Public Policies

The lack of patents reflects barriers to innovation.



Impact on Public Health

Promotes sustainability and values traditional knowledge.

ACKNOWLEDGEMENTS







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RHEOLOGICAL AND TEXTURAL PROPERTIES OF EMULSION GELS COMPOSED BY LENTIL PROTEINS

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ABSTRACT

Emulsion gels (EG) made from plant ingredients present a promising alternative to animal fats. The characteristics of EG are influenced by the functional properties of the protein layer stabilizing the oil droplets, which can be affected by the drying method used to process the proteins. This study evaluated the rheological and textural properties of EG prepared with freeze-dried (FP) and spray-dried (SP) lentil proteins at different oil concentrations. Results showed that FP EG exhibited higher hardness values than SP EG at both oil fractions, with an increased hardness at 50% oil fraction. A gel-like structure was observed in all of the EG tested. These findings suggest that freeze drying could be a more suitable drying method for the development of EG, although further investigation is needed.

Keywords: *Emulsion gels, freeze-dried, spray-dried, lentil, protein*.

1. INTRODUCTION

The creation of "healthier" products involves altering their composition and/or processing methods to reduce or eliminate potentially harmful compounds (Jiménez-Colmenero et al., 2001). In this matter, emulsion gels (EG) are an interesting approach, as they can be used to replace animal fats and proteins, providing a versatile matrix whose structural and functional properties can be modified by selecting different ingredients and preparation conditions. EG, composed of polymeric gel matrices with incorporated oil droplets, is valued in the food industry for its thermodynamic stability (McClements, 2016). They serve as effective fat substitutes, enhancing fat content and fatty acid profiles to meet nutritional needs. The choice of oil, protein-polysaccharide interactions, and gelation conditions affect the EG structure, impacting its sensory and structural qualities (Ren et al., 2022). Typically, a protein layer stabilizes the oil droplets, influencing the EG properties (Dickinson, 1994, 1998). Drying methods, such as freeze-drying and spray-drying, further affect protein functionality and emulsifying properties (Cui et al., 2021; Hernández-García et al., 2016; Liu et al., 2015).

Legume protein isolates, such as lentil protein isolates, are typically processed into dry powder to ensure stable, long-term storage and facilitate their use in food applications. Joshi et al. (2011) found that both spray-drying and freeze-drying resulted in better solubility and gelling properties than vacuum-drying for lentil proteins. However, these proteins were not further examined in a cold-set EG system. Therefore, this study aims to evaluate the differences between the two drying methods and oil fractions in terms of their impact on the viscoelastic properties and texture parameters of the resulting EG.

2. MATERIALS AND METHODS

2.1. Materials

Lentil flour of the Laya brand and sunflower oil of the Natura brand were purchased from a local market. Sodium alginate and glucono-δ-lactone (GDL) were provided by Bio Vanda S.A. (Rafaela, Argentina). Calcium citrate was bought from Biopack S.A. (Buenos Aires, Argentina). All other chemicals used were of analytical grade.

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2.2. Methods

2.2.1 Freeze-dried and spray-dried lentil protein concentrates

Lentil protein concentrate (PC) was prepared from lentil flour, following the procedures detailed by Shrestha et al. (2023) with minor modifications. Lentil proteins were extracted from a lentil flour aqueous dispersion (100 g/L), keeping the pH at 8.0 with 2 mol/L NaOH (Cicarelli, San Lorenzo, Argentina), and stirred for 60 min. The supernatant, obtained after centrifugation at 1800×g for 30 min at 20 °C, was acidified to pH 4.5 with HCl 2 mol/L (Cicarelli, San Lorenzo, Argentina). The resulting precipitate was left in contact with the supernatant overnight, followed by another centrifugation step at 1800×g for 30 minutes at 20 °C. The precipitate was then solubilized by adjusting the pH to 8.0 with 2 mol/L NaOH and subsequently freeze-dried (FP) in a 24 h cycle, with a working pressure of 50 µm Hg (LIOTOP L101 equipment; LIOBRAS LTDA., Brazil) or spray dried (SP) at T_{in}= 130 °C and T_{out}= 70 °C according to Cui et al. (2021) using a Mini Spray Dryer B-290 (BÜCHI Labortechnik AG, Flawil, Suiza).

2.2.3 EG preparation

EG was prepared using an aqueous phase composed of alginate (1% w/v) and FP or SP (1.2% w/v). This aqueous phase was homogenized with sunflower oil (30% or 50% v/v) to form a stable EG by an OMNI GLH-220 for 60 seconds at 18500 rpm. GDL (30 g/kg) and calcium citrate (75 mM) were added to induce acid gelation. The mixture was left to rest at 25°C overnight.

2.2.3 Rheology

EG was prepared as described before, with GDL carefully added just before the start of the measurement to prevent premature gelation. Frequency sweeps were performed over a range of 0,01 to 100 rad/s, within the linear viscoelastic region of the samples using an HR-30 Oscillating Rheometer (TA Instruments, DE, United States).

2.2.4 Texture

Double compression tests to 50% of the height were performed on 10 mm thick EG samples using a TVT 6700 Texture Analyzer (PerkinElmer, Bs. As., Argentina) with a cylindrical geometry of 25 mm in diameter at an initial and retraction velocity of 1 mm/s. The evaluated parameters included hardness, adhesiveness, and cohesiveness.

2.2.4 Statistical analysis

Determinations were performed at least in triplicate for rheology and quintuplicate for texture analysis. Results were expressed as mean ± standard deviation. Data was analyzed through two-way ANOVA and the Tukey test; differences were considered significant when $p<0.05$. Normality and homoscedasticity assumptions were tested before performing parametric tests. All statistical analyses were made using SigmaPlot 12 software.

3. RESULTS AND DISCUSSION:

Rheology analysis was made by a frequency sweep within the linear viscoelastic region of the samples, shown in Figure 1 and Figure 2. It can be observed that in all cases, the storage modulus (G') is higher than the loss modulus (G") throughout the range of frequencies analyzed. For FP and SP EG, G’ and G’’ values increase as the oil fraction increases. SP and FP EG present similar G’ and G’’ values at 50% oil fraction. At the lower oil fraction, gels made from FP have higher G’ and G’’ values than those made from SP.

Regarding the texture analysis, Table 1 presents the mean values for the textural parameters of the different EG formulations. Hardness varied significantly ($p < 0.05$) depending on the drying method and the oil fraction, with the highest value observed in FP 50% and the lowest in SP 50%. The greater hardness observed in FP at both oil fractions may probably be attributed to higher protein solubility, which could enhance the gel structure. Additionally, as the oil fraction increases, the morphology of protein-coated oil droplets may potentially form a gel-like network with closely packed oil droplets, as suggested by Yang et al. (2013). This could explain the higher hardness at the 50% oil fraction for FP. To further validate this hypothesis, confocal laser scanning microscopy should be conducted, along with an evaluation of the covalent and hydrophobic interactions within the protein network. Other textural parameters, including adhesiveness, cohesiveness, stringiness, stickiness, and springiness, did not show significant differences among the samples ($p < 0.05$).

4. CONCLUSIONS:

As seen in the frequency sweep assay, the predominance of the storage modulus (G') over the loss modulus (G") suggests a typical gel

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structure. According to texture analysis, the effect of the drying method is highly significant in the hardness outcome. The interaction between the protein type and the oil fraction is significant, suggesting that the influence of the drying method is not the same for both oil fractions. Neither the protein type, the oil fraction, nor their interaction has a significant effect on adhesiveness, cohesiveness, stickiness, and springiness. Overall, these findings suggest that freeze-drying may be more effective for improving the structural integrity of EG, particularly at higher oil fractions. Further studies are needed to expand knowledge of these systems.

5. DECLARATIONS

5.1. Acknowledgments

This work was supported by the Agencia Nacional de Promoción de la Investigación, el Desarrollo Tecnológico y la Innovación under project PICT-2021-GRF-TII-00239, which also provided a scholarship, and by CONICET under project PIP 2021-2023 GI 11220200101351CO.

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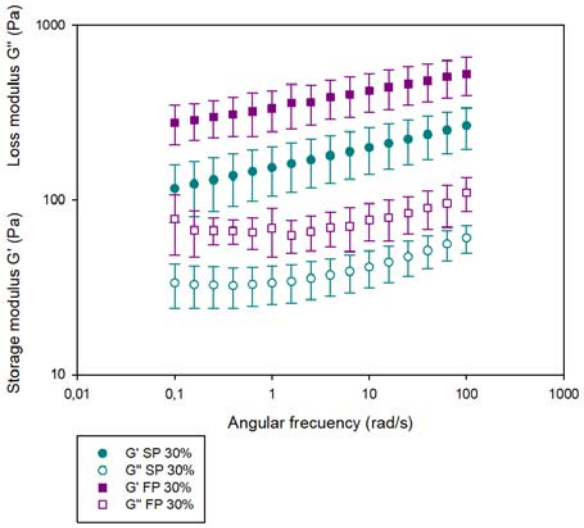


Figure 1. *Frequency sweep for EG from FP and SP, both with an oil fraction of 30%*

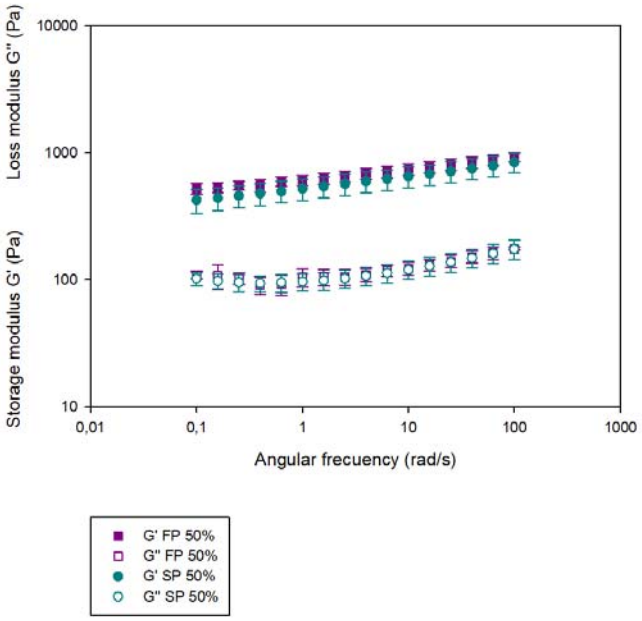


Figure 2. *Frequency sweep for EG from FP and SP, both with an oil fraction of 50%*

Table 1. Textural parameters of emulsion gels with different drying methods and oil fractions.

Drying method	FP	FP	SP	SP
Oil Fraction	30%	50%	30%	50%
Hardness (g)	170 ± 20	200 ± 20	140 ± 30	120 ± 20
Adhesiveness	110 ± 50	80 ± 10	110 ± 20	100 ± 10
Cohesiveness	0.3 ± 0.1	0.2 ± 0.2	0.4 ± 0.0	0.2 ± 0.1
Stringiness	7 ± 1	5.0 ± 0.4	6 ± 1	6.0 ± 0.2
Stickiness (g)	-20 ± 2	-20 ± 1	-20 ± 2	-20 ± 0
Springiness	0.4 ± 0.1	0.3 ± 0.4	1.0 ± 0.4	0.4 ± 0.3

Values are presented as mean ± standard deviation (n=5). FP: freeze-dried protein; SP: spray-dried protein.

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RHEOLOGICAL AND TEXTURAL PROPERTIES OF EMULSION GELS COMPOSED BY LENTIL PROTEINS

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INTRODUCTION

- The prevalence of obesity and non-communicable chronic diseases is increasing due to unhealthy diets and sedentary lifestyles.
- Plant-based diets are gaining recognition for their potential health benefits, including the prevention and management of chronic diseases.
- Emulsion gels (EGs), which can mimic the properties of animal fats, offer a promising alternative for developing healthier food products.
- This study investigates the effect of different drying methods at different oil fractions on the properties of lentil protein-based EG.



BACKGROUND

- EGs are valued for their thermodynamic stability and fat substitution potential in food products.
- The structural and functional properties of EGs depend on protein-polysaccharide interactions, gelation conditions, and the drying method used.
- Previous studies have shown that drying methods like freeze-drying and spray-drying influence the emulsifying and gelling properties of proteins.



OBJECTIVE

Evaluate the impact of freeze-drying (FP) and spray-drying (SP) on the rheological and textural properties of lentil protein emulsion gels at different oil concentrations.



METHODOLOGY

- Lentil protein concentrates (PC) were prepared by alkaline extraction
- PC were then dried using freeze-drying or spray-drying techniques, respectively
- The mixtures were gelled using glucono-δ-lactone (GDL) and calcium citrate
- Rheological measurements were performed, at least by triplicate, using a frequency sweep test over a range of 0,01 to 100 rad/s, within the linear viscoelastic region of the samples
- Textural parameters were evaluated through double compression tests to 50% of the height were performed on 10 mm thick EG, with a cylindrical geometry of 25 mm in diameter, at an initial and retraction velocity of 1 mm/s. Measurements were performed in quintuplicate



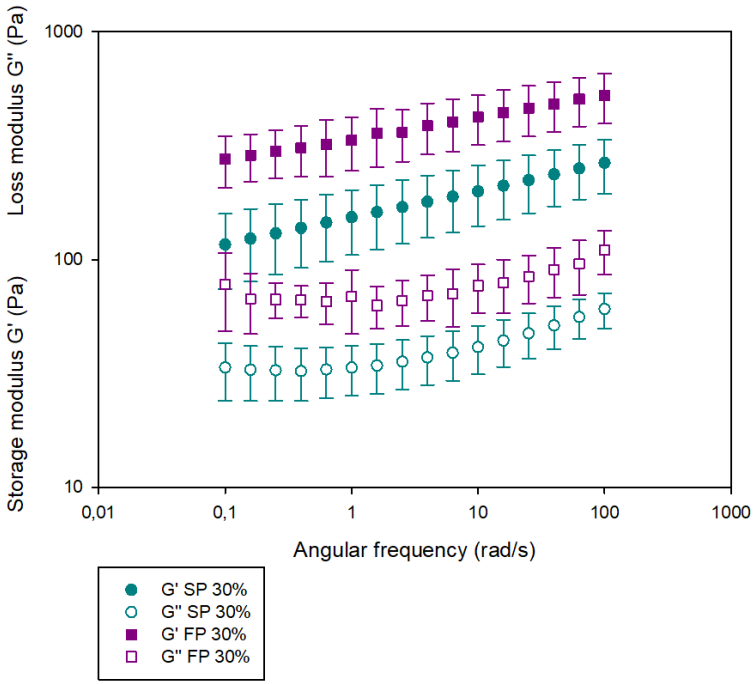
RESULTS AND DISCUSSION

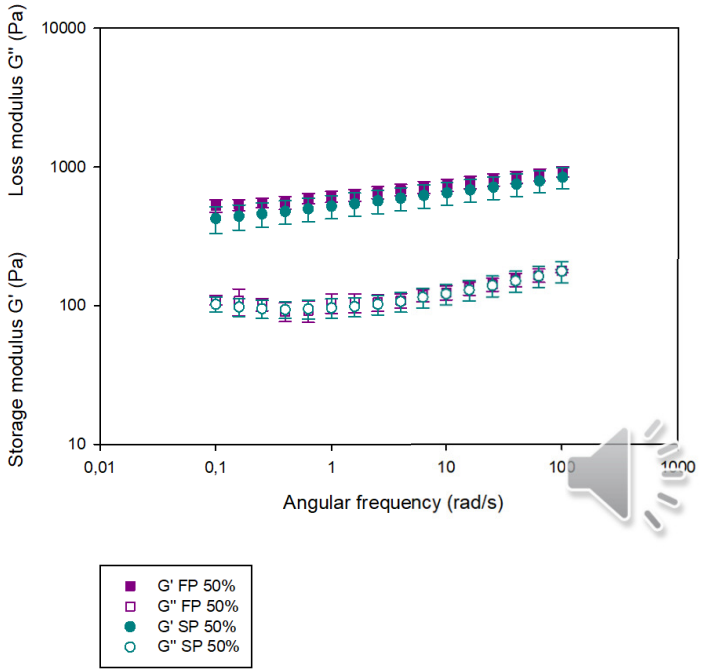
Rheology

- Higher oil concentrations resulted in increased G' and G'' values for both drying methods.

- At 30% oil fraction, freeze-dried samples exhibited higher values than spray-dried ones.

- At 50% oil fraction, the differences in G’ and G’’ were less pronounced





RESULTS AND DISCUSSION

Texture

- Hardness was significantly higher in freeze-dried samples, particularly at 50% oil, indicating a stronger gel network.

- Other textural parameters like adhesiveness and cohesiveness showed no significant differences.

DM	OF	H (g)	A	Co	Str	Sti (g)	Spr
FP	30	170 ± 20	110 ± 50	0.3 ± 0.1	7 ± 1	-20 ± 2	0.4 ± 0.1
FP	50	200 ± 20	80 ± 10	0.2 ± 0.2	5.0 ± 0.4	-20 ± 1	0.3 ± 0.4
SP	30	140 ± 30	110 ± 20	0.4 ± 0.0	6 ± 1	-20 ± 2	1.0 ± 0.4
SP	50	120 ± 20	100 ± 10	0.2 ± 0.1	6.0 ± 0.2	-20 ± 0	0.4 ± 0.3

These results could be attributed to to **better protein solubility** achieved through freeze-drying, which enhances gel structure. Additionally, as the oil fraction increases, the morphology of protein-coated oil droplets may potentially form a gel-like network with **closely packed oil droplets**, as suggested in previous work.

CONCLUSIONS

- Freeze-drying could be more effective than spray-drying in enhancing the structural integrity of emulsion gels, especially at higher oil fractions.

- Further studies should focus on understanding the molecular interactions within the gel matrix.



ACKNOWLEDGEMENTS

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EXTRACTION AND CHARACTERIZATION OF BIXIN (BIXA ORELLANA L.): CLINICAL IMPACT AND ITS PHARMACOLOGICAL APPLICATIONS

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RESUMO

The annatto plant (*Bixa orellana* L.), from the Bixaceae family, is widely recognized as the source of the most used natural dye in the world. The extracts obtained from its fruits can be water-soluble or fat-soluble, positioning annatto as one of the main natural products for the food industry, besides its applications in pharmacology, cosmetics, and technology. Carotenoids extracted from annatto are vulnerable to degradation when exposed to light, high temperatures, or sulfur dioxide. This degradation can compromise the effectiveness of carotenoids, which demonstrate significant potential in clinical treatments. Bixin, one of the main compounds extracted from annatto seeds, can contribute to reducing cholesterol levels, preventing cardiovascular diseases, decreasing inflammation in lung injuries, influencing motor activity in mice, and inhibiting gastric secretion without impacting acid production. Additionally, bixin presents antispasmodic and hypotensive properties, potentially improving health and well-being, especially when applied in biomedical devices. The analysis of bixin by UV-visible spectroscopy, in the range of 200 to 900 nm, using chloroform as a solvent, indicated that the peaks observed in the spectrum vary according to the solvent used. Infrared spectroscopy revealed a band between 772.4 and 778.8 cm^{-1}, associated with hydrogen vibration of a cis-C-CH=CH-C structure, with a strong peak at 754 cm^{-1}. The presence of a peak at 1159 cm^{-1} strongly suggests the cis structure of bixin. Future studies are fundamental to deepen the understanding of how these characteristics influence the efficacy and safety of bixin in specific applications.

Keywords: *Annatto plant, Bixin extract, Carotenoids, Spectroscopic analysis, Pharmaceutical applications*.

1. INTRODUÇÃO:

A planta urucum (*Bixa orellana* L.), da família Bixáceas, é exclusivamente reconhecida pela restrição de um corante natural, a bixina, que possui aplicações específicas nas indústrias alimentícias e farmacêuticas (OZAKI; DUARTE, 2006; ZARRINGHALAMI; SAHARI; HAMIDI-ESFEHANI, 2009). Este corante é extraído dos frutos da planta e pode resultar em produtos hidrossolúveis e lipossolúveis, destacando-se como um dos principais carotenoides, com 80% de sua composição formada por carotenoides identificados (SATYANARAYANA; PRABHAKARA RAO; RAO, 2003).

A bixina é aprovada pela FDA para uso na indústria alimentícia e cosmética, apresentando características lipossolúveis devido à presença de éster metílico em sua estrutura (GARCIA *et al.*, 2012). Além disso, a bixina é estável na presença de agentes redutores e oxidantes, o que a torna útil em diversas formulações. Em termos de atividade farmacológica, a bixina possui propriedades antioxidantes, antimicrobianas e antitumorais (COSTA; CHAVES, 2005).

Estudos demonstram seus efeitos anti-inflamatórios, genotóxicos e hepatoprotetores. A planta também apresenta potencial no tratamento

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da asma brônquica e na modulação de comportamentos relacionados ao diabetes. Contudo, sua baixa solubilidade em água limita seu uso, incentivando pesquisas em técnicas de encapsulamento para melhorar sua eficácia como biomaterial (RIOS; MERCADANTE, 2004).

2. MATERIAIS E MÉTODOS

2.1 Materiais

Cloroformio UV HPLC - Espectroscopico 1000ml – Dinâmica®; Hexano PA 1000ml - Dinâmica®; Acetonitrila HPLC (Gradiente) 4000ml - PANREAC®; Ácido Acético Glacial PA ACS 1000ml - VETEC®.

2.2 Métodos

A bixina, uma matéria-prima extraída das sementes do urucum (Bixa orellana L.), foi obtida no município de Agricolândia – PI, região nordeste do Brasil (Latitude: 5° 48' 1" Sul, Longitude: 42° 40' 6" Oeste), seguindo um procedimento adaptado ao método proposto (BARBOSA-FILHO *et al.*, 1998). Aproximadamente 200 g de sementes de urucum, previamente limpas de folhas e cascas, foram colocadas em um extrator Soxhlet com 1000 mL de hexano (C_6H_{14}) sob agitação constante por 24 horas. Após esse período, o hexano foi removido e, em seguida, adicionou-se clorofórmio ($CHCl_3$) a 70°C durante mais 24 horas. O precipitado resultante foi filtrado e seco em estufa a 60 °C por 24 horas (figura 1).

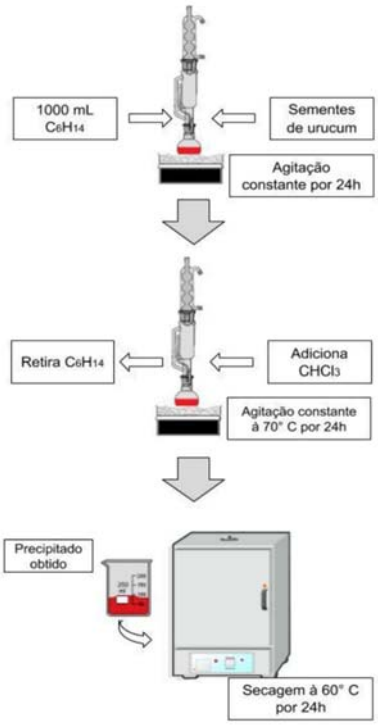


Figura 1. Fluxograma da síntese da Bixina.

Para caracterizar a amostra de bixina, diversos métodos foram aplicados. A análise por espectroscopia UV-Visível foi realizada em um espectrofotômetro Shimadzu UV-1800, cobrindo a faixa de 200 a 900 nm, utilizando $CHCl_3$ como solvente para diluição da bixina. A morfologia da bixina foi analisada por Microscopia Eletrônica de Varredura (MEV) com um equipamento modelo SSX-550 da Shimadzu. A amostra foi submetida à secagem a 60 ºC por 24 horas e coberta com uma fina camada de ouro para garantir condutividade, sendo a análise realizada com uma tensão de 15 kV.

A composição química foi determinada por Fluorescência de Raios-X (FRX) de energia dispersiva, utilizando um espectrômetro Epsilon 30 da Panalytical, empregando um método semiquantitativo em atmosfera de vácuo. O difratograma da amostra foi obtido através da técnica de Difração de Raios-X (DRX), utilizando um difratômetro Shimadzu XRD-6000 com radiação CuKα (40 kV e 30 mA), sendo o intervalo de varredura entre 10º e 90º com uma taxa de 0,014 º/min.

As mudanças estruturais e funcionais na amostra foram avaliadas por Espectroscopia de Infravermelho (FTIR) com um espectrômetro Shimadzu IRA Ftinity-1, na faixa de 400 a 4000 cm^{-1}. A estabilidade térmica foi investigada por Análise Termogravimétrica (TGA) no modelo Shimadzu TGA-51, abrangendo uma faixa de temperatura de 25 °C a 1000 °C, enquanto a Calorimetria Exploratória Diferencial (DSC) foi conduzida com o modelo DSC 60 PLUS da Shimadzu, entre 25 °C e 600 °C.

Para a separação cromatográfica da bixina, foi utilizada a técnica de Cromatografia Líquida de Alta Eficiência (HPLC), com uma coluna Lichrospher 100 RP-18. A fase móvel foi composta de acetonitrila e ácido acético (75:25). As amostras foram previamente filtradas e injetadas em um cromatógrafo LC-10 AD VP da Shimadzu, com detecção em 460 nm por UV-visível. A identificação dos picos de bixina foi baseada tanto no comportamento cromatográfico quanto na comparação dos espectros obtidos.

3. RESULTADOS E DISCUSSÃO:

A análise por espectrofotometria UV/Visível revelou picos em 470 e 502 nm, em concordância com os resultados experimentais obtidos (figura 2). Esses picos de absorção da bixina podem variar de acordo com o solvente

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empregado, e, neste estudo, o clorofórmio foi utilizado, resultando em um pico mais intenso em 470 nm (SCOTTER, 2016).

A bixina diluída em clorofórmio apresenta picos próximos, em 471 nm e 503 nm (RAHMALIA; FABRE; MOULOUNGUI, 2015), que explica que as duplas ligações conjugadas da bixina formam um grupo cromóforo responsável por absorver luz, resultando em uma forte banda de absorção acima de 400 nm, como também foi observado nesta análise.

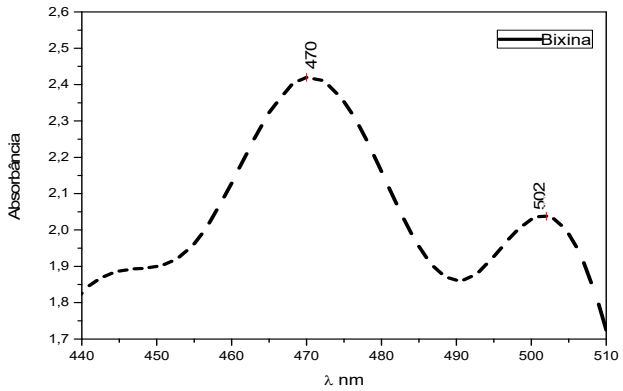


Figura 2. Espectro UV-vis da Bixina diluída em $CHCl_3$.

Na análise por MEV, após a deposição de uma fina camada de ouro de 14 nm para aumentar a condutividade e facilitar a visualização, foi identificada a presença de cristais de bixina cercados por aglomerados de impurezas, como mostrado na figura 3. Esses aglomerados podem ser consequência do processamento e manipulação durante a restrição do material.

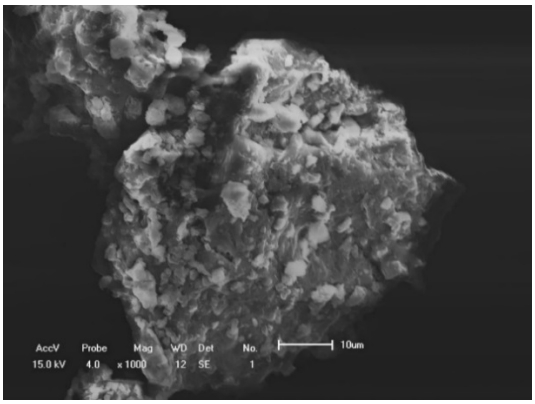


Figura 3. Micrografia da Bixina.

A FTIR da bixina revelou uma forte banda em 1159 cm^{-1}, característica de um grupo éster CO típico de espécies cis. Além disso, uma banda entre 772,4 e 778,8 cm^{-1} foi associada à vibração de hidrogênio fora do plano do grupo cis-C-CH=CH-C, com um pico forte em 754 cm^{-1}, indicando a presença da estrutura cis na bixina (figura 4). Quando protegida em clorofórmio, observou-se uma banda larga em 3349 cm^{-1}, atribuída à vibração de alongamento dos grupos OH, além de uma banda em 1716 cm^{-1} referente ao grupo C=O. Outras bandas incluíram vibrações de CO entre 1285 e 1159 cm^{-1}, e vibrações de C=C em 1610 cm^{-1}, dados que estão de acordo com a literatura científica disponível (BARBOSA-FILHO *et al.*, 1998; YUSÁ-MARCO *et al.*, 2008; OLIVEIRA JÚNIOR *et al.*, 2019).

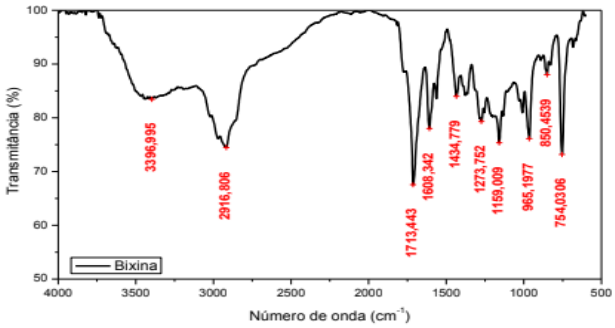


Figura 4. Espectroscopia de infravermelho da Bixina.

Na análise da TG e DSC, a curva TG da bixina, realizada sob atmosfera de nitrogênio, mostrou perda de massa em diferentes faixas de temperatura. A primeira perda, de 2,35%, ocorreu entre 20-120 °C devido à umidade, seguida por uma perda de 9,02% entre 120-200 °C, e uma perda significativa de 38,41% entre 200-400 °C. A isomerização da cis-bixina para trans ocorre entre 200-240 °C, com fusão observada por volta de 200 °C.

A análise DSC confirmou eventos endotérmicos e exotérmicos, com um pico endotérmico entre 142,59 e 196,52 °C, atribuído à fusão da bixina, corroborando os dados da TG. Eventos térmicos adicionais entre 348,03-384,54 °C e 450,45-505,37 °C foram relacionados à manipulação térmica da bixina.

A cromatografia líquida de alta eficiência foi validada para a análise, uma vez que não apresentou picos de interferência significativos (figura 5), conforme descrito no estudo de (SILVA *et al.*, 2005) Esse método foi utilizado para purificar, identificar e quantificar os pigmentos de urucum por técnicas espectroscópicas e cromatográficas. Nos cromatogramas, foram observados picos minoritários com tempos de retenção próximos ao da bixina (19,792 min), sugerindo a presença de isômeros geométricos.

4. CONCLUSÃO:

Os resultados indicam que a bixina é uma promessa de biomaterial para a indústria

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farmacêutica, devido à sua estrutura bem definida, estabilidade térmica em temperaturas moderadas e composição química conhecida. No entanto, a presença de isômeros e a manipulação em temperaturas mais baixas podem ser especificações que precisam ser comprovadas antes de sua utilização em produtos farmacêuticos. Estudos adicionais são essenciais para entender como essas características influenciam a eficácia e a segurança da bixina em aplicações específicas.

5. DECLARAÇÕES

5.1. Agradecimentos

Agradecimento à CAPES. Ao IFPI, UFPI e ao Laboratório de Inovação Tecnologica e Empreendedorismo – Medicamentos e Correlatos.

5.2. Acesso Aberto

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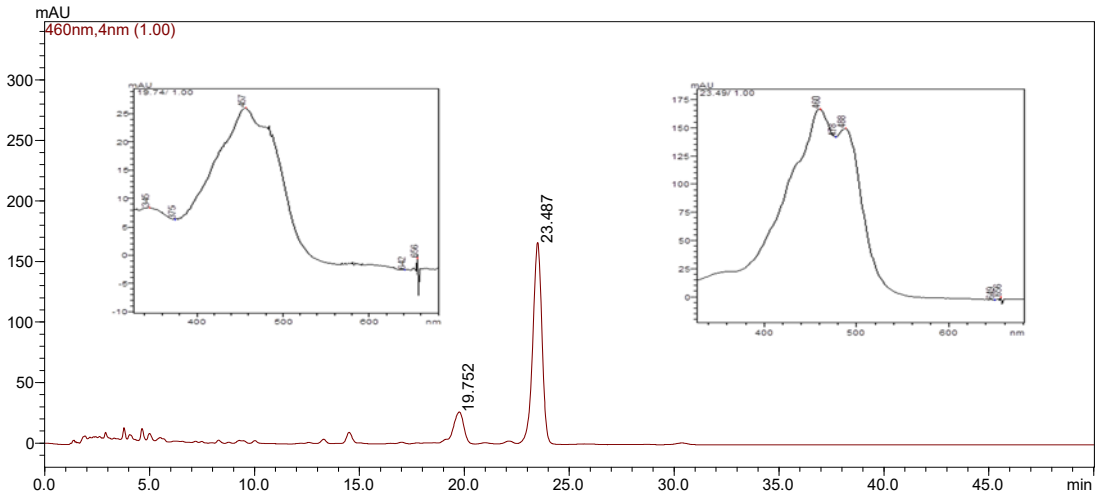


Figura 5. Cromatograma, obtido por CLAE, do padrão de bixina. Condições cromatográficas: coluna Lichrospher 100 RP-18 e acetonitrila:ácido acético 5% (75:25) como fase móvel com fluxo de 1 mL/min. Detecção a 460 nm.

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Southern Science Conference, 2024.

EXTRAÇÃO E CARACTERIZAÇÃO DA BIXINA (*BIXA ORELLANA* L.): IMPACTO CLÍNICO E APLICAÇÕES FARMACOLÓGICAS

EXTRACTION AND CHARACTERIZATION OF BIXIN (*BIXA ORELLANA* L.): CLINICAL IMPACT AND PHARMACOLOGICAL APPLICATIONS

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October/2024

SUMÁRIO

- Introdução
- Objetivos
- Materiais e Métodos
- Resultados e Discussão
- Conclusão
- Agradecimentos
- Referências

INTRODUÇÃO

1

- Planta Urucum (*Bixa orellana* L.) da família Bixáceas.
- Utilizada em aplicações alimentícias e farmacêuticas
- Apresenta em sua composição 80% de carotenoides.

2

- Apresenta em sua composição éster etílico.
- Além disso, apresenta-se estável na presença de agentes redutores e oxidantes.

3

- Entre suas propriedades farmacológicas, pode-se destacar atividades antioxidantes, antimicrobianas e antitumorais.

4

- Apresenta potencial no tratamento da asma e na modulação de comportamentos relacionados a diabetes.

OBJETIVOS

- Extrair e caracterizar a bixina proveniente da semente de urucum.
- Compreender as carateristicas da bixina e suas aplicações farmacológicas.
- Aprofundar sobre a segurança e eficácia em aplicações específicas .

MATERIAIS E MÉTODOS

2.1 Materiais

Clorofórmio UV HPLC- Espectroscopio 1000 mL - Dinâmica®; Hexano PA 1000 mL- Dinâmica®; Acetonitrila HPLC (Gradiente) 4000 mL- PANREAC®; Ácido Acético Glacial PA ACS 1000 mL- VETEC®.

2.2 Métodos

- A bixina, extraída das sementes do urucum *(Bixa orellana* L.), foi obtida no municipio de Agricolândia- PI.
- Seguindo o procedimento adaptado ao método proposto por Barbosa filho et al [6].

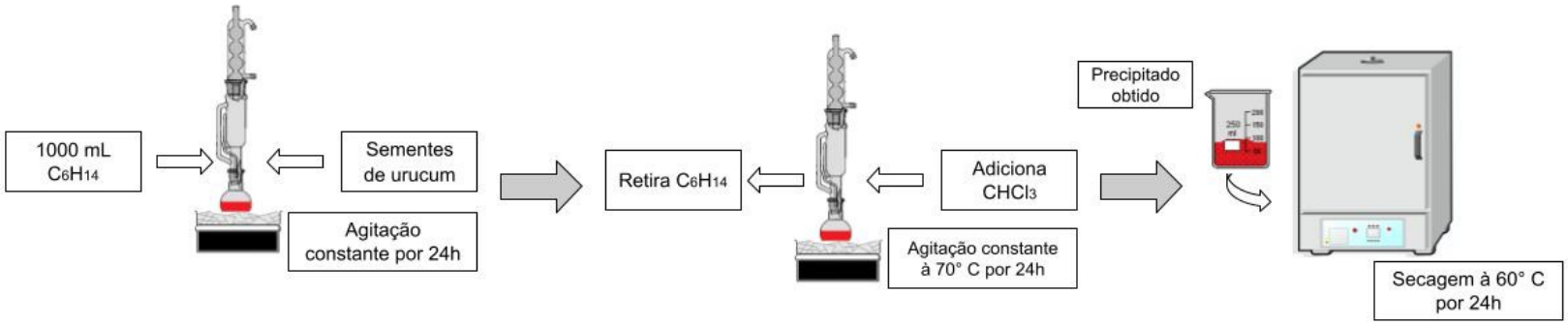


Figura 1 - Fluxograma da síntese da Bixina

MATERIAIS E MÉTODOS

2.2 Métodos	Espectroscopia UV-VIS
	Microscopia Eletrônica de Varredura (MEV)
	Fluorêscencia de Raio- X (FRX)
	Difração de Raio- X (DRX)
	Espectroscopia de Infavermelho (FTIR)
	Análise Termogravimétrica (TGA) e Calorimetria Exploratória Diferencial (DSC)
	Cromatografia Líquida de Alta Eficiência (HPLC)

RESULTADOS E DISCUSSÃO

A análise por espectrofotometria UV/Visível revelou picos em 470 e 502 nm, em concordância com os resultados experimentais obtidos (figura 2). Esses picos de absorção da bixina podem variar de acordo com o solvente empregado, e, neste estudo, o clorofórmio foi utilizado, resultando em um pico mais intenso em 470 nm [7].

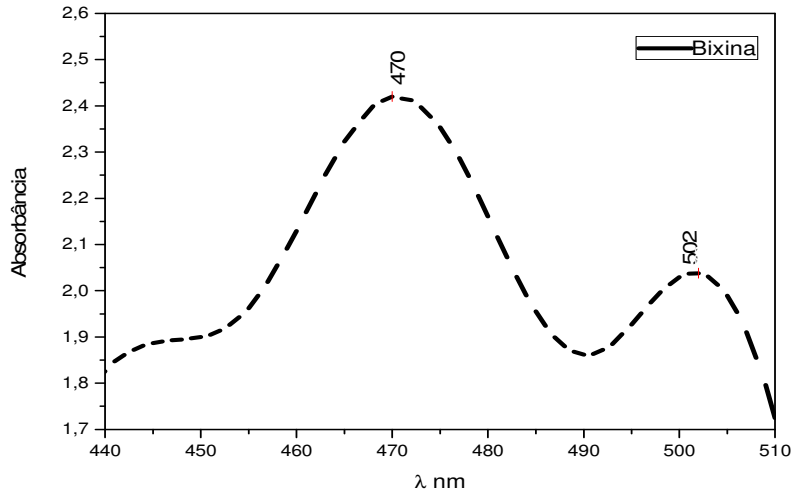


Figura 2. Espectro UV-vis da Bixina diluída em $CHCl_3$ (P.A.).

Na análise por MEV, após a deposição de uma fina camada de ouro de 14 nm para aumentar a condutividade e facilitar a visualização, foi identificada a presença de cristais de bixina cercados por aglomerados de impurezas, como mostrado na figura 3.

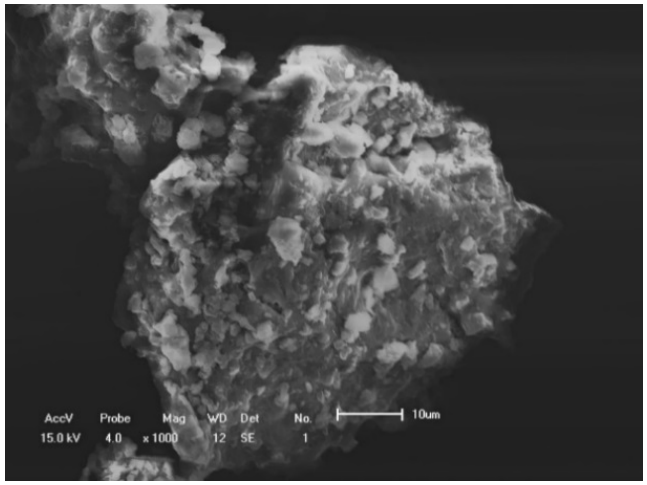


Figura 3. Micrografia da Bixina.

RESULTADOS E DISCUSSÃO

- A FTIR da bixina revelou uma forte banda em 1159 cm^{-1}, característica de um grupo éster CO típico de espécies cis. Além disso, uma banda entre 772,4 e 778,8 cm^{-1} foi associada à vibração de hidrogênio fora do plano do grupo cis-C-CH=CH-C, com um pico forte em 754 cm^{-1}, indicando a presença da estrutura cis na bixina .
- Quando protegida em clorofórmio, observou-se uma banda larga em 3349 cm^{-1}, atribuída à vibração de alongamento dos grupos OH, além de uma banda em 1716 cm^{-1} referente ao grupo C=O.

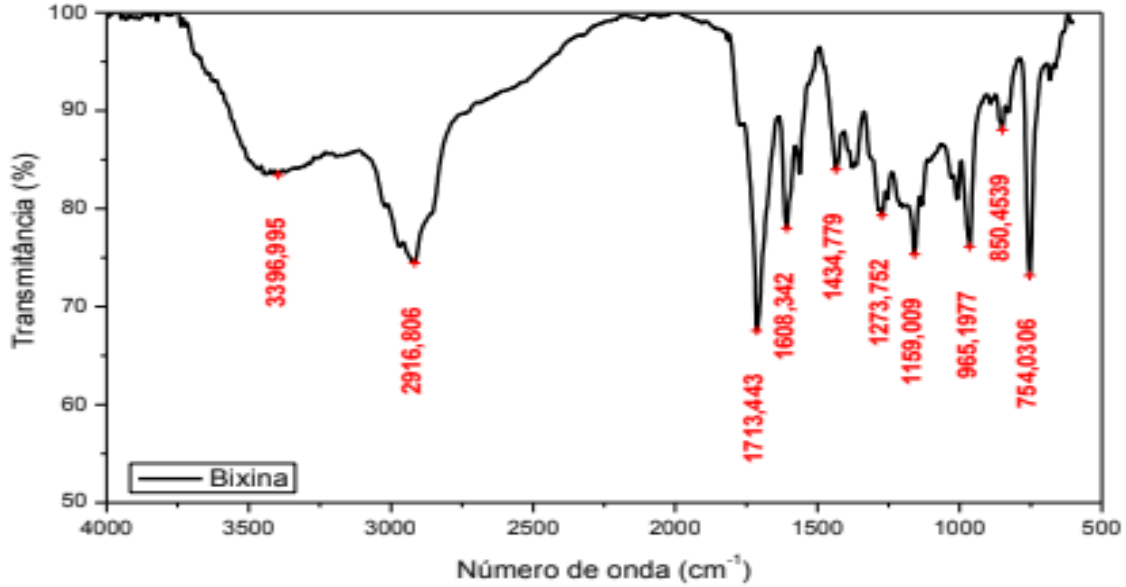
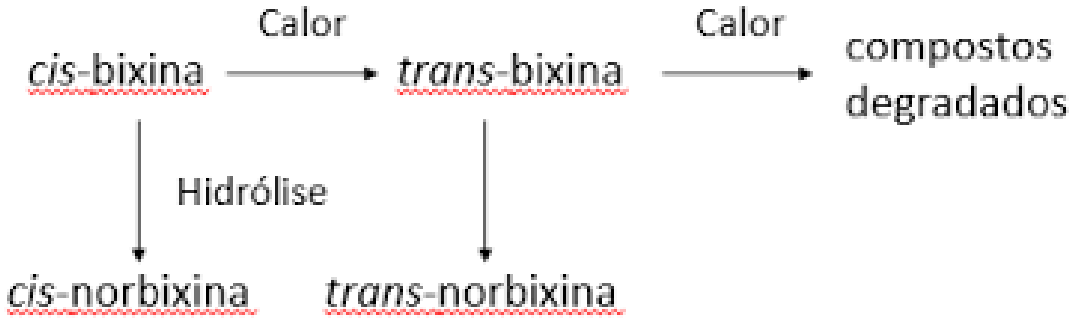


Figura 4. Espectroscopia de infravermelho da Bixina.

RESULTADOS E DISCUSSÃO

Na análise da TG e DSC, a curva TG da bixina, realizada sob atmosfera de nitrogênio, mostrou perda de massa em diferentes faixas de temperatura. A primeira perda, de 2,35%, ocorreu entre 20-120 ˚C devido à umidade, seguida por uma perda de 9,02% entre 120-200 ˚C, e uma perda significativa de 38,41% entre 200-400 ˚C. A isomerização da cis-bixina para trans ocorre entre 200-240 ˚C, com fusão observada por volta de 200 ˚C.

Figura 5. Alteração química causada por temperatura



Fonte: UFV, 2021

RESULTADOS E DISCUSSÃO

A cromatografia líquida de alta eficiência foi validada para a análise, uma vez que não apresentou picos de interferência significativos (figura 5), conforme descrito no estudo de Silva [12]. Nos cromatogramas, foram observados picos minoritários com tempos de retenção próximos ao da bixina (19,792 min), sugerindo a presença de isômeros geométricos.

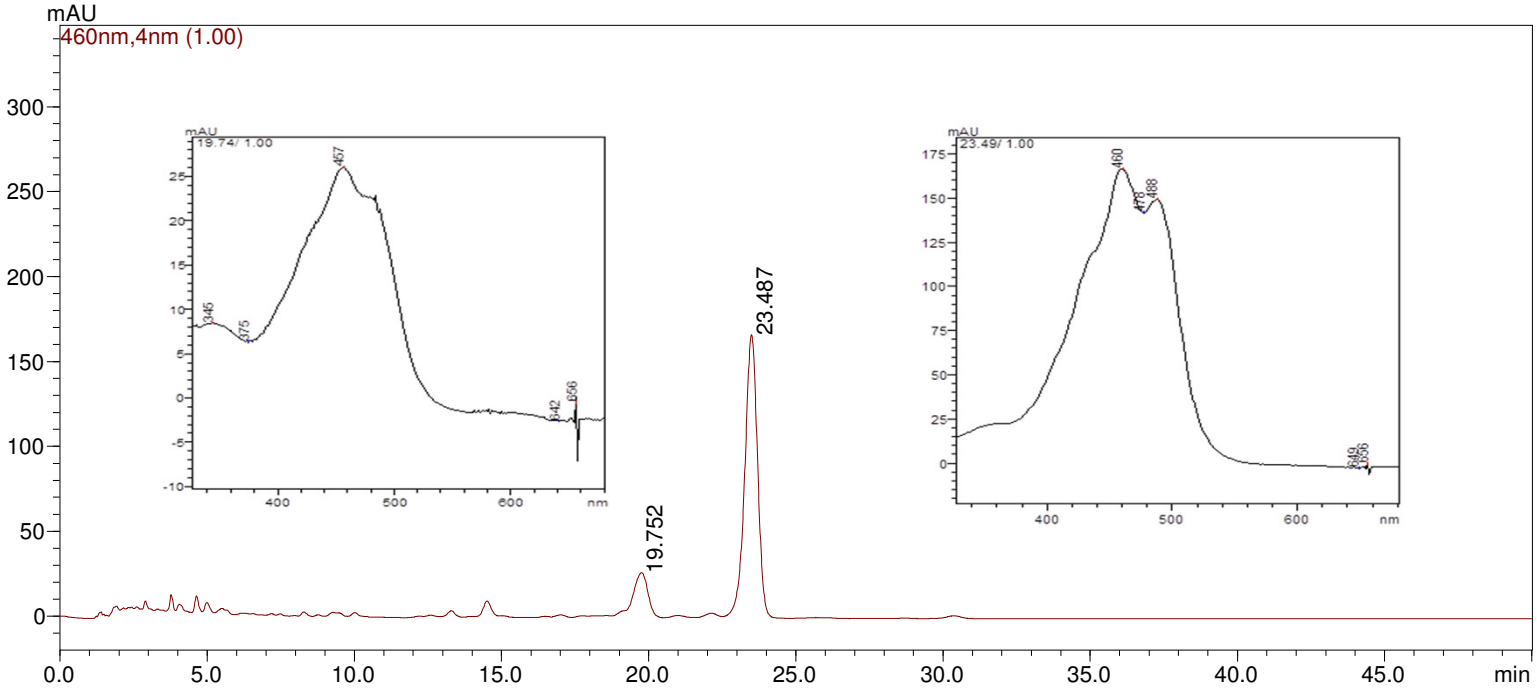


Figura 6. Cromatograma, obtido por CLAE, do padrão de bixina. Condições cromatográficas: coluna Lichrospher 100 RP-18 e acetonitrila:ácido acético 5% (75:25) como fase móvel com fluxo de 1 mL/min. Detecção a 460 nm.

CONCLUSÃO

- Os resultados indicam que a bixina é uma promessa de biomaterial para a indústria farmacêutica, devido à sua estrutura bem definida, estabilidade térmica em temperaturas moderadas e composição química conhecida.
- No entanto, a presença de isômeros e a manipulação em temperaturas mais baixas podem ser especificações que precisam ser comprovadas antes de sua utilização em produtos farmacêuticos.
- Estudos adicionais são essenciais para entender como essas características influenciam a eficácia e a segurança da bixina em aplicações específicas.

AGRADECIMENTOS

Agradecimento à CAPES. Ao IFPI, UFPI e ao Laboratório de Inovação Tecnológica e Empreendedorismo – Medicamentos e Correlatos.

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QUANTITATIVE ASSESSMENT OF ENVIRONMENTAL LICENSING IN NON-LICENSING MUNICIPALITIES OF RIO DE JANEIRO: A COMPARATIVE STUDY BETWEEN 2022 AND 2023.

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ABSTRACT

Human development generates both positive and negative environmental impacts. Negative impacts include soil, air, and water pollution, as well as ecosystem degradation, while positive impacts involve job creation, economic and technological development, and sustainable practices. Environmental licensing is an essential administrative procedure to ensure that potentially polluting activities are conducted in a way that harmonizes economic development with environmental preservation. This study aims to analyze the licenses issued by the State Institute for the Environment of Rio de Janeiro (INEA) in the years 2022 and 2023 across nineteen non-licensing municipalities, seeking to understand the challenges they face. The research is based on data collected through the transparency platform "Ambiente +" and analysis using Minitab software. The results of this study highlight the need to strengthen the institutional and technical capacity of non-licensing municipalities, promoting awareness of the importance of environmental licensing and providing the necessary support so that these municipalities can fully assume their responsibilities in local environmental management.´

Keywords: *Municipal public management; Environmental licensing; Competent authority.*

1. INTRODUÇÃO

O licenciamento ambiental é fundamental para proteger o meio ambiente e garantir a conformidade legal de atividades potencialmente poluidoras, conciliando crescimento econômico com preservação ambiental (Sánchez, 2013; Fiorillo, 2013).

No Brasil, esse instrumento faz parte da Política Nacional de Meio Ambiente (PNMA), conforme a Lei 6.938/1981, e visa assegurar que o desenvolvimento econômico ocorra em harmonia com a proteção ambiental (CONAMA, 1997).

Rio de Janeiro, o licenciamento ambiental iniciou com o Decreto 1.633/77. Atualmente a gestão dessas atividades é regida pelas resoluções CONEMA 92/21 e 95/22, as quais estabelecem a relação das atividades de competência dos municípios e os critérios para seu enquadramento. No entanto, para que os municípios exerçam plenamente a função de órgão ambiental licenciador, devem cumprir requisitos como possuir um órgão ambiental capacitado, um Conselho Municipal de Meio Ambiente ativo, legislação própria disciplinando os procedimentos de licenciamento ambiental e fiscalização com a previsão de sanções administrativas, além de um Fundo Municipal do Meio Ambiente implantado.

Apesar dos avanços na descentralização do licenciamento ambiental, ainda existem desafios a serem superados. Segundo dados do Portal de Licenciamento do INEA (2024), dos 92 municípios do estado do Rio de Janeiro, 19 ainda não estão aptos a realizar o licenciamento ambiental por não atenderem aos requisitos

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necessários.

Diante deste cenário, este trabalho tem como objetivo analisar as licenças emitidas pelo INEA em 2022 e 2023 nos municípios não licenciadores, buscando compreender os desafios enfrentados e contribuir para o fortalecimento da gestão ambiental local no estado do Rio de Janeiro.

2. MATERIAL E MÉTODOS

2.1 Materiais

- Plataforma Ambiente + do Instituto Estadual do Ambiente (INEA): utilizada para coleta de dados sobre licenças ambientais emitidas nos anos de 2022 e 2023 para os municípios não licenciadores.
- Portal de Licenciamento INEA: consultado para verificar a situação dos municípios em relação à aptidão para licenciamento ambiental.
- Software Minitab (versão 20.0): utilizado para análise estatística, geração de gráficos e testes de hipóteses.

Legislação: A pesquisa se baseou nas seguintes normas:

- Lei Federal 6.938/1981 (PNMA);
- Resolução CONAMA 237/1997;
- Decreto Estadual 1.633/1977;
- Lei Estadual 5.101/2007;
- Resoluções CONEMA 92/2021 e 95/2022.

Esses materiais permitiram a coleta e análise dos dados sobre as licenças ambientais nos municípios não licenciadores.

2.2 Métodos

Para a realização deste estudo, foram adotadas as seguintes etapas metodológicas:

Revisão de literatura: Foi realizada uma pesquisa na base de dados do Google Acadêmico, utilizando a seguinte string de busca: “(licença ambiental) AND (INEA) AND (descentralização) AND (órgão não licenciador) AND (gestão pública) AND (CONMA 95) AND (impacto ambiental local)”. Essa string foi elaborada com o objetivo de encontrar artigos relevantes que abordassem o tema do licenciamento ambiental no estado do Rio de Janeiro, com foc Revisão de Literatura: Pesquisas no Google Acadêmico com a string “(licença ambiental) AND (INEA) AND (descentralização) AND (órgão não licenciador)” resultaram em 27 artigos, dos quais 5 foram selecionados para embasamento teórico.

- Coleta de Dados: Os dados de licenciamento ambiental de 2022 e 2023 foram extraídos da plataforma Ambiente +.

A seleção incluiu:

a) Licenciamento Ambiental e Acompanhamento de licenças;
Licenças e instrumentos de controle emitidos;
Filtragem por municípios não licenciadores,
b) Intervalo de tempo: 01/01/2022 a 31/12/2022 e 01/01/2023 a 31/12/2023, Figura 1.



***Figura 1**. Figura 1. Licenças e instrumentos de controle emitidos - Plataforma Ambiente +.*
Fonte: INEA, 2024.

Análise Estatística: Usou-se o Minitab para calcular estatísticas descritivas e gerar um gráfico de BoxPlot. O teste de normalidade de Shapiro-Wilk (α = 0,05) foi aplicado, seguido do teste não paramétrico de Mann-Whitney para comparar as medianas dos anos de 2022 e 2023. Esses métodos possibilitaram a análise dos dados e elaboração de conclusões sobre o licenciamento ambiental nos municípios do Rio de Janeiro.

3. RESULTADOS E DISCUSSÃO

Após a coleta e organização dos dados referente às licenças ambientais emitidas pelo INEA nos anos de 2022 e 2023 para os municípios não licenciadores, foram obtidos os resultados apresentados na Tabela 1.

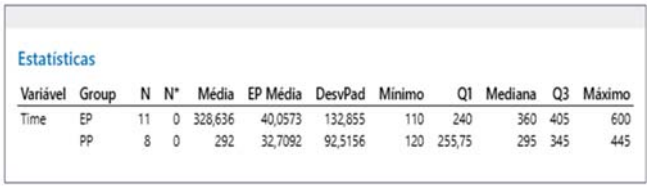
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Tabela 1. *Relação das Licenças ambientais emitidas pelo INEA, referente aos anos de 2022 e 2023.*

Municípios	Licenças emitidas em 2022	Licenças emitidas em 2023
Bom Jardim	13	3
om Jesus do Itabapoana	3	1
nceição de Macabu	7	1
Duas Barras	5	2
Engenheiro Paulo de Frontin	0	1
Italva	1	3
Itaocara	6	5
Itaperuna	16	6
Itatiaia	5	2
Laje do Muriaé	1	1
Macuco	2	2
Natividade	5	3
Pinheiral	13	3
Porciúncula	4	1
Quissamã	6	5
anta Maria Madalena	9	0
Sumidouro	6	0
rajano de Moraes	8	0
Varre-Sai	3	1
Total	**113**	**40**

Fonte: Elaborado pelo autor.

Observou-se um decréscimo total de licenças emitidas no ano de 2023 em relação a 2022. A Figura 2 apresenta as estatísticas descritivas dos conjuntos de dados analisados, incluindo médias, mediana e desvio padrão.



Estatísticas

Variável	Group	N	N*	Média	EP Média	DesvPad	Mínimo	Q1	Mediana	Q3	Máximo
Time	EP	11	0	328,636	40,0573	132,855	110	240	360	405	600
	PP	8	0	292	32,7092	92,5156	120	255,75	295	345	445

Figura 2. *Estatísticas descritivas.*

Em seguida, foi aplicado o gráfico de BloxPlot (Figura 3) para visualizar a distribuição e os valores discrepantes dos dados.

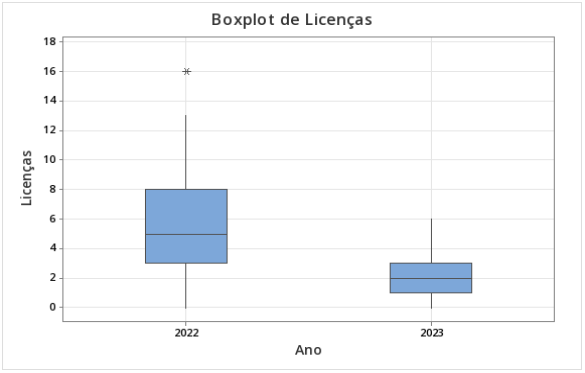


Figura 3. BloxPlot das amostras consideradas

Para determinar se os dados seguiam uma distribuição normal, foi realizado o teste de normalidade de Shapiro-Wilk (Figura 4), considerando um nível de significância de 5% (α=0,05). O resultado indicou que os dados não possuíam distribuição normal (p-value <0,005).



Figura 4. Teste de normalidade

Devido a não normalidade dos dados, aplicou-se o teste não paramétrico de Mann-Whitney (Figura 5) para comparar as medianas das licenças emitidas entre os anos de 2022 e 2023. As hipóteses testadas foram:

- H0: As medianas das licenças emitidas em 2022 e 2023 são iguais.
- H1: As medianas das licenças emitidas em 2022 e 2023 são diferentes.

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Teste

Hipótese nula	H_0: $\eta_1 - \eta_2 = 0$
Hipótese alternativa	H_1: $\eta_1 - \eta_2 \neq 0$

Método	Valor W	Valor-p
Não ajustado para empates	478,50	0,002
Ajustado para empates	478,50	0,002

Figura 5. *Teste Mann Whitney.*

Os dados oficialmente informados demostram uma redução significativa no número de licenças ambientais emitidas pelo INEA em 2023, em comparação com 2022. Esse descréscimo pode ser atribuído a alguns fatores, incluíndo a limitação de recursos financeiro e técnicos capacitados nos municípios, bem como a diminuição da demanda por licenças ambientais para atividades econômicas locais.

Ademais, a ausência do licenciamento ambiental local pode resultar na incapacidade de cumprir com as exigências legais e na exclusão de uma etapa fundamental para a gestão ambiental municipal (Faria, 2019). Além disso, a falta de conscientização e prioridade das administrações municipais sobre a importância de assumir o licenciamento ambiental pode reforçar essa lacuna, uma vez que a elaboração e implementação de legislações e políticas públicas voltadas ao meio ambiente ainda não são vistas com prioridade em muitos casos (Bursztyn, M, 2012).

4. CONCLUSÃO

A análise dos dados apresentados neste trabalho evidencia a necessidade de fortalecer a capacidade institucional e técnica dos municípios não licenciadores do estado do Rio de Janeiro. Essa capacitação é essencial para que esses municípios possam efetivamente assumir suas responsabilidades ambientais, promovendo um equilíbrio sustentável entre o desenvolvimento econômico local e a preservação dos recursos naturais. Além disso, é fundamental valorizar as particularidades de cada região, garantindo que as atividades propostas sejam adequadas a realidade local, respeitando a diversidade ecológica e socioeconômica local.

5. DECLARAÇÕES

5.1. Agradecimentos

Os autores agradecem à Universidade de Vassouras e ao Programa de Mestrado Profissional em Ciências Ambientais, assim como à Fundação Carlos Chagas Filho de Amparo à Pesquisa do Estado do Rio de Janeiro pelo apoio e incentivo à pesquisa. Agradecem também à Universidade de Mendoza pela organização do evento enriquecedor.

5.2. Acesso Aberto

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4. Fiorillo, C. A. P. Curso de direito ambiental brasileiro.14. ed. São Paulo: Saraiva, **2013**.
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Southern Science Conference, 2024.

AVALIAÇÃO QUANTITATIVA DO LICENCIAMENTO AMBIENTAL NOS MUNICÍPIOS NÃO LICENCIADORES DO RIO DE JANEIRO: UM ESTUDO COMPARATIVO ENTRE OS ANOS DE 2022 E 2023.

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October/2024

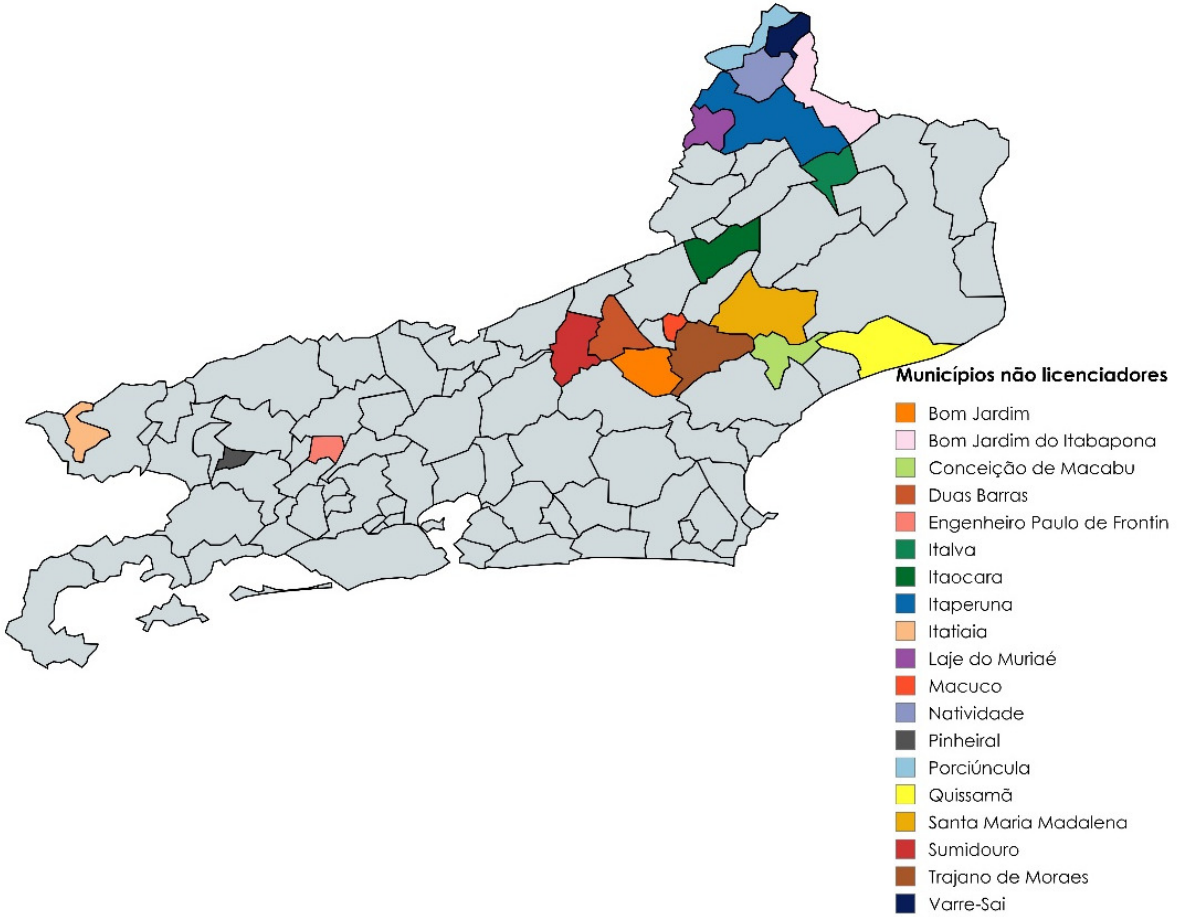
INTRODUÇÃO

- O licenciamento ambiental é fundamental para proteger o meio ambiente e garantir a conformidade legal de atividades potencialmente poluidoras, conciliando crescimento econômico com preservação Ambiental.

- No Rio de Janeiro, atualmente a gestão dessas atividades é regida pelas resoluções CONEMA 92/21 e 95/22, que definem as competências municipais.

INTRODUÇÃO

- Apenas 19 dos 92 municípios do estado não estão aptos a licenciar, uma vez que não cumprem com os requisitos necessários.



OBJETIVO

Este estudo tem como objetivo analisar as licenças emitidas pelo INEA em 2022 e 2023 nos municípios não licenciadores, buscando compreender os desafios enfrentados e contribuir para o fortalecimento da gestão ambiental local no estado do Rio de Janeiro.

METODOLOGIA

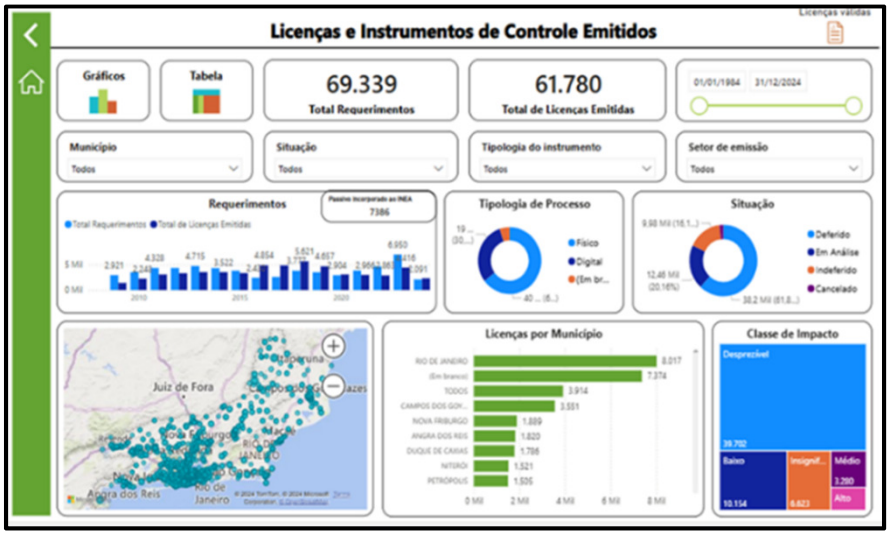
- Pesquisa e Coleta de Dados:

- Fonte: Google Acadêmico e Plataforma Ambiente + (INEA).

- Dados: Licenciamento ambiental e instrumentos de controle para municípios não licenciadores.

- Período: 01/01/2022 a 31/12/2022 e 01/01/2023 a 31/12/2023.

- Análise: Minitab (versão 20.0).



Licenças e instrumentos de controle emitidos - Plataforma Ambiente +.
Fonte: INEA, 2024.

RESULTADOS E DISCUSSÕES

- Relação das Licenças ambientais emitidas pelo INEA, referente aos anos de 2022 e 2023.

Municípios	Licenças emitidas em 2022	Licenças emitidas em 2023
Bom Jardim	13	3
Bom Jesus do Itabapoana	3	1
Conceição de Macabu	7	1
Duas Barras	5	2
Engenheiro Paulo de Frontin	0	1
Italva	1	3
Itaocara	6	5
Itaperuna	16	6
Itatiaia	5	2
Laje do Muriaé	1	1
Macuco	2	2
Natividade	5	3
Pinheiral	13	3
Porciúncula	4	1
Quissamã	6	5
Santa Maria Madalena	9	0
Sumidouro	6	0
Trajano de Moraes	8	0
Varre-Sai	3	1
Total	113	40

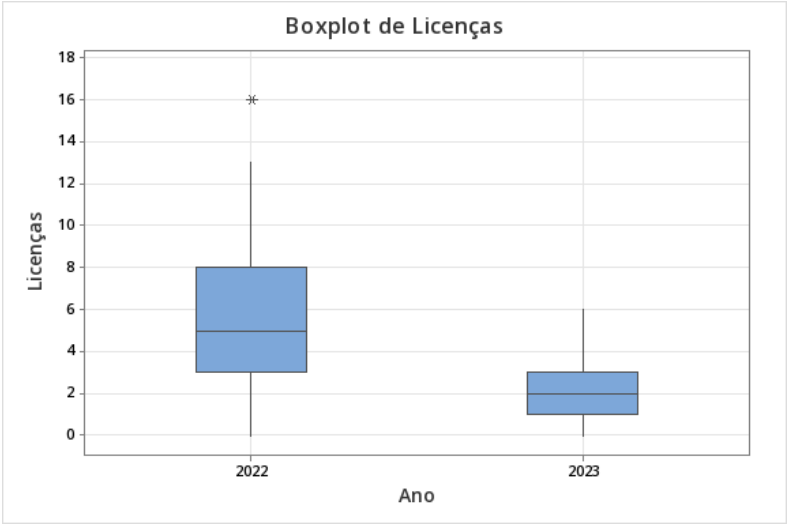
RESULTADOS E DISCUSSÕES

- Decréscimo total de licenças emitidas no ano de 2023 em relação a 2022.

Estatísticas

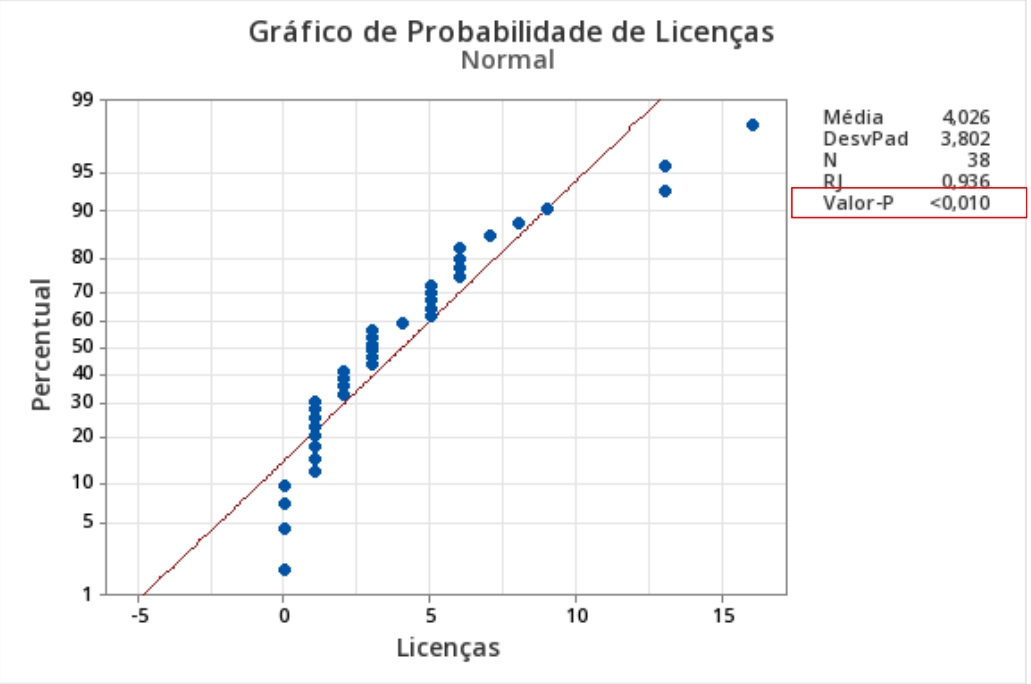
Variável	Ano	N	N*	Média	EP Média	DesvPad	Mínimo	Q1	Mediana	Q3	Máximo
Licenças	2022	19	0	5,94737	0,995527	4,33940	0	3	5	8	16
	2023	19	0	2,10526	0,403890	1,76052	0	1	2	3	6

- Aplicação do gráfico de BloxPlot para visualizar a distribuição e os valores discrepantes dos dados.



RESULTADOS E DISCUSSÕES

- Aplicação do teste de normalidade de Shapiro-Wilk para determinar se os dados seguiam uma distribuição normal, considerando o nível de significância de 5% (α=0,05).



RESULTADOS E DISCUSSÕES

- Foi aplicado o teste não paramétrico de Mann-Whitney para comparar as medianas das licenças emitidas entre 2022 e 2023, devido à não normalidade dos dados.

- Houve uma redução significativa no número de licenças ambientais emitidas pelo INEA em 2023 em comparação a 2022 para municípios não licenciadores no Rio de Janeiro

Teste

Hipótese nula	$H_0: \eta_1 - \eta_2 = 0$
Hipótese alternativa	$H_1: \eta_1 - \eta_2 \neq 0$

Método	Valor W	Valor-p
Não ajustado para empates	478,50	0,002
Ajustado para empates	478,50	0,002

RESULTADOS E DISCUSSÕES

- Ausência de licenciamento ambiental local:

- Pode resultar na incapacidade de cumprir exigências legais.

- Exclui uma etapa fundamental para a gestão ambiental municipal (Faria, 2019).

- Falta de conscientização e prioridade pelas administrações municipais:

- Desconsideram a importância do licenciamento ambiental.

- A elaboração e implementação de legislações e políticas ambientais ainda não são prioridades em muitos casos (Bursztyn, 2012).

CONCLUSÕES

- A transparência da Plataforma Ambiente + do INEA facilita o conhecimento das licenças concedidas para atividades de impacto local.
- Faz necessário fortalecer a capacidade institucional e técnica dos municípios não licenciadores, promovendo a conscientização sobre a importância do licenciamento ambiental e fornecendo suporte para que assumam suas responsabilidades na gestão ambiental local.

AGRADECIMENTOS

- Universidade de Vassouras e ao Programa de Mestrado, Profissional em Ciências Ambientais, assim como à Fundação Carlos Chagas Filho de Amparo à Pesquisa do Estado do Rio de Janeiro pelo apoio e incentivo à pesquisa.
- Agradecem também à Universidade de Mendoza pela organização do evento enriquecedor.

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SOUTHERN SCIENCE CONFERENCE
2024 - VIRTUAL CONFERENCE AND IN PERSON EDITION

STATISTICAL ANALYSIS OF BIODIESEL CONSUMPTION GROWTH IN BRAZIL IN 2022 AND 2023 AND HOW THE ROLE OF THE IMMERSIVE VIRTUAL ENVIRONMENT CAN SUPPORT BEST PRACTICES FOR THIS BIOFUEL

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ABSTRACT

Biodiesel consumption in Brazil has shown immense growth in recent years. In 2022, consumption reached approximately 6.27 million cubic meters. In 2023, there was a significant increase, with consumption reaching around 7.34 million cubic meters, reflecting a growth of 19.4%, according to data provided by the National Agency for Petroleum, Natural Gas and Biofuels (ANP). This value was driven by the increase in mandatory mixing to 12% from April 2023, as stipulated by CNPE Resolution No. 3/2023.The use of the metaverse as an interactive virtual environment aims to broadly promote the concepts of environmental sustainability, creating a dynamic platform for user awareness and education. In this immersive environment, detailed virtual models of the biodiesel production process will be developed, allowing users to explore the process in an interactive and practical way. Additionally, the metaverse will enable simulations that highlight the benefits and advantages of biodiesel compared to fossil fuels, making the learning experience more engaging and effective.With the help of Minitab Software, it was possible to design and simulate scenarios that demonstrate the positive impact of virtual reality on the increase in biodiesel consumption in Brazil in 2022 and 2023. Interaction with the metaverse enhances the implementation of good practices in the biofuels sector, creating a new level of engagement and understanding for companies, governments and consumers, accelerating the use of renewable fuels.

keywords: *Biodegradable; Education; Interactivity; Simulation; Sustainability*.

1. INTRODUÇÃO

De acordo com Pacific Biodiesel, o termo “biodiesel” originou-se pela primeira vez em 1853, quando Patrick Duffy da Irlanda patenteou o processo de transesterificação de óleo vegetal em biodiesel. O combustível foi reconhecido e adicionado durante o início de 1941 a 1945 no tempo da Segunda Guerra Mundial na Europa devido à baixa disponibilidade de petróleo.

No Brasil, especificamente, o biodiesel ganhou destaque significativo desde os anos 2000, com o programa de biodiesel sendo implementado para promover o desenvolvimento regional e a sustentabilidade ambiental através do uso de recursos locais. Nos últimos anos, o Brasil tem testemunhado um crescimento notável no consumo de biodiesel, impulsionado por políticas públicas que incentivam a produção e o uso de biocombustíveis como parte de sua estratégia energética sustentável.

Mais precisamente em 2022 e 2023, o país registrou marcos significativos nesse setor, refletindo não apenas um aumento na produção, mas também uma conscientização crescente sobre a importância de reduzir as emissões de gases de efeito estufa e promover a segurança

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energética.

O ambiente virtual imersivo surgiu como uma ferramenta promissora para disseminar boas práticas e promover a educação sobre biocombustíveis. .

Através dessa iniciativa ocorrerá a construção desse processo do biodiesel dentro de um ambiente virtual conhecido como metaverso, que por si mesmo é um espaço que simula um tipo de mundo virtual que tenta replicar a realidade por meio de dispositivos digitais. Com isso, a forma de se entender a fabricação do biodiesel será interativa e imersivo. Além disso, é uma forma sustentável de desenvolver novas tecnologias e práticas de produção, sem a necessidade de recursos físicos.

Com base no exposto, este trabalho tem como objetivo realizar uma simulação interativa do processo de produção da planta do biodiesel. Este presente artigo foi organizado em três etapas distintas: pesquisa bibliográfica e revisão da literatura; coleta e análise dos dados direcionados usando a ferramenta Minitab.

2. MATERIAL E MÉTODOS

O levantamento de dados e informações é uma das principais maneiras de começar a realização de um projeto. A primeira coisa a fazer é coletar informações detalhadas sobre como fazer o biodiesel. Isso inclui todas as etapas, equipamentos, insumos e fornecedores envolvidos através do produto. Após a coleta de bases, é feita a modelagem do processo de fabricação de biodiesel, levando em consideração a aplicação, sustentabilidade e qualidade do produto final. É feito também um ambiente virtual e de modelagem 3D (Silva, P. R. 2021) que simula a produção de biodiesel. Para a construção deste cenário no metaverso é necessário o conhecimento detalhado da produção e da planta do biodiesel (FIGURA 1), desde as etapas de prepare da matéria-prima até a obtenção do produto final, utilizando recursos como vídeos de tutorias interativos para a melhor compreensão do usuário ao utilizar os óculos VR ou o ambiente do metaverso com fácil acesso a dispositivos móveis, desktop ou notebook.

No entanto, o modelo virtual é testado e validado para validar o produto, garantindo sua eficácia e veracidade em comparação ao processo real de produção de biodiesel. Com isso o modelo virtual está implementado e disponível após sua validação. Estudantes, pesquisadores, profissionais da indústria e outros interessados no assunto podem usá-lo. Quanto à viabilidade do projeto, é importante pensar no investimento inicial em tecnologia e nas possíveis vantagens do projeto. As vantagens incluem custos reduzidos com os devidos experimentos físicos, a oportunidade de treinar e capacitar profissionais de forma remota através do ambiente de simulação e a redução dos efeitos ambientais ao simular práticas sustentáveis. Além disso, o futuro produto tem a capacidade de atrair parcerias com empresas do setor de biocombustíveis (Almeida, A. B. 2019) que podem estar interessadas em inovações tecnológicas e sustentáveis.

Existe um grande potencial para inovação e sustentabilidade do desenvolvimento de modelos virtuais do processo de produção de biodiesel como por exemplo a parceria com a Univassouras no metaverso, que através de lá, poderá ser feito o laboratório de biodiesel dentro do ambiente imersivo, visto que a Universidade oferece esse recurso para ser feito o combustível fisicamente.

Para melhor fundamentação, foi realizada uma revisão sistemática, onde o presente trabalho obteve resultados mais objetivos e refinados de materiais já publicados, essa pesquisa foi feita pelo Google acadêmico usando uma String de busca BIODIESEL AND SUSTENTABILIDADE AND REALIDADE AUMENTADA AND MODELAGEM 3D.



Figura 01: *A planta do biodiesel*

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3. RESULTADOS E DISCUSSÃO

Os dados fornecidos pelo site da ANP (Agência Nacional do Petróleo, Gás Natural e Biocombustíveis) referente ao consumo de milhões de litro de biodiesel no ano de 2022 e 2023.

Tabela 1: *Dados referente ao consumo por mês e ano do Biodiesel.*

Ano	Mês	Consumo de biodiesel milhões/Litros
2022	Janeiro	500
2022	Fevereiro	480
2022	Março	520
2022	Abril	530
2022	Maio	540
2022	Junho	550
2022	Julho	560
2022	Agosto	570
2022	Setembro	580
2022	Outubro	590
2022	Novembro	600
2022	Dezembro	610
2023	Janeiro	615
2023	Fevereiro	620
2023	Março	625
2023	Abril	630
2023	Maio	635
2023	Junho	640
2023	Julho	645
2023	Agosto	650
2023	Setembro	655
2023	Outubro	660
2023	Novembro	665
2023	Dezembro	670

Logo depois de uma análise estatística descritivas com a utilização do Software Minitab sobre o aumento do consumo por milhões de litros do biodiesel no Brasil, fornecido pelo site da ANP (Agência Nacional do Petróleo, Gás Natural e Biocombustíveis) obteve-se o resultado na tabela... com a análise foi possível identificar a Média, a Ep Média, Desvio Padrão, Mínimo, Q1, Mediana, Q3 e Máximo.

Tabela 2: A*presenta as estatísticas descritivas para conjuntos de dados no estudo*.

Estatísticas

Variável	Ano	N	N*	Média	EP Média	DesvPad	Mínimo	Q1	Mediana	Q3	Máximo
milhões de litros	2022	12	0	552,5	11,6206	40,2549	480	522,5	555	587,5	610
	2023	12	0	642,5	5,20416	18,0278	615	626,25	642,5	658,75	670

Com os dados, pode-se perceber que a média entre os anos de 2022 e 2023 do consumo de biodiesel por milhos de litros apresentam diferença.

Para determinar o teste de normalidade foi utilizado Kolmogorov-Smirnov para obter o valor-p, considerando que as ocorrências não ultrapassaram 50 observações. Para tanto, estabeleceu-se um teste de hipótese para testar a normalidade dos dados p

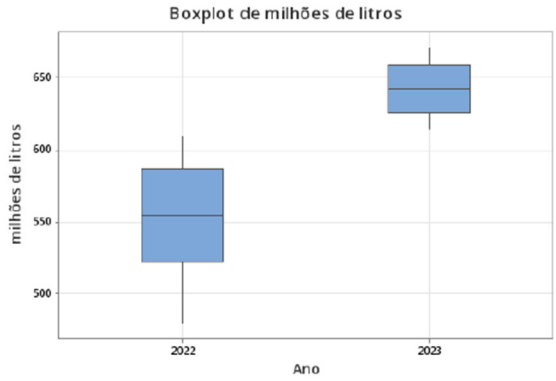


Grafico 1: *BoxPlot das amostras consideradas.*

Para verificar se as amostras tinham a distribuição normal foi realizado o Teste de Normalidade.

Significância = 5%
Teste de hipótese
H0: Os dados apresentam distribuição normal
H1: Os dados não apresentam distribuição normal

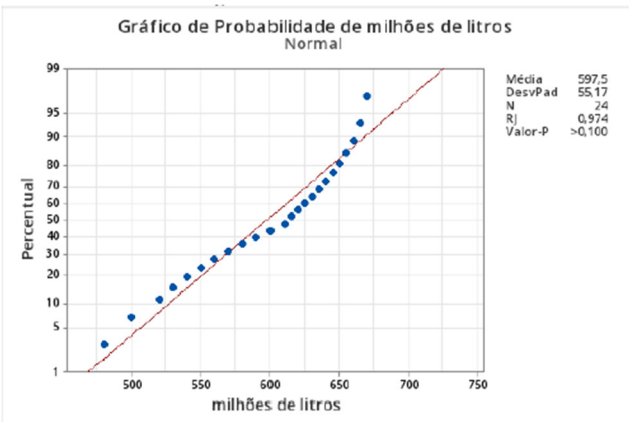


Grafico 2: *Teste de Normalidade*

Pelo método de Shapiro-Wilk, como p-value > 0,100 é superior ao nível de significância estabelecido de 5% (= 0,05) então aceita-se a Hipótese Nula de que os dados possuem distribuição normal.

Pelo Teste não paramétrico Mann-

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Whitney, como p-value = 0,000 é inferior ao nível de significância estabelecido de 5% (= 0,05), então aceita-se a hipótese alternativa de que existe diferença significativa entre as médias.

Tabela 5: *Teste não paramétrico*

Teste

Hipótese nula H_0: $\eta_1 - \eta_2 = 0$
Hipótese alternativa H_1: $\eta_1 - \eta_2 \neq 0$

Método	Valor W	Valor-p
Não ajustado para empates	300,00	0,000
Ajustado para empates	300,00	0,000

4. CONCLUSÕES

A análise acima mostra um aumento significativo no consumo de biodiesel no Brasil em 2023. Como tal crescimento é essencial para a promoção de práticas mais sustentáveis no contexto energético, auxiliando na redução das emissões de gases de efeito estufa e na diversificação da matriz energética do Brasil. Por outro lado, ambientes virtuais imersivos surgem como uma ferramenta vital para a disseminação de boas práticas no que tange aos biocombustíveis.

Por meio de simulações práticas, aprendizado interativo e modelagem de cenários, essas tecnologias promovem uma educação mais eficaz e um treinamento mais seguro, além de aumentar e se cria novas ideias e ajuda na consciência ambiental. Se amplamente adotados, tais recursos terão a capacidade de impulsionar a transição para um futuro mais sustentável e eficiente no consumo de biocombustíveis.

5. DECLARAÇÕES

5.1. Agradecimentos

Os autores agradecem a Universidade de Vassouras pela disponibilidade de aprendizagem. Agradecem ao Programa de Mestrado Profissional em Ciências Ambientais pelo apoio e incentivo à pesquisa. E agradecem a FAPERJ pela ajuda da bolsa técnica ao autor principal.

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Southern Science Conference, 2024.

STATISTICAL ANALYSIS OF THE GROWTH IN BIODIESEL CONSUMPTION IN BRAZIL IN THE YEARS 2022 AND 2023 AND HOW THE ROLE OF AN IMMERSIVE VIRTUAL ENVIRONMENT CAN ASSIST IN THE GOOD PRACTICES OF THIS BIOFUEL.

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November/2024

INTRODUÇÃO

- Criado em 1853 por Patrick Duffy, Irlanda.
- Utilização reconhecida durante a Segunda Guerra Mundial (1941-1945) devido à escassez de petróleo.
- Programa de biodiesel visa promover desenvolvimento regional e sustentabilidade ambiental.
- Aumento na produção e consumo em 2022 e 2023.
- Enfoque em redução de emissões de gases de efeito estufa e promoção da segurança energética.
- Metaverso como ferramenta para disseminar boas práticas e promover a educação sobre biocombustíveis.

INTRODUÇÃO

- Abordagem interativa e imersiva.
- Desenvolvimento de novas tecnologias e práticas de produção de forma sustentável.

OBJETIVO

Este trabalho tem como objetivo realizar uma simulação interativa do processo de produção da planta do biodiesel. Este presente artigo foi organizado em três etapas distintas: pesquisa bibliográfica e revisão da literatura; coleta e análise dos dados direcionados usando a ferramenta Minitab.

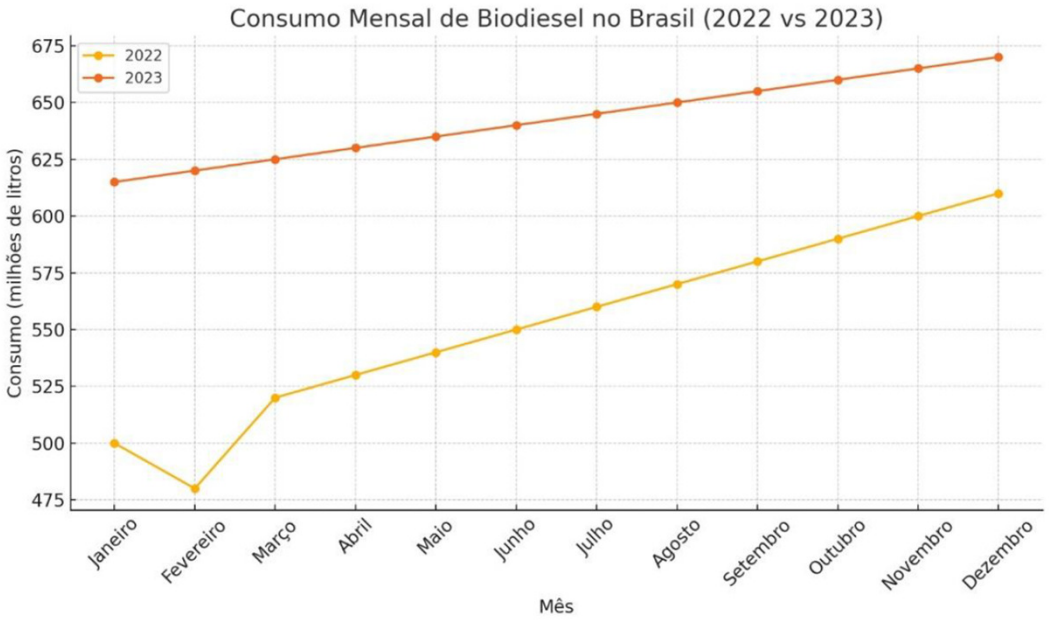
METODOLOGIA

- Foi realizado uma pesquisa no site do Gov (Agência Nacional do Petróleo, Gás Natural e Biocombustíveis) para a realização dos dados
- Dados entre 01/01/2022 até 01/01/2023
- Foi ultilizado a ferramente Minitab versão 20.0

RESULTADOS E DISCUSSÕES

- Os dados fornecidos pelo site da ANP (Agência Nacional do Petróleo, Gás Natural e Biocombustíveis) referente ao consumo de milhões de litro de biodiesel no ano de 2022 e 2023.

Ano	Mês	Consumo de biodiesel milhões/Litros
2022	Janeiro	500
2022	Fevereiro	480
2022	Março	520
2022	Abril	530
2022	Maio	540
2022	Junho	550
2022	Julho	560
2022	Agosto	570
2022	Setembro	580
2022	Outubro	590
2022	Novembro	600
2022	Dezembro	610
2023	Janeiro	615
2023	Fevereiro	620
2023	Março	625
2023	Abril	630
2023	Maio	635
2023	Junho	640
2023	Julho	645
2023	Agosto	650
2023	Setembro	655
2023	Outubro	660
2023	Novembro	665
2023	Dezembro	670



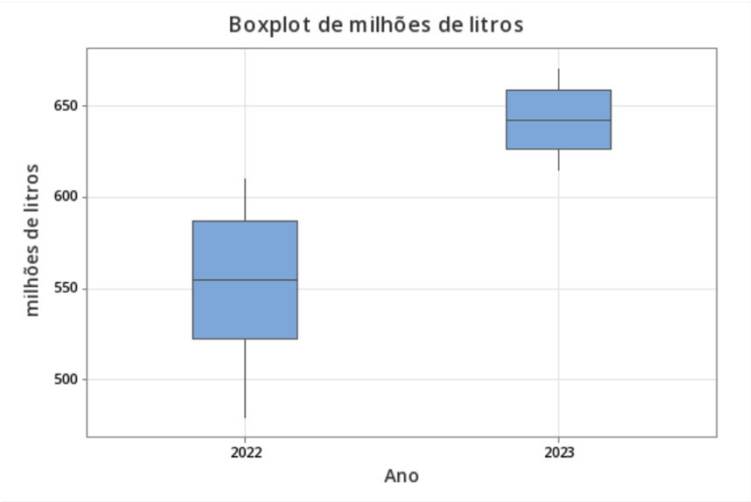
RESULTADOS E DISCUSSÕES

- Com os dados, pode-se perceber que a média entre os anos de 2022 e 2023 do consumo de biodiesel por milhos de litros apresentam diferença.

Estatísticas

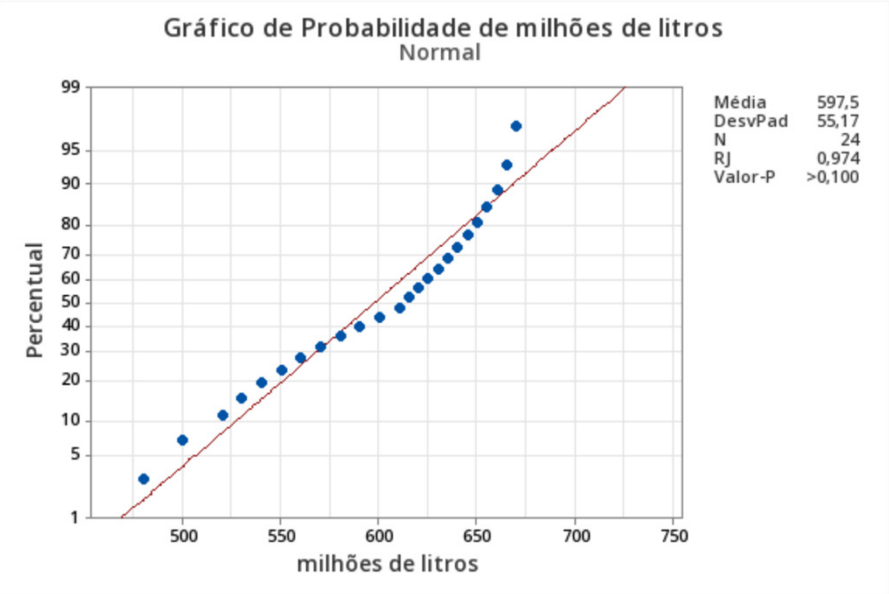
Variável	Ano	N	N*	Média	EP Média	DesvPad	Mínimo	Q1	Mediana	Q3	Máximo
milhões de litros	2022	12	0	552,5	11,6206	40,2549	480	522,5	555	587,5	610
	2023	12	0	642,5	5,20416	18,0278	615	626,25	642,5	658,75	670

- Para determinar o teste de normalidade foi utilizado Kolmogorov-Smirnov para obter o valor-p, considerando que as ocorrências não ultrapassaram 50 observações. Para tanto, estabeleceu-se um teste de hipótese para testar a normalidade dos dados



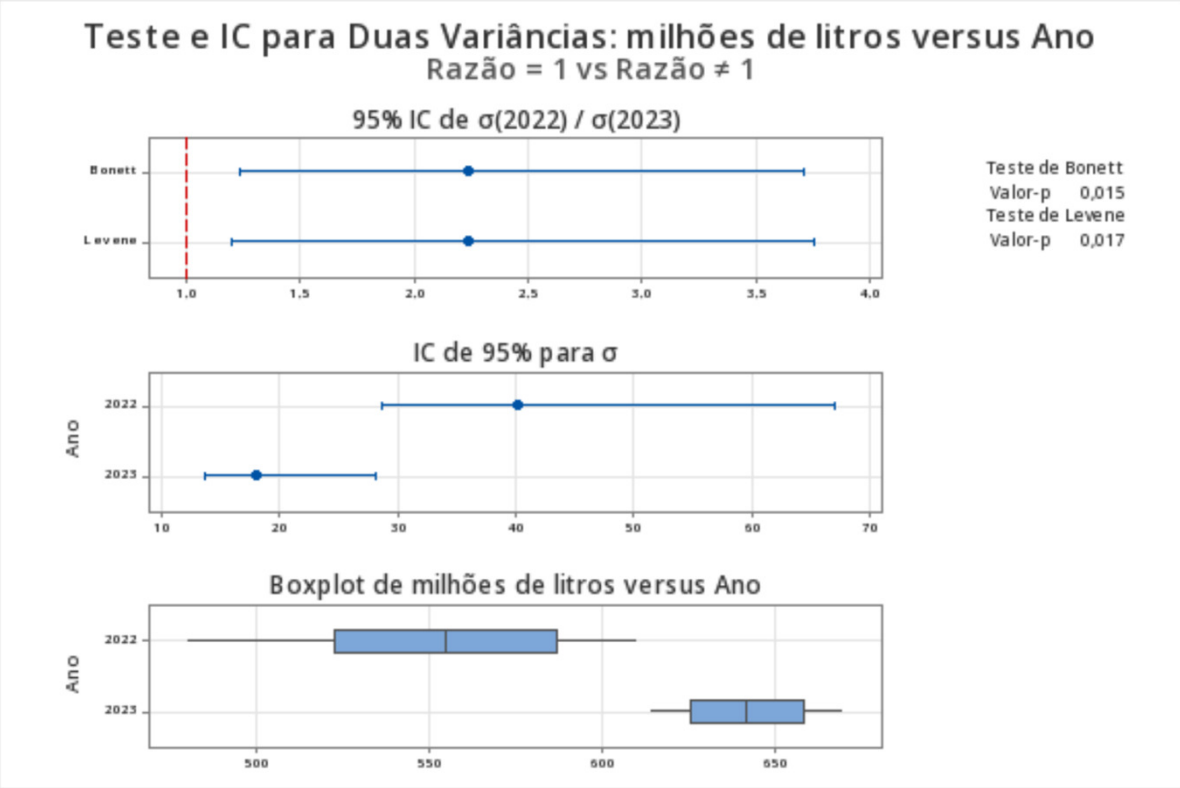
RESULTADOS E DISCUSSÕES

- Pelo método de Shapiro-Wilk, como p-value > 0,100 é superior ao nível de significância estabelecido de 5% (= 0,05) então aceita-se a Hipótese Nula de que os dados possuem distribuição normal.
- Significância = 5%
- Teste de hipótese
- H0: Os dados apresentam distribuição normal
- H1: Os dados não apresentam distribuição normal



RESULTADOS E DISCUSSÕES

- Pelo teste de Levene, como p-value = 0,017 e com Bonett 0,015 é inferior ao nível de significância estabelecido de 5% (= 0,05), então aceita-se a hipótese alternativa de que os grupos não possuem igualdade de variâncias, ou seja, são Heterocedástico



RESULTADOS E DISCUSSÕES

- Pelo Teste não paramétrico Mann-Whitney, como p-value = 0,000 é inferior ao nível de significância estabelecido de 5% (= 0,05), então aceita-se a hipótese alternativa de que existe diferença significativa entre as médias.

Teste

Hipótese nula	$H_0: \eta_1 - \eta_2 = 0$
Hipótese alternativa	$H_1: \eta_1 - \eta_2 \neq 0$

Método	Valor W	Valor-p
Não ajustado para empates	300,00	0,000
Ajustado para empates	300,00	0,000

CONCLUSÕES

- Aumento significativo no consumo de biodiesel no Brasil.
- Contribuição para a promoção de práticas sustentáveis no setor energético.
- Auxílio na redução das emissões de gases de efeito estufa.
- Diversificação da matriz energética do Brasil.
- Estímulo à criação de novas ideias e aumento da consciência ambiental.
- Potencial de impulsionar a transição para um futuro mais sustentável e eficiente no consumo de biocombustíveis se amplamente adotadas.

AGRADECIMENTOS

- A Universidade de Vassouras
- A FAPERJ por me apoiar com um incentivo a bolsa de estudos
- O Programa de Mestrado Profissional em Ciências Ambientais

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PUBLIC POLICIES FOR SUSTAINABLE PROCUREMENT: EVALUATION AND IMPROVEMENT PROPOSALS IN THE CAFÉ'S VALEY REGION, A CASE STUDY IN THE MUNICIPALITY OF VASSOURAS, RIO DE JANEIRO, BRAZIL

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[1,2] Universidade de Vassouras, Pró-Reitoria de Pós-Graduação e Capacitação Profissional, Programa de Mestrado Profissional em Ciências Ambientais

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ABSTRACT

Sustainability has emerged as a critical global agenda, particularly in public procurement, where it significantly influences market trends and sustainable practices. The objects of this study are the public policies for sustainable public acquisition in the Vale do Café region. A case study methodology was employed to analyze the municipality of Vassouras, Rio de Janeiro, Brazil. It evaluates the impact of current sustainable procurement policies and highlights the main challenges to their implementation. The research also proposes improvements, including to draft and propose a normative instruction and a digital tool to guide stakeholders. In line with the Sustainable Development Goals (SDGs), the study underscores the importance of sustainability in fostering economic growth, responsible consumption, and climate action.
.

Keywords*: Environmental Policy; Public Administration; Sustainable Development Goals*.

1. INTRODUCTION

In recent years, the concern for sustainable development has become a central focus in global politics. Balancing economic growth with environmental preservation and social well-being is now imperative for governments and international organizations. Sustainable public procurement (SPP) serves as a key tool, influencing markets and promoting sustainable practices (UNEP, 2015). The term 'sustainability' gained traction after the 1987 United Nations Conference, and though its definition remains fluid, it is now integral to modern policies.

The focus of this research is the municipality of Vassouras, located in the Vale do Café region, with a strong agricultural tradition, particularly in coffee cultivation. The region faces challenges in integrating sustainable practices into public procurement, given its unique socio-economic and environmental context. This study evaluates existing sustainable procurement policies in Vassouras, identifies implementation challenges, and proposes practical solutions for improvement. It also aims to contribute to several Sustainable Development Goals (SDGs), particularly responsible consumption (SDG 12), climate action (SDG 13), and sustainable cities (SDG 11). The central issue of this research is to understand how public procurement in Vassouras can promote sustainability and what barriers hinder its implementation. This is a critical question due to the transformative potential of public procurement in driving sustainable development.

2. MATERIALS AND METHODS

This research adopts a qualitative approach, combining document analysis and case studies. Primary sources include legislation, municipal procurement reports, and relevant academic literature. Content analysis was conducted on public procurement documents from Vassouras, focusing on tenders from 2019 to 2023.

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Additionally, semi-structured interviews were held with key stakeholders involved in procurement processes, including public officials, contractors, and environmental consultants. This identified both the practical challenges faced by these actors and the policy gaps in promoting sustainable procurement. The analysis followed Bardin's methodology (2011), with thematic categorization and comparative analysis of the collected data. The normative and legislative framework referenced includes Brazil's Constitution (1988), Law 14.133/21 (New Public Procurement Law), and municipal regulations on environmental protection and sustainable procurement. The study also considers the integration of international sustainability standards, such as the United Nations' SDG.

3. RESULTS AND DISCUSSION:

The Brazilian legislative framework for public procurement is comprehensive, particularly with the introduction of Law 14.133/21, which incorporates sustainability as a key principle in procurement. Article 225 of the Brazilian Constitution guarantees the right to an ecologically balanced environment, requiring the state to protect it. Additionally, the National Solid Waste Policy (Law 12.305/10) and the National Policy on Sustainable Procurement (Decree 7.746/12) set guidelines for integrating sustainability into procurement processes.

At the state level, the Constitution of the State of Rio de Janeiro (Article 258) mandates the promotion of environmental preservation and the recovery of natural resources. Vassouras' municipal regulations, such as the Municipal Solid Waste Management Program and the Sustainable Procurement Policy, offer additional guidance, though their practical implementation remains limited.

3.2. Analysis of Sustainable Procurement in Vassouras

The analysis of procurement documents from Vassouras between 2019 and 2023 reveals that although sustainability is acknowledged as a key goal, its implementation remains inconsistent. The table 1 summarizes the inclusion of sustainability clauses in public tenders.

Table 1 - Inclusion of Sustainability Clauses in Public Tenders in Vassouras (2019-2023).

Year	Number of Tenders	Environmental Licensing (%)	Use of Sustainable Materials (%)	Social Responsibility Clauses (%)
2019	66	5%	10%	8%
2020	84	6%	12%	9%
2021	97	7%	15%	10%
2022	286	9%	18%	12%
2023	214	8%	16%	11%

Source: Author's elaboration, 2024.

The table shows that sustainability criteria in public tenders are rarely included, particularly regarding environmental licensing and the use of sustainable materials. Despite the existing legislation, only a small percentage of tenders explicitly incorporate sustainability.

3.3. Challenges and Barriers

The implementation of sustainable procurement in Vassouras faces several key challenges. One significant issue is the lack of awareness and proper training among public officials responsible for procurement processes.

Without adequate knowledge of sustainability principles, they often omit relevant clauses from tenders. Another challenge is resistance from suppliers, many of whom are hesitant to adopt sustainable practices due to perceived higher costs and the complexity of complying with environmental standards.

Furthermore, the lack of effective mechanisms for monitoring and enforcing sustainability clauses weakens their impact. Even when such clauses are included in contracts, enforcement is often insufficient, with limited consequences for non-compliance.

Lastly, economic constraints at the municipal level pose additional barriers, as there is a prevailing belief that sustainable products and services are more expensive, which discourages their adoption.

3.4. Proposed Improvements

To address these challenges, this research proposes several key improvements. First, a formal normative instruction should be developed to standardize the inclusion of sustainability criteria in all public procurement processes in Vassouras, providing clear guidelines for both public officials and suppliers.

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Additionally, a digital tool incorporating artificial intelligence could assist stakeholders by offering step-by-step guidance on how to meet sustainability requirements, simplifying the process for both parties.

Finally, regular training sessions should be organized to enhance the understanding of sustainable procurement among public officials, while workshops could help suppliers transition to more sustainable practices.

To address these challenges, this research proposes the following improvements:

Development of a Normative Instruction

A formal instruction should be developed to standardize the inclusion of sustainability criteria in all public procurement processes in Vassouras. This would provide clear guidelines for public officials and suppliers.

4. CONCLUSIONS:

This study underscores the important role of sustainable public procurement in promoting environmental and economic sustainability in Vassouras. While the legislative framework provides a solid foundation, its practical implementation is hindered by a lack of awareness, supplier resistance, and insufficient monitoring mechanisms. The proposed improvements, such as developing a normative instruction and creating a digital tool, aim to address these issues and integrate sustainability into procurement processes.

By enhancing the capacity of public officials and suppliers, Vassouras can make notable progress toward achieving the SDG, particularly those related to responsible consumption, climate action, and sustainable cities. Future research should focus on developing quantitative measures of sustainability in procurement and exploring the long-term economic benefits of sustainable practices.

5. DECLARATIONS

5.1. Open Access

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Southern Science Conference, 2024.

"PUBLIC POLICIES FOR SUSTAINABLE PROCUREMENT: EVALUATION AND IMPROVEMENT PROPOSALS IN THE CAFÉ'S VALEY REGION, A CASE STUDY IN THE MUNICIPALITY OF VASSOURAS, RIO DE JANEIRO, BRAZIL"

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November/2024

INTRODUCTION

In recent years, the concern for sustainable development has become a central focus in global politics. Balancing economic growth with environmental preservation and social well-being is now imperative for governments and international organizations. Sustainable public procurement (SPP) serves as a key tool, influencing markets and promoting sustainable practices (UNEP, 2015). The term 'sustainability' gained traction after the 1987 United Nations Conference, and though its definition remains fluid, it is now integral to modern policies.

The focus of this research is the municipality of Vassouras, located in the Vale do Café region, with a strong agricultural tradition, particularly in coffee cultivation. The region faces challenges in integrating sustainable practices into public procurement, given its unique socio-economic and environmental context. This study evaluates existing sustainable procurement policies in Vassouras, identifies implementation challenges, and proposes practical solutions for improvement. It also aims to contribute to several Sustainable Development Goals (SDGs), particularly responsible consumption (SDG 12), climate action (SDG 13), and sustainable cities (SDG 11). The central issue of this research is to understand how public procurement in Vassouras can promote sustainability and what barriers hinder its implementation. This is a critical question due to the transformative potential of public procurement in driving sustainable development.

AIM/OBJETIVE/PURPOSE

Evaluate public policies for sustainable bidding in the municipality of Vassouras, which is part of the Vale do Café Region, and propose improvements that can increase the effectiveness of these policies by preparing a draft Normative Instruction for the standardization of work routines and the creation of control procedures, in order to formalize bidding processes with sustainable practices, making the entire process clear, efficient and effective.

METHODOLOGY

This research adopts a qualitative approach, combining document analysis and case studies. Primary sources include legislation, municipal procurement reports, and relevant academic literature. Content analysis was conducted on public procurement documents from Vassouras, focusing on tenders from 2019 to 2023.

Additionally, semi-structured interviews were held with key stakeholders involved in procurement processes, including public officials, contractors, and environmental consultants. This identified both the practical challenges faced by these actors and the policy gaps in promoting sustainable procurement. The analysis followed Bardin's methodology (2011), with thematic categorization and comparative analysis of the collected data. The normative and legislative framework referenced includes Brazil’s Constitution (1988), Law 14.133/21 (New Public Procurement Law), and municipal regulations on environmental protection and sustainable procurement. The study also considers the integration of international sustainability standards, such as the United Nations’ SDG.

RESULTS AND DISCUSSION

The Brazilian legislative framework for public procurement is comprehensive, particularly with the introduction of Law 14.133/21, which incorporates sustainability as a key principle in procurement. Article 225 of the Brazilian Constitution guarantees the right to an ecologically balanced environment, requiring the state to protect it. Additionally, the National Solid Waste Policy (Law 12.305/10) and the National Policy on Sustainable Procurement (Decree 7.746/12) set guidelines for integrating sustainability into procurement processes.

At the state level, the Constitution of the State of Rio de Janeiro (Article 258) mandates the promotion of environmental preservation and the recovery of natural resources. Vassouras' municipal regulations, such as the Municipal Solid Waste Management Program and the Sustainable Procurement Policy, offer additional guidance, though their practical implementation remains limited.

3.2. Analysis of Sustainable Procurement in Vassouras

The analysis of procurement documents from Vassouras between 2019 and 2023 reveals that although sustainability is acknowledged as a key goal, its implementation remains inconsistent. The table 1 summarizes the inclusion of sustainability clauses in public tenders.

Table 1 - Inclusion of Sustainability Clauses in Public Tenders in Vassouras (2019-2023).

Year	Number of Tenders	Environmental Licensing (%)	Use of Sustainable Materials (%)	Social Responsibility Clauses (%)
2019	66	5%	10%	8%
2020	84	6%	12%	9%
2021	97	7%	15%	10%
2022	286	9%	18%	12%
2023	214	8%	16%	11%

Source: Author's elaboration, 2024.

The table shows that sustainability criteria in public tenders are rarely included, particularly regarding environmental licensing and the use of sustainable materials. Despite the existing legislation, only a small percentage of tenders explicitly incorporate sustainability.

3.3. Challenges and Barriers

The implementation of sustainable procurement in Vassouras faces several key challenges. One significant issue is the lack of awareness and proper training among public officials responsible for procurement processes.

Without adequate knowledge of sustainability principles, they often omit relevant clauses from tenders. Another challenge is resistance from suppliers, many of whom are hesitant to adopt sustainable practices due to perceived higher costs and the complexity of complying with environmental standards.

Furthermore, the lack of effective mechanisms for monitoring and enforcing sustainability clauses weakens their impact. Even when such clauses are included in contracts, enforcement is often insufficient, with limited consequences for non-compliance.

Lastly, economic constraints at the municipal level pose additional barriers, as there is a prevailing belief that sustainable products and services are more expensive, which discourages their adoption.

3.4. Proposed Improvements

To address these challenges, this research proposes several key improvements. First, a formal normative instruction should be developed to standardize the inclusion of sustainability criteria in all public procurement processes in Vassouras, providing clear guidelines for both public officials and suppliers.

Additionally, a digital tool incorporating artificial intelligence could assist stakeholders by offering step-by-step guidance on how to meet sustainability requirements, simplifying the process for both parties.

Finally, regular training sessions should be organized to enhance the understanding of sustainable procurement among public officials, while workshops could help suppliers transition to more sustainable practices.

To address these challenges, this research proposes the following improvements:

Development of a Normative Instruction:

A formal instruction should be developed to standardize the inclusion of sustainability criteria in all public procurement processes in Vassouras. This would provide clear guidelines for public officials and suppliers.

CONCLUSIONS

This study underscores the important role of sustainable public procurement in promoting environmental and economic sustainability in Vassouras. While the legislative framework provides a solid foundation, its practical implementation is hindered by a lack of awareness, supplier resistance, and insufficient monitoring mechanisms. The proposed improvements, such as developing a normative instruction and creating a digital tool, aim to address these issues and integrate sustainability into procurement processes.

By enhancing the capacity of public officials and suppliers, Vassouras can make notable progress toward achieving the SDG, particularly those related to responsible consumption, climate action, and sustainable cities. Future research should focus on developing quantitative measures of sustainability in procurement and exploring the long-term economic benefits of sustainable practices.

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ANALYSIS OF USED COOKING OIL COLLECTION IN VASSOURAS - RJ (2021-2023)

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ABSTRACT

Improper disposal of used cooking oil represents a significant environmental challenge, contributing to the pollution of water resources and escalating water treatment costs. The recycling of waste oil aligns with several Sustainable Development Goals (SDGs) articulated in the commitments established by the 2030 Agenda during the United Nations Summit in 2015. The primary objective of this study was to conduct a statistical analysis of waste oil collection in Vassouras, RJ, over the period from 2021 to 2023. The descriptive statistical analysis was performed using the Minitab software to examine the normality of the monthly quantity using the Anderson-Darling method, homogeneity of variances by Levene's test, and comparison of the means of the volume of oil collected by Analysis of Variance (ANOVA). The results obtained indicated a p-value of 0.123 in the Anderson-Darling normality test, a p-value of 0.425 in the Levene test, and a p-value of 0.592 in the ANOVA test. These values suggest that, in the last three years, the collection of residual oil has remained stable, without the presence of extreme patterns or severe asymmetries, presenting minimal monthly variations at a significance level of 5%. On average, 1,012.97 liters/month were collected, equating to approximately 34 mL per inhabitant, a marginal figure when evaluating the total population of the city, which is approximately 34,000 inhabitants. The expansion of the network of voluntary delivery points, the training of environmental agents, and the encouragement of reverse logistics initiatives can also contribute to the increase in the volume collected and the proper disposal of this waste. Additional awareness-raising initiatives by governmental bodies, corporations, and educational institutions be implemented to enhance public awareness and improve the collection of this waste, thereby conserving water resources.

Keywords: *Descriptive Statistics, MINITAB, Sustainability, Environmental Education.*

1. INTRODUCTION

Environmental issues are becoming increasingly relevant, and studies indicate that waste management is one of the greatest challenges for society within the sustainable action agenda. The correct disposal and reuse of waste are of extreme importance for human survival and the mitigation of environmental impacts (Morais, Santos, and Silva, 2024).

The proper reuse of waste oil can generate valuable products, such as biodiesel, paints, varnishes, soap, and animal feed, among others (Kaurav *et al.,* 2024). The production of biodiesel has proven to be a sustainable form of reuse, in addition to adding value to this waste. However, for reuse to be effective, greater attention is needed to collection logistics (Lago and Rocha Jr., 2016).

The proper disposal and reuse of waste oil collaborate with several Sustainable Development Goals (SDGs) described in the commitment made in the 2030 Agenda during the United Nations Summit in 2015 (Morais, Santos, and Silva, 2024). Related goals include poverty eradication, responsible consumption and production, sustainable cities and communities, quality education, clean water and sanitation, life on water and land, affordable and clean energy, and partnerships and means of implementation (Morais, Santos, and Silva, 2024).

Despite advances in environmental

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legislation, such as the National Solid Waste Policy (Law No. 12,305/2010), there is still no national policy specifically aimed at the collection and reuse of residual frying oil in Brazil (Brazil, 2010). In the city of Vassouras - RJ, the Environmental Education Plan (Law No. 30,200/2020) was created to raise awareness among the population about the importance of preserving the environment and reducing pollution from household, commercial, and institutional waste (Vassouras, 2020).

The company analyzed in this article provides collection containers in commercial establishments, public institutions, partner condominiums, cooperatives, and collection at homes in neighborhoods, days, and times previously determined and published on the municipality's social networks (Taveira, 2016).

In descriptive statistics, the Anderson-Darling normality test verifies whether the data follow a normal distribution, a necessary premise for the application of parametric tests. The equality of variances test, such as the Levene test, compares the variances of the groups and returns a p-value, which, if it is greater than the established significance level, indicates that the hypothesis of equality of variances cannot be rejected (Anselmo, 2016; Torman, V. B. L., Coster, R. and Riboldi, J., 2012).

On the other hand, analysis of variance (ANOVA) is a widely used statistical test to determine if there is a significant difference between the means of three or more groups. ANOVA compares the variability between the means of the groups with the variability within each group (Pagotto *et al*., 2021).

The present study aimed to statistically analyze, using the Minitab software, the collection of residual oil in the city of Vassouras - RJ during the years 2021, 2022, and 2023, based on data obtained from the city hall.

2. MATERIALS AND METHODS:

2.1. Materials

For the preparation of this study, data obtained from reports sent by the company responsible for the collection of household waste oil in the city of Vassouras - RJ to the city hall were used, referring to the years 2021, 2022, and 2023.

2.2. Methods

2.2.1. Data Collection and Analysis

The data obtained in the reports were submitted to a descriptive statistical analysis using the Minitab software, a program composed of several basic statistical tools (Anselmo, 2016).

2.2.2. Statistical Analysis

Initially, the Anderson-Darling Normality Test was performed with a significance level α = 5% to verify whether the data followed a normal distribution. Once normality was confirmed, the Equality of Variances Test (α = 5%) was performed to assess homoscedasticity between the groups. Finally, Analysis of Variance (ANOVA) was applied with a significance level of 5% to compare the means of the volume of oil collected between the three years.

The decision was based on the analysis of the p-value obtained, considering a significance level of 5%. In case p-value > α, the null hypothesis (H_0) of equality of the averages of the volume of oil collected between the years 2021, 2022, and 2023 was accepted. Otherwise, H_0 was rejected, and the alternative hypothesis (H_1) that at least one mean differs was accepted.

3. RESULTS AND DISCUSSION:

3.1. Results

Table 1 shows a total of 36,467 liters, on average 1,012.97 liters of residual cooking oil collected by the private company responsible for this service in the city of Vassouras – RJ during the 2021-2023 triennium.

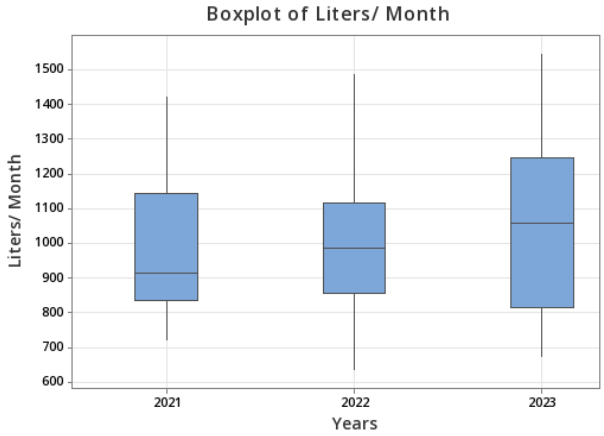
***Table 1**: Residual frying oil collected by the responsible company in the period 2021-2023.*

Month	2021 (L)	2022 (L)	2023 (L)
Jan	840	1,150	1,047
Feb	900	1,027	1,260
Mar	1,150	855	1,210
Apr	1,230	1,485	675
May	725	755	1,072
Jun	930	910	910
Jul	795	640	795
Aug	875	1,145	1,482
Sep	1,420	865	1,190
Oct	980	1,000	878
Nov	1,123	1,015	1,543
Dec	835	975	780
Total	11,803	11,822	12,842
Mean	983.58	985.17	1,070.17

Reference: Authors.

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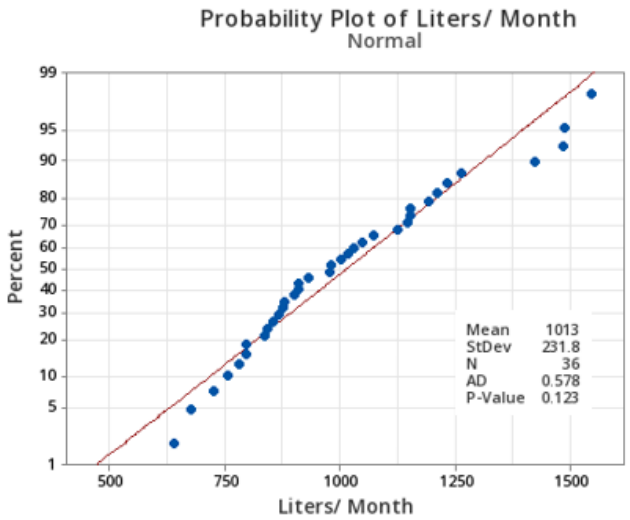
The analysis of the Box Plot graph (Graph 1) indicates that the distribution of residual oil collection in 2023 exhibited greater dispersion in the volumes collected, as evidenced by the higher frequency of extreme values (outliers) and a more pronounced variation in the amount of oil collected across the months of that year. Conversely, the years 2021 and 2022 demonstrated reduced dispersion, suggesting that the monthly volumes recorded were more consistent. Notably, the year 2022 displayed a monthly collection with the smallest deviation relative to the annual average, indicating greater stability in the volumes of oil collected during that period.



***Graph 1**: Monthly variation in the volume of waste oil collected in Vassouras - RJ (2021-2023).*

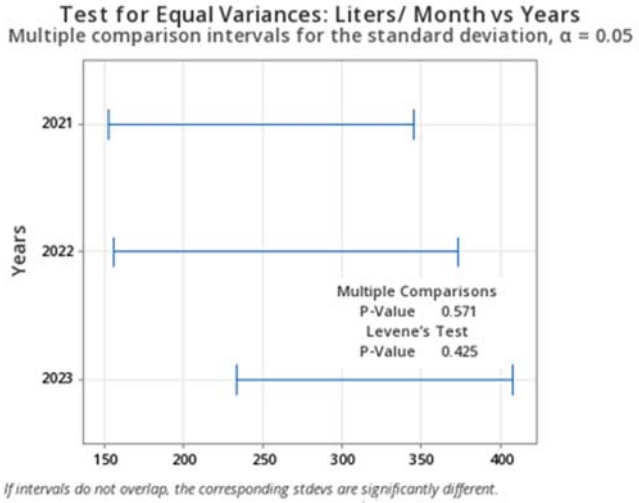
3.1.1. Statistical Analysis

The Anderson-Darling normality test (Graph 2) indicated that the waste oil collection data follow a normal distribution (p-value = 0.123 > α = 0.05), meeting the premise for performing subsequent parametric tests.



***Graph 2**: Anderson-Darling Normality Test.*

The test of equality of variances (Graph 3) showed that the groups are homoscedastic (p-value = 0.425 > α = 0.05); that is, the collection of residual oil in the period analyzed did not present significant variations.



***Graph 3**: Equality of Variances Test.*

Finally, ANOVA (Table 2) revealed that there was no significant difference between the means of the volume of oil collected in the three years analyzed (p-value = 0.592 > α = 0.05). Therefore, the null hypothesis (H_0) that the means are statistically equal is accepted.

Table 2: Analysis of Variance (ANOVA).

Source	DF	SS	MS
Year	2	58897	29448
Error	33	1822078	55214
Total	35	1880975	
F-Value		**P-Value**	
0.53		0.592	

DF: freedom, SS: sum of the square, MS: mean square, F-Value: valor de F, P-Value: Valor de p.

3.2.Discussion

The results obtained demonstrate that, despite the efforts of the private company and the local government, there was no significant increase in the volume of residual cooking oil collected in Vassouras - RJ during the 2021-2023 triennium.

Considering that the city has an estimated population of 34,000 inhabitants (IBGE, 2022), the average monthly volume of 1,012.97 liters corresponds to only 34 mL per inhabitant.

Corroborating with Lago and Rocha Jr

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(2016), the expansion of the network of voluntary delivery points, the training of environmental agents, and the encouragement of reverse logistics initiatives can also contribute to the increase in the volume collected and the proper disposal of this waste.

4. CONCLUSIONS:

The statistical analysis of the collection of residual cooking oil in Vassouras - RJ (2021-2023) revealed that there was no significant increase in the volume collected despite the efforts of the private company and the local government.

The tests indicated that the data followed a normal distribution with equal variances, and ANOVA confirmed that there was no significant difference between the averages of the volume collected in the three years by the company analyzed.

Therefore, the collection of residual oil in Vassouras by the company analyzed did not show significant growth in the period assessed, and greater engagement of all sectors of society is necessary to reverse this scenario, preserve natural resources, and promote the sustainable development of the city.

5. DECLARATIONS

5.1. Acknowledgments

The authors wish to express their gratitude to the private company responsible for collecting waste cooking oil in Vassouras – RJ for the information provided in this study and the University of Vassouras and the University of Mendoza for organizing this enriching event.

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Southern Science Conference, 2024.

ANALYSIS OF USED COOKING OIL COLLECTION IN VASSOURAS - RJ (2021-2023)

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November/2024

INTRODUCTION

- Waste oil is a major environmental challenge ;
- It has high potential for reuse in the manufacture of various products, such as biodiesel, detergents, etc;
- The reuse of waste oil is directly aligned with the Sustainable Development Goals (SDGs) of the 2030 Agenda.





AIM/OBJETIVE/PURPOSE

The present study aimed to statistically analyze, using the Minitab software, the collection of residual oil in the city of Vassouras - RJ during the years 2021, 2022 and 2023.

METHODOLOGY

- **Bibliographic Review;**
- **Data Collection and Analysis** ;
- **Descriptive Statistical Analysis :**
  - **Minitab Software;**
    - **Normality Test** ($\alpha = 5\%$) - Anderson-Darling;
    - **Equality of Variances Test** ($\alpha = 5\%$) - Levene Test;
    - **Analysis of Variance** ($\alpha = 5\%$) - ANOVA.

H_0 = The null hypothesis is accepted.
H_1 = The alternative hypothesis is accepted.

RESULTS AND DISCUSSION

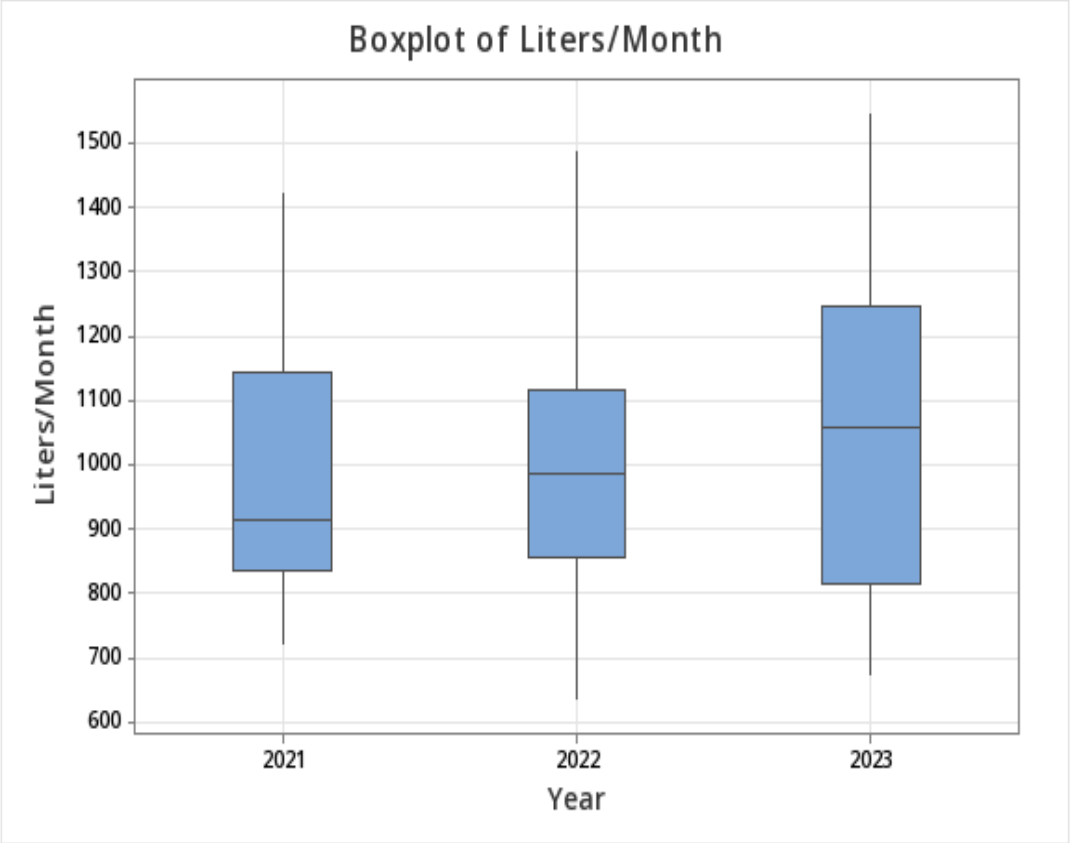
***Table 1**: Quantity of residual frying oil collected by the responsible company in the three year period (2021-2023).*

Month	2021 (L)	2022 (L)	2023 (L)
January	840	1,150	1047
February	900	1,027	1,260
March	1,150	855	1,210
April	1,230	1,485	675
May	725	755	1,072
June	930	910	910
July	795	640	795
August	875	1,145	1,482
September	1420	865	1,190
October	980	1,000	878
November	1,123	1,015	1,543
December	835	975	780
Total	11,803	11,822	12,842

According to the data in Table 1, the private waste oil collection company collected an average of 12,156, totaling 36,467 liters of residual cooking oil in the city of Vassouras – RJ during the 2021-2023 triennium.

RESULTS AND DISCUSSION

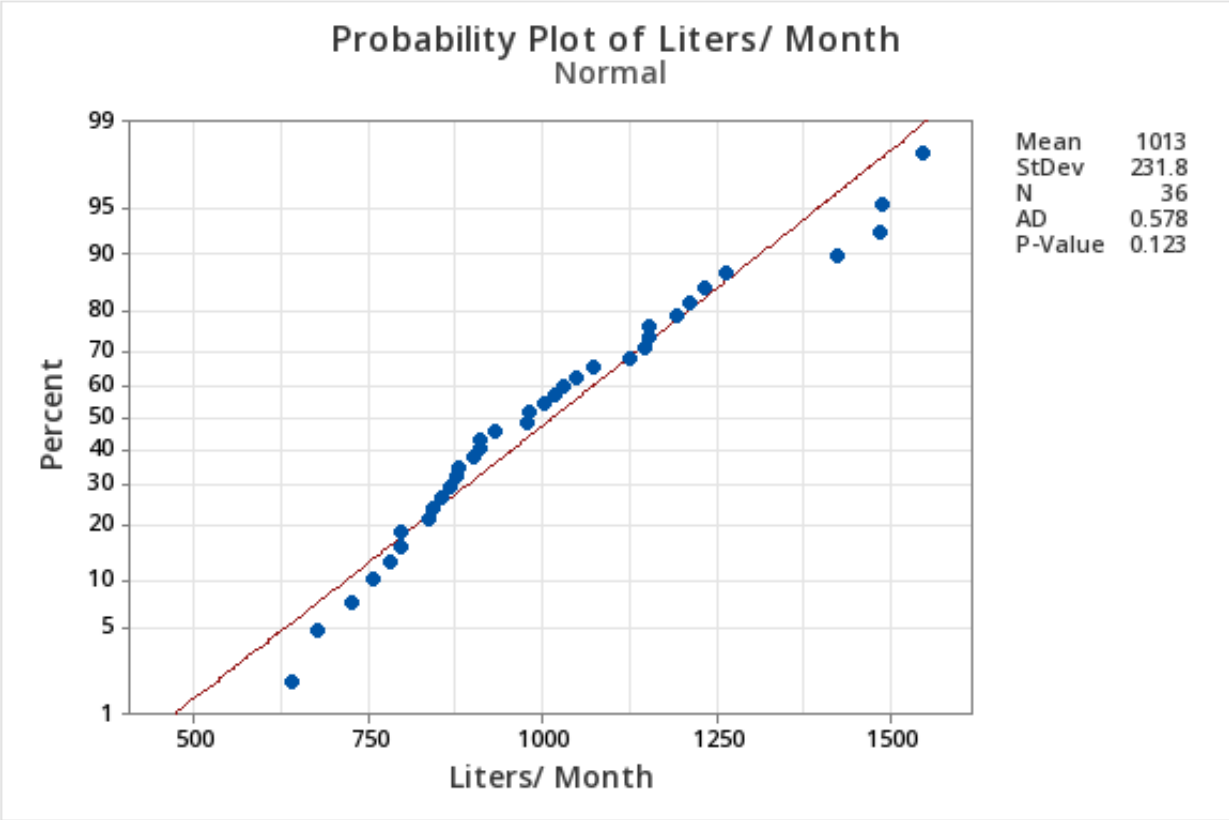
The analysis of the Box Plot graph indicated that the distribution of residual oil collection in 2023 exhibited greater dispersion in the volumes collected, characterized by a higher frequency of extreme values. Conversely, the years 2021 and 2022 demonstrated reduced dispersion, particularly in 2022, which showed greater stability in the volumes of oil collected during this period.



***Graph 1**: Monthly variation in the volume of residual cooking oil collected in Vassouras - RJ (2021-2023).*

RESULTS AND DISCUSSION

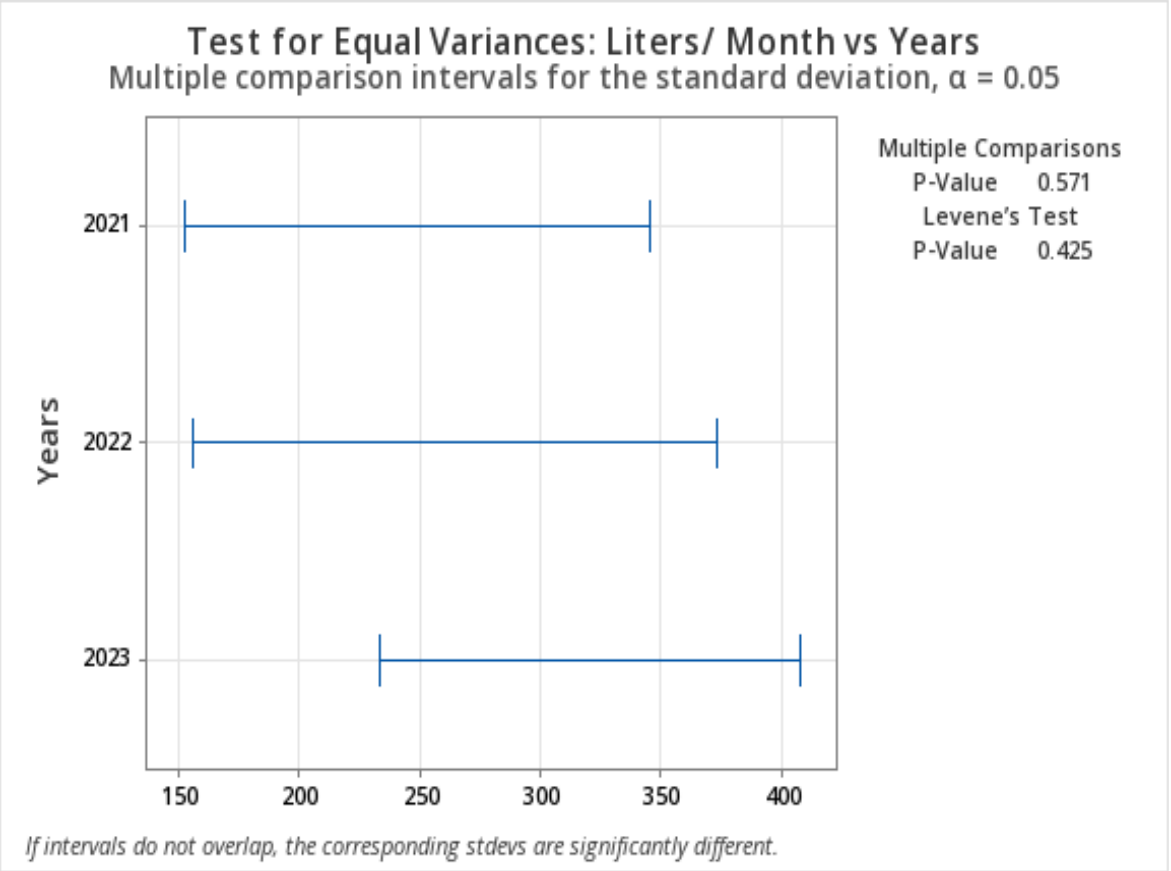
The Anderson-Darling normality test indicated that the data followed a normal distribution (p-value = 0.123 > α = 0.05), meeting the premise for subsequent parametric tests.



Graph 2: Anderson – Darling NormalityTest

RESULTS AND DISCUSSION

The test of equality of variances (Graph 3) showed that the groups are homocedastic (p-value = 0.425 > α = 0.05), that is, they have statistically equal variance.



Graph 3: Equality of Variances Test

RESULTS AND DISCUSSION

Table 2: Analysis of Variance (ANOVA).

Source	DF	SS	MS	F-Value	P-Value
Year	2	58897	29448	0.53	0.592
Error	33	1822078	55214		
Total	35	1880975			

DF: Degree of freedom, SS: sum of the square, MS: mean square, F-Value: valor de F, P-Value: Valor de p.

Finally, ANOVA (Table 2) revealed that there was no significant difference between the means of the volume of oil collected in the three years analyzed (p-value = 0.592 > α = 0.05).

RESULTS AND DISCUSSION

Considering that the city of Vassouras has an estimated population of 34,000 inhabitants (IBGE, 2022), the average monthly volume of 1,012.97 liters corresponds to only 34 mL per inhabitant.

Corroborating with Lago & Rocha Jr (2016), the expansion of the network of voluntary delivery points, the training of environmental agents and the encouragement of reverse logistics initiatives can also contribute to the increase in the volume collected and to the proper disposal of this waste .

CONCLUSIONS

- .The tests indicated that the data followed a normal distribution with equal variances, and ANOVA confirmed that there was no significant difference between the averages of the volume collected in the three years by the company analyzed.

- Therefore, the collection of residual oil in Vassouras, by the company analyzed, did not show significant growth in the period analyzed, and greater engagement of all sectors of society is necessary to reverse this scenario, preserve natural resources and promote the sustainable development of the city.

ACKNOWLEDGEMENTS

- The authors wish to express their gratitude to the private company responsible for collecting waste cooking oil in Vassouras - RJ for the information provided in this study and the University of Vassouras and the University of Mendoza for organizing this enriching event.

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BIOCOMPATIBLE GELATIN/CURCUMIN DRESSINGS FOR POTENTIAL USE IN ANTIMICROBIAL PHOTODYNAMIC THERAPY

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ABSTRACT

Chronic wound infections caused by antibiotic-resistant bacteria have become a significant problem for modern healthcare systems, often associated with high costs and requiring intensive topical wound management. Successful wound healing is achieved by reducing bacterial load and providing an environment conducive to cell growth. Nanofibers demonstrate remarkable success in wound healing due to their structure, which offers a promising platform for drug delivery that can mimic the native extracellular matrix and accelerate cell proliferation. In this study, cytocompatible gelatin plus curcumin nanofibrous membranes were obtained by electrospinning. The combination of these nanofibers with antimicrobial photodynamic therapy, a promising procedure that does not induce antibiotic resistance, aims to enhance the antimicrobial effect through the activation of curcumin. The membranes were crosslinked with glutaraldehyde vapors to improve their stability in aqueous media. The hydrophilicity of the membranes were determined by measuring the water contact angle, and cytotoxicity was evaluated. Smooth and homogeneous nanofibers formed gelatin/curcumin membranes. The addition of curcumin did not decrease membrane hydrophilicity, which exhibited good cytocompatibility to Vero cells. These results demonstrate the potential of gelatin/curcumin nanofibrous membranes as a promising strategy in antimicrobial photodynamic therapy, providing a valuable option for controlling bacterial infections and antibiotic resistance.

Keywords: *Nanofibrous, gelatin, curcumin, antimicrobial photodynamic therapy, electrospinning*

1. INTRODUCTION

Antimicrobial resistance is a major public health problem (Rossolini & Mantengoli, 2008). In 2014, the World Health Organization estimated that, by 2050, deaths related to resistant bacteria will exceed those caused by cancer (WHO, 2021). This increase in resistance is not only a natural biological phenomenon but is also the result of multiple factors, such as overuse of antibiotics, inappropriate prescribing, over-the-counter sales of drugs, and lack of interest by the pharmaceutical industry in developing new treatments.

Therefore, there is an urgent need to study new compounds and find innovative therapeutic strategies (Lazovski et al., 2017). Antimicrobial photodynamic therapy (APDT) has emerged as a promising alternative for the treatment of microbial infections, gaining relevance in different health fields (Pérez-Laguna et al., 2019). In addition to combating antimicrobial resistance, APDT can offer potent antibiotic action by inhibiting a broad spectrum of pathogens, thanks to the production of reactive oxygen species induced by a photochemical reaction (Polat & Kang, 2021).

Curcumin, a natural photosensitizer isolated mainly from the rhizome of turmeric (*Curcuma Longa*), possesses antiviral, anti-inflammatory, antitumor, and antibacterial properties. Its activation with blue light (λ= 405 at 435 nm) makes it an ideal candidate for APDT, although its hydrophobic structure requires modification for effective use in this context

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(Abrahamse & Hamblin, 2017).

Electrospinning is a fabrication technique that uses an electric field to produce nanofibrous membranes with fiber diameters on the nanometer scale and high surface-to-volume ratio (Li et al., 2002). Another advantage of electrospinning is the possibility of dispersing, solubilizing, and releasing bioactive molecules from these nanofibrous membranes. It has been reported that different bioactive molecules can be incorporated into electrospun membranes with maintenance of their bioactivity (Nie et al., 2008). Gelatin (Gel), a versatile polymeric biomaterial, has been widely used in wound dressings and tissue engineering (Figueroa-Lopez et al., 2018; Miguez et al., 2022). Its low cost, non-toxicity, and ease of preparation make it suitable for these types of applications (Topuz & Uyar, 2017).

This work proposes the development and characterization of a new material for use in biomedicine aimed at overcoming the limited efficiency of conventional treatments against antibiotic resistance. It is proposed to obtain a dressing for wound healing formed by nanofibrous membranes composed of Gel and curcumin by electrospinning.

2. MATERIALS AND METHODS

2.1. Materials

All the chemicals obtained from Sigma-Aldrich (Milwaukee, WI) were used without further purification. Solvents (GR grade) from Merck were distilled. The curcumin solution (3.2mM) was obtained from *Curcuma Longa*. Fetal bovine serum, penicillin, and streptomycin were purchased from Gibco.

2.2. Singlet oxygen ($^1O_2$) in solution of DMF

To evidence the production of singlet oxygen ($^1O_2$) by curcumin solution, the indirect method of 9,10-dimethylanthracene (DMA) decay was employed. For this purpose, 2.5 ml of DMF was placed in a quartz cuvette, and 120 µl of DMA was added. 50 µl of curcumin solution 3.2 mM was added, and the spectrum was taken. It was irradiated with an H5 LED (λmax = 460 nm) for 1-minute intervals. The kinetics of the decay was studied by following the decrease in absorbance at 379 nm for DMA. The log (A_0/A_t) was plotted as a function of irradiation time. The value obtained from the slope represents the decay rate constant (k_{obs}) of DMA by the action of $^1O_2$ generated by irradiation of the photosensitizer (Curcumin in DMF solution).

2.3 Electrospun membranes

2.3.1 Preparation

Solutions of Gel and curcumin/Gel in 1:1 acetic acid (20 % v/v):DMF was used for electrospinning. In all cases, the gelatin (30 % w/v) was fully dissolved in acetic acid and yielded a clear solution [10]. Then, solutions of 3.2 mM of curcumin in DMF were added to the gelatin-acetic acid solution. The resulting solutions were loaded into a 5 ml plastic syringe with a 21G gauge stainless steel blunt needle at its tip, which was then connected to a syringe pump. Each solution was delivered at a constant feed rate of 5.0 µl/min, and a high voltage of 15 kV was applied to prepare the GEL and CUR nanofibrous membranes. The electrospun fibers were deposited on a static collector covered with aluminum foil. The distance between the needle and the collector was maintained at 15 cm. electrospinning was carried out at 25 °C and 40 % relative humidity. The resulting electrospun membranes were vacuum-dried for 24 hours to eliminate the remaining solvent. Then, the meshes were removed from the aluminum foil and cut into 1x1 cm^2 squares. Finally, fibrous membranes were crosslinked with glutaraldehyde vapor (GTA, 5 wt.% in H_2O). Then, the crosslinked membranes were placed in a vacuum desiccator for 24 hours to remove any residual GTA.

2.3.2 Characterization

2.3.2.1 Scanning Electron Microscopy

The size and morphology of the nanofiber membranes were analyzed by Scanning Electron Microscopy (SEM, LAMARX, IFEG-FaMAF-UNC). The diameter distribution of the fibers was measured from the micrographs using ImageJ software, with the diameter being measured on 100 fibers chosen at random in each sample.

2.3.2.2 Water contact angle

The hydrophilicity of electrospun membranes was investigated by water contact angle measurement with a homemade contact angle goniometer. A drop of deionized water was dropped on the surface of each nanofibrous membrane, and a video was recorded immediately. The contact angle was measured using the images captured in the video by ImageJ software. Each sample was measured at least three times at different locations for average.

2.3.2.4 Cytotoxicity assay

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To assess the cytocompatibility of the membranes, extracts of them were prepared according to the International Organization for Standardization 10993–part 12-2012 (ISO) (ISO 10993-12, 2012), and the MTT assay was carried out using epithelial Vero cell lines (ISO 10993–5-2009), as we have previously described (Bavaresco et al., 2020)

3. RESULTS AND DISCUSSION

The detection of singlet oxygen was followed by the decay of DMA, which has a high reaction rate and specificity with singlet oxygen. The obtained decay kinetics is shown in Figure 1. The black colored curve shows the absorption spectrum of the employed solution containing DMA and curcumin at time 0, while the other curves correspond to the measurements performed after irradiation intervals of 1-minute. The absorbance values decreased as the irradiation time increased. This graph shows that the curcumin solution irradiated with blue light generates singlet oxygen, determining a decay rate constant (k_{obs}) of curcumin in DMF solution: 2.893 x 10^{-3} M^{-1} s^{-1} (figure inset in Figure 1).

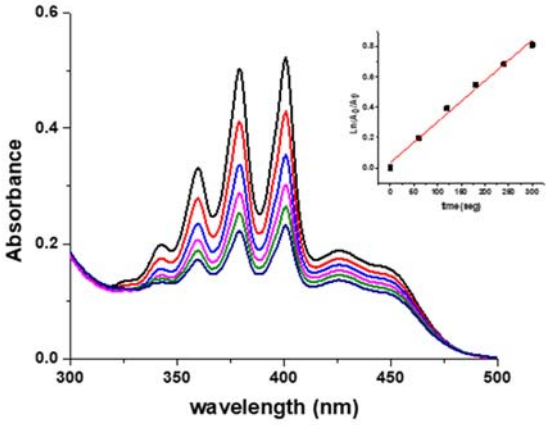


Figure 1. *Decay kinetics of DMA (DMF, 379 nm)*

The morphology of the prepared SEM examined non-crosslinked and crosslinked nanofibrous membranes (Figure 2)

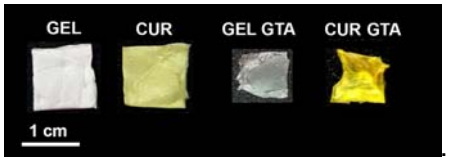


Figure 2. *Macroscopy images of electrospun membranes*

The micrographs show that non-crosslinked membranes had highly uniform and smooth nanofibers without the occurrence of bead defects. While crosslinked, nanofibers were fused together, forming bondings at junctions (Figure. 3A). The diameter distribution of the fibers was measured from the SEM images using ImageJ software. The most frequent fiber diameters were in the range of 90 to 520 nm and 150 to 1150 nm for non-crosslinked GEL and CUR membranes, respectively (Figure 3B). Crosslinked GEL and CUR had fiber diameters in the range: 65 a 610 nm and 110 a 800 nm, respectively. Thus, it can be observed that CUR non-crosslinked and crosslinked membranes have significantly bigger fiber diameters compared to GEL membranes due to the incorporation of curcumin into the GEL nanofibers (Gulsun et al., 2022).

The mass of curcumine incorporated in non-crosslinked CUR was 1.79 ± 0.07 mg curcumin / g CUR membrane.

The hydrophilicity of the GEL and CUR membrane was examined by static water contact angle analysis. As expected, the GEL membrane had a low contact angle: 64.63°, due to the hydrophilicity of gelatin (Tang et al., 2019). The CUR membrane had a water contact angle of 66.79°. A Student's T-test showed no significant differences between the mean fiber diameter of GEL and CUR membranes ($t(4)=1.354$; $p=0.2471$), indicating that curcumin did not decrease the hydrophilicity of the GEL membrane.

Finally, the cytotoxicity of the nanofibrous membranes of GEL and CUR was evaluated *in vitro* by measuring Vero cell viability after incubation with the membrane extracts for 24 hours. This test protocol was used to evaluate the dark toxicity of the membranes (Grinholc et al., 2008). Vero cell viability was greater than 70% in all cases, indicating a lack of extract membrane toxicity to this cell line. According to ISO 10993 (ISO 10993-5, 2009), samples are considered to be non-toxic whenever cell viability is greater than 70%. All groups revealed percentages higher than that of the positive control (phenol solution 0.2%).

4. CONCLUSIONS:

In this study, gelatin plus curcumin membranes for application in antimicrobial photodynamic therapy were developed by electrospinning. The membranes were successfully produced and characterized. All nanofibrous membranes exhibited a smooth surface with homogeneous fiber distribution. The membranes showed a low contact angle, which would give them optimal characteristics as wound dressings. Additionally, cytocompatibility was confirmed by MTT assay in the Vero cell line.

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Overall, the CUR membrane obtained and characterized in this work has a promising use in antimicrobial photodynamic therapy.

5. DECLARATIONS

5.1. Acknowledgments

This work was supported by Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) of Argentina, Secretaría de Ciencia y Tecnología, Universidad Nacional de Córdoba (SECYT-UNC) and Fondo para la Investigación Científica y Tecnológica (FONCYT).

5.2. Open Access

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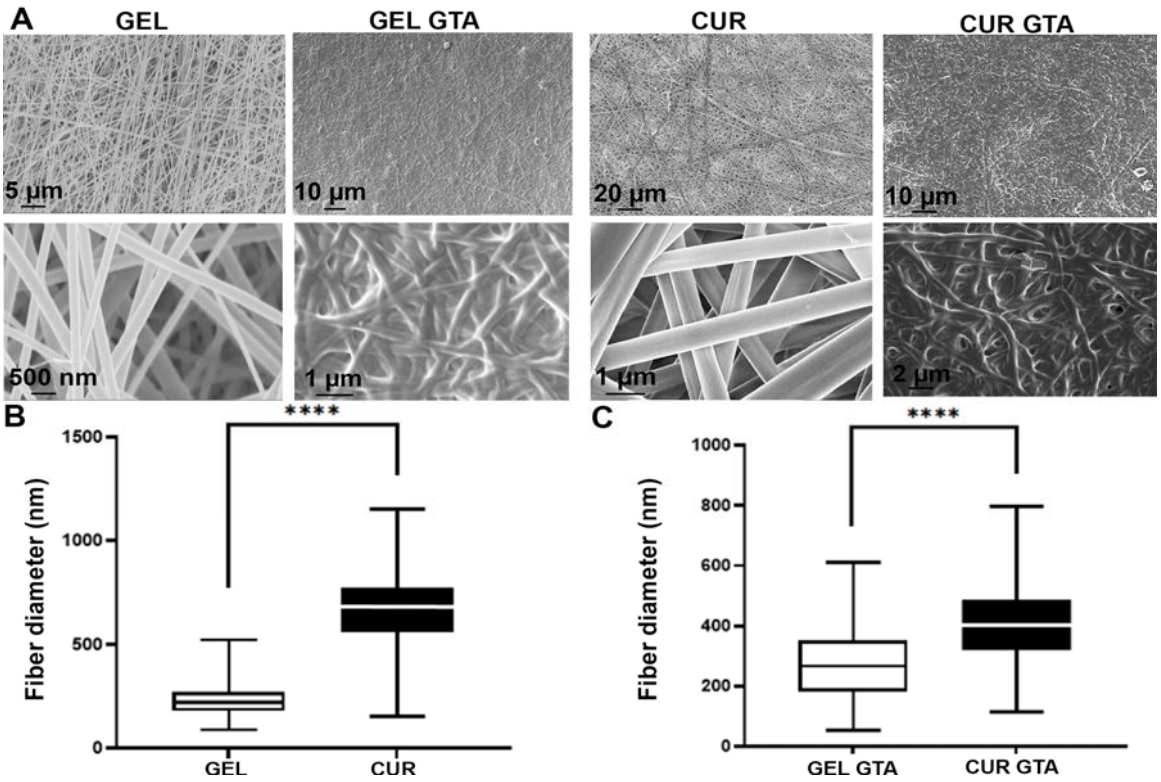


Figure 3. *Representative SEM micrographs of the membrane surfaces (A). Fiber diameter of non-crosslinked membranes (B). Fiber diameter of crosslinked membranes (C). ****p < 0,0001 (Kruskal-Wallis test)*

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BIOCOMPATIBLE GELATIN/CURCUMIN DRESSINGS FOR POTENTIAL USE IN ANTIMICROBIAL PHOTODYNAMIC THERAPY

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November/2024

INTRODUCTION

2024 - Southern Science Conference

* Antimicrobial resistance is a major public health problem [1]. In 2014, the World Health Organization estimated that, by 2050, deaths related to resistant bacteria will exceed those caused by cancer [2].

*** Antimicrobial photodynamic therapy (APDT) has emerged as a promising alternative for the treatment of microbial infections, gaining relevance in different health fields [3].**

* Curcumin, a natural photosensitizer, possesses antiviral, anti-inflammatory, antitumor, and antibacterial properties. Its activation with blue lightmakes it an ideal candidate for APDT.

*** Gelatin (Gel), a versatile polymeric biomaterial, has been widely used in wound dressings and tissue engineering [4,5]. Its low cost, non-toxicity and ease of preparation make it suitable for these types of applications [6].**

PURPOSE

2024 - Southern Science Conference

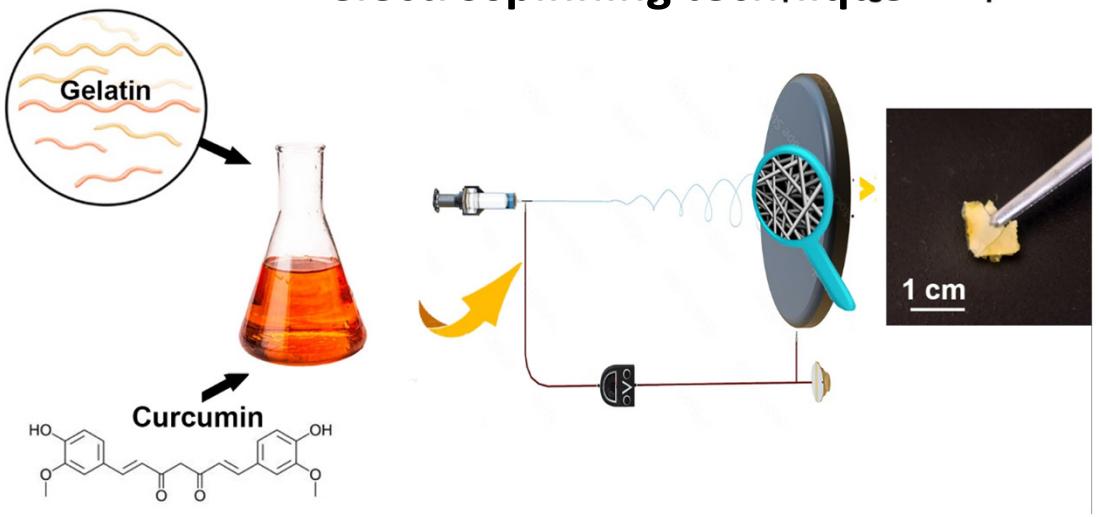
- This work proposes the development and characterization of a new material for use in biomedicine, aimed at overcoming the limited efficiency of conventional treatments against antibiotic resistance.

- **We are proposed to obtain a dressing for wound healing, formed by nanofibrous membranes composed of Gel and curcumin by electrospinning.**

METHODOLOGY

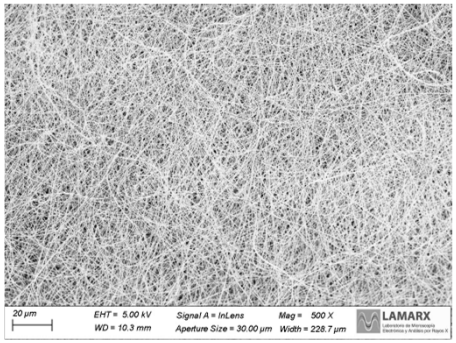
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Curcumin/Gelatin nanofibrous membranes obtained by electrospinning technique

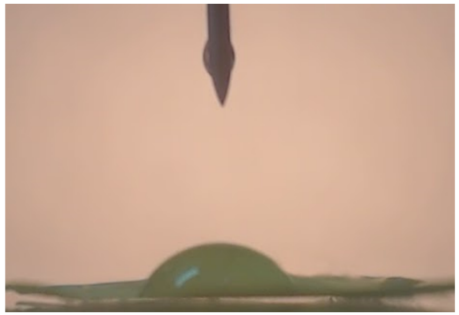


Membranes characterization

SEM analysis



Water contact angle

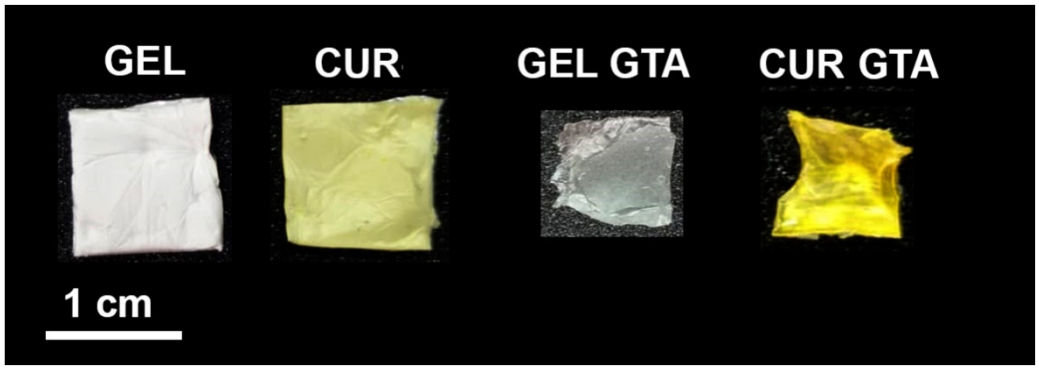


Cytotoxicity assay

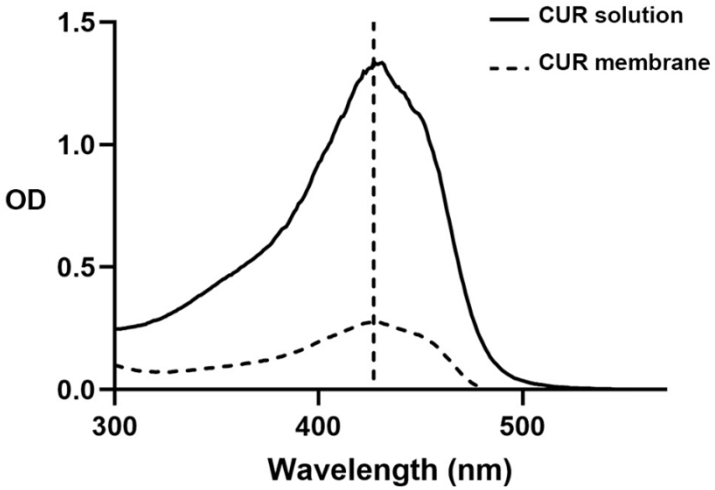


RESULTS AND DISCUSSION

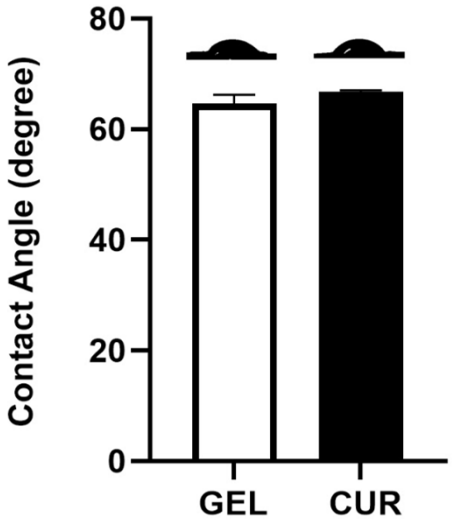
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Macroscopy images of electrospun membranes



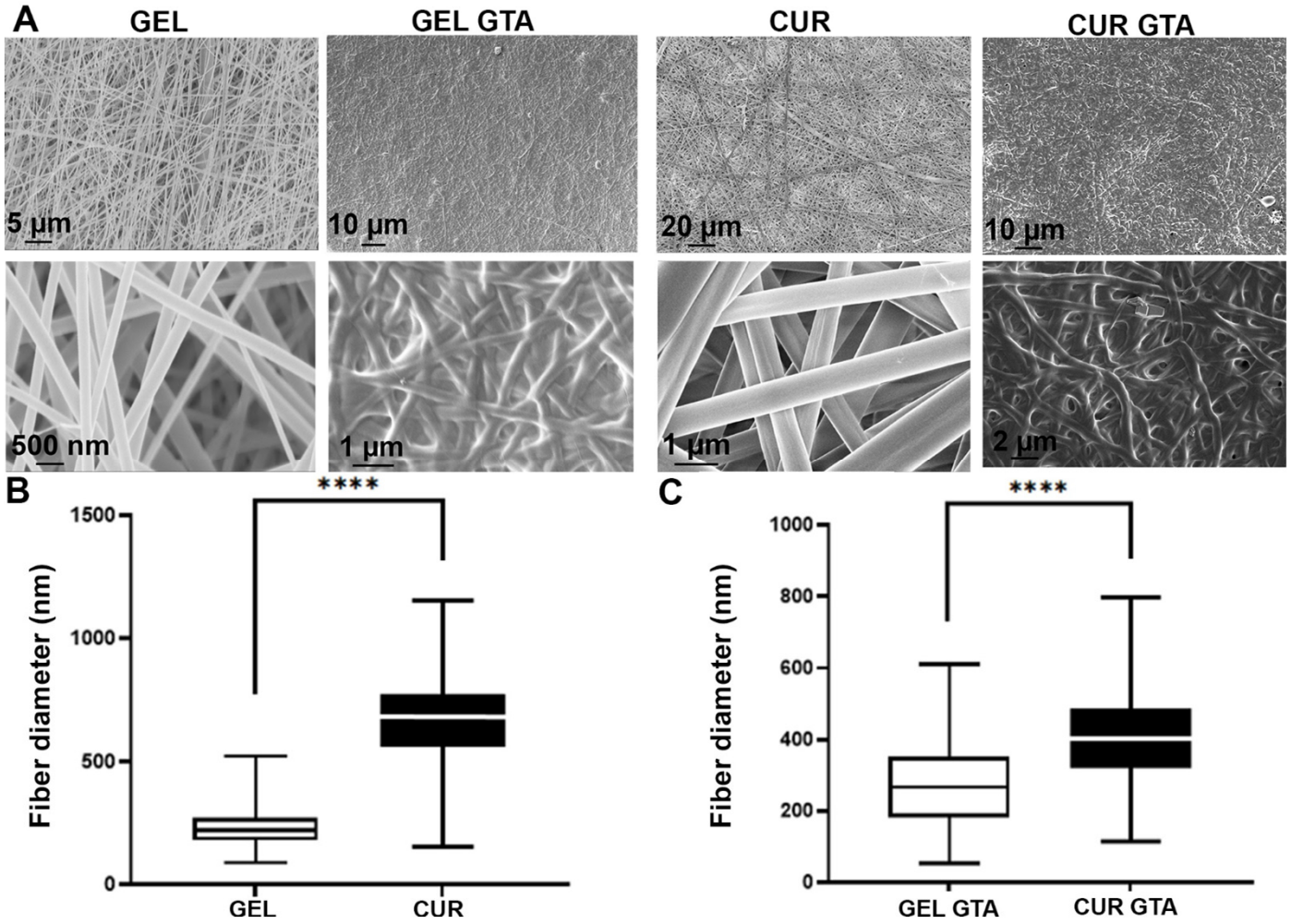
UV-vis in DMF for curcumin solution and for desorption of CUR electrospun membrane in the region of the spectrum between 300 and 500 nm.



Averaged water contact angles. The shapes above the bars are the images captured after the water droplet dripped on the surface of composite fibrous membranes

RESULTS AND DISCUSSION

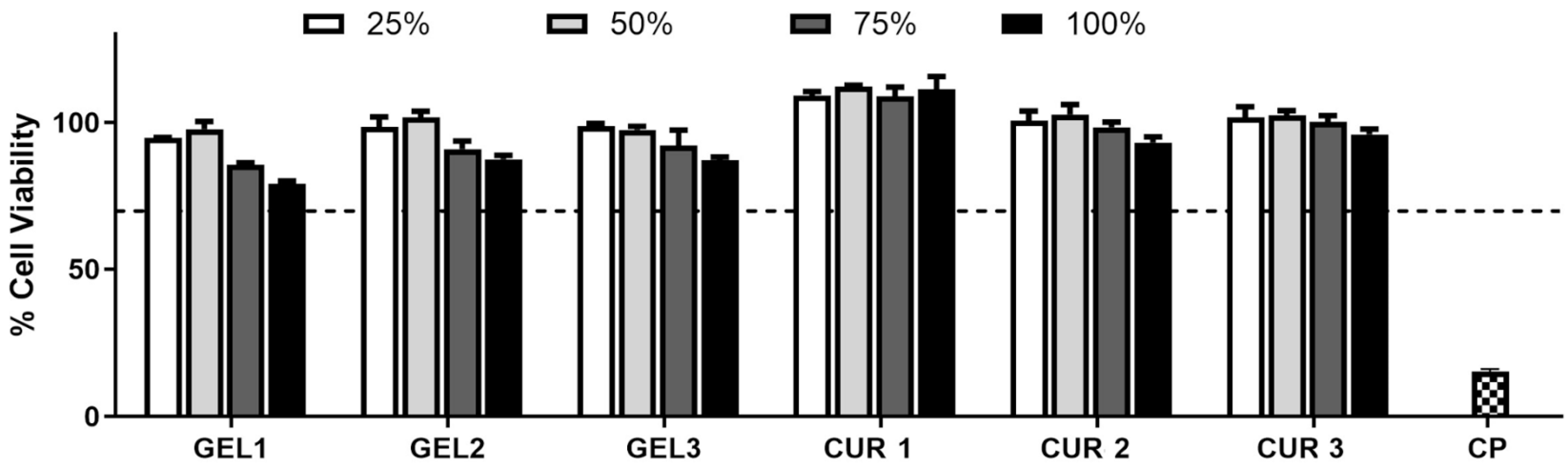
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Representative SEM micrographs of the membrane surfaces (A). Fiber diameter of non-crosslinked membranes (B). Fiber diameter of crosslinked membranes (C). ****p < 0,0001 (Kruskal-Wallis test)

RESULTS AND DISCUSSION

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Vero Cell viability for diluted extracts (25%, 50%, 75% and 100%) from GEL and CUR membranes after cell culture for 24 hours. Vero cell viability was greater than 70% in all cases, indicating a lack of extract membrane toxicity to this cell line (according to ISO 10993)

CONCLUSIONS

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- In this study, gelatin plus curcumin membranes for application in antimicrobial photodynamic therapy were developed by electrospinning. The membranes were successfully produced and characterized.

- All nanofibrous membranes exhibited a smooth surface with homogeneous fiber distribution. The membranes showed a low contact angle, which would give them optimal characteristics as wound dressings.

- Additionally, cytocompatibility was confirmed by MTT assay in the Vero cell line. Overall, the CUR membrane obtained and characterized in this work has a promising use in antimicrobial photodynamic therapy.

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- Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) of Argentina
- Secretaría de Ciencia y Tecnología, Universidad Nacional de Córdoba (SECYT-UNC)
- Fondo para la Investigación Científica y Tecnológica (FONCYT)

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SYSTEMATIC LITERATURE MAPPING ON SOCIO-ENVIRONMENTAL IMPACTS ON FOOD AND NUTRITION SECURITY

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ABSTRACT

Over the last two centuries, the relationship between man and the environment has intensified, resulting in a negative deficit that has been seen to the detriment of our planet. This has led to the high consumption of renewable and non-renewable natural resources, in addition to the impacts generated by population growth and the increased demand for subsistence in societies, which has led to a major imbalance in observed natural phenomena. Studies and reports have shown how climate and environmental changes, directly and indirectly, interfere with production systems, especially food systems, causing the environmental decharacterization of food production sites, forcing them to migrate in search of areas with better environmental and climate quality. Furthermore, it is increasingly observed that environmental changes cause major problems in the nutritional composition of food, impacting the Food and Nutrition Security of several countries and, as a consequence, impacting the health quality of these societies.

Keywords: *Climate Change; Environment; Food and Nutrition Security.*

1. INTRODUCTION

Over the last two centuries, the relationship between humans and the environment has intensified, resulting in a negative deficit for the planet. The Industrial Revolution led to a demographic impact in the 19th century, where the population doubled, and what we saw in the 20th century was that it tripled, reaching 6 billion people in the year 2000. According to the German Foundation for World Population – DSW (2024), it is currently estimated that there are 8 billion people.

Malthus (1798) presented a pessimistic scenario in which the world would not be able to sustain human subsistence.

The Malthusian Theory (Malthus, 1798) predicted that population growth would follow a geometric progression while food production would grow in an arithmetic progression.

Malthus was partly right; the population grew, and there was scarcity. However, he did not account for wars, epidemics, and natural disasters, which balanced things out.

Medical, scientific, and economic advances enabled this exponential population growth and increased human life expectancy, which at the time was around 40 years (Freire, 2022) and is now 73.4 years, according to the Global Data website (2024).

Environmental changes and the impacts generated by population growth and increased demand for subsistence have caused imbalances in natural phenomena, thus altering food production systems.

The planet is changing, and the environment, climate, and natural phenomena are increasingly showing signs of this imbalance, characterized by events such as heatwaves, floods, droughts, erratic seasons, changes in ocean water temperature systems, rising sea levels, and atmospheric pollution. These issues compromise food and nutritional security, directly or indirectly affecting human health.

Jared Diamond (DIAMOND, 2005) (DIAMOND, 2018) describes in his books how societies caused natural changes in the environments where they were located and how they suffered from the impacts of their interactions with the environment, wasting resources and ignoring natural signs when they intervened rapidly and recklessly in the environment.

Some societies found solutions to environmental damage and rapid population growth, managing to prosper to some extent, while others did not heed nature's warnings and collapsed.

New information, still under development, shows that even with technological advancements that maintain balanced food production, the nutritional quality of the food produced is lower than the food produced when the impacts of climate change and environmental damage caused by humanity are still

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DOI: 10.48141/SSCON_29_2024.pdf

minimal (Myers et al., 2014).

Other factors, such as changes in seasonal characteristics, increasingly lead to the need to relocate crops to places never previously considered, which lack the natural conditions for their production. Thus, there is a growing reliance on genetic modification techniques for these developments.

The question that remains is: "Will food have the same nutritional quality as those produced before in places suitable for their cultivation?"

2. MATERIALS AND METHODS

This study was developed in three stages: systematic literature mapping, thorough evaluation of the bibliographies, and the creation of a synthesis in the form of an article.

First, a search for bibliographic content was conducted on Google Scholar and through bibliographic research with professionals in the fields of nutrition, medicine, and engineering.

All bibliographic material was analyzed to verify how humans impact climate characteristics and environmental quality, how these human-induced changes affect food production, the nutritional quality of food, and how this can impact food and nutritional security as well as the health quality of a society.

3. RESULTS AND DISCUSSION:

Using the search engine Google Scholar and the string: "Food Security" AND "Climate Change" AND "Nutritional Quality" AND (Environment OR "Environmental") AND ("food and nutritional security" OR FNS), 196 articles were identified, of which only 94 (47.96%) were archived for having information aligned with the theme of this study.

The 94 (100%) selected articles were fully analyzed, with 34 (36.17%) found to be relevant and compatible with the study's theme. The other 60 (63.83%) articles were discarded.

In addition to Google Scholar, through consultations with professionals in the fields of Nutrition, Engineering, and Medicine, another 21 articles were recommended, of which 10 (42.62%) were aligned with the study's theme, while 11 (52.38%) were discarded for lacking alignment.

The selected articles, theses, dissertations, and books were chosen as the bibliographic basis due to their content corroborating, either entirely or in part, with valuable information on how climate and environmental changes can directly or indirectly affect food production and the nutritional quality of food. Furthermore, they provide insights into how the decline in nutritional quality can impact human health, posing risks to our well-being.

After analyzing the theoretical content of the selected bibliography, it is evident that concerns about the impacts of climate and environmental changes on Food and Nutritional Security have existed since the 1990s. According to Alpino et al. (2022), this concern can be divided into two phases. The first, between 1990 and 2005, is classified as the neutral phase, where it was believed that climate change would neither negatively nor positively impact Food and Nutritional Security, meaning that food production and the impacts of climate change would be balanced out. The second phase, classified as the negative phase, spans from 2005 to the present and marks the beginning of a search for knowledge and understanding of the interfaces between climate change and its effects on food production and quality.

According to Myers et al. (2014), in a study published in the journal Nature, the nutritional content of edible portions from six major staple crops was analyzed. These crops were produced under two conditions: (i) exposed to elevated environmental CO_2 concentrations and (ii) under normal concentration conditions. A reduction in the content of minerals and proteins in the food was observed, thereby compromising their nutritional quality.

This occurs because variations in atmospheric CO_2 concentration can affect the biochemical processes of plants, as plant production capacity is directly linked to CO_2 through photosynthesis, which plays a role in altering nutrient levels. This triggers various health impacts on societies that depend on these crops for critical nutrients.

Below are some crops analyzed by Myers et al. (2014) that showed a reduction of 5-15% in nutrient concentrations:

- Wheat: proteins, zinc, iron, phytate;
- Soybeans: zinc, iron, magnesium, copper, calcium, sulfur, phosphate, and boron;
- Rice: zinc, iron, manganese, copper, calcium, sulfur, phosphate, and proteins;
- Corn: iron, magnesium, potassium, and phosphate.

However, it is not only climate change that

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currently impacts food production and nutritional quality. When we analyze food produced in poor or contaminated soils or when we consider food grown in areas with atmospheric or water pollutants (PASCHOAL et al., 2018), we also observe impacts on both productivity and nutritional quality.

Soil degradation directly affects food production and can also interfere with the nutritional quality of food. Regarding water issues, in addition to the impacts previously mentioned, these foods can become contaminated, and these contaminants, in turn, are absorbed by the human body through ingestion. This list of pollutants includes antibiotics, heavy metals, pesticides, chemical additives, and pathogenic microorganisms.

In Brazil, according to the Ministry of Health, there are more than 250 types of Water and Foodborne Diseases caused by bacteria and their toxins, viruses, parasites, or chemical substances such as lead and pesticides.

Thus, it is necessary to deepen our understanding of how environmental changes affect food production and quality, the consequences for human health, and how we can assist farmers, particularly subsistence farmers, in adapting and preparing to find ways to maintain productivity and nutritional quality in their crops.

It is, therefore, essential to identify the primary foods in the Brazilian diet and understand how environmental impacts alter their nutritional quality, as well as the potential health consequences due to the lack of essential nutrients for the human body.

4. CONCLUSION:

Considering the analyzed bibliography, it is evident that the environmental changes caused by humans and the intensification of Climate Change are significantly affecting food production, not only quantitatively but also in terms of nutritional composition, thereby intensifying food insecurity among populations that are directly and indirectly impacted by negative social and environmental effects.

As this topic is dynamic and new factors continually emerge in the realm of Food and Nutritional Security, often negatively, it is important to continue studies aimed at deepening our understanding of the relationships between the Environment and Food and Nutritional Security, as well as to understand how the impacts on food, especially regarding their nutritional composition, affect human health.

In order to deepen the knowledge of how the nutritional quality of food is affected by environmental changes, a laboratory analysis of the nutritional chemical composition of foods, such as vegetables and legumes, produced in the South Fluminense region of the State of Rio de Janeiro is proposed. This will take place in two scenarios: one near anthropized areas and one in a location with a low index of anthropization. These types of food are indicated as part of a suitable daily diet.

Based on the results, correlations will be made to other food production scenarios to assess impacts on food and nutritional security as well as health.

All knowledge produced from these efforts will serve as a basis for developing a product for the master's thesis, which aims to assist food producers in decision-making regarding the preliminary analyses of production location, crop choices, and exposure to socio-environmental risks in order to produce food with nutritional quality and ensure safety in their production.

5. DECLARATIONS

5.1. Acknowledgments

I thank my wife for encouraging me to continue learning and seeking new knowledge and for her partnership. To my children, the reasons for my life. To my advisor, Prof. Dr. Marco Antônio Pereira Araújo, for sharing his knowledge and encouraging me, and to Vassouras University for providing my development.

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Southern Science Conference, 2024.

Systematic Literature Mapping on Socio-environmental Impacts on Food and Nutrition Security

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Marco Antonio Pereira Araújo
Vassouras University, Master's in Environmental Science, Brazil.

November/2024

SUMMARY

2024 - Southern Science Conference

change by your text

Introduction ---------- 3

Objective ---------- 8

Methodology ---------- 9

Results and Discussion ---------- 11

Conclusions ---------- 13

References ---------- 14

INTRODUCTION

- The relationship between man and the environment and its consequences;
- The relationship between environmental quality and food and nutrition security;
- Increased risk of food insecurity resulting from food unavailability and nutritional insecurity resulting from the low nutritional quality of food;
- Risks associated with low nutritional quality and food contamination.

INTRODUCTION

Over the last two centuries, the relationship between man and the environment has intensified, resulting in a negative deficit unfavorable to the planet.

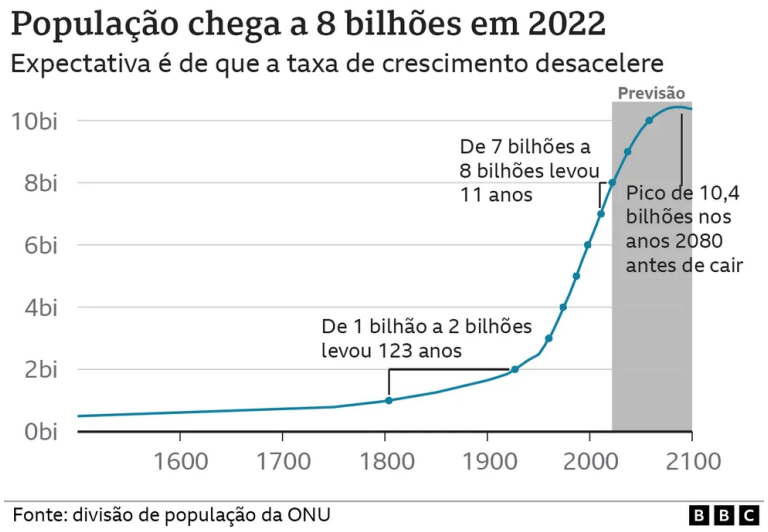


Image 1: Population Growth Chart
https://g1.globo.com/mundo/noticia/2022/11/15/mundo-chega-a-8-bilhoes-de-habitantes-quem-sao-as-criancas-nascidas-no-5o-6o-e-7o-bilhao.ghtml

INTRODUCTION

Malthusian Theory: Population growth occurs in geometric progression (2, 4, 8, 16, 32...), while food production would follow arithmetic progression (2, 4, 6, 8, 10...). Thus, every 25 years, the world population would double.

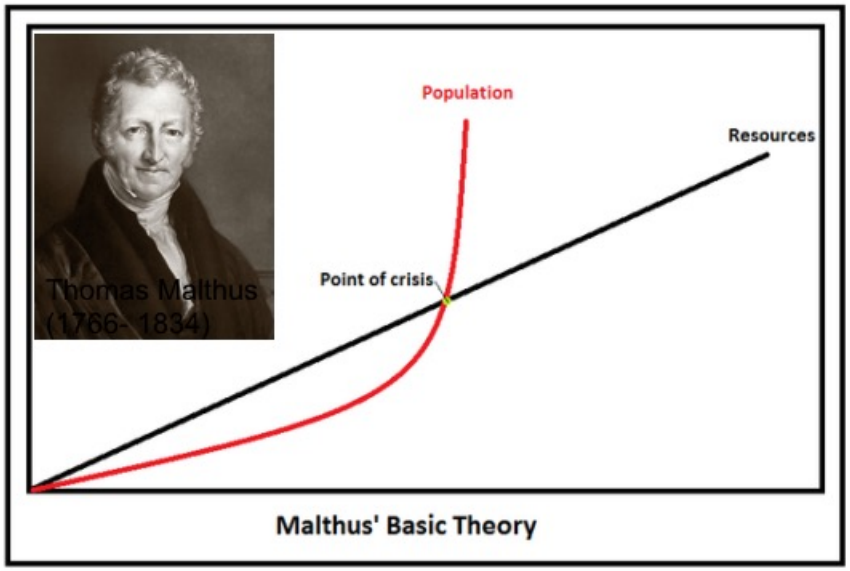


Image 2: Malthus Theory
(https://mun.ca)

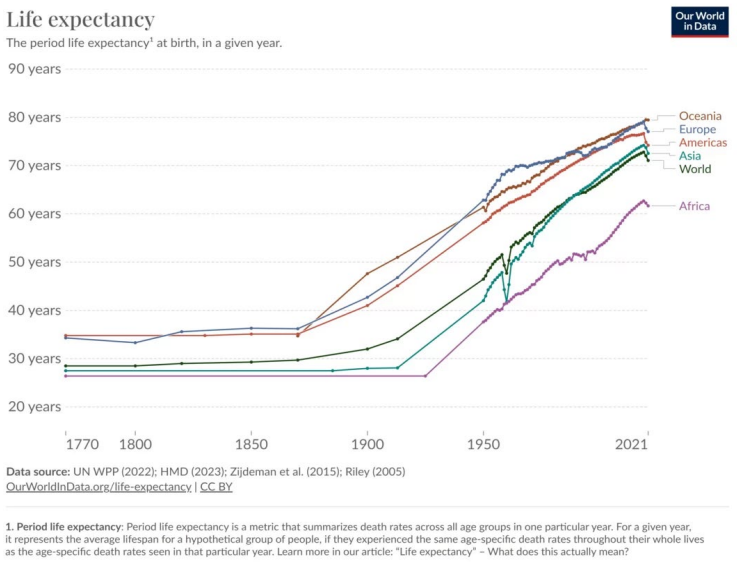


Image 3: Life Expectancy
(https://academiamedica.com.br/blog/longevidade-como-a-expectativa-de-vida-global-se-transformou-desde)

INTRODUCTION

The impacts generated by population growth and the increased demand for the subsistence of societies.



Photo 1: Waterspout – Chopperguy Jerry Fergusun and Pilot Andrew Park

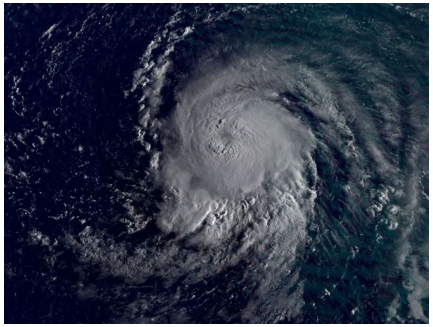


Photo 2: Satellite images show Hurricane Lee in the Atlantic Ocean - CNN



Photo 3: Drought - Gustavo Mansur/ Palacio Piratini (Proj. Colabora)



Photo 4: Flood– Jovem Pan / Créditos: Leo Piva/Agencia Estado

INTRODUCTION

Drought in RS: Over 200,000 producers affected, with losses exceeding R$ 33 billion.



Seca no RS: mais de 200 mil produtores atingidos, e prejuízos acima de R$ 33 bilhões

Estiagem que assola o estado derruba a produção de soja, milho e leite, e deixa propriedades sem acesso à água

Ayrton Centeno
Brasil de Fato | Porto Alegre (RS) | 14 de fevereiro de 2022 às 18:19

Salvar

Noventa e oito mil produtores de milho registram prejuízos, crescimento de quase cinco mil plantadores desde o boletim anterior da Emater/RS, datado de 3 de fevereiro - Reprodução

Photo 5: Drought
https://www.brasildefato.com.br/2022/02/14/seca-no-rs-mais-de-200-mil-produtores-atingidos-e-prejuizos-acima-de-r-33-bilhoes 14/02/2022

Billion-dollar losses in agribusiness: with a strong El Niño and excessive rainfall, damages increase in Southern Brazil.



Prejuízo bilionário no agronegócio: com forte El Niño e chuvas em excesso, danos aumentam no Sul do Brasil

Produtores rurais no Sul do Brasil seguem contabilizando os danos e prejuízos causados pela chuva em excesso. Safra atual já soma cerca de 2 bilhões de reais em prejuízos.

Excesso de chuva no Sul do Brasil continua provocando danos e prejuízos bilionários na agricultura.

Photo 6 : Flood
https://www.tempo.com/noticias/actualidade/prejuizo-bilionario-no-agronegocio-com-forte-el-nino-e-chuvas-em-excesso-danos-aumentam-no-sul-do-brasil.html
25/11/2023

Losses in agriculture caused by the rains in RS have already exceeded R$ 1 billion.



Prejuízos na agropecuária causados pelas chuvas no RS já passam de R$ 1 bilhão

Segundo a Confederação Nacional de Municípios (CNM), R$ 1,1 bilhão é apenas na agricultura. Danos na pecuária chegam a R$ 61 milhões. Dados são parciais, uma vez que nem todos os municípios conseguem contabilizar perdas.

Por g1
10/05/2024 17h47 · Atualizado há 3 semanas

Vista aérea de Porto Alegre (RS) mostra diversas áreas de alagamentos em toda a cidade com destaque para a zona sul, na manhã desta quinta-feira, 2 de Maio de 2024, devido às fortes chuvas ocorridas em todo o Estado, no últimos dias. — Foto: MIGUEL NORONHA/ENQUADRAR/ESTADÃO CONTEÚDO

Photo 7: Flood
https://g1.globo.com/economia/agronegocios/noticia/2024/05/10/prejuizos-na-agropecuaria-causados-pelas-chuvas-no-rs-ja-passam-de-r-1-bilhao.ghtml
10/05/2024

OBJETIVE

Evaluate, through bibliographic data, books, dissertations, theses, and academic articles, how environmental and social changes affect the productivity and nutritional quality of food and how this can impact the food and nutritional security (FNS) of a given society.

METHODOLOGY

This study was developed in 2 (two) stages: systematic mapping of the literature; evaluation and synthesis of the selected articles.

- 1st - Literature mapping (books, theses, dissertations, articles).

- String: **"Food Security" AND "Climate Change" AND "Nutritional Quality" AND (Environment OR "Environmental") AND ("food and nutritional security" OR FNS)**;

- 2nd - Evaluation: 196 articles were identified, of which 94 (47.96%) were analyzed after the final definition of the string. Of the 94 (100%) articles analyzed, 34 (36.17%) are aligned with the theme of this project, and 60 (63.83%) were discarded.

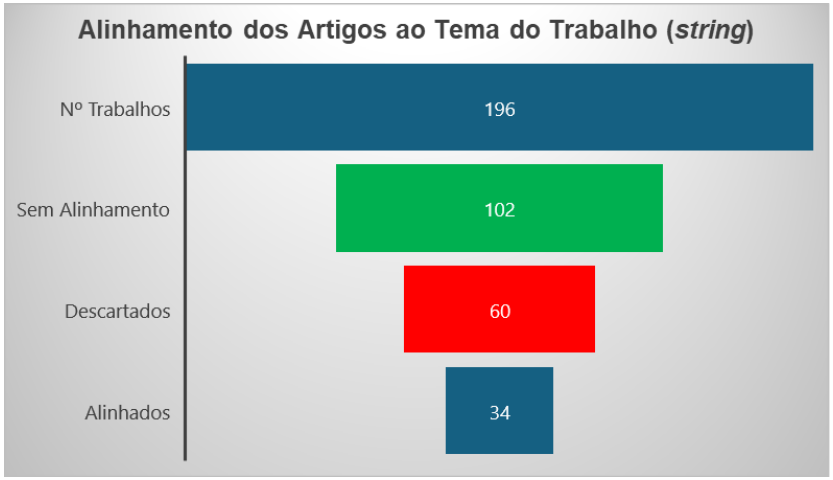


Figure 1: Distribution of work



Figure 2: Number of works analyzed

METHODOLOGY

Other sources of research:

- Conferences with professionals in the fields of Nutrition, Engineering, and Medicine;

- Articles and publications recommended and/or researched on other platforms (Nature, Scielo, etc.): 21 articles, of which 10 (42.62%) are aligned with the theme of the project, and 11 (52.38%) were discarded.

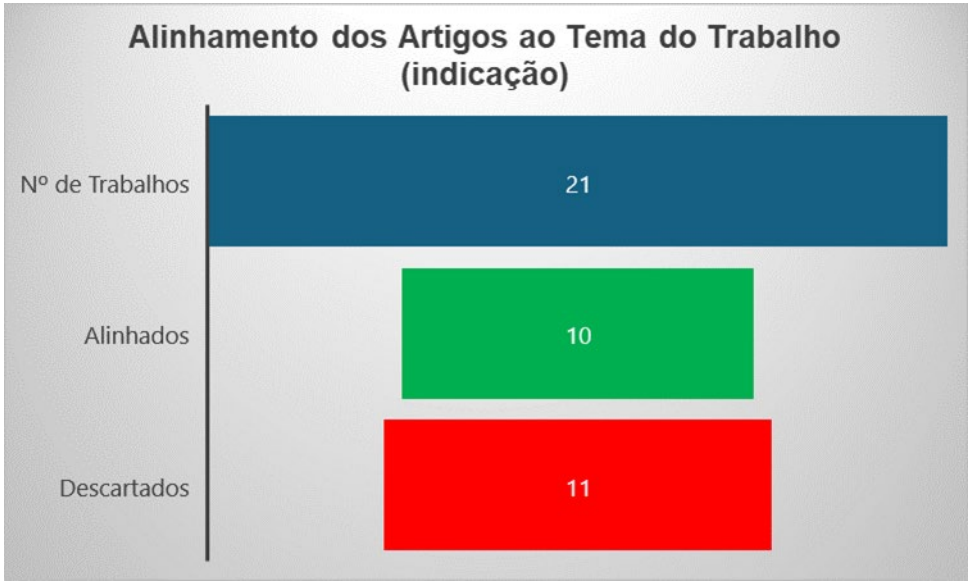


Figure 3: Distribution of received and recommended works

RESULTS AND DISCUSSION

The analyzed literature indicates significant concern regarding the consequences of negative environmental impacts on Food and Nutritional Security (FNS).

- Alpino et al. (2022) divides the concern about environmental impacts into two phases:

✓ The **first phase**, from 1990 to 2005, is classified as the neutral phase;
✓ The **second phase** is classified as the negative phase.

- Myers et al. (2014), in a study published in the journal Nature, showed how the increase in CO2 affects the nutritional composition of major crops, indicating reductions of 5 to 15% in concentrations:

- **Wheat**: proteins, zinc, iron, phytic acid;
- **Soy**: zinc, iron, magnesium, copper, calcium, sulfur, phosphate, and boron;
- **Rice**: zinc, iron, manganese, copper, calcium, sulfur, phosphate, and proteins;
- **Corn**: iron, magnesium, potassium, and phosphate.

RESULTS AND DISCUSSION

- Valéria (PASCHOAL et al., 2018) analyzes that the same effect is expected in crops produced in poor, contaminated soils or in areas with the presence of atmospheric or water pollutants.

In this case, these foods become contaminated and consequently are assimilated by the human body through ingestion. This list of pollutants includes antibiotics, heavy metals, pesticides, and chemical additives.

- How do environmental changes impact food production and quality, and what are the consequences for human health? Additionally, how can we assist producers, particularly subsistence farmers, in adapting and preparing to find ways to produce their crops while maintaining productivity and nutritional quality?

CONCLUSIONS

The analyzed literature demonstrates that environmental changes have significantly affected:

- food production; and
- its nutritional composition.

This intensifies food insecurity for populations directly and indirectly affected by negative social and environmental impacts.

It is important to continue studies aimed at deepening the relationships between the Environment and Food and Nutritional Security while seeking to understand how the impacts on the nutritional composition of food affect the quality of human health. Next steps:

- ✓ Study the composition of foods exposed to anthropization and those not exposed;
- ✓ Study the consequences for human health;
- ✓ Propose solutions

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II SOUTHERN SCIENCE CONFERENCE
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CONCENTRATION-DEPENDENT EFFECTS OF ALLOPREGNANOLONE ON FOLLICULAR MORPHOMETRY IN BOVINE PREANTRAL FOLLICLES

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ABSTRACT

Allopregnanolone (ALLO) is a neurosteroid with potential roles in ovarian function, but its effects on bovine preantral follicles remain unexplored. In this study, we examined the concentration-dependent effects of ALLO on bovine preantral follicles cultured *in vitro* for 24 hours at concentrations ranging from 5 to 1000 nM. Follicular morphometry, including follicle, oocyte, and chromatin diameters, as well as follicular density and degeneration, were evaluated. Primordial follicle density did not exhibit significant alterations, but primary follicle density increased at 100 nM , while secondary follicle density augmented at 50 nM. Degeneration of primordial follicles increased at 100 nM and decreased at 1000 nM. In primary follicles, degeneration was significantly higher at 100 nM, 500 nM, and 1000 nM, whereas secondary follicle degeneration significantly increased at 10 nM. Morphometric analysis showed that primordial follicle diameters were reduced at 5 nM and 500 nM, but increased at 10 nM. Primary follicle diameters significantly decreased at 5 nM and 500 nM and increased at 100, while secondary follicle diameters were reduced at 50 nM, 100 nM , and 500 nM . Oocyte and chromatin diameters also showed significant reductions across different concentrations. These findings provide the first evidence of ALLO's role in modulating the morphometry of bovine preantral follicles, suggesting its potential involvement in bovine reproductive physiology. Further research is needed to elucidate the molecular mechanisms underlying these effects and their implications for reproductive biotechnologies.

Keywords: *Preantral follicles, ovary, bovine, allopregnanolone*

1. INTRODUCTION

Neurosteroids, particularly allopregnanolone (ALLO), are synthesized de novo in the brain and are crucial modulators of a variety of physiological processes, including reproductive functions. These steroids are produced in both the central nervous system and peripheral nervous system, operating independently of conventional steroidogenic organs (Baulieu, 1997; Melcangi et al., 2011). ALLO, an endogenous metabolite of progesterone, is synthesized through a series of enzymatic conversions within astrocytes and oligodendrocytes, highlighting its role as a neuroactive compound (Majewska et al., 1986; Mensah-Nyagan et al., 1999). Literature indicates that ALLO exerts significant effects on ovarian physiology, influencing apoptosis, cell proliferation, and folliculogenesis (Cáceres et al., 2021). However, research com ALLO's impact on bovine preantral follicles remains scarce, despite preatral follicles comprise Around 90% of the total ovarian folicular population and serving as a primary resource of oocytes (Lucci et al., 2002). Although various studies have assessed the morphometric characteristics of preantral follicles

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in different species (Alves et al., 2018), the specific effects of ALLO on the morphology and functionality of bovine preantral follicles have yet to be explored. Considering the physiological effects of ALLO on ovarian tissue, this study aims to analyze the effects of six distinct ALLO concentrations on histological morphometric parameters. We hypothesize that ALLO induces concentration-dependent effects on bovine preantral follicles *in vitro*. Identifying optimal concentrations could enhance follicle activation, growth, and development in bovine ovarian cortex tissue during *in vitro* experiments, contributing to improved follicle development strategies and fertility preservation in cattle.

2. MATERIALS AND METHODS

2.1. Materials

ALLO (Steraloids Inc) was dissolved in methanol. ALLO concentrations (5 nM - 1000 nM) were prepared by diluting in M199 culture medium (Gibco) supplemented with 3 mM glutamine, 2 mM hypoxanthine, 1% BSA, 10 ng/mL insulin, 2.5 mg/mL transferrin, 4 ng/mL selenium, and 50 mg/mL ascorbic acid. Bouin's solution (Biopur Diagnostics), hematoxylin and eosin (Biopack) were used for histological procedures.

2.2. Methods

Ovaries were collected from 8 Bos taurus heifers within 30 minutes of slaughter from a local abattoir. Within 2 hours *post-mortem*, the cortex was dissected into 5x5x1 mm pieces and cultured in supplemented M199 medium for 24 hours in 5% CO2 at 37°C, with twelve fragments per ovary exposed to different ALLO concentrations. The chosen concentrations were based on physiological levels around 5 nM in bovine oviductal fluid (Lamy et al., 2016).

After incubation, the cultured fragments were fixed and embedded in paraffin for histological analysis.

Follicles were recorded under a light microscope, quantified, and classified morphologically as primordial, primary, and secondary. They were further differentiated into (i) normal (spherical follicles with intact theca and oocytes) and (ii) degenerated (pyknotic oocytes, eosinophilic ooplasm, chromatin shrinkage, and detached granulosa cells).

Follicle density and major diameters of follicles, oocytes, and visible chromatin were calculated using Image J software.

Statistical analysis was performed using GraphPad Prism 8, applying the Kruskal-Wallis test for non-parametric data and Dunn's post-hoc test for comparisons with control groups.

Results were presented as mean ± S.E.M.

3. RESULTS AND DISCUSSION:

In this study, ALLO significantly influenced follicular and oocyte diameters as well as follicular densities in bovine ovarian tissue after 24 hours of *in vitro* culture. Primordial follicles showed no significant differences in density. However, primary follicle density increased significantly at 100 nM ($p<0.01$), as well as secondary follicles density at 50 nM ($p<0.01$).

Primordial follicles showed an increased degeneration at 100 nM ($p<0.001$), but it decreased at 1000 nM ($p<0.05$). Primary follicles also exhibited significant degeneration at 100 nM ($p<0.001$), 500 nM, and 1000 nM ($p<0.01$), while secondary follicles had higher degeneration rates at 10 nM ($p<0.01$).

Follicular diameters showed notable changes: primordial follicles decreased at 5 nM ($p<0.001$), increased at 10 nM ($p<0.01$), and decreased again at 500 nM ($p<0.001$). Primary follicles exhibited decreases at 5 nM ($p<0.001$) and 500 nM ($p< 0.001$), while an increase occurred at 100 nM ($p< 0.001$). Secondary follicles also experienced diameter reductions at 50 nM ($p< 0.01$), 100 nM ($p<0.001$), and 500 nM ($p<0.05$).

Oocyte diameters significantly decreased at 5, 10, 50, and 500 nM ($p<0.001$) and 100 nM ($p<0.01$), with similar trends in primary and secondary follicles. Additionally, nuclei diameters were reduced in primordial and primary follicles at several concentrations ($p<0.001$), and secondary follicles nucleus showed a decrease at 5 nM ($p<0.001$). Detailed results are summarized in Table 1.

Early follicular development is regulated by hormonal factors and various local influences. ALLO exhibited significant, concentration-dependent effects on follicular morphometry and density, indicating its potential to influence follicular maturation. While some observed parameters may enhance *in vitro* culture systems, others could adversely affect follicular growth.

The number of primordial follicles in the ovary influences its functionallity and individual fertility (Findlay et al., 2015). Any factor inhibiting primordial follicle formation or transition can reduce the ovarian reserve at birth and impair

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fertility throughout life.

The variability in responses found in this study may be attributed to the types of follicles analyzed and their hormonal microenvironments. Primordial follicles, with flattened pregranulosa cells in a dormant phase, may respond differently due to their inmaturity and lack of receptors. In contrast, primary and secondary follicles, are metabolically active, with effective intercellular communication and a more complex ultrastructure (Kere et al., 2020).

Evaluating morphometric parameters in preantral follicles is crucial, as they represent critical stages in ovarian development. Understanding how ALLO influences these parameters can provide insights for optimizing bovine reproductive efficiency and follicular maturation *in vitro*.

4. CONCLUSIONS:

This study demonstrates that ALLO has distinct effects on bovine ovarian follicles, influencing key aspects of early folliculogenesis that directly impact reproductive efficiency. While certain morphometric changes suggest potential benefits for *in vitro* follicular development, other findings indicate possible negative effects. The variability in response across different follicular stages highlights the need for further research to optimize the use of ALLO in reproductive biotechnologies and better understand its role in supporting or inhibiting follicular maturation.

5. DECLARATIONS

5.1. Acknowledgments

We thank our colleagues, Daniel Alvarez and Analía V. Juan, for providing access to slaughterhouse samples and for their willingness and collaboration. This work was partially supported by grants from Universidad de Mendoza (UUMM2019-00022) and a grant from the National Scientific and Technical Research Council of Argentina (CONICET, PIP N° 11220200100969CO).

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Follicle type	Treatment	Diameters		
Primordial		**Follicular diameter**	**Oocyte diameter**	**Nuclear diameter**
	Control	ns	ns	ns
	5 nM	$p < 0.001$	$p < 0.001$	$p< 0.001$
	10 nM	ns	$p < 0.001$	ns
	50 nM	ns	$p < 0.001$	ns
	100 nM	ns	$p < 0.01$	$p < 0.001$
	500 nM	$p < 0.001$	$p < 0.001$	$p < 0.001$
	1000 nM	ns	ns	ns
Primary		**Follicular diameter**	**Oocyte diameter**	**Nuclear diameter**
	Control	ns	ns	ns
	5 nM	$p < 0.001$	$p < 0.001$	$p < 0.001$
	10 nM	ns	$p < 0.001$	ns
	50 nM	ns	$p < 0.001$	ns
	100 nM	$p < 0.001$	ns	$p < 0.001$
	500 nM	$p < 0.001$	$p < 0.001$	$p < 0.001$
	1000 nM	ns	$p < 0.01$	ns
Secondary		**Follicular diameter**	**Oocyte diameter**	**Nuclear diameter**
	Control	ns	ns	ns
	5 nM	ns	$p < 0.001$	$p < 0.001$
	10 nM	ns	$p < 0.001$	ns
	50 nM	$p < 0.01$	$p < 0.001$	ns
	100 nM	$p < 0.001$	$p < 0.001$	ns
	500 nM	$p < 0.05$	$p < 0.001$	ns
	1000 nM	ns	ns	ns

Table 1. *p*-values for the diameters of primordial, primary, and secondary follicles, as well as oocyte and visible nuclear diameters, after 24 hours of *in vitro* culture with different concentrations of ALLO. Significant differences compared to the control were determined using the Kruskal-Wallis test followed by Dunn's *post hoc* test (ns: not significant).

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CONCENTRATION-DEPENDENT EFFECTS OF ALLOPREGNANOLONE ON FOLLICULAR MORPHOMETRY IN BOVINE PREANTRAL FOLLICLES

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November/2024

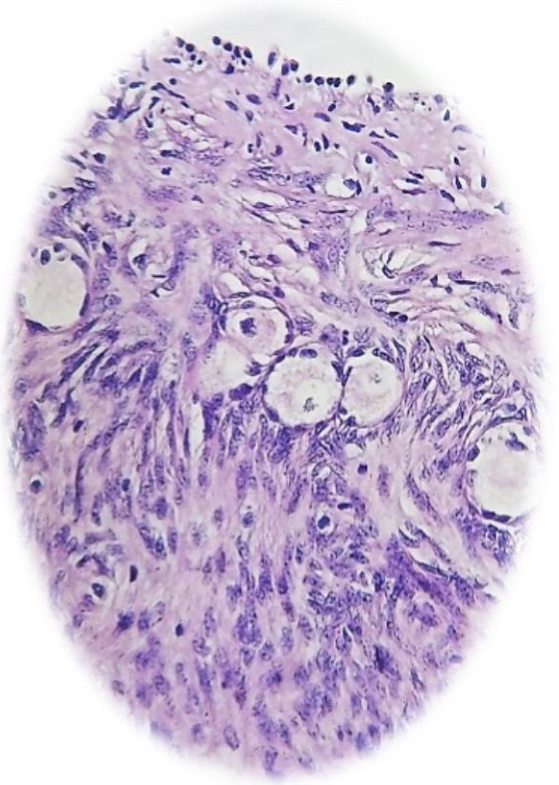
INTRODUCTION

Preantral follicles

This term include primordial, primary, and secondary follicular stages

Preantral follicles comprise about 90% of the ovarian follicle population and are essential for the female ovarian reserve established at birth.

In vitro follicle culture technology allows for the observation of structural and morphometric changes in preantral follicles; it is a biotechnological approach increasingly used to preserve fertility and conserve ovarian tissue.



BACKGROUND

Allopregnanolone (ALLO)

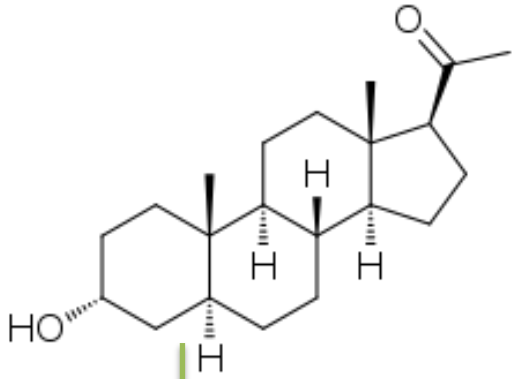
Most active metabolite of Progesterone.

Its concentrations fluctuate under conditions of stress, pregnancy, and during the estrous and menstrual cycles.

Positive allosteric modulator of $GABA_A$ receptor

It acts as a neuromodulator in ovarian physiology

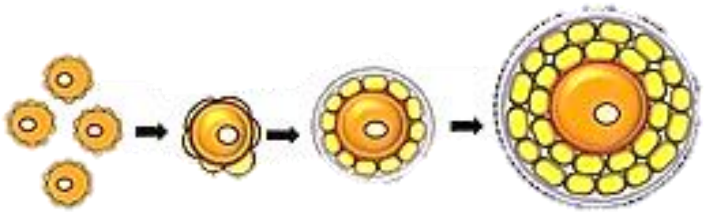
ALLO **exerts dose-dependent effects on ovarian functions in female rats**

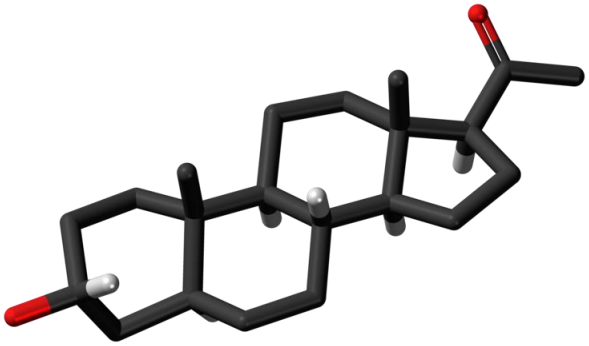




BACKGROUND

Allopregnanolone and preantral follicles





Folliculogenesis involves the transition from primordial to preantral and antral stages, which are critical for ovarian function.

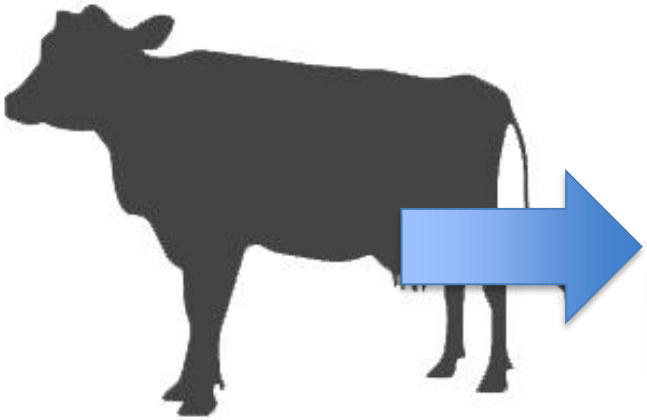
Previous studies in farm animals have focused on the neurophysiological effects of ALLO and its role in stress responses, with limited research on its reproductive implications.

The specific effects of ALLO on preantral follicle development have not yet been studied

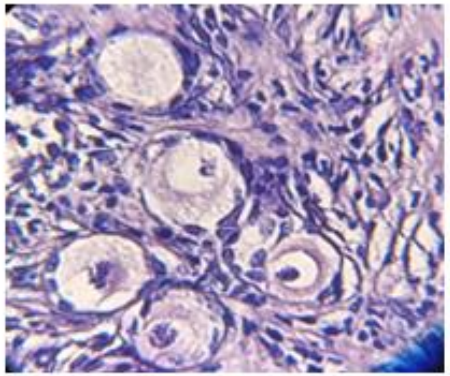
AIM/OBJETIVE/PURPOSE

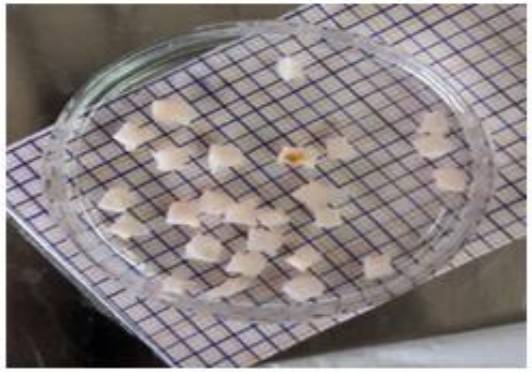
This study aims to investigate the concentration-dependent effects of ALLO on follicular density and the diameters of follicles , oocytes and nuclei in bovine preantral follicles cultured *in vitro*.

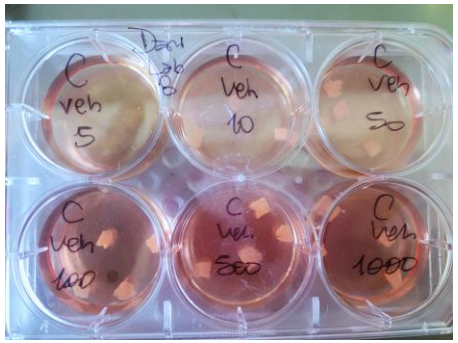
METHODOLOGY











Ovarian source: slaughterhouse (Aberdeen Angus heifers)

METHODOLOGY

In vitro culture

Glutamine
- 3 mM

Hypoxanthine
- 2 mM

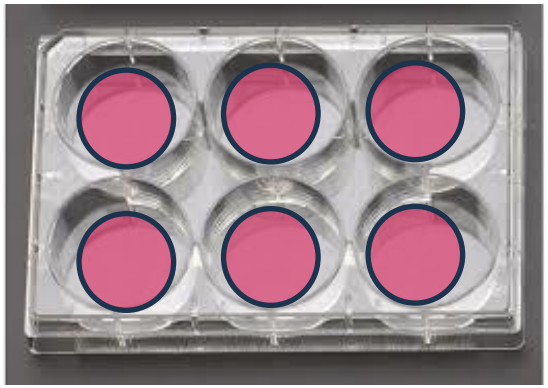
BSA
- 1%

Insulin
- 10 ng/mL

Transferrin
- 2.5 mg/mL

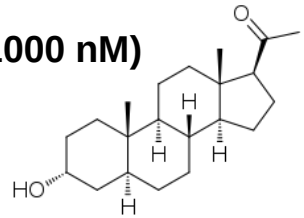
Selenium
- 4 ng/mL

Ascorbic acid
- 50 mg/mL





1. **M199 + vehicle (control)**
2. **M199 + ALLO (5 nM – 1000 nM)**



37°C
5% CO_2

24 h

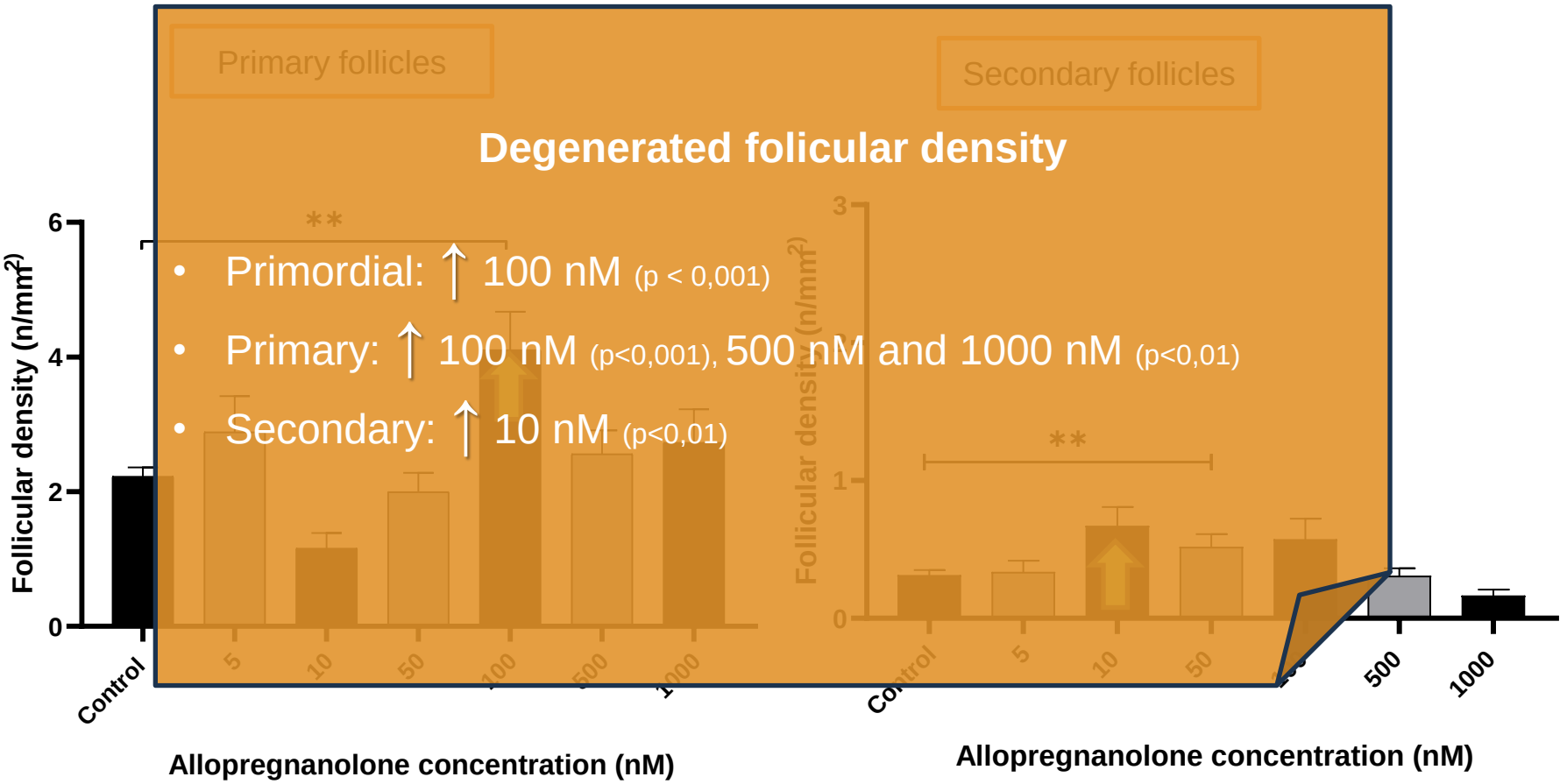
Histology and image analysis

Endpoints:

- Classification: normal - degenerated
- Follicular density
- Diameter of follicles, oocytes and nuclei

RESULTS AND DISCUSSION

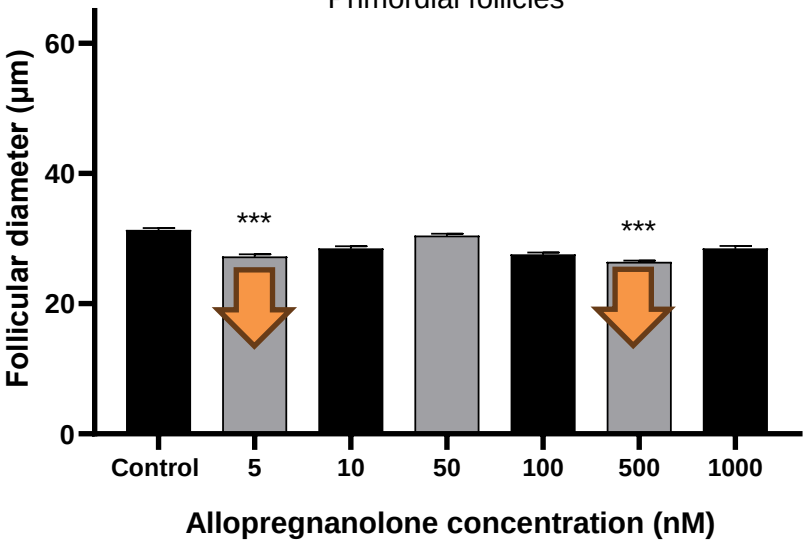
Follicular density



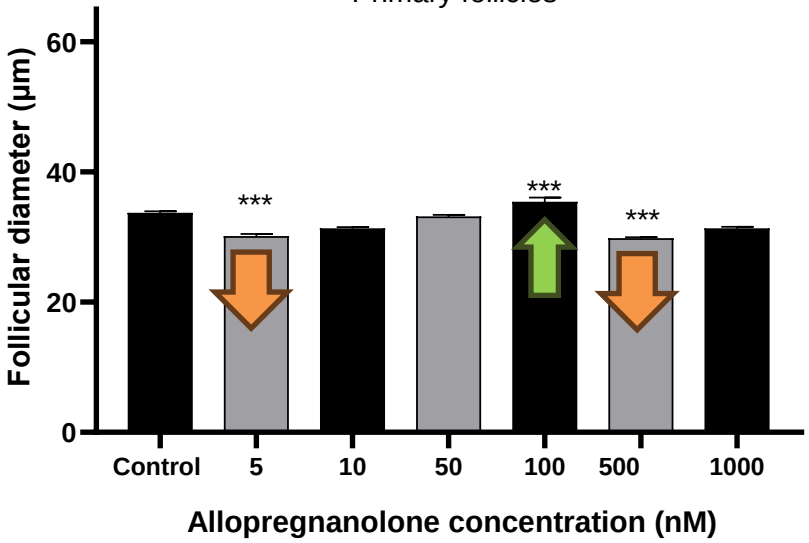
RESULTS AND DISCUSSION

Follicular Diameter

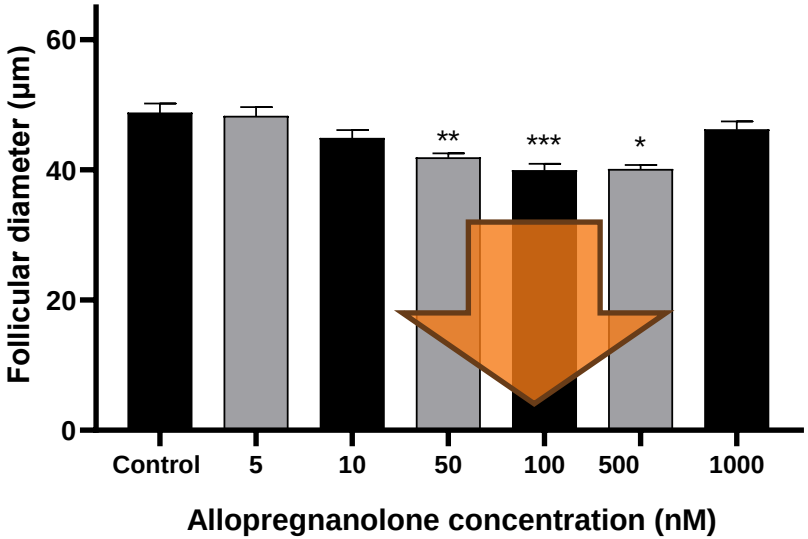
Primordial follicles



Primary follicles



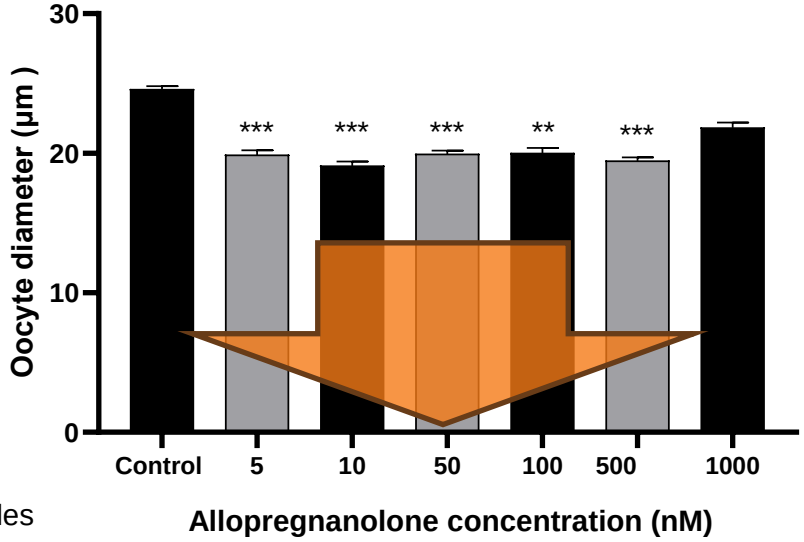
Secondary follicles



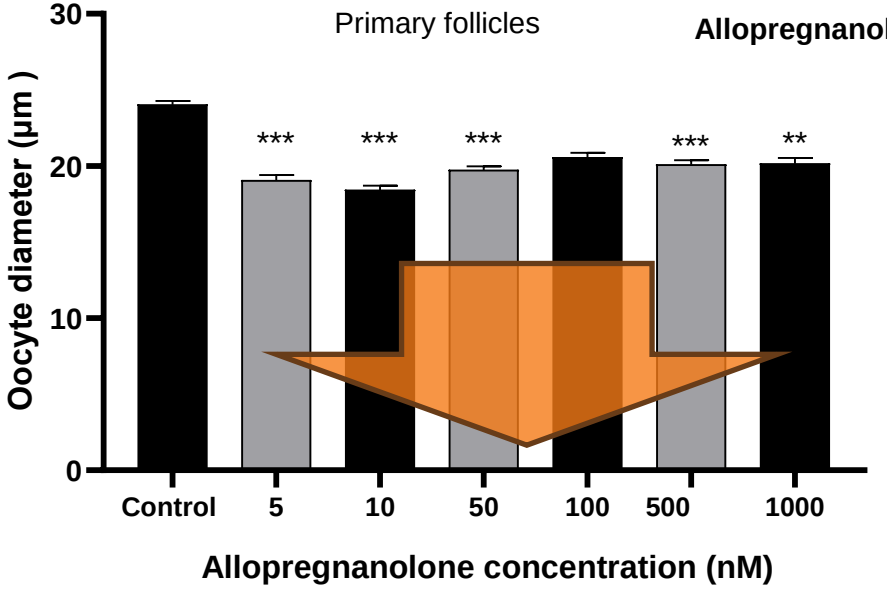
RESULTS AND DISCUSSION

Oocyte Diameter

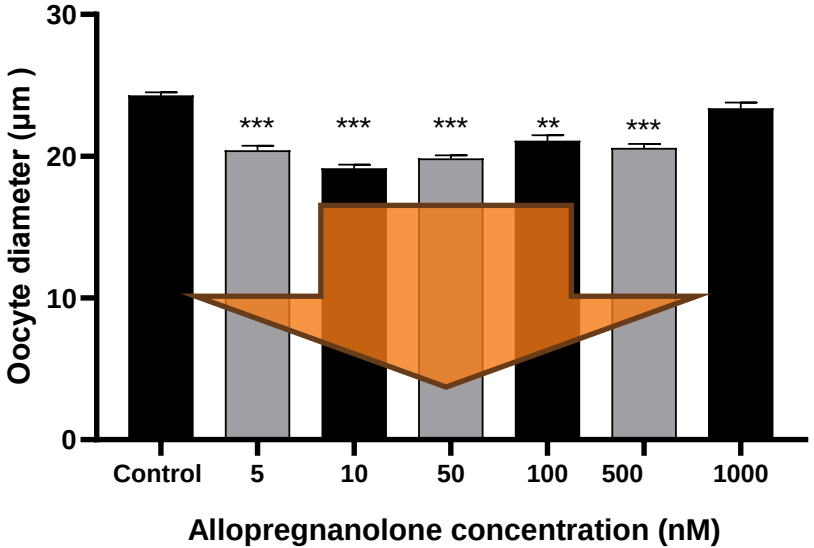
Primordial follicles



Primary follicles



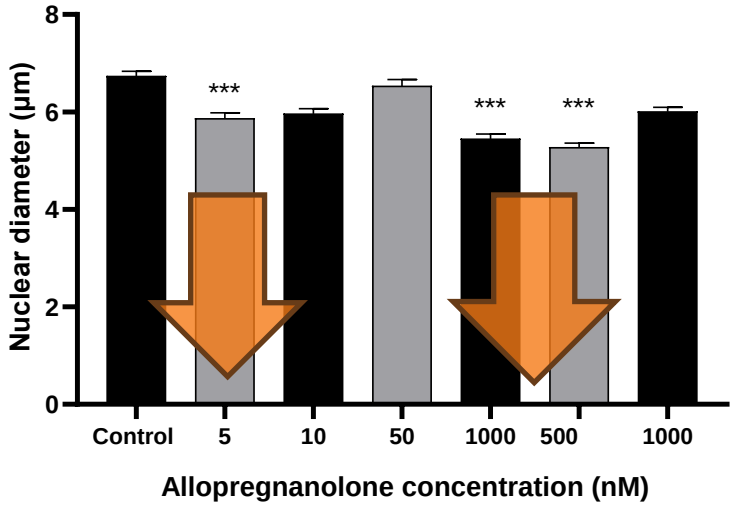
Secondary follicles



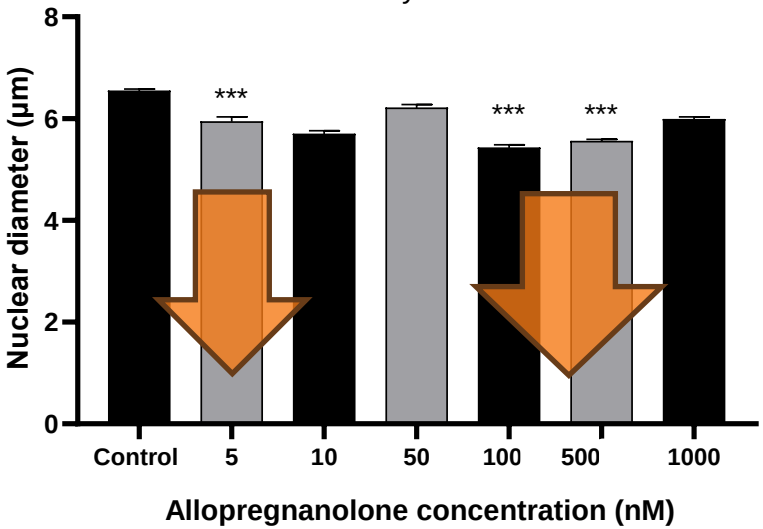
RESULTS AND DISCUSSION

Nuclear Diameter

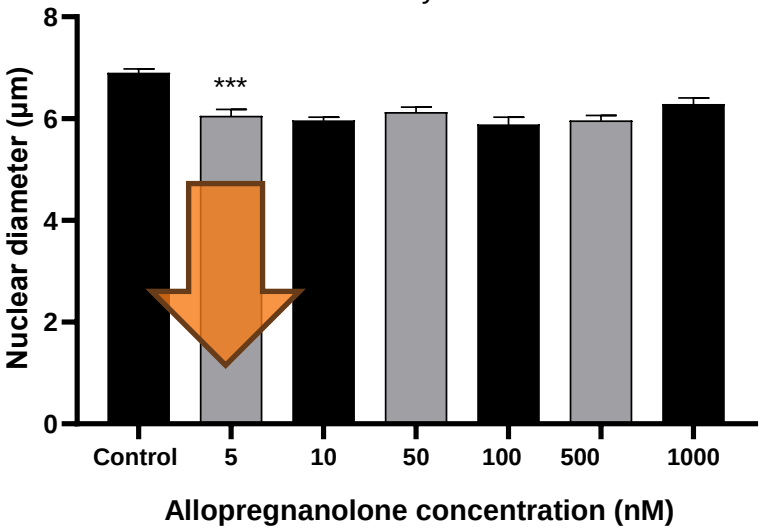
Primordial follicles



Primary follicles



Secondary follicles

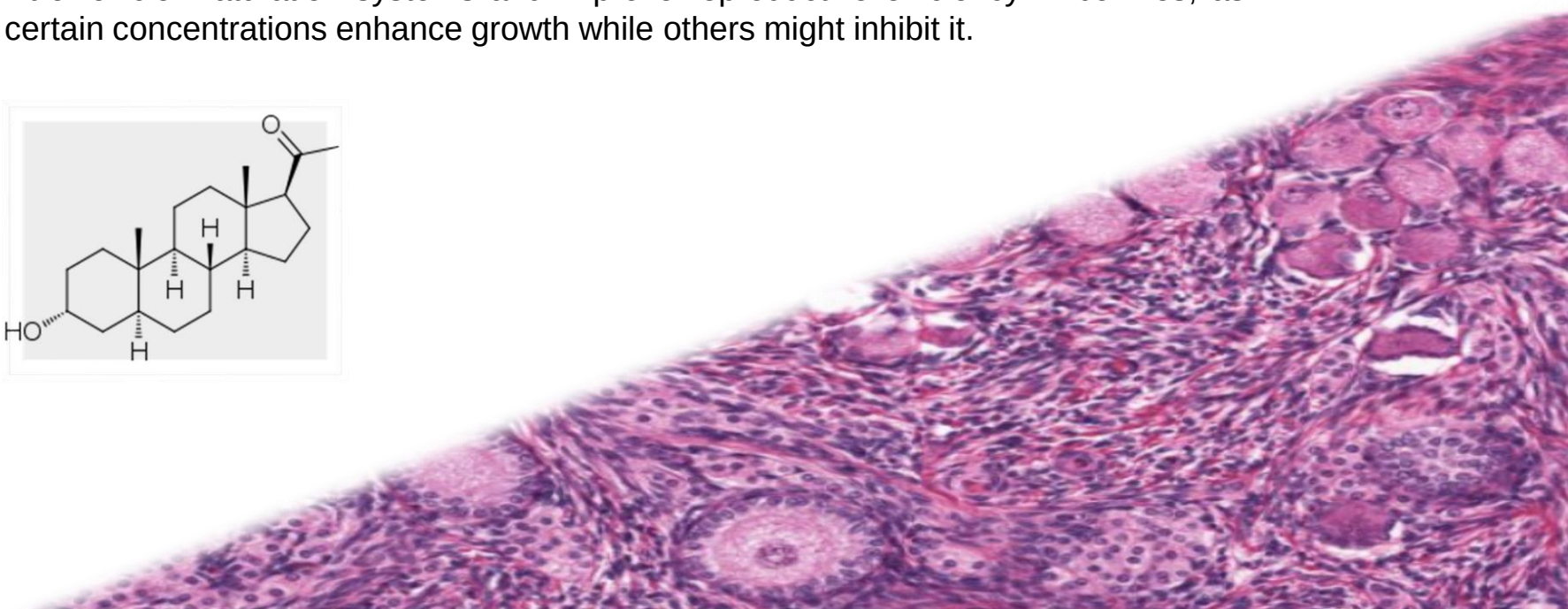


CONCLUSIONS

- ALLO exhibited concentration-dependent effects on follicular density and morphometry, suggesting its potential role in regulating follicular development.

- Differences in response to ALLO may arise from the distinct hormonal environments of primordial, primary, and secondary follicles, with more mature follicles being more responsive due to their higher metabolic activity.

- Understanding how ALLO influences follicular morphometry could help optimize in vitro follicle maturation systems and improve reproductive efficiency in bovines, as certain concentrations enhance growth while others might inhibit it.



ACKNOWLEDGEMENTS

We thank our colleagues, Daniel Alvarez and Analía V. Juan, for providing access to slaughterhouse samples and for their willingness and collaboration.

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DENSE CLUSTERS OF RAW SEWAGE LOCATIONS ON MINNA NEIGHBOURHOOD GIS MAPS ARE POINTERS TO VERITABLE URBAN DECAY AND MOSQUITO-BREEDING GROUNDS

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ABSTRACT

Raw sewage discharge points in the Minna urban area are significant mosquito breeding sites. This study aims to use georeferencing and descriptive observations to identify these locations within Minna, creating maps with the Geographic Information System. Crew members surveyed sectors for sewage discharge points, collecting data and taking photographs. The Minna township map was georeferenced in ArcGIS®10.8, leading to the creation of raw sewage pollution layers for five sectors. These clusters often appeared in low-income neighborhoods, where economic status influenced proper sewage management. The study suggests using the results as a medical information resource for public health interventions. It also recommends periodic sewage pollution audits and expanding the study to cover more areas in future research.

Keywords: *Sewage-pollution; cesspit; georeferencing; GIS; sanitation*

1. INTRODUCTION

The result of the limited-extent pilot study of 2012 (Jonah *et al.*, 2015) to determine the spatial spread of raw sewage discharge over the built-up area of Minna was significant in its novelty because raw sewage discharge points are veritable mosquito breeding sites in the urban area. It is known that mosquitoes are active vector parasites that transmit malarial disease.

The term “sewage” describes raw sewage, sewage sludge, or septic tank waste. Raw sewage is mainly water containing excrement, industrial release, and debris such as sanitary towels, condoms, and plastic. Excrement is the major source of harmful microorganisms, including bacteria, viruses, and parasites. It is also water-carried waste, in solution or suspension, that is intended to be removed from a community. It is more than 99% water and is characterized by volume or rate of flow, physical condition, chemical constituents, and the bacteriological organisms that it contains. Sewage treatment reduces the water content and removes debris but does not kill or remove all the microorganisms (www. hss.delaware.gov).

According to the Encyclopaedia Britannica (2014), malaria is a serious relapsing infection in humans, characterized by periodic attacks of chills and fever, anemia, splenomegaly (enlargement of the spleen), and often fatal complications. It is caused by one-celled parasites of the genus *Plasmodium* that are transmitted to humans by the bite of *Anopheles* mosquitoes. Malaria can occur in temperate regions, but it is most common in the tropics and subtropics. In many parts of sub-Saharan Africa, entire populations are infected more or less constantly. Malaria is also common in Central America, the northern half of South America, and in South and Southeast Asia. The disease also occurs in countries bordering on the Mediterranean, in the Middle East, and in East Asia. In Europe, North America, and the developed countries of East Asia, malaria is still encountered in travelers arriving or returning from affected tropical zones.

The Geographic Information System (GIS) provides an interactive platform by which maps that have been created of geospatial attributes can be queried in sort of user-friendly interfaces such that a “deep-mine” of acquired geospatial data can be readily processed and the result displayed in rapid relatable formats that constitutes the basis of a veritable audit mechanism. Jonah *et al.* (2011), Jonah and Jimoh (2013), Jonah and Ayofe (2014),

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Jonah and Saidu (2018), Jonah and Sunday (2021) have employed this audit mechanism characteristic of the GIS in their works on urban built-up landmarks, site-specific topographic, natural-material economic-resource, raw sewage, and air pollution inquiries.

2. METHOD

2.1 Study Area Segmentation and Pre-Survey.

At the outset, Minna township built-up areas, shown in Figure 1, were segmented into five sectors, namely: Greater Bosso, Minna Central, Greater Maitumbi, Tunga, and Greater Chanchaga. Subsequently, the pre-survey stage, whence the survey party visited random segment locations for site familiarisation and testing of the hand-held Geographic Information System unit especially, was initiated.

2.2 Principal Survey Procedures.

Upon the familiarisation trips to the broader survey area, the main exercise kicked in. Crew members investigate every acre of assigned sectors for locations where sewage water freely flows out of households into the neighborhood, forming slow-moving puddles. At such a location, geographic information coordinates are taken along with the date of survey, time of the survey, weather at the time of the survey, name of recorder or data specialist, and information about the defaulter householder (where this is volunteered). The survey party also takes photographs of the point of interest. This process is repeated for as many points as can be accessed by the data specialists. All this germane information is recorded on a purpose-specific datasheet.

3. RESULTS AND DISCUSSION

3.1 Analyses of Data

3.1.1 Importing Latitude and Longitude Information at Each Survey Point into ArcGIS®10.8.

From each data sheet corresponding to a distinct raw sewage pollution point, latitude and longitude (x-y) information was extracted and imported into the ArcGIS®10.8 software. Next, the World Geodetic System (WGS 1984) platform was chosen as the default coordinate system for the x-y information.

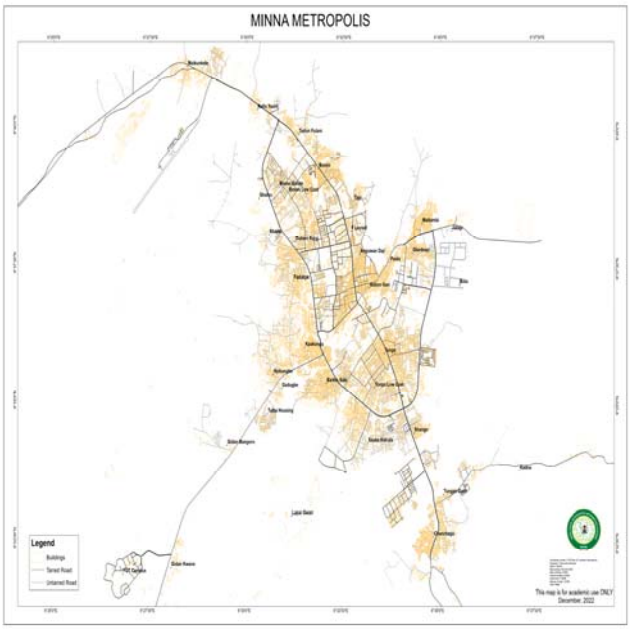


Figure 1. *Map of Minna township*

3.1.2 Acquisition of the Minna Township Built-up and Settlement Shapefiles.

The Minna township built-up and settlement shapefiles were duly acquired and imported into the ArcGIS®10.8 software. By merging the two distinct shapefiles, the required substrate of major and minor roads and settlements was activated, thus defining a collage of the Minna township map.

3.1.3 Creation of the Minna Raw Sewage Pollution Layer.

It is necessary to create polygons for locations with identified raw sewage pollution menace so as to separate these regions from other unpolluted zones. For the five sectors, distinct polygons were also created to segment the respective sub-study areas. This means that the road networks and settlements in these sectors are emphasized on the collaged Minna township map. Each georeferenced location is consequently highlighted on its true placement point in the respective sub-study areas. Figures 2 to 6 show the raw sewage pollution layers on the Minna GIS map for the different sectors of the town.

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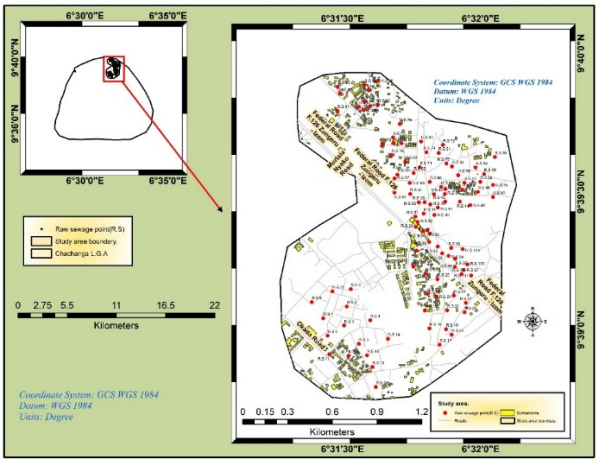


Figure 2. *The raw sewage pollution layer for Greater Bosso shows more sanitation default zones at the central to the north-northcentral portions*

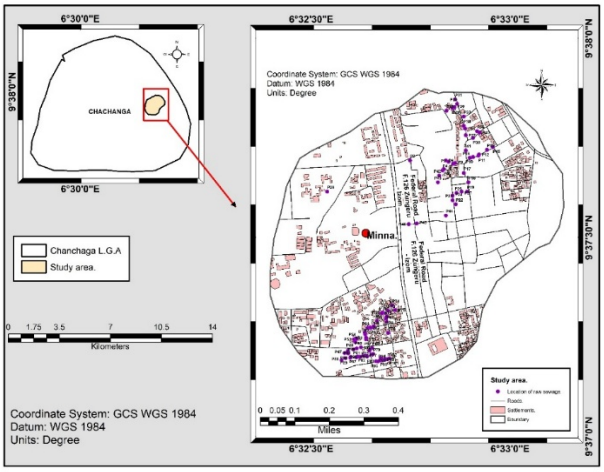


Figure 3. *Composite raw sewage pollution layer for Minna Central showing zones of obvious mosquito breeding sites at the southwest and northeast*

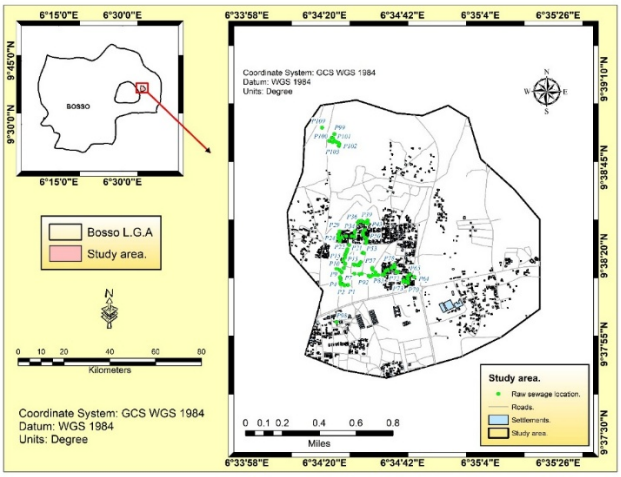


Figure 4. *Composite raw sewage pollution layer for Greater Maitumbi showing preponderance of slum settlements at the central to the northwest portions*

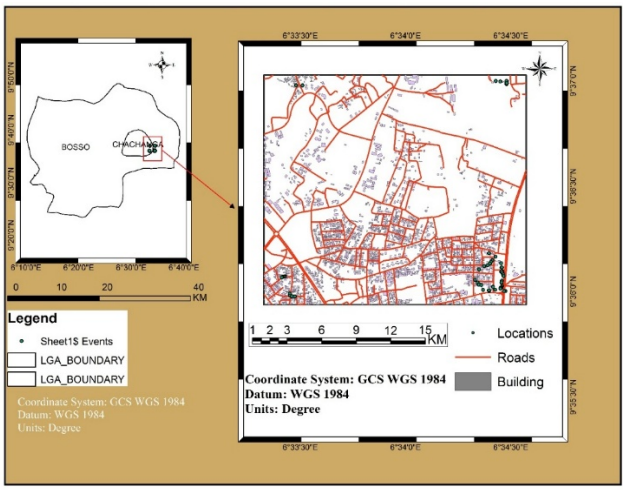


Figure 5. *Composite raw sewage pollution layer for Tunga with no defined slum-settlement clusters or mosquito-breeding locations except at a tiny segment of the southeast portion of the neighborhood as well as at the extreme southwest*

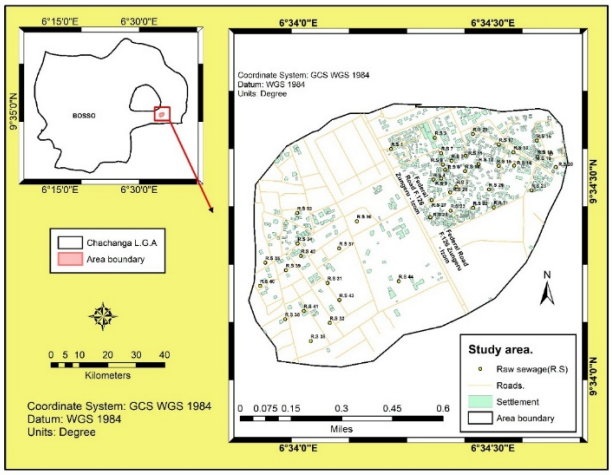


Figure 6. *The composite raw sewage pollution layer for Greater Chanchaga indicates that poor housing settlements that favor mosquito-breeding locations are concentrated to the northeast and southwest of the federal highway bisecting this neighborhood*

3.2 Discussion

The composite raw sewage pollution maps for the neighborhoods of Greater Bosso, Minna Central, Greater Maitumbi, Tunga, and Greater Chanchaga form the contiguous collaged map of Minna's built-up township. Representative dots at their true latitude-longitude positions on each sectored polygon area have been colored-coded to represent a raw sewage pollution point, although the use of different color schemes for the different sectors was just a mere aesthetic excursion. Figure 2 indicates that more than 50% of the households visited are at default of sewage

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sanitation. The southern one-half of the Greater Bosso neighborhood, which indicates fewer clusters, is the portion that very influential government functionaries and businessmen have built their dwellings in spite of cultural norms.

The information gleaned from Figure 3 indicates less than 25% raw sewage pollution regime for the Minna Central neighborhood.

The fact known to residents of Minna is that the proportion of green-clustered dots for the core Greater Maitumbi sub-study area of Figure 4 should be 95%-plus. The core built-up neighborhood is one large expanse of slum-infested portion of town. Alas, investigations for this study were limited to tiny portions of the northwest and the west-central neighborhoods of Greater Maitumbi, where the proportion of of households at default of sewage sanitation was over 90%. Wide expanses of undeveloped bushlands ring off the core Greater Maitumbi sub-study area at the heart of Minna.

At the Tunga neighborhood, heavily built-up at the southern sector, as indicated in Figure 5, survey density does not correspond to housing density (this was due to survey resources constraints), but for the locations visited at the built-up zones of the northwest, northeast, southwest, and southeast, green-dot clusters overlap in regimes or patterns that will be nightmarish for town planners. The northern sector of the Tunga neighborhood is characterized by open spaces of undeveloped fields with wild vegetation growing there.

The densely built-up northeast zone characterizes the Greater Chanchaga neighborhood of Figure 6 and the comparatively spaced-out southwest zone, conveniently separated by the arterial F126 highway that traverses Minna town. Clusters of yellow dots in higher proportion are the norm for the northeast zone vis-à-vis the southwest zone.

4. CONCLUSIONS

Greater Bosso has its share of raw sewage pollution spots that form clusters in poor and low-income neighborhoods. Overall, economic status is a very important factor governing household sewage piping and proper collection in purpose-built cesspits. However, there are, regrettably, relatively affluent homes that still elect to pipe wastewater through orifices bored through the bottom of their brick fence. In Figure 2, the red clusters at the northeast are the slum settlement of Angwan Biri and its outlying neighborhood, whilst those traversing the F126 are the contiguous slum settlements of Hayin Gwari and Central Bosso built-up areas. The scattered red dots in the southeast zone correspond to the relatively well-planned Okada Road neighborhood. Stagnant pools of wastewater that correlate with the red dots in Figure 2 are the media that encourage mosquitoes to breed perennially in this neighborhood. It is no surprise that endemic malarial infestations are commonplace in the Angwan Biri, Hayin Gwari, and Central Bosso built-up areas. The Bosso Campus of the Federal University of Technology, Minna, is actually located in the Central Bosso sector.

The contiguous low-income slum settlements of Limawa and Makera are recognized in Figure 3 by the clusters of purple dots at the south end of the sector, whilst the clusters at the northeast are the densely-populated, unplanned Angwan Sarki-Angwan Daji sectors. There cannot be much surprise here because the clusters observed here correspond to frontier settlements of Minna township from over 80 years ago. It is within the Minna Central neighborhood that the Government Reservation Area (GRA) neighborhood is located at the northwest and where retired army generals' (including two former heads of state) homes fuse with government offices and the Central Bank's offices plus other commercial banks' operation offices at the east-central portion. The northwest and southeast portions of the Minna Central neighborhood are the "cleanest" habitable built-up areas because of the absence of sewage sludge that encourages mosquitoes and other vermin to breed. This situation sharply contrasts those of the Limawa, Makera, and Angwan Sarki-Angwan Daji sectors.

The predominance of clusters of green dots in Figure 4 for Greater Maitumbi indicates obvious slum settlements. Were available resources to permit a full-scale house-to-house survey, there is no doubt Figure 4 will be one green-dot clustered map.

Obviously, the slum-dwelling conclusion associated with dot clusters can be made for the northwest, northeast, southwest, and southeast portions of Figure 5. These relatively small segments forming a veritable disconnected "ring" over the wider Tunga neighborhood will lead to the obvious subjective conclusion that Inner Tunga suffers raw sewage sanitation default.

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Nonetheless, a purpose-specific study must be conducted in this regard. The Tunga sector is one of two “old town” neighborhoods (the other being Minna Central) of Minna from over 80 years ago, and not having a built-up segment designated for GRA, it is a veritable sewage-sludge-cum-mosquito-breeding built-up neighborhood.

Yellow-dot spread corresponds to residential densities in the two zones of interest in the Greater Chanchaga sector of Figure 6, and this pattern appears to be the norm. Clustered, poorly-spaced homesteads are at the default of raw sewage sanitation, and thus, these homesteads provide a convenient breeding ground for mosquitoes, thereby engendering endemic malarial infestation.

5. DECLARATIONS

5.1. Acknowledgements

The author is grateful to Professor Luis De Boni for his untiring patience and helpful editorial insights in providing appropriate guides to prepare this material.

5.2. Open Access

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DENSE CLUSTERS OF RAW SEWAGE LOCATIONS ON MINNA NEIGHBOURHOOD GIS MAPS ARE POINTERS TO VERITABLE URBAN DECAY AND MOSQUITO-BREEDING GROUNDS

Sunday Adole Jonah

Federal University of Technology, Department of Physics, Nigeria

November/2024

INTRODUCTION

- **Information 1;** Result of limited-extent pilot study of 2012 (Jonah *et al.*, 2015) to determine the spatial spread of raw sewage discharge over the built-up area of Minna was significant in its novelty because raw sewage discharge points are veritable mosquito breeding sites in the urban area
- **Information 2;** Mosquitoes are active vector parasites that transmit malarial disease
- **Information 3;** Raw sewage is mainly water containing excrement, industrial release, and debris such as sanitary towels, condoms, and plastic
- **Information 4;** According to the Encyclopaedia Britannica (2014), malaria is a serious relapsing infection in humans, characterised by periodic attacks of chills and fever, anemia, splenomegaly (enlargement of the spleen), and often fatal complications
- **Information 5;** The Geographic Information System (GIS) provides an interactive platform by which maps that have been created of geospatial attributes can be queried in sort of user-friendly interfaces such that a "deep-mine" of acquired geospatial data can be readily processed and the result displayed in rapid relatable formats that constitutes the basis of a veritable audit mechanism (Jonah *et al.*, 2011; Jonah and Jimoh, 2013)

AIM/OBJECTIVE/PURPOSE

Knowing the extent of this raw sewage discharge will be the basis for evolving measures to adopt pro-active approach in the quest to tackle this menace that is related to the malarial scourge, for raw sewage discharge points provide the environment that plasmodium-carrying mosquitoes breed.

METHODOLOGY

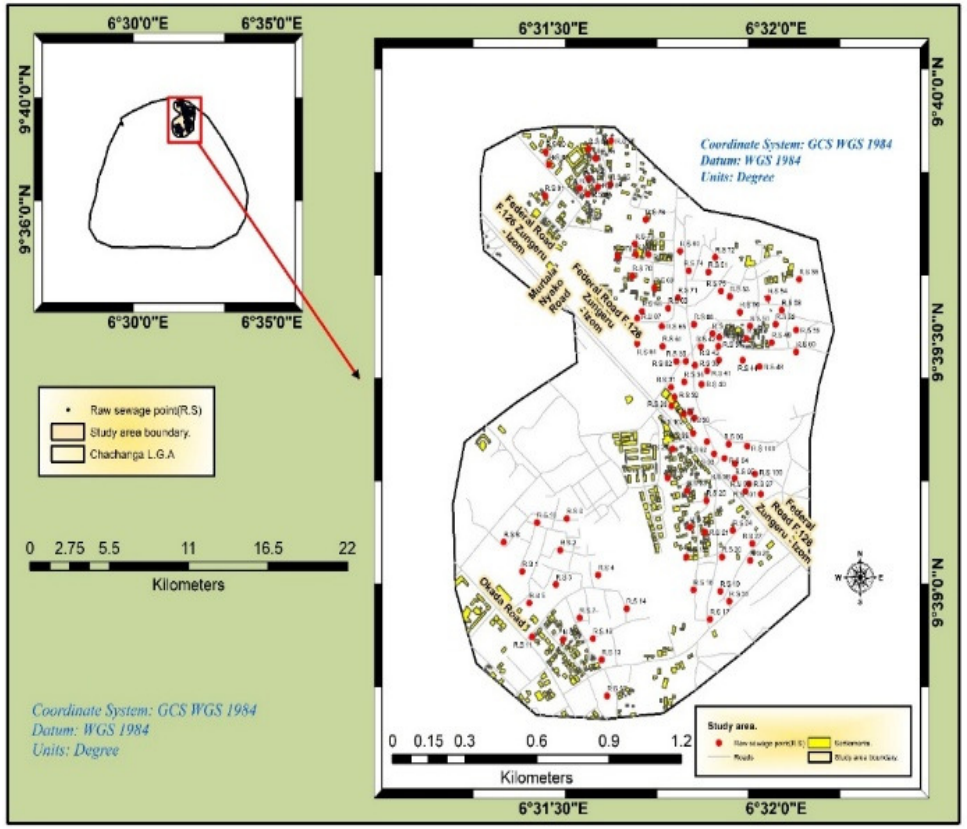
- At the outset, Minna township built-up areas was segmented into five sectors, namely: Greater Bosso, Minna Central, Greater Maitumbi, Tunga, and Greater Chanchaga
- Subsequently, the pre-survey stage, whence the survey party visited random segment locations for site familiarisation and testing of the hand-held Geographic Information System unit especially, was initiated
- Upon familiarisation trips to the broader survey area, the main exercise kicked in: crew members investigate every acre of assigned sectors for locations where sewage water freely flows out of households into the neighbourhood, forming slow-moving puddles
- At such a location, geographic information coordinates are recorded along with other germane information
- This process is repeated for as many points as can be accessed by the data specialists
- Information thus acquired is recorded on a purpose-specific datasheet

RESULTS (1)

- **Importing Latitude and Longitude Information at Each Survey Point into ArcGIS®10.8:** From each data sheet corresponding to a distinct raw sewage pollution point, latitude and longitude (x-y) information was extracted and imported into the ArcGIS®10.8 software. Next, the World Geodetic System (WGS 1984) platform was chosen as the default coordinate system for the x-y information.
- **Acquisition of the Minna Township Built-up and Settlement Shapefiles:** The Minna township built-up and settlement shapefiles were duly acquired and imported into the ArcGIS®10.8 software. By merging the two distinct shapefiles, the required substrate of major and minor roads and settlements was activated, thus defining a collage of the Minna township map.
- **Creation of the Minna Raw Sewage Pollution Layer:** It is necessary to create polygons for locations with identified raw sewage pollution menace so as to separate these regions from other unpolluted zones. For the five sectors, distinct polygons were also created to segment the respective sub-study areas. This means that the road networks and settlements in these sectors are emphasised on the collaged Minna township map. Each georeferenced location is consequently highlighted on its true placement point in the respective sub-study areas.
- Figures hence show raw sewage pollution layers on the Minna GIS map for the different sectors of the town.

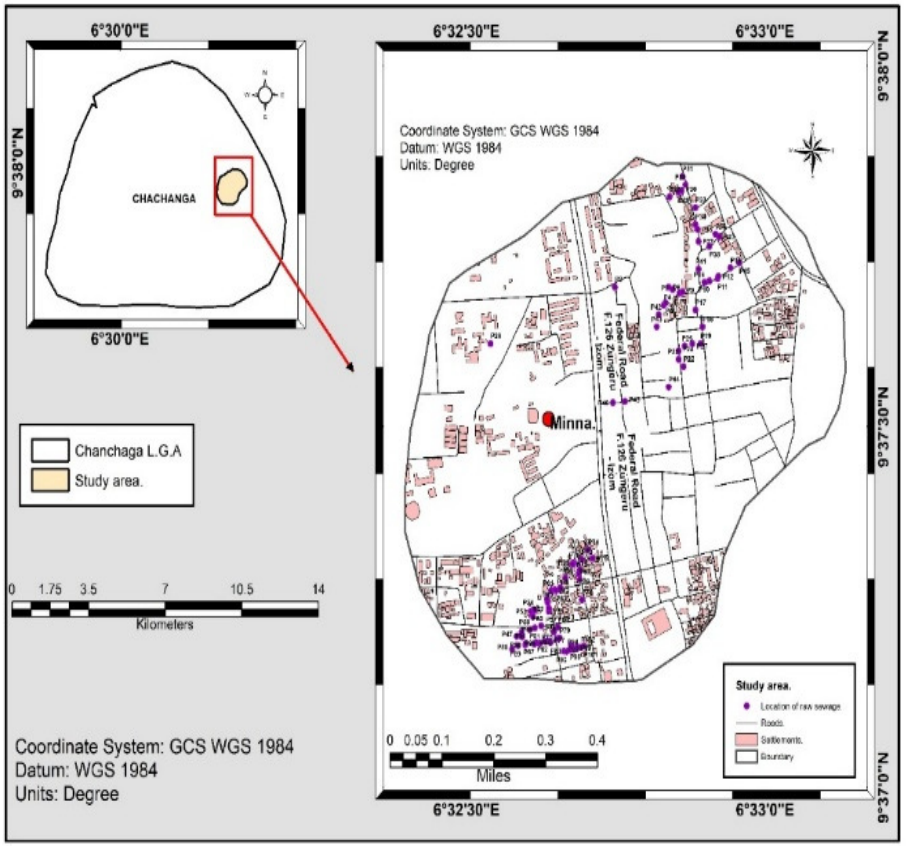
RESULTS (2)

Raw sewage pollution layer for Greater Bosso showing more sanitation default zones at the central to the north-northcentral portions



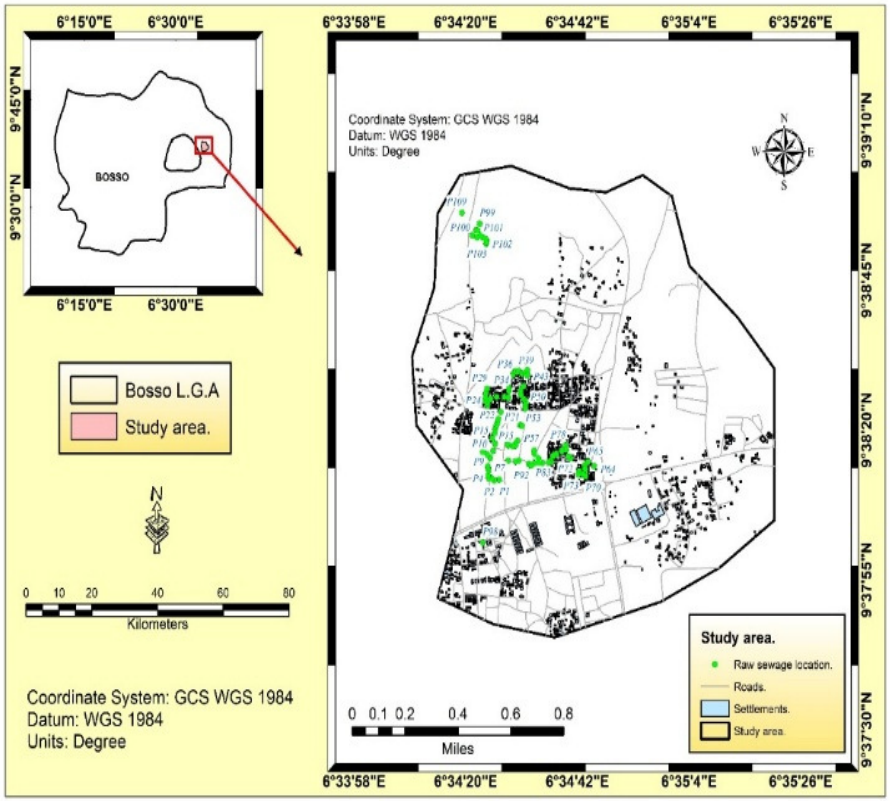
RESULTS (3)

Composite raw sewage pollution layer for Minna Central showing zones of obvious mosquito breeding sites at the southwest and northeast



RESULTS (4)

Composite raw sewage pollution layer for Greater Maitumbi showing prepoderance of slum settlements at the central to the northwest portions



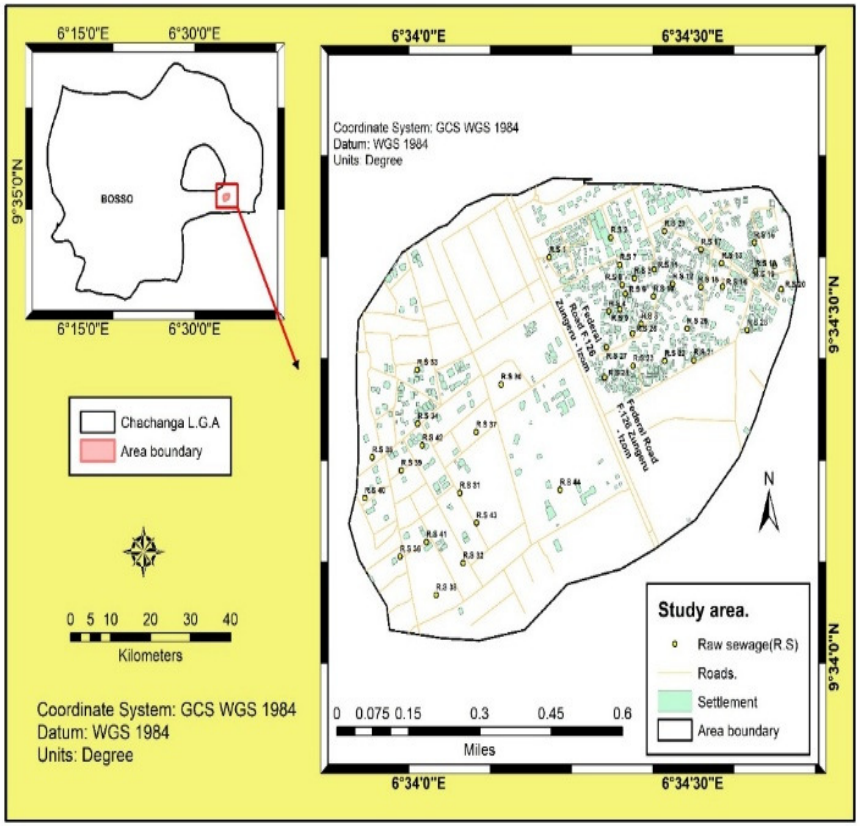
RESULTS (5)

Composite raw sewage pollution layer for Tunga with no defined slum-settlement clusters or mosquito-breeding locations except at a tiny segment of the southeast portion of the neighbourhood as well as at the extreme southwest



RESULTS (6)

Composite raw sewage pollution layer for Greater Chanchaga indicates that poor housing settlements that favour mosquito-breeding location are concentrated to the northeast and southwest of the federal highway bisecting this neighbourhood



DISCUSSION

- The Greater Bosso raw sewage pollution layer map indicates that more than 50% of the households visited are at default of sewage sanitation.
- The Minna Central neighbourhood raw sewage pollution layer map indicates less than 25% raw sewage pollution regime for this built-up area
- The fact known to residents of Minna is that that the proportion of green-clustered dots for the core Greater Maitumbi neighbourhood should be 95%-plus. The core built-up neighbourhood is one large expanse slum-infested portion of town.
- At the Tunga neighbourhood, heavily built-up at the southern sector, the locations visited at the built-up zones of the northwest, northeast, southwest, and southeast indicate that clusters corresponding to sewage locations overlap in regimes or patterns that will be nightmarish for town planners.
- The densely built-up northeast zone characterises the Greater Chanchaga neighbourhood and the comparatively spaced-out southwest zone. Clusters of yellow dots indicating raw sewage discharge locations-cum-mosquito breeding sites in higher proportion are the norm for the northeast zone vis-à-vis the southwest zone.

CONCLUSIONS

- **Conclusion 1;** Greater Bosso has its share of raw sewage pollution spots that form clusters in poor and low-income neighborhoods. Overall, economic status is a very important factor governing household sewage piping and proper collection in purpose-built cesspits.
- **Conclusion 2;** The contiguous low-income slum settlements of Limawa and Makera are recognised by the clusters of purple dots at the south end of the sector whilst the clusters at the northeast are the densely-populated, unplanned Angwan Sarki-Angwan Daji sectors. The northwest and southeast portions of the Minna Central neighbourhood are the "cleanest" habitable built-up areas because of absence of sewage sludge that encourage mosquitoes and other vermin to breed.
- **Conclusion 3;** Were available of resources to permit a full-scale house-to-house survey, there is no doubt that the Greater Maitumbi pollution layer map will be one green-dot clustered map.
- **Conclusion 4;** The Tunga sector is one of two "old town" neighbourhoods of Minna from over 80 years ago, and not having a built-up segment designated for GRA, it a veritable sewage-sludge-cum-mosquito-breeding built-up neighbourhood.
- **Conclusion 5;** Yellow-dot spread correspond to residential densities in the two zones of interest in the Greater Chanchaga neighbourhood. Clustered, poorly-spaced homesteads are at default of raw sewage sanitation and thus these homesteads provide convenient breeding ground for mosquitoes thereby engendering endemic malarial infestation.

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ASSESSMENT OF THE PRESENCE OF HEAVY METALS IN THE WATERS OF THE PARAÍBA DO SUL RIVER IN THE CITY OF VOLTA REDONDA, RJ - BRAZIL

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ABSTRACT

Drinking quality water is a fundamental human right, although many individuals still lack access to this resource due to several factors. One major factor is the inadequate disposal of domestic and industrial sewage, as well as the storage of industrial solid waste along riverbanks, which contaminates the soil and water with heavy metals and other emerging pollutants. This is particularly evident in the Paraíba do Sul River (RPS) in the city of Volta Redonda, Rio de Janeiro, Southeastern Brazil. This study aims to assess ore processing waste impacts present on RPS banks on this river's waters. A quantitative methodology was employed by analyzing water samples with an atomic absorption spectrophotometer (AAS) to quantify metal concentrations in RPS water samples in accordance with current Brazilian legislation (CONAMA 357/2005).

Keywords: *Paraíba do Sul River; Heavy Metals; Emerging Contaminants; bioaccumulator.*

1. INTRODUCTION

Potable and quality water is a fundamental human right, although many individuals do not have access to this resource due to various factors, including the inadequate disposal of domestic and industrial sewage, as well as industrial solid waste stored along riverbanks, contaminating soil and water with heavy metals and other emerging pollutants. As has taken place in several rivers globally, Brazilian rivers are extremely impacted, including the Paraíba do Sul River (RPS), certainly one of the most affected throughout Brazilian history, mainly due to its location between the Rio-São Paulo axis, a connection and development vector for one of the most important economic regions in South America. The mid-Paraíba region deserves attention, especially the municipality of Volta Redonda, in the state of Rio de Janeiro, Southeastern Brazil, due to an industrial park where industries with a high potential for contaminating the RPS, particularly due to heavy metals, are concentrated. This river is of utmost importance as it serves as a water supply source for several cities in this region.

Effluents do not usually receive adequate treatment, resulting in high pollutant loads that rivers are not always able to absorb, significantly affecting their quality (Araújo et al., 2007). The release of metals into water intended for human consumption can lead to significant health risks, including various diseases and disorders related to metal toxicity (RIBEIRO, 2013). Although Brazilian legislation establishes permissible limits for several metals in both drinking water and wastewater, their toxic effects vary based on the specific type and concentration of each metal (BRAGA et al., 2009).

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2. MATERIAL AND METHODS

Herein, a qualitative-quantitative and instrumental methodology was employed comprising metal determinations employing an atomic absorption spectrophotometer, pHmeter, analytical balance, and standard pH solutions. All experimental tests were conducted at the Centro Universitário Geraldo Di Biase chemistry laboratory, Volta Redonda Campus, Rio de Janeiro. A bibliographic research was carried out to identify effective methods for detecting heavy metals at low concentrations. Atomic Absorption Spectrometry (AAS) was noted as a feasible and highly accessible method and, according to Sibal and Espino (2018), the main laboratory technique for measuring metals in water.

Water samples were obtained in the city of Volta Redonda along the RPS. The sample storage bottles were rinsed with concentrated nitric acid and left to rest for 24 hours. They were then rinsed with distilled water and filled with the water samples collected at two different points along the RPS. Each collected sample was acidified with 10% nitric acid and stored in refrigerators prior to the metal determination analyses.

3. RESULTS AND DISCUSSION

The overload of pollutants released into RPS waters, especially untreated sanitary effluents and industrial effluents containing heavy metals, along with waste storage from mineral processing along the banks of the RPS and the substantial increase in water extraction for urban population supply, have caused significant negative water quality impacts (Table 1).

***Figure 1**. Solid waste from the mineral processing along the banks of the Paraíba do Sul River, Rio de Janeiro, Southeastern Brazil*.



Reference: The authors (2024).

***Table 1**. Metal concentrations were determined in water samples from the Paraíba do Sul River through Atomic Absorption Spectrometry, the scanning wavelength for each metal, and CONAMA limits.*

Metal	ʎ (nm)	Concentration ($mg.L^{-1}$)	CONAMA 357 ($mg.L^{-1}$)
Zn	213	0.05	0.18
Mn	279.48	0.05	0.10
Cu	324.75	0.11	0.009
Cr	235.87	0.20	0.05
Ni	232	0.53	0.025
Co	240.73	0.87	0.05
Pb	273.31	1.10	0.01
Fe	248.33	2.54	0.30

Reference: The authors (2024).

Only manganese (Mn) and zinc (Zn) met the tolerance limits established by the CONAMA legislation 357/2005, while the other determined elements exceeded maximum permissible levels in freshwater for Pb (0.01 $mg.L^{-1}$), Zn (0.18 $mg.L^{-1}$), and Cr (0.05 $mg.L^{-1}$). This may directly affect the quality of RPS waters and cause serious harm to the local biota and human health.

This corroborates previous assessments, such as Barreto et al. (2024), who surveyed pollutants present in RPS water column and sediment samples in the Médio Paraíba do Sul and Baixo Paraíba do Sul areas from 2005 to 2023. A literature review carried out by the authors indicated a Pb level reported by Tonhá et al. (2021) in the Médio Paraíba do Sul region of 0.00014 $mg.L^{-1}$, much lower than that observed herein, of 1.10 $mg.L^{-1}$. Lead is a bioaccumulative metal that poses serious health risks, including cancer.

In addition to impacts caused by the discharge of untreated effluents, the dispersion of solid waste, such as mining waste, which contains high Fe levels, along the banks is also observed, which is occasionally carried into the river (Costa et al., 2022). Iron, although not a toxic metal, poses several problems for public water supplies, as it imparts color and taste to the water, causing stains on clothes and sanitary fixtures. It also leads to the development of deposits in pipelines and iron bacteria, resulting in biological contamination of the water within distribution networks. Thus, iron

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constitutes a potable water standard. Nickel, on the other hand, is of environmental concern due to its carcinogenic properties and its potential to cause respiratory and heart problems in humans. Cobalt toxicity is considered relatively low, although excessive doses can lead to goiter, hypothyroidism, heart failure, and pulmonary fibrosis (hardening of the lungs), which can be fatal (Ambiente Brasil, 2007).

Cobalt (Co) is a relatively scarce metal in nature, but when found, it comes from the burning of fossil fuels pigment manufacturing and is in the composition of metallic alloys and phosphate fertilizers. In excess, it can cause lung diseases and skin inflammation (dermatitis contact details).

4. CONCLUSIONS

This assessment indicates several metals above established CONAMA guidelines in RPS waters alongside other pollutants, with only Mn and Zn within tolerance limits. The most concerning finding was the presence of Pb at concentrations exceeding CONAMA guidelines. Interventions are necessary to assess whether the solid waste resulting from mineral processing along the banks of the Paraíba do Sul River in the city of Volta Redonda, Rio de Janeiro, Southeastern Brazil, is contributing to the significant increase of metals in RPS waters, given that Pb is a bioaccumulative metal and its presence in the river can result in various environmental problems and human health issues.

To study the risks that a given population maybe running research is needed for in-depth investigations into the contamination of the soil along the banks of the river, sediments, and fish, as well as assessment of the health of the population, in order to have an idea about the level of contamination by heavy metals that were caused by pollution. It is important to inform responsible authorities about domestic waste and industrial, sewage, and other sources of pollution so that they can take the appropriate measures, thus preventing these waste and pollutants from reaching the river without adequate treatment. It also requires awareness on the part of the population so that they do not throw waste into rivers, which, as a consequence, can affect the environment and will directly affect mainly through the consumption of contaminated fish.

For the population supposedly contaminated by heavy metals requires health monitoring to prevent and reduce long-term effects.

In view of the above, it is clear that the Pollution of water systems is a problem for society as a whole. And suppose this society intends to own potable water drinks that can be consumed in the future. In that case, it must above review your activities, be they domestic, commercial, or industrial, as they all have implications that end up directly or indirectly degrading the available water sources.

5. DECLARATIONS

5.1. Open Access

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Southern Science Conference, 2024.

ASSESSMENT OF THE PRESENCE OF HEAVY METALS IN THE WATERS OF THE PARAÍBA DO SUL RIVER IN THE CITY OF VOLTA REDONDA, RJ - BRAZIL

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November/2024

INTRODUCTION

CHALLENGES OF CONTAMINATION IN THE PARAÍBA DO SUL RIVER

- The Paraíba do Sul River has been impacted throughout Brazilian history, due to its location between the Rio - São Paulo axis, a vector of connection and development of one of the most important economic regions in South America.

- The region of middle Paraíba deserves attention, especially in the municipality of Volta Redonda, with emphasis on the industrial park where industries with high potential for contaminating the river, including heavy metals, are concentrated.

OBJETIVE

- The objective of the research was to analyze the heavy metals present in the waters of the Paraíba do Sul River in the city of Volta Redonda using the atomic absorption spectrometer method and compare with the CONAMA 357/2005 legislation.

METHODOLOGY

- Qualitative-quantitative methodology, equipment (atomic absorption spectrometer - model PinAAcle 900T, Perkin Elmer);
- The experimental tests were conducted in the Chemistry laboratory at UGB, (Centro Universitário Geraldo Di Biase) - Campus Volta Redonda - Rio de Janeiro;
- The waters were collected in the city of Volta Redonda, RJ (as shown in Figures 1, 2 and 3).

Figure 1. Sample collection in the city of Volta Redonda



The authors

Figure 2. Sample preparation at the time of collection.



The authors

Figure 3. Prepared samples



The authors

RESULTS AND DISCUSSION

- The load of pollutants, including untreated sanitary and industrial effluents, negatively impacts the water quality of the Paraíba do Sul River;
- Table 1 presents concentrations of metals in water samples, Figure 4, compared to the allowable limits set by CONAMA legislation 357/2005;
- Exposure to heavy metals, such as lead and nickel, poses significant risks to human health and the ecosystem.
- The presence of iron, although non-toxic, causes water quality issues, while cobalt contamination is a concern due to adverse effects in high doses.

Figure 4. Solid waste from ore processing on the banks of the Paraíba do Sul River in the city of Volta Redonda - sample collection point



Reference: The authors (2024).

Table 1 - Concentration of metals found in the analysis of water from the Paraíba River and CONAMA legislation 357

Metals	λ (nm)	Concentration ($mg.L^{-1}$)	CONAMA 357 ($mg.L^{-1}$)
Zn	213	0,05	0,18
Mn	279,48	0,05	0,10
Ag	328,07	0,10	0,01
Cu	324,75	0,11	0,009
Cr	235,87	0,20	0,05
Ni	232	0,53	0,025
Co	240,73	0,87	0,05
Pb	273,31	1,10	0,01
Fe	248,33	2,54	0,30

Reference: The authors (2024).

CONCLUSIONS

After the approach of this study, the work demonstrated the occurrence of metals in the water. It was found that, in addition to the waters of the Paraíba do Sul River presenting various pollutants, contamination by metals was also detected, with the most concerning finding being the identification of lead in concentrations exceeding the tolerance limits required by legislation. An intervention is necessary to assess whether the solid waste resulting from mineral processing along the banks of the Paraíba do Sul River in the city of Volta Redonda is contributing to this significant increase, given that lead is a bioaccumulative metal and its presence in the river can lead to various environmental problems and health issues for humans.

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COST-EFFECTIVE AND RELIABLE BITE FORCE MEASUREMENT APPARATUS

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ABSTRACT

Bite force measurements are particularly important across different age groups. By analyzing bite force in these specific contexts, clinicians can better tailor treatments and improve patient outcomes in terms of comfort and functionality. To develop a low-cost and effective bite force device. Central to the apparatus is the load cell, which is meticulously milled from stainless steel to ensure durability and accuracy. The load cell serves as the primary sensor for measuring bite force, utilizing a full-bridge strain gauge configuration. The developed bite force apparatus demonstrates a significant advantage over commercial models in terms of cost and accessibility. Initial tests show less than 2% variance in repeated measurements, confirming the device's accuracy. The next step is to proceed with testing and validation. This study presents a cost-effective and reliable bite force measurement apparatus that enhances accessibility for clinical and research applications.

Keywords: *Bite force, dental health, load cell, strain gauge, clinical applications*

1. INTRODUCTION

Bite force refers to the amount of force exerted by the masticatory muscles during the process of biting or chewing. It is a critical parameter in both clinical and dental research, as it provides valuable insights into the functionality of the jaw muscles, teeth, and overall oral health. The measurement of bite force is widely used to assess the strength and endurance of the masticatory system, as well as to diagnose various dental and musculoskeletal conditions. Clinically, bite force measurement helps in evaluating the efficiency of prosthetic appliances.

To develop a low-cost and effective bite force device that can serve as a facilitator in the diagnosis, monitoring, and treatment of vulnerable populations.

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2. MATERIALS AND METHODS

2.1. Materials

The development involved a load cell (primary sensor) utilizing a full-bridge strain gauge configuration; a CAD model of the load cell was simulated on a computer to withstand an equivalent load of 75 kg; a 10-bit Analog-to-Digital Converter; a microcontroller system based on Arduino technology, and a mobile application, developed using the AI2 MIT App Inventor.

2.1. Methods

Central to the apparatus is the load cell, which is meticulously milled from stainless steel to ensure durability and accuracy. To enhance the accuracy and resolution of the measurements, the apparatus incorporates a 10-bit Analog-to-Digital

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Converter (ADC). By employing amplification circuitry, the weak signals from the strain gauge are boosted to ensure that even subtle changes in bite force can be accurately captured.

2.2.1. Microcontroller system

At the heart of the bite force measurement apparatus is a microcontroller system based on Arduino technology. The microcontroller processes the digitized bite force data and prepares it for transmission. A Bluetooth module is incorporated to facilitate real-time monitoring.

The microcontroller software is designed to efficiently manage the process of bite force measurement. The software operates by waiting for a command from the mobile application, which initiates the entire measurement process. The app sends a word command via Bluetooth to the microcontroller.

3. RESULTS AND DISCUSSION:

3.1. Results

The developed bite force apparatus demonstrates a significant advantage over commercial models in terms of cost and accessibility. Initial tests show less than 2% variance in repeated measurements, confirming the device's accuracy. Its adaptability allows it to accommodate various dental structures, ensuring comprehensive data collection across different populations. Regular assessments can help tailor prosthetic devices or treatments for elderly patients and guide early interventions for children. Furthermore, the device's affordability enables large-scale testing, facilitating studies on age-related dental changes and improving overall oral health strategies. The next step is to proceed with testing and validation.

3.2. Discussions

The next phase will involve comparing the results obtained from our device with those produced by commercial apparatuses, such as the Kratos DMD model. These comparisons will help assess the accuracy, reliability, and overall performance of the developed apparatus. Successful validation will ensure that the device meets clinical standards and is ready for broader application, offering a cost-effective and accessible tool for precise bite force measurement across diverse populations.

4. CONCLUSIONS:

This study presents a cost-effective and reliable bite force measurement apparatus that improves accessibility for both clinical and research applications, integrating advanced sensor technology with user-friendly software.

5. DECLARATIONS

5.1. Acknowledgements

Dental professionals and participants involved in the study for their cooperation and support.

5.2. Funding source

FAPERGS for the financial support received for this research project.

5.3. Open Access

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Cost-effective and reliable bite force measurement apparatus



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November/2024

Introduction

Bite force refers to the amount of force exerted by the masticatory muscles during the process of biting or chewing;

It is a critical parameter in both clinical and dental research, as it provides valuable insights into the functionality of the jaw muscles, teeth, and overall oral health;

The measurement of bite force is widely used to assess the strength and endurance of the masticatory system, as well as to diagnose various dental and musculoskeletal conditions;

By analyzing the bite force in these specific contexts, clinicians can better tailor treatments and improve patient outcomes in terms of comfort and functionality.



Objective

- The primary objective of this project is to develop a cost-effective bite force measurement apparatus utilizing a stainless steel load cell.

Materials and Methods

- **Development of the Load Cell**

Central to the apparatus is the load cell, which is meticulously milled from stainless steel to ensure durability and accuracy.

The load cell serves as the primary sensor for measuring bite force, utilizing a full-bridge strain gauge configuration. This setup effectively converts mechanical strain into electrical signals, allowing for precise measurement of the force exerted during biting.

Materials and Methods

• The CAD model of the load cell was simulated on a computer to withstand an equivalent load of 75 kg without material yielding, and after optimization, the prototype was manufactured:

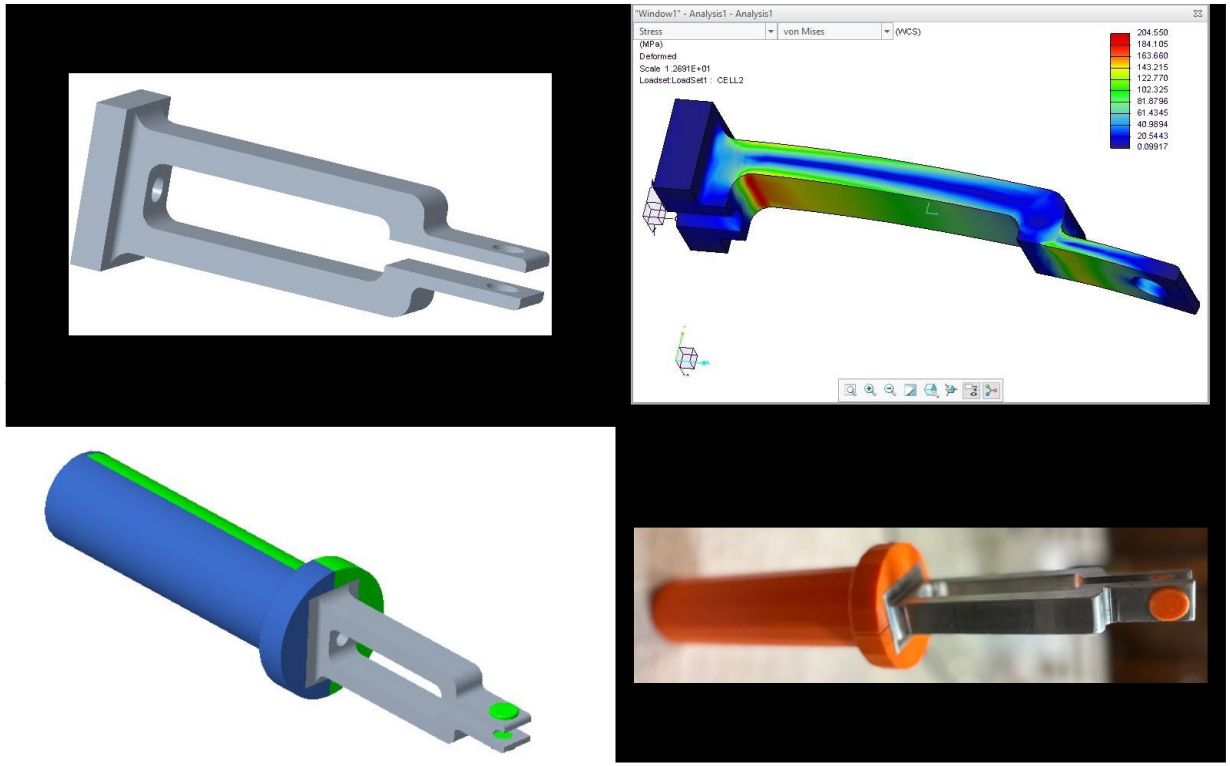


Figure 1. Proposed design for the load cell.

Materials and Methods

To enhance the accuracy and resolution of the measurements, the apparatus incorporates a 10-bit Analog-to-Digital Converter (ADC).

The ADC plays a crucial role in translating the analog signals generated by the load cell into digital data that can be processed by the microcontroller.

By employing amplification circuitry, the weak signals from the strain gauge are boosted to ensure that even subtle changes in bite force can be accurately captured.

At the heart of the bite force measurement apparatus is a microcontroller system based on Arduino technology.

The microcontroller processes the digitized bite force data and prepares it for transmission. To facilitate real-time monitoring, a Bluetooth module is incorporated, allowing the device to wirelessly transmit bite data to a mobile device

Materials and Methods

• The mobile application, developed using the AI2 MIT App Inventor, provides a user-friendly interface for visualizing and analyzing bite force data

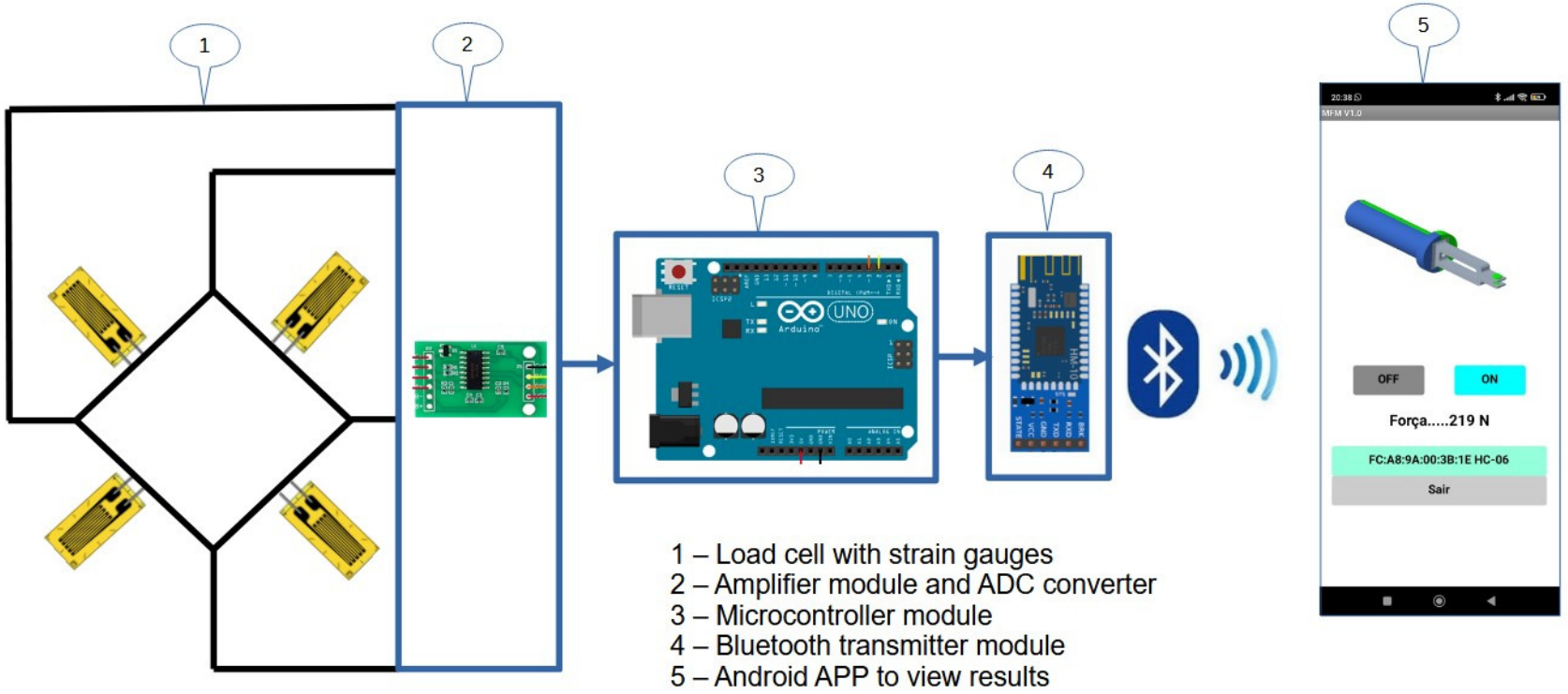


Figure 2. The electronic and software parts.

• Microcontroller Software Overview

The software operates by waiting for a command from the mobile application, which initiates the entire measurement process. The app sends a word command via Bluetooth to the microcontroller, signaling the start of the acquisition.

```
Start system:
  Initialize scale with DT and SCK pins
  Start USB and Bluetooth communication
  Send "Starting..." via USB and Bluetooth
  Set default scale and adjust tare (subtract current weight)

Main loop:
  Clear Bluetooth data buffer

  Check for received Bluetooth data:
    If data is available:
      Read character
      If character == 's':
        Do nothing
      If character == 'm':
        Start data capture for 5 seconds
        Store maximum value during that time
        Send maximum value via USB and Bluetooth

  Clear USB data buffer
```

Figure 3. The microcontroller main routines.

• Android Application Overview

The app requires the user to select a Bluetooth device for connection, establishing communication with the microcontroller system embedded in the bite force measurement apparatus. This initial step is crucial, as it ensures that the app is linked to the correct hardware for data acquisition.

Figure 4. shows the block design for the application buttons.

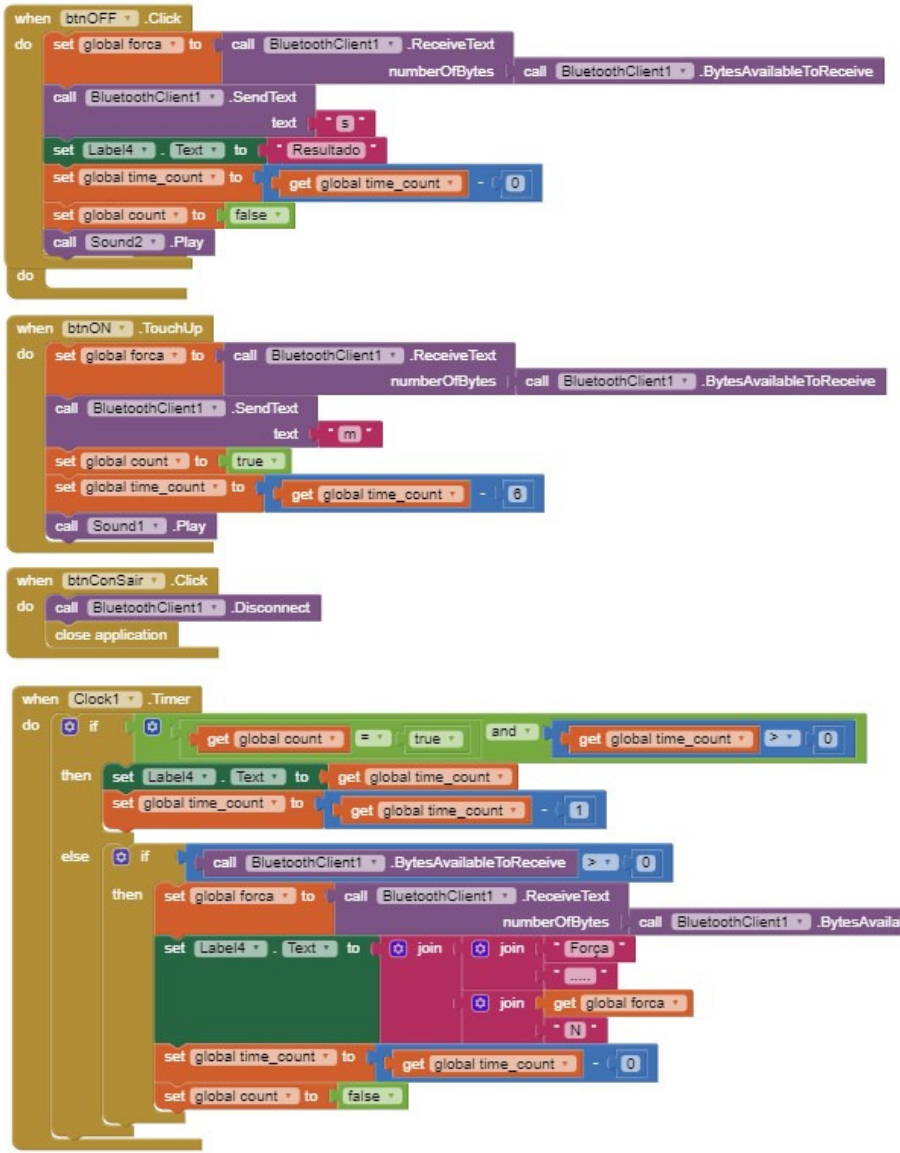


Figure 5. The block design for the routine to collect data via Bluetooth.

Results and Discussions

- The developed bite force apparatus demonstrates a significant advantage over commercial models in terms of cost and accessibility. Initial tests show less than 2% variance in repeated measurements, confirming the device's accuracy.

- Its adaptability allows it to accommodate various dental structures, ensuring comprehensive data collection across different populations.

- Regular assessments can help tailor prosthetic devices or treatments for elderly patients and guide early interventions for children.



Results and Discussions

- The next phase will involve comparing the results obtained from our device with those produced by commercial apparatuses, such as the Kratos DMD model.

- These comparisons will help assess the accuracy, reliability, and overall performance of the developed apparatus. Successful validation will ensure that the device meets clinical standards and is ready for broader application, offering a cost-effective and accessible tool for precise bite force measurement across diverse populations.

Conclusions

• This study presents a cost-effective and reliable bite force measurement apparatus that enhances accessibility for clinical and research applications.

• By integrating advanced sensor technology and user-friendly software, the device provides valuable insights into oral health, particularly in vulnerable populations. Regular bite force assessments can facilitate early diagnosis and effective treatment planning, ultimately improving patient outcomes.

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EFFECT OF INCREASING SOIL BULK DENSITY AND ORGANIC AMENDMENT ON SELECTED SOIL PROPERTIES, GROWTH, AND YIELD OF COWPEA

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ABSTRACT

A study at the Department of Agronomy, University of Ilorin, Nigeria examined the effect of bulk density and organic amendment on soil properties and cowpea yield using a two factorial Randomized Complete Block Design. Treatments included six levels of imposed bulk density (1.0, 1.20, 1.40, 1.60, 1.80 and 2.0 g×cm^{-3}) and two types of organic amendments (poultry droppings and cattle dung), applied at 10% per pot, with an un-amended control, replicated twice. The experiment was conducted twice during 2023. Parameters measured included total porosity, organic matter content, germination percentage, and yield. As soil bulk density increased from 1.2 to 2.0 g×cm^{-3}, total porosity declined by at least 7% for every 0.2 g×cm^{-3} increase; however, organic amendment significantly increased porosity by 18%. Increasing bulk density from 1.4 to 2.0 g×cm^{-3} reduced soil organic matter. Soil reaction changed significantly only at 2.0 g×cm^{-3} bulk density. Bulk density beyond 1.40 g×cm^{-3} significantly reduced cowpea germination by 10-28%. Bulk density from 1.40 to 2.0 g×cm^{-3} reduced cowpea yields by 16% per 0.2 g×cm^{-3} increase, with 1.40 g×cm^{-3} established as critical bulk density. Organic amendment significantly doubled cowpea yield, with no significant difference between poultry droppings and cattle dung effects.

Keywords: *Soil compaction; Organic manure; Sandy loam; Soil properties; Crop productivity*

1. INTRODUCTION

An increase in soil bulk density is a consequence of land intensification for crop farming. Among the efforts made to improve the food security of staple crops is the use of machines for farming activities. However, continuous use of these machines deforms the soil structure and increases soil bulk density, which negatively impacts soil porosity, seed germination rate, seedling emergence, impedance of root penetration, growth, and yield. Legumes are rich in protein and have become substitutes for animal protein (Bolarinwa et al., 2019), which has led to the intensification of land to increase their production. In the same vein, cowpea is an important legume used as food in almost all households and as animal feed in Africa (Mary et al., 2019), and to keep up with its increasing demands, there is, therefore, a need for sustainable soil management. Tillage practices are a crucial part of soil management systems that create ideal soil conditions for seed germination, seedling emergence, plant development, and unrestricted root growth (Licht and Al-Kaisi, 2005). However, when not well managed, tillage increases the soil bulk density, which can result to delayed seedling emergence, restricted root development, and poor growth and yield of crops (Igoni and Ayotamono, 2016).

Odey (2018) reported a positive correlation between tractor traffic with bulk density and a negative correlation with total porosity, whereas Thadshaini et al. (2018) observed a reduction in the yield of cowpea with an increase in soil bulk density to 1.6g/cm3. Amauri et al. (2007) reported that compaction of an Oxisol to penetration resistance greater than 2.33 Mpa and a bulk density greater than 1.51 g·cm^{-3} decreased soybean root development and consequently reduced yield. Igwe (2005) observed that the bulk density of soil can change if the packing arrangement of the soil aggregates changes, and the packing arrangement can be altered by changes in the soil aggregate shape and size (Blaire et al., 2003). Replacement of soil inorganic materials of high density with organic materials of low density can also lead to a change in the soil bulk density to a lesser extent

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(Igwe, 2005). The addition of organic matter to the topsoil by incorporating plant residues has been widely studied, and it is reported to improve bulk density and soil porosity (Ohu and Mamman, 2014; Shahgoli & Jannatkhah, 2018). Sustainability needs to be considered for food security to succeed. Therefore, it is pertinent to study the effect of increasing bulk density on soil and ways of ameliorating such effects, hence ensuring sustainable cowpea production.

2. MATERIALS AND METHODS

A two-factorial experiment in Randomized Complete Block Design was conducted twice during 2023 at the Agronomy Nursery Pavilion, University of Ilorin, Nigeria (N 8˚2910.788" E 4˚4038.5788"). Treatments included six bulk density levels (1.0, 1.2, 1.4, 1.6, 1.8, and 2.0 g×cm^{-3}) and two organic amendments (poultry dropping and cattle dung) with an unamended control. Soil masses were manually compacted into 3485 cm³ pots to achieve desired bulk densities, calculated as soil mass to volume ratio. Organic amendments were applied at 10% by soil mass per pot. Soil analysis included particle size (hydrometer method), pH (1:2.5 soil-liquid ratio), and organic carbon (dichromate wet digestion method), with organic matter calculated using 1.724 multiplication factor.

Plant data collected at maturity included height, leaf count, germination percentage, flowering time, pod count, and yield. Plant height was measured from soil surface to shoot tip. Data underwent analyses of variance using GenStat 17th edition, with means separated using least significant difference (5% probability). Regression analysis examined bulk density effects on cowpea grain yield.

Table 1: Quantity of the experimental soil and organic amendment

Bulk density (g·cm^{-1})	**Mass of soil (g)**	**Mass of Organic amendment (g)**
1.00	3119	311.9
1.20	3743	374.3
1.40	4367	436.7
1.60	4991	499.1
1.80	5615	561.5
2.00	6239	623.9

3. RESULTS AND DISCUSSION:

3.1 Characterization of the studied soil

Table 2 shows the experimental soil was a sandy loam (79.08% sand, 4% silt, and 16.92% clay) with a bulk density of 1.24 g·cm^{-3} which is below the critical values of bulk density at which root penetration is likely to be severely restricted in sandy loams (Jones, 1983). The soil was of high porosity (53.21%), which implies adequate aeration in the soil. The saturated hydraulic conductivity (Ksat) of the soil was moderately rapid with a slightly acidic (6.2) soil reaction, while poultry droppings (8.4) and cattle dung (8.1) were moderately alkaline. According to Metson (1961) rating of exchangeable bases, the concentration of calcium in the soil was low (3.64 cmol/kg) but moderate in poultry droppings (8.66 cmol/kg) and cattle dung (7.85 cmol/kg); magnesium concentration was moderate in soil (2.26 cmol/kg) but high in poultry droppings (4.39 cmol/kg) and cattle dung (4.18 cmol/kg); sodium concentration was moderate in soil (0.42 cmol/kg), poultry dropping (0.56 cmol/kg), and cattle dung (0.52 cmol/kg); while potassium was moderate in soil (0.37 cmol/kg) and high in both poultry droppings (0.91 cmol/kg) and cattle dung (0.76 cmol/kg). Using Bruce and Rayment (1982) rating, the soil total nitrogen (0.18%) was rated medium, while total nitrogen in poultry droppings (0.34%) and cattle dung (0.31%) was high. Available phosphorus in soil was low (6.81 mg/kg) but moderate in poultry droppings (10.72 mg/kg) and cattle dung (12.37 mg/kg).

Increasing bulk density and organic amendment significantly affected soil total porosity in both trials. As soil bulk density increased from 1.2 to 2.0 gcm^{-3}, total porosity declined by at least 7% for every 0.2 gcm^{-3} increase, similar to effects seen with repeated traffic over soils, reducing pore volume and causing soil degradation. Bulk density from 1.60 to 2.0 gcm^{-3} reduced soil total porosity from 36.92% to 30.70% across trials. While ideal soil porosity for crops varies by soil type, species, and climate, optimal ranges are typically 40-60%, with soybeans requiring 45-55%. Studies show bulk density fundamentally relates to soil porosity and hydraulic conductivity. Managing bulk density below 1.60 gcm^{-3} through reduced traffic and organic amendment positively affects soil porosity.

Organic amendment significantly increased porosity by minimum 18%, with poultry

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manure showing superior effects compared to cattle dung. The interaction between bulk density and amendments showed soils at 1.0 gcm^{-3} with poultry droppings achieved highest porosity (48.05% and 47.80% in trials), while 2.0 gcm^{-3} without amendments had lowest (25.91% and 25.66%). The 1.0 gcm^{-3} treatment involved soil loosening rather than compaction, creating more void space. Organic materials improve soil porosity, nutrient cycling, and water retention while reducing erosion.

Table 2: Characterization of soil in University of Ilorin and Properties of Soil Amendments

Properties	Soil	Poultry dropping	Cattle dung
Sand (%)	79.08	-	-
Silt (%)	4	-	-
Clay (%)	16.92	-	-
Textural class	Sandy loam	-	-
Bulk density (g/cm^3)	1.24	-	-
Total porosity (%)	53.21	-	-
Ksat (mm/hr)	66.3	-	-
MWD (mm)	84.8	-	-
pH (H_2O)	6.2	8.4	8.1
Ca (cmol/kg)	3.64	8.66	7.85
Mg (cmol/kg)	2.26	4.39	4.18
K (cmol/kg)	0.37	0.91	0.76
Na (cmol/kg)	0.42	0.56	0.52
Exchangeable acidity (cmol/kg)	0.63	1.12	1.25
N (%)	0.18	0.34	0.31
P (mg/kg)	6.81	10.72	12.37

N=Nitrogen; P=Phosphorus; Ca=Calcium; Mg: Magnesium; K=Potassium; Na=Sodium

3.2 Effects of increasing soil bulk density and organic amendment on soil properties

Increasing bulk density from 1.4 to 2.0 gcm^{-3} significantly reduced soil organic matter, but organic amendments increased it by factor of 2.5 from 1.36% in control soils. Poultry droppings produced higher organic matter (3.47% and 3.49%) compared to cattle dung (3.30% and 3.33%). Decreased organic matter at higher bulk densities relates to reduced pore spaces housing decomposer microorganisms. Organic manure application commonly increases soil organic matter and fertility, with organic matter showing negative correlation to bulk density and contributing to improved soil structural stability.

3.3 Effects of increasing Soil Bulk Density and Organic Amendment on Germination percentage and Yield of Cowpea

Bulk density beyond 1.40 gcm^{-3} significantly reduced cowpea seed germination by 10-28%, with maximum reduction at 2.0 gcm^{-3}. Organic amendment improved germination by 16-20% across trials. Control soils showed 100% germination at 1.0-1.4 gcm^{-3}, cattle dung-amended soils at 1.0-1.60 gcm^{-3}, and poultry dropping-amended soils at 1.0-1.80 gcm^{-3}. Lowest germination occurred in control soils at 2.0 gcm^{-3}. Reduced pore volume from increased bulk density decreased water and air availability, creating anoxic conditions and higher penetration resistance, affecting seed emergence.

Bulk density from 1.40-2.0 gcm^{-3} reduced cowpea yields by 16% per 0.2 gcm^{-3} increase. Peak yields occurred at 1.20 gcm^{-3}, with lower yields at 1.0 gcm^{-3} due to poor anchorage and nutrient leaching. Critical bulk density was 1.40 gcm^{-3}, beyond which maximum yield loss occurred. Yield reduction stemmed from poor water/nutrient mobility, aeration, root development, and physiological activities.

Organic amendment doubled cowpea yield, with no significant difference between poultry droppings and cattle dung. Amendment effectiveness was higher at bulk densities below 1.60 gcm^{-3}. Best yields occurred with 1.20 gcm^{-3} bulk density plus poultry droppings, while lowest yields were in unamended soils at 2.0 gcm^{-3}. A strong negative correlation ($r = 0.96$) between bulk density and yield produced the equation $y = -0.1063+1.0553$ ($R2 = 0.9293$). Maintaining bulk density between 1.20-1.40 gcm^{-3} with organic amendments increased yields 50-80% above regional potential. Improved physical properties enhanced soil fertility and crop productivity.

4. CONCLUSIONS:

This study concludes that (1) increasing bulk density beyond a critical value of 1.40 $g{\cdot}cm^{-3}$ significantly reduced soil organic matter content, total porosity, cowpea germination percentage, and yield, (2) organic amendment of compacted soils improves the bulk density, porosity, soil organic matter, germination percentage and yield of cowpea and (3) Poultry droppings significantly improved selected physical and chemical properties of the soil compared to cattle dung.
Based on the findings of this study, the application of either poultry dropping or cattle

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dung (10% of soil mass) should be used to ameliorate the effect of increasing bulk density on soil properties and, subsequently on cowpea yield. Further study should be done to examine the quantity of organic amendment that can improve cowpea yield at bulk density 2.0 g·cm^{-3}.

5. DECLARATIONS

5.1. Open Access

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Table 3: Effect of imposed bulk density and organic amendment on total porosity (%) of a soil in University of Ilorin, Nigeria

Factor A (Bulk Density gcm^{-3})	Trial 1				Trial 2			
	Factor B (Organic Amendment)				Factor B (Organic Amendment)			
	CO	**PD**	**CD**	**Mean**	**CO**	**PD**	**CD**	**Mean**
1.00	35.72^{gh}	48.05^{a}	44.78^{c}	**42.85**	36.48^{f}	47.80^{a}	44.91^{b}	**43.06**
1.20	42.14^{d}	46.67^{b}	41.64^{de}	**43.48**	41.89^{cd}	46.16^{b}	41.64^{cd}	**43.23**
1.40	34.72^{h}	42.39^{d}	41.51^{de}	**39.54**	34.34^{g}	42.64^{c}	41.51^{cd}	**39.50**
1.60	31.82^{i}	40.50^{e}	38.24^{f}	**36.86**	31.82^{h}	40.50^{d}	38.62^{e}	**36.98**
1.80	28.18^{j}	38.62^{f}	36.35^{g}	**34.38**	27.67^{i}	38.87^{e}	36.86^{f}	**34.47**
2.00	25.91^{k}	34.59^{h}	31.57^{i}	**30.69**	25.66^{j}	34.72^{g}	31.82^{h}	**30.73**
Mean	**33.08**	**41.80**	**39.01**		**32.98**	**41.78**	**39.22**	
	LSD$_{(0.05)}$ Factor A= 0.66 Factor B= 0.47 A x B= 1.14				**LSD$_{(0.05)}$ Factor A= 0.84 Factor B= 0.59 A x B= 1.46**			

Means with the same letter are not significantly different at 95% probability
CO=Control, PD=Poultry dropping, CD=Cattle dung

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Southern Science Conference, 2024.

EFFECT OF INCREASING SOIL BULK DENSITY AND ORGANIC AMENDMENT ON SELECTED SOIL PROPERTIES, GROWTH AND YIELD OF COWPEA

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September/2024

INTRODUCTION

- Increase in soil bulk density is a consequence of land intensification for crop farming;
- High demand for cowpea led to intensification of land for its production;
- Increased soil bulk density impaired soil and cowpea productivity (Igoni and Ayotamono, 2016);
- Incorporation of organic matter in soil is said to improve soil bulk density (Shahgoli & Jannatkhah, 2018);
- For food security to succeed, soil management sustainability should be considered.

OBJETIVE

To determine the effect of increasing bulk density and organic amendment on soil properties and cowpea production

METHODOLOGY

- A two factorial experiment in Randomized Complete Block Design
- The treatments we're six levels of bulk density (1.0 gcm-3, 1.2 gcm^{-3}, 1.4 gcm^{-3}, 1.6 gcm^{-3}, 1.8 gcm^{-3} and 2.0 gcm^{-3}) imposed and two types of organic amendments (poultry dropping and cattle dung) with an unamended treatment (control).
- Soil masses were manually compacted into pots of known volume (3485cm^3), the desired bulk density was then determined as a fraction of mass of the soil to its volume.
- The quantity of organic amendments applied was 10% percent by mass of soil per pot
- Parameters measured included, total porosity, organic matter content, germination percentage and yield.
- The data obtained were subjected to analyses of variance (ANOVA) using GenStat 17th edition and pertinent means were separated using the least significant difference (LSD) at 5% probability level.
- Regression of the soil bulk density against cowpea grain yield was also carried out.

RESULTS AND DISCUSSION

Table 1: Characterization of a soil in University of Ilorin and Properties of Soil Amendments

Properties	Soil	Poultry dropping	Cattle dung
Sand (%)	79.08	-	-
Silt (%)	4	-	-
Clay (%)	16.92	-	-
Textural class	Sandy loam	-	-
Bulk density (g/cm^3)	1.24	-	-
Total porosity (%)	53.21	-	-
Ksat (mm/hr)	66.3	-	-
MWD (mm)	84.8	-	-
pH (H_2O)	6.2	8.4	8.1
Ca (cmol/kg)	3.64	8.66	7.85
Mg (cmol/kg)	2.26	4.39	4.18
K (cmol/kg)	0.37	0.91	0.76
Na (cmol/kg)	0.42	0.56	0.52
Exchangeable acidity (cmol/kg)	0.63	1.12	1.25
N (%)	0.18	0.34	0.31
P (mg/kg)	6.81	10.72	12.37

RESULTS AND DISCUSSION

Table 2: Effect of imposed bulk density and organic amendment on total porosity (%) of a soil in University of Ilorin, Nigeria

Factor A (Bulk Density gcm^{-3})	Trial 1				Trial 2			
	Factor B (Organic Amendment)				Factor B (Organic Amendment)			
	CO	PD	CD	Mean	CO	PD	CD	Mean
1.00	35.72^{gh}	48.05^{a}	44.78^{c}	**42.85**	36.48^{f}	47.80^{a}	44.91^{b}	**43.06**
1.20	42.14^{d}	46.67^{b}	41.64^{de}	**43.48**	41.89^{cd}	46.16^{b}	41.64^{cd}	**43.23**
1.40	34.72^{h}	42.39^{d}	41.51^{de}	**39.54**	34.34^{g}	42.64^{c}	41.51^{cd}	**39.50**
1.60	31.82^{i}	40.50^{e}	38.24^{f}	**36.86**	31.82^{h}	40.50^{d}	38.62^{e}	**36.98**
1.80	28.18^{j}	38.62^{f}	36.35^{g}	**34.38**	27.67^{i}	38.87^{e}	36.86^{f}	**34.47**
2.00	25.91^{k}	34.59^{h}	31.57^{i}	**30.69**	25.66^{j}	34.72^{g}	31.82^{h}	**30.73**
Mean	**33.08**	**41.80**	**39.01**		**32.98**	**41.78**	**39.22**	
	$LSD_{(0.05)}$ Factor A= 0.66 Factor B= 0.47 A x B= 1.14				**$LSD_{(0.05)}$ Factor A= 0.84 Factor B= 0.59 A x B= 1.46**			

Means with the same letter are not significantly different at 95% probability
CO=Control, PD=Poultry dropping, CD=Cattle dung

- As the soil bulk density increased from 1.2 gcm^{-3} to 2.0 gcm^{-3}, total porosity continued to decline by at least 7% for every 0.2 gcm^{-3} increase in the two trials
- Subjecting the soil to organic amendment significantly ($p<0.05$) increased total porosity by a minimum of 18%
- The effect of poultry manure was significantly ($p<0.05$) higher than that of cattle dung.

RESULTS AND DISCUSSION

Table 3: Organic matter (%) of a soil in University of Ilorin as affected by increasing bulk density and organic amendments

Factor A (Bulk Density gcm^{-3})	Trial 1				Trial 2			
	Factor B (Organic Amendment)				Factor B (Organic Amendment)			
	CO	PD	CD	Mean	CO	PD	CD	Mean
1.00	1.89	4.12	3.84	**3.28**	1.92	4.18	3.87	**3.32**
1.20	1.95	4.25	3.99	**3.40**	1.97	4.31	4.05	**3.44**
1.40	1.78	4.38	4.06	**3.41**	1.83	4.32	4.06	**3.41**
1.60	1.36	3.51	3.41	**2.76**	1.40	3.51	3.43	**2.78**
1.80	0.62	2.25	2.18	**1.68**	0.65	2.30	2.22	**1.72**
2.00	0.56	2.29	2.30	**1.72**	0.53	2.35	2.32	**1.73**
Mean	**1.36**	**3.47**	**3.30**		**1.38**	**3.49**	**3.33**	
	$LSD_{(0.05)}$	**Factor A= 0.23 Factor B= 0.16 A x B= ns**			**$LSD_{(0.05)}$**	**Factor A= 0.22 Factor B= 0.15 A x B= ns**		

CO=Control, PD=Poultry dropping, CD=Cattle dung

- Increasing bulk density from 1.4 – 2.0 gcm^{-3} significantly reduced the soil organic matter
- Application of organic amendments increased the soil organic matter by at least a factor of about 2.5 from 1.36% in control soils.
- Soils amended with poultry droppings (3.47% and 3.49%) had higher organic matter content compared to those under cattle dung (3.30% and 3.33%) amendment in trial 1 and 2 respectively.

RESULTS AND DISCUSSION

Table 4: Germination percentage (%) of cowpea seed in a soil in University of Ilorin as affected by increasing bulk density and organic amendments

Factor A (Bulk Density gcm^{-3})	Trial 1				Trial 2			
	Factor B (Organic Amendment)				Factor B (Organic Amendment)			
	CO	PD	CD	Mean	CO	PD	CD	Mean
1.00	100.0^{a}	100.0^{a}	100.0^{a}	**100.0**	100.0^{a}	100.0^{a}	100.0^{a}	**100.0**
1.20	100.0^{a}	100.0^{a}	100.0^{a}	**100.0**	100.0^{a}	100.0^{a}	100.0^{a}	**100.0**
1.40	100.0^{a}	100.0^{a}	100.0^{a}	**100.0**	100.0^{a}	100.0^{a}	100.0^{a}	**100.0**
1.60	78.0^{b}	100.0^{a}	100.0^{a}	**92.7**	67.0^{cd}	100.0^{a}	100.0^{a}	**89.0**
1.80	55.7^{c}	100.0^{a}	89.0^{ab}	**81.6**	55.7^{de}	100.0^{a}	78.0^{bc}	**77.9**
2.00	44.3^{c}	89.0^{ab}	89.0^{ab}	**74.1**	44.3^{e}	89.0^{ab}	78.0^{bc}	**70.4**
Mean	**79.7**	**98.2**	**96.3**		**77.8**	**98.2**	**92.7**	
	$LSD_{(0.05)}$ Factor A= 10.9 Factor B= 7.7 A x B= 18.9				**$LSD_{(0.05)}$ Factor A= 9.96 Factor B= 7.04 A x B= 17.25**			

Means with the same letter are not significantly different at 95% probability
CO=Control, PD=Poultry dropping, CD=Cattle dung

- Increasing bulk density beyond 1.40 gcm^{-3} significantly ($p<0.05$) reduced germination percentage of cowpea seed by a minimum of 10% on the average and a maximum of 28% when the imposed bulk density was increased to 2.0 gcm^{-3}
- Subjecting such soils under bulk density treatment to organic amendment led to a minimum of 16% and a maximum of 20% increase in germination count on the average for the two trials.

RESULTS AND DISCUSSION

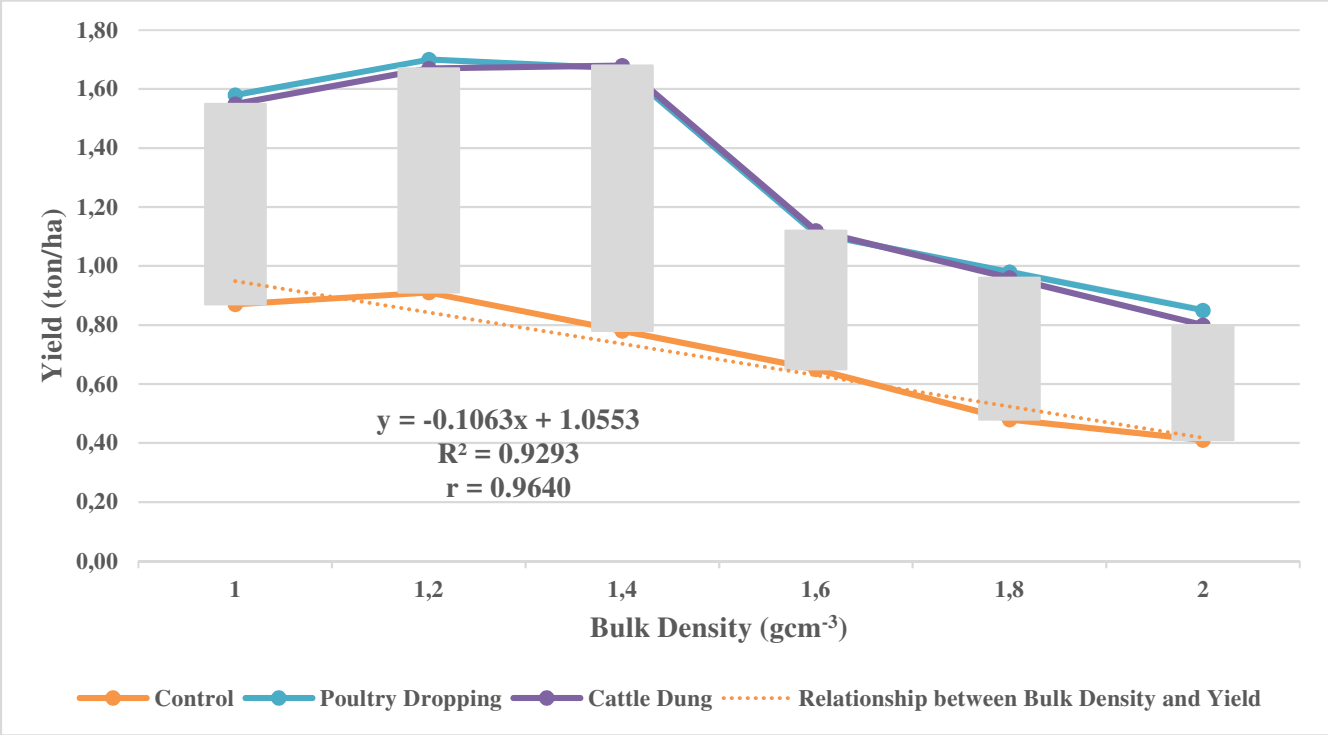


Figure 1: Relationship between bulk density and cowpea yield in amended and non-amended soil

- Imposed bulk density in the range of 1.40 – 2.0 gcm^{-3} significantly reduced cowpea yields by at least 16% for every 0.2 gcm^{-3} increases in bulk density.
- Yield was lower in soils under 1.0 gcm^{-3} bulk density treatment compared to those obtained in soils treated with 1.20 and 1.40 gcm^{-3}
- Organic amendment significantly ($p<0.05$) increased cowpea yield by a factor of two (2), with no significant difference between the effect of poultry droppings and cattle dung.

CONCLUSIONS

- Increasing bulk density beyond a critical value of 1.40 gcm-3 significantly reduced soil organic matter content, total porosity, cowpea germination percentage and yield;
- Organic amendment of compacted soils improves the bulk density, porosity, soil organic matter, germination percentage and yield of cowpea;
- Poultry droppings significantly improved selected physical and chemical properties of the soil compared to cattle dung;
- application of either poultry dropping or cattle dung (10% of soil mass) should be used to ameliorate effect of increasing bulk density on soil properties and subsequently on cowpea yield.

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STATISTICAL ANALYSIS OF BIOGAS PRODUCTION BETWEEN 2022 AND 2023 IN THE STATE OF RIO DE JANEIRO

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ABSTRACT

According to Cibiogás and the Energy Research Company, biomethane gas production is expanding in Brazil. It is estimated that the production value has increased by 87% over the past 10 years, with the largest production volume associated with the sanitation sector (74%), notably with landfills responsible for 96% of biogas production in this category. According to data from the National Petroleum Agency (ANP), in the years 2022 and 2023, there was an increase in biomethane gas production in the northeast and southeast regions. This study investigates the impact of increased biomethane gas production capacity in 2022 and 2023 specifically in the state of Rio de Janeiro. In 2022, a new government cycle began, so using Minitab software, we conducted a statistical analysis to determine if there were significant changes in biomethane production in landfills in the state of Rio de Janeiro, given recent developments in Brazil's sanitation sector.

Keywords: *Sanitary; Minitab; Solid Waste; Renewable Energy*

1. INTRODUÇÃO

A produção de biometano tem se destacado globalmente como fonte renovável de energia para redução de gases de efeito estufa, com aterros sanitários sendo cruciais na produção de biogás no Brasil.

Segundo a Agência Nacional de Petróleo, a produção de biometano cresce mais de 20% anualmente, principalmente na Europa e Estados Unidos, com Brasil, China e Índia triplicando sua produção desde 2015.

O Relatório Técnico 02-2021 do Programa de Energia Para o Brasil (BEP) indica que em 2019, o Brasil gerou 79 milhões de toneladas de resíduos urbanos, com 59,5% destinados a aterros sanitários (ABRELPE, 2020). A fração orgânica poderia produzir 1,9 bilhões de Nm³ de biogás anualmente em 811 aterros, com São Paulo, Minas Gerais e Rio de Janeiro tendo maior potencial.

Segundo o Banco Nacional de Desenvolvimento (2024), em 2022, vinte plantas (2,2% do total) produziam 22% do biogás nacional. Seis plantas receberam autorização da ANP desde 2021: Gás Verde, GNR Dois Arcos, GNR Fortaleza, ZEG Biogás e Energia, Cocal Energia e Sinergás GNV do Brasil (Cibiogás, 2022; IEA, 2023a).

O estudo analisa a produção de biometano no Rio de Janeiro em 2022-2023, usando software Minitab para análise estatística, com metodologia incluindo revisão bibliográfica e coleta de dados do período.

2. MATERIAIS E MÉTODOS

2.1. Materiais

1. Painel Dinâmico de Produtores de Biometano da ANP: Uma ferramenta interativa que fornece dados de produção de biometano declarados pelos agentes via

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Sistema de Informações de Movimentação de Produtos (Simp). Este painel inclui informações sobre a localização dos produtores, capacidades de produção autorizadas e matéria-prima utilizada.

2. Software Minitab: Utilizado para realizar análises estatísticas dos dados coletados. O Minitab foi empregado para testes de normalidade, homocedasticidade e comparação de médias entre os anos analisados.

3. Revisão Bibliográfica: Pesquisa realizada no Google Acadêmico para explorar a literatura sobre aterros sanitários e produção de biogás, abrangendo o período de 2020 a 2024. Foram identificados e utilizados registros relevantes para contextualizar o estudo, dando ênfase ao intervalo entre os anos de 2022 e 2023.

2.2. Métodos

A Agência Nacional de Petróleo (ANP) lançou o Painel Dinâmico de Produtores de Biometano, uma ferramenta interativa que permite visualizar dados de produção de biometano declarados pelos agentes via Sistema de Informações de Movimentação de Produtos (Simp).



Figura 1: Painel Dinâmico- Produtores de biometano

O painel inclui um mapa interativo com a localização de todos os produtores regulados pela ANP, suas capacidades de produção autorizadas e informações sobre a matéria-prima utilizada, com filtros disponíveis para análise por período específico.

Tendo como base estes dados, verifica-se o aumento da capacidade instalada de plantas de geração de biogás nas regiões nordeste e sudeste no período dos anos de 2022 e 2023 para verificar se o estado do Rio de Janeiro teve uma contribuição relevante.

Segundo a Revista Casa (2019), como apresentado na Figura 2, o aterro sanitário local em Seropédica é considerado o maior da América Latina, recebendo cerca de 10 mil toneladas de lixo diariamente. Estima-se que, quando estiver em operação constante, a usina produza cerca de 73 milhões de metros cúbicos de gás natural renovável por ano.



Figura 2: O aterro sanitário de Seropédica (Reprodução/Casa.com.br)

Dessa forma, a análise dos dados primeiramente com a apuração da capacidade de produção de biogás conforme os dados apresentados no Quadro 1.

Quadro 1 - Produção de biogás – região nordeste e sudeste

CAPACIDADE DE PRODUÇÃO (Milhões m³/dia)		
ANO	**MÊS**	**QUANTIDADE**
2022	JANEIRO	330.000
2023	DEZEMBRO	417.122

Fonte: Dados obtidos Painel Dinâmico Produtores de biometano - ANP (2024)

Neste quadro, estão disponibilizadas a capacidade de produção diária do gás de biometano em milhões por m³/dia.

Depois, utilizando ainda os dados do painel da ANP, foi gerado o segundo levantamento de dados, que apurou a produção de biogás no estado do Rio de Janeiro conforme dados do Quadro 2:

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Quadro 2 – Produção de biometano no Rio de Janeiro

ANO	MÊS	QUANTIDADE GÁS (m³/mês)
2022	JANEIRO	3161343250,000
2022	FEVEREIRO	2805443000,000
2022	MARÇO	2976531270,000
2022	ABRIL	3164608360,000
2022	MAIO	3119032110,000
2022	JUNHO	2596059140,000
2022	JULHO	2643183001,000
2022	AGOSTO	3099926000,000
2022	SETEMBRO	3212714250,000
2022	OUTUBRO	3651424010,000
2022	NOVEMBRO	3095227870,000
2022	DEZEMBRO	3384189770,000
2023	JANEIRO	3036906490,000
2023	FEVEREIRO	3191145180,000
2023	MARÇO	3441360350,000
2023	ABRIL	3454918780,000
2023	MAIO	3225840420,000
2023	JUNHO	4012685540,000
2023	JULHO	4028086730,000
2023	AGOSTO	3724225240,000
2023	SETEMBRO	3380932950,000
2023	OUTUBRO	3897429900,000
2023	NOVEMBRO	3544679294,000
2023	DEZEMBRO	3671877540,000

Fonte: Dados obtidos Painel Dinâmico Produtores de biometano - ANP (2024)

Para realização deste artigo foi feita uma pesquisa no Google Acadêmico para explorar a literatura sobre aterro sanitário e produção de biogás. A string de pesquisa utilizada foi (a evolução da produção de gás biometano no estado do Rio de Janeiro), abrangendo o período de 2020 a 2024.

Foram identificados 491 registros relevantes, após a primeira triagem a segunda triagem, analisando os títulos, a quantidade de registros ficou em 48. Na terceira triagem, com a análise dos resumos a quantidade foi para 5 registros, sendo que foram utilizados 2 neste artigo, e além destes dados, também foi utilizado literatura de apoio.

3. RESULTADO E DISCUSSÃO:

Ao tratar os dados disponíveis com o software do Minitab sobre a produção de gás biometano fornecido pela ANP, utilizando a tabela de estatística descritiva no Minitab para a análise exploratória de dados, obteve-se um resumo claro e detalhado das características dos dados para facilitar interpretações e decisões analíticas. Na Tabela 1, já com a análise realizada no citado aplicativo foi possível identificar a média, EP média, desvio padrão, mínimo, Q1, mediana, Q3 e máximo dos dados.

Com os dados, pode-se perceber que a média entre os anos de 2022 e 2023, do estado do Rio de Janeiro aparentemente apresentam diferença, porém para a afirmar é necessário elucidar através de dados utilizando o BoxPlot, apresentado na Tabela1.

O gráfico 1 do boxplot no Minitab é uma representação visual útil para visualizar a distribuição e a dispersão dos dados, além de identificar possíveis outliers.

Ele permite visualizar de forma rápida como os dados estão distribuídos em termos de quartis e mediana, facilita a identificação de valores atípicos que podem distorcer a análise estatística e é útil para comparar a distribuição de variáveis entre diferentes grupos ou categorias.

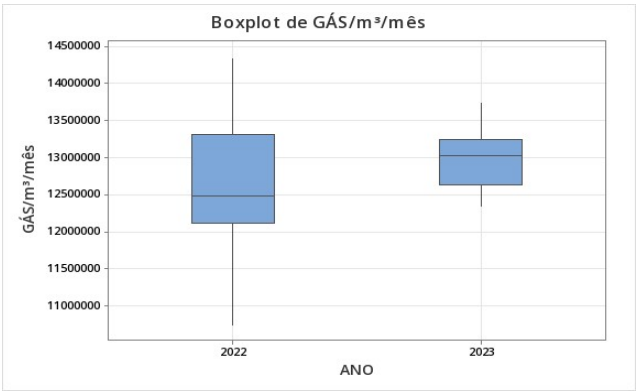


Gráfico 1. *Boxplot de gás/m³/mês*

Não foram observados outliers na análise.

Para o teste de normalidade foi utilizado Shapiro-Wilk devido ao número de observações ser menor que 50. Com valor-p maior que o nível de significância (0,05), não rejeitamos a hipótese nula, indicando consistência com distribuição normal. Em 2023, observou-se menor variação nos valores.

O valor p de 0,1 indica ausência de evidências significativas de desvio da normalidade, permitindo uso de métodos paramétricos para verificar homocedasticidade.

Teste para Duas Variâncias (gás/m³/mês versus ano): Nível de significância = 5%

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Hipóteses: H0: Grupos possuem igualdade de variâncias H1: Grupos não possuem igualdade de variâncias.

Os testes de Bonett e Levene, com valor p maior que o nível de significância, sugerem homocedasticidade. Os níveis de significância aproximaram-se do limiar entre 2022 e 2023.

Como os dados apresentam distribuição normal e igualdade de variâncias, utiliza-se o Teste T para comparação dos dois grupos.

Gráfico 3. Teste T para Duas Variâncias: gás/m³/mês versus ano

Hipótese nula H_0: $\mu_1 - \mu_2 = 0$

Hipótese alternativa H_1: $\mu_1 - \mu_2 \neq 0$

Valor-T	GL	Valor-p
-1,30	15	0,214

Por meio do resultado do Gráfico 3, como p-value = 0,214 é superior ao nível de significância estabelecida de 5% (0,05), aceita-se a hipótese nula de que não houve diferença significativa entre os anos de 2022 e 2023.

4. CONCLUSÃO:

Os aterros sanitários representam um grande desafio para os governos, mas também oferecem alternativas para a utilização do gás biometano gerado nesses locais. Neste estudo, observou-se que, embora a capacidade de produção de gás biometano tenha aumentado no biênio 2022/2023 nas regiões nordeste e sudeste, especificamente no estado do Rio de Janeiro, a análise estatística realizada não indicou uma diferença estatisticamente significativa na produção de biogás em comparação ao biênio 2021-2022.

5. DECLARAÇÕES

5.1. Acesso Aberto

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Tabela 1.

Variável	ANO	N	Nº	Média	EP Média	DesvPad	Mínimo	1º tri	Mediana	3º tri	Máximo
GÁS/m³/mês	2022	12	0	12640428	263456	912640	10752000	12125098	12482513	13308712	14329756
GÁS/m³/mês	2023	12	0	12979045	118941	409945	12351661	12642720	13028790	13253919	13734565

Gráfico 2. Teste de normalidade

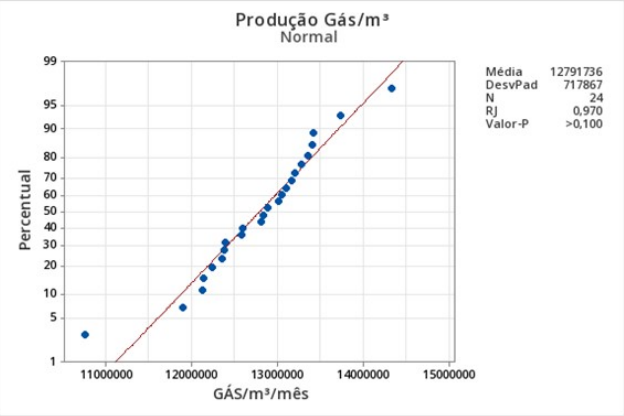
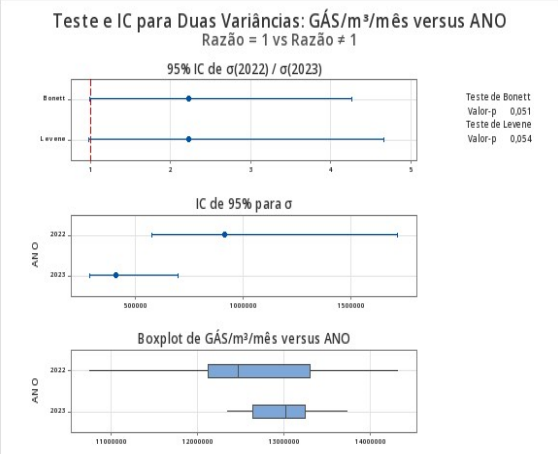


Gráfico 3. Teste e IC para Duas Variâncias: gás/m³/mês versus ano



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Southern Science Conference, 2024.

STATISTICAL ANALYSIS OF BIOGAS PRODUCTION BETWEEN 2022 AND 2023 IN THE STATE OF RIO DE JANEIRO

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Novembro/2024

INTRODUÇÃO

- A crescente produção de biometano tem se destacado globalmente, com um aumento anual superior a 20%, conforme relatado pela Agência Nacional de Petróleo.

- No contexto brasileiro, a gestão de resíduos sólidos urbanos é um tema crucial, evidenciado pelo Relatório Técnico 02-2021 do Programa de Energia Para o Brasil (BEP), que revela que, em 2019, apenas 59,5% dos 79 milhões de toneladas de resíduos urbanos gerados foram adequadamente destinados a aterros sanitários.

- Dentre esses resíduos, a fração orgânica, que totaliza cerca de 24,5 milhões de toneladas anuais, tem um potencial significativo para a produção de biogás, especialmente nos estados de São Paulo, Minas Gerais e Rio de Janeiro.

OBJETIVO

Este estudo analisa o impacto do aumento da capacidade de produção de biogás nos anos de 2022 e 2023, com foco no estado do Rio de Janeiro. Utilizando o software Minitab, a pesquisa realiza uma análise estatística para verificar se ocorreram mudanças significativas na produção de biogás.

METODOLOGIA

MATERIAIS E MÉTODOS

- Para este estudo, foram utilizados os materiais e métodos conforme descrito a seguir, sendo que a abordagem adotada incluiu uma revisão bibliográfica abrangente para contextualizar o tema, seguida pela coleta de dados relevantes sobre a produção de biometano no estado do Rio de Janeiro.

- Em seguida, os dados foram analisados utilizando o software Minitab, permitindo uma avaliação estatística rigorosa.

- A descrição detalhada dos materiais e métodos utilizados é apresentada a seguir, garantindo a transparência e a reprodutibilidade da pesquisa.

METODOLOGIA

Materiais

- Painel Dinâmico de Produtores de Biometano da ANP
- Software Minitab;
- Revisão Bibliográfica.

METODOLOGIA

- Dessa forma, a análise dos dados iniciou-se com a apuração da capacidade de produção de biogás conforme a Quadro 1 abaixo

- Com base nesses dados, o estudo examina o aumento da capacidade instalada de plantas de geração de biogás nas regiões Nordeste e Sudeste entre 2022 e 2023, focando na relevância da contribuição do estado do Rio de Janeiro.

Quadro 1 - Produção de biogás – região nordeste e sudeste

CAPACIDADE DE PRODUÇÃO (Milhões m³/dia)		
ANO	MÊS	QUANTIDADE
2022	JANEIRO	330.000
2023	DEZEMBRO	417.122

Fonte: Dados obtidos Painel Dinâmico Produtores de biometano - ANP (2024)

- Neste quadro estão disponibilizada a capacidade de produção diária do gás de biometano em milhões por m³/dia.

METODOLOGIA

- Depois, utilizando ainda os dados do painel da ANP, foi gerado o segundo levantamento de dados, que apurou a produção de biogás no estado do Rio de Janeiro conforme dados do quadro 2 ao lado:

- Para realização deste artigo, em conjunto, foi feita uma pesquisa no Google Acadêmico para explorar a literatura sobre aterro sanitário e produção de biogás. A string de pesquisa utilizada foi (a evolução da produção de gás biometano no estado do Rio de Janeiro), abrangendo o período de 2020 a 2024.

Quadro 2 – Produção de biometano no Rio de Janeiro

ANO	MES	QUANTIDADE GAS (m^3/mês)
2022	JANEIRO	3161343250,000
2022	FEVEREIRO	2805443000,000
2022	MARÇO	2976531270,000
2022	ABRIL	3164608360,000
2022	MAIO	3119032110,000
2022	JUNHO	2596059140,000
2022	JULHO	2643183001,000
2022	AGOSTO	3099926000,000
2022	SETEMBRO	3212714250,000
2022	OUTUBRO	3651424010,000
2022	NOVEMBRO	3095227870,000
2022	DEZEMBRO	3384189770,000
2023	JANEIRO	3036906490,000
2023	FEVEREIRO	3191145180,000
2023	MARÇO	3441360350,000
2023	ABRIL	3454918780,000
2023	MAIO	3225840420,000
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2023	JULHO	4028086730,000
2023	AGOSTO	3724225240,000
2023	SETEMBRO	3380932950,000
2023	OUTUBRO	3897429900,000
2023	NOVEMBRO	3544679294,000
2023	DEZEMBRO	3671877540,000

Fonte: Dados obtidos Painel Dinâmico Produtores de biometano - ANP (2024)

RESULTADOS E DISCUSSÃO

- Através da tabela de estatísticas descritivas, gerada através do Minitab, foi possível obter um resumo detalhado das características dos dados, facilitando assim as interpretações e decisões analíticas.

- Na Tabela 1, que apresenta os resultados da análise, foram identificados os seguintes parâmetros estatísticos: média, erro padrão da média (EP média), desvio padrão, valor mínimo, primeiro quartil (Q1), mediana, terceiro quartil (Q3) e valor máximo.

Tabela 1. Estatística descritiva: gás/m³/mês

Variável	ANO	N	N*	Média	EP Média	DesvPad	Mínimo	1º tri	Mediana	3º tri	Máximo
GÁS/m³/mês	2022	12	0	12604428	263456	912640	10752000	12125098	12482513	13308732	14329756
	2023	12	0	12979045	118341	409945	12351661	12642720	13028790	13253919	13734565

Fonte: os autores (2024)

RESULTADOS E DISCUSSÃO

- Com os dados, pode-se perceber que a média entre os anos de 2022 e 2023, do estado do Rio de Janeiro aparentemente apresentam diferença, porém para a afirmar é necessário elucidar através de dados utilizando o BoxPlot, apresentado na Figura1.

- Neste caso, podemos observar que não houve outliers.

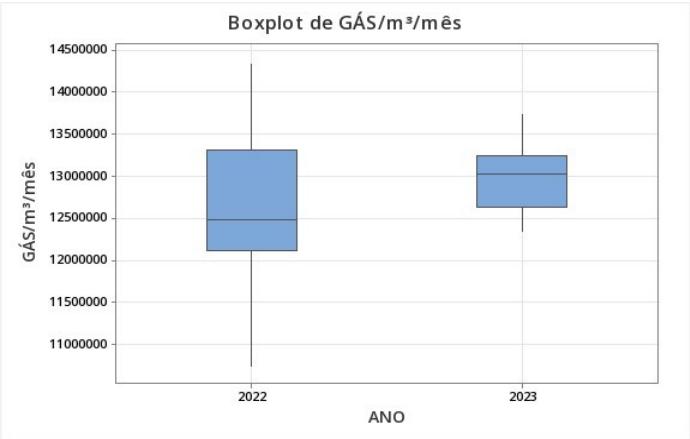
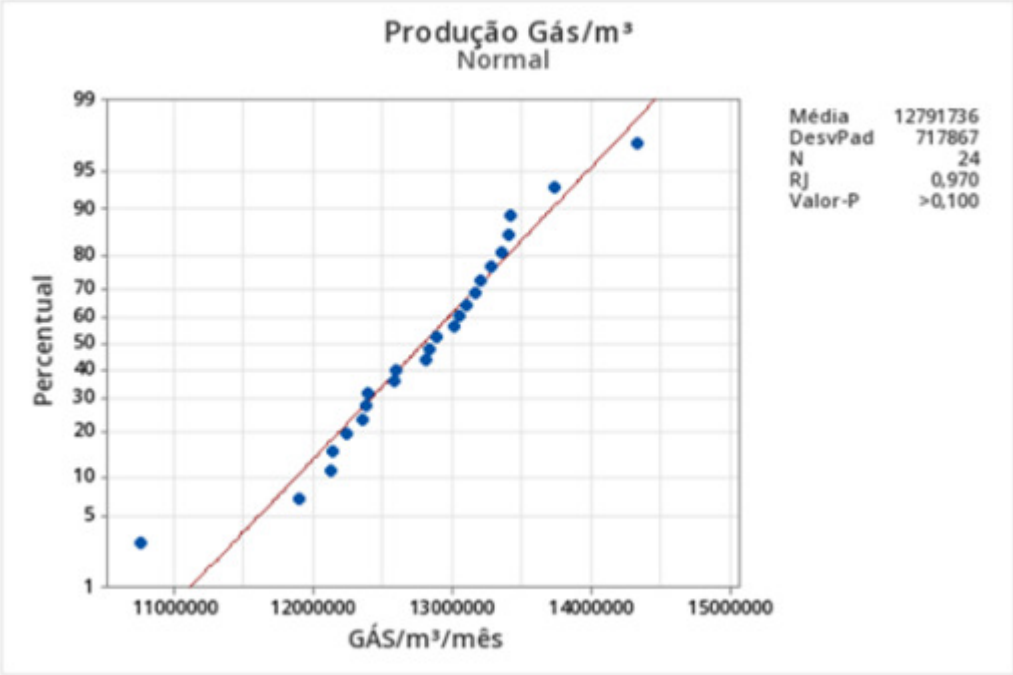


Figure 1. *Boxplot de gás/m³/mês*

RESULTADOS E DISCUSSÃO

. Para determinar o teste de normalidade (gráfico 2) foi utilizado shapiro wilk para obter o valor-p, considerando que as ocorrências não ultrapassam 50 observações. .

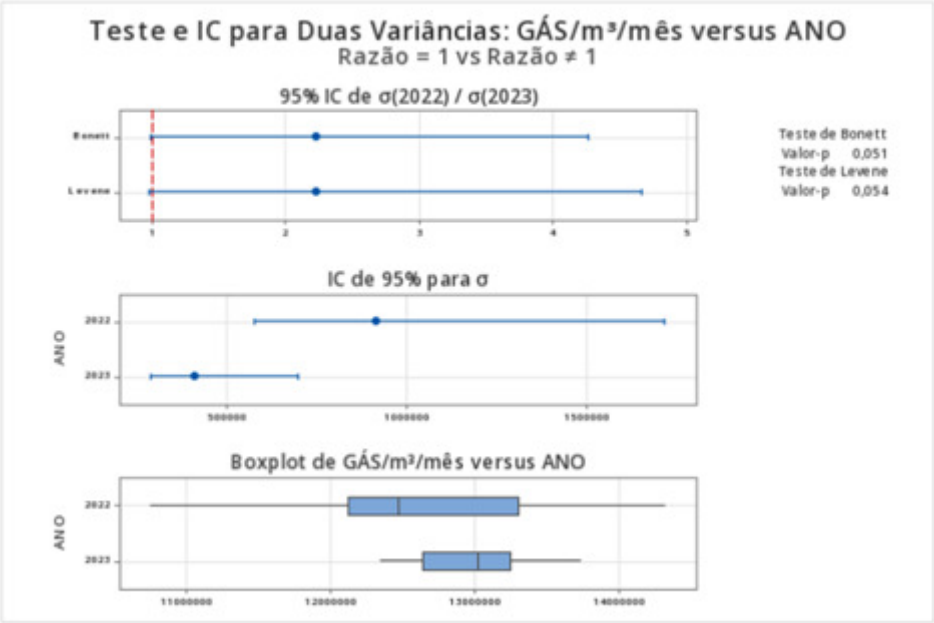
Gráfico 2. Teste de normalidade



RESULTADOS E DISCUSSÃO

Para finalizar o estudo e verificar se as amostras são paramétricas, como os dados apresentam distribuição normal e igualdade de variâncias, deve-se utilizar um método estatístico paramétrico para a comparação dos grupos.

Gráfico 3. teste e IC para Duas Variâncias: gás/m³/mês versus ano



Através do resultado do Gráfico 3, como p-value = 0,214 é superior ao nível de significância estabelecida de 5% (0,05), aceita-se a hipótese nula de que não houve diferença significativa entre os anos de 2022 e 2023.

CONCLUSÕES

- Os aterros sanitários representam um grande desafio para os governos, mas também oferecem alternativas para a utilização do gás biometano gerado nesses locais.

- Neste estudo, observou-se que, embora a capacidade de produção de gás biometano tenha aumentado no biênio 2022/2023 nas regiões nordeste e sudeste, especificamente no estado do Rio de Janeiro, a análise estatística realizada não indicou uma diferença estatisticamente significativa na produção de biogás em comparação ao biênio 2022-2023.

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II SOUTHERN SCIENCE CONFERENCE
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SIMULTANEOUS DETERMINATION OF ASCORBIC ACID, URIC ACID, AND DOPAMINE ON CARBON NANOTUBE PASTE ELECTRODE

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ABSTRACT

Ascorbic acid (AA), uric acid (UA), and dopamine (DA) play crucial roles in human metabolism. These substances coexist in biological fluids, and their levels are directly associated with various pathologies. A significant problem encountered in the direct and simultaneous electrochemical detection of AA, UA, and DA is that these species present very close oxidation potentials on most electrode materials, leading to an overlap in the voltammetric response. The goal of this work was to determine the concentration of AA, UA, and DA in a natural water sample on a carbon nanotube paste electrode (CNTPE). All voltammetric measurements were performed on a μAutolab potentiostat/galvanostat (Metrohm) connected to an electrochemical cell of three electrodes: working, reference (Ag/AgCl, $KCl_{3.0M}$), and auxiliary (platinum). The working electrode was handmade in our laboratory. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were used for the electroanalytical study. The linear ranges for the simultaneous determination of AA, DA, and UA by DPV were 0.45 – 1.0 mM, 50 – 200 μM, and 10 – 90 μM, respectively. The limits of detection for AA, DA, and UA were 7.97 mM; 8.57 μM, and 5.96 μM, respectively. Relative standard deviations (RSD) were 4.6; 2.8, and 1.6% for 0.45 mM of AA, 50 μM of DA, and 50 μM of UA. The oxidation mechanism of AA, UA, and DA involves 2 electrons and 2 protons. Electrochemical detection of DA in the presence of high levels of AA on carbon-based electrodes becomes difficult due to the catalytic oxidation of AA by DA. For these three molecules, it was observed that the oxidation peak currents increased with increasing concentration. CNTPE allowed the separation of ternary mixture oxidation peaks of the AA, UA, and DA by CV and, when associated with DPV, allowed the simultaneous quantitative determination of AA, UA, and DA.

Keywords: *catecholamines; cyclic voltammetry; differential pulse voltammetry*.

1. INTRODUCTION

Ascorbic acid (AA), uric acid (UA), and dopamine (DA) play crucial roles in human metabolism. These substances coexist in biological fluids (e.g., blood and urine), and their levels are directly associated with various pathologies. Thus, individual or simultaneous determination of these molecules is an essential issue in biomedical chemistry and pathological and diagnostic research. A significant problem encountered in the direct and simultaneous electrochemical detection of AA, AU, and DA is that they present very close oxidation potentials on most electrode materials, leading to an overlap in the voltammetric response (Oliveira, 2012).

The multiwalled carbon nanotubes (MWCNTs) are produced at low cost, and compared to most commercially available sensors based on metal oxides, silicon, and other materials, sensors based on carbon nanotubes (CNT) have the following advantages: high electrical conductivity and consequently decreased resistance to charge transfer; excellent chemical stability; broad application potential as molecular electronic components; the possibility of functionalization due to the presence of carboxylic groups; high sensitivity, because of large surface area, CNT can be used to immobilize enzymes, to maintain high biological activity; fast response time, have a remarkable ability to mediate electron transfer kinetics quickly; lower redox reaction potential and less surface fouling effects and high

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stability and lifetime (Pinho Júnior, 2016).

To this end, several techniques have been used to detect DA, AA, and UA, such as fluorimetry, chemiluminescence, ion exchange chromatography, high-performance liquid chromatography, ultraviolet-visible spectroscopy, and capillary electrophoresis. These techniques may present some disadvantages or inconveniences, as they are often complicated and often require pre-treatment of the sample, long analysis time, or a large number of organic solvents, which, in addition to being expensive, lead to the generation of a large amount of toxic waste. In this sense, electrochemical methods have received great attention due to their various advantages, such as low cost, high sensitivity and selectivity, speed of analysis, and ease of operation. Furthermore, these methods can be miniaturized and automated, enabling the construction of portable devices that allow rapid and efficient analysis of substances *in situ* (Oliveira, 2012).

The main goal of this work was to determine the concentration of ascorbic acid, uric acid, and dopamine on carbon nanotube paste electrodes (CNTPE).

2. MATERIALS AND METHODS

2.1. Materials

Potassium ferricyanide $K_4[Fe(CN)_6]$, NaOH, KNO_3, dibasic sodium phosphate, monobasic potassium phosphate, ascorbic acid, and H_3PO_4, purchased from Vetec®; HNO_3, dopamine (DA), multiwalled carbon nanotubes, and mineral oil (Nujol) purchased from Sigma-Aldrich®, all reagents were grade P.A.

Phosphate buffers 0.10 M (pH = 7.0) and 50 mM (pH = 4.0), KCl 0.1 M, $K_4[Fe(CN)_6]$ 1.0 mM, stock solutions of ascorbic acid (AA) 200 ppm, 1762 ppm and 10 mM (phosphate buffer 50 mM), dopamine (DA) 200 ppm, and 0.010 M (phosphate buffer 0.050 M), uric acid (UA) 1.0 mM (NaOH 0.1 M) and NaOH 2.0 M. All solutions were prepared with deionized water and pH were measured in a pHmeter (Metrohm).

2.2. Methods

All voltammetric measurements were performed on a μAutolab potentiostat/galvanostat (Metrohm) connected to an electrochemical cell (25.0 mL) of three electrodes: working, reference (Ag/AgCl, $KCl_{3.0M}$) and auxiliary (platinum). Voltammetric measurements were recorded with the Nova 2.1.5 software. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were used for the electroanalytical study. Before each test, the solutions were always purged with N_2 gas for 5 minutes.

The working electrode was handmade in our laboratory by introducing a brass wire into a Teflon® cylinder, leaving a small space for placing the electrode material paste: carbon nanotubes (CNT) + mineral oil. A preliminary study optimized the voltammetric working conditions: better buffer, CNT + oil ratio, and sweeping speed. The phosphate buffer was chosen because several authors (Yao et al., 2007; Lin et al., 2008) claim to be the most used and appropriate for this study.

Another optimized condition was the proportion of CNT and mineral oil for paste formation. The proportion chosen was 50%CNT: 50%mineral oil (m/m), as in this case, the paste had better adhesion and consistency than the proportion 65%CNT: 35%mineral oil (m/m). Regarding the scanning speed, due to the oxidation of DA presenting a slow electron transfer kinetics, the voltammetric recordings were carried out at 10 $mV \cdot s^{-1}$. The following proportions were used to prepare the paste: 50% CNT + 50% mineral oil and 65% CNT + 35% mineral oil.

Before using CNTPE, it is necessary to estimate the effective surface area of this electrode, as the surface area occupied by carbon nanotubes is unknown. The area was estimated from data obtained by cyclic voltammetry for the reversible pair $Fe(CN)_6^{4-}/Fe(CN)_6^{3-}$ and Randles-Sevcik equation (Brett & Brett, 1996). The effective area (*A*) of the CNTPE was estimated to be 0.084 cm^2.

3. RESULTS AND DISCUSSION

3.1. Results

In the study of electrochemical behavior, 50 mM phosphate buffer (pH = 4.0) was used as a supporting electrolyte; according to Yao et al. (2007), under these conditions, there is an improvement in the electrocatalytic activity for the oxidations of dopamine (DA), uric acid (UA) and ascorbic acid (AA), facilitating the lowering of the excess potential of DA. Initially, this study was carried out using cyclic voltammetry. A mixture of these three analytes with concentrations: AA 70 μM; UA 10 μM, and DA 20 μM were used to observe each species' individual behavior.

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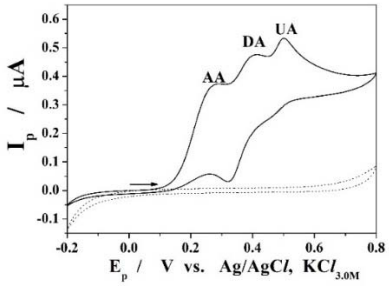


Figure 1. Cyclic voltammograms were recorded on CNTPE in 50 mM phosphate buffer (pH = 4.0) and mixture: 70 µM AA + UA 10 µM + DA 20 µM. Experimental: $E_i = E_f = 0.0$ V; $E_{\lambda1} = -0.20$ V; $E_{\lambda2} = 0.80$ V, and $\nu = 10$ mV.s^{-1}. Source: the authors.

It's possible to observe in Figure 1 the presence of all perfectly separated oxidation and reduction peaks. However, they present low currents. Therefore, this CNTPE, without chemical modification, could reproduce the records of modified electrode surfaces described in the literature (Yao et al., 2007; Lin et al., 2008).

As can be seen in Figure 2, three AA, DA, and UA oxidation peaks can be observed at different potentials of 200 mV, 380 mV, and 470 mV, respectively, with a potential difference between AA and DA of 180 mV and 90 mV between DA and UA. Since differential pulse voltammetry (DPV) has higher current sensitivity and better resolution than cyclic voltammetry, DPV was used for the electroanalytical determination of DA, AA, and UA on the CNTPE.

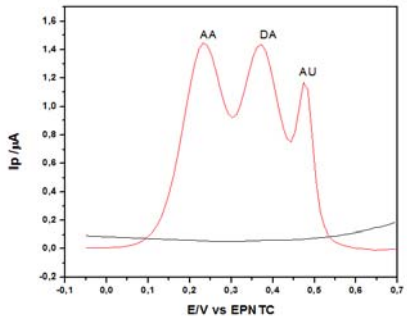


Figure 2. Differential pulse voltammograms were recorded over CNTPE in 50 mM phosphate buffer (pH = 4.0) containing 70 µM AA, 10 µM UA, and 20 µM DA. Experimental: $\nu = 5.0$ mV·s^{-1}, $A_p = 20$ mV, and $\Delta E_i = 10$ mV. Source: the authors.

Three separate recordings were made once the experimental parameters for using DPV were defined. For each one, the concentration of one of the analytes was increased with successive additions of the solution of one of the analytes. In contrast, the concentrations of the other two species were maintained constants. The results are shown in Figure 3.

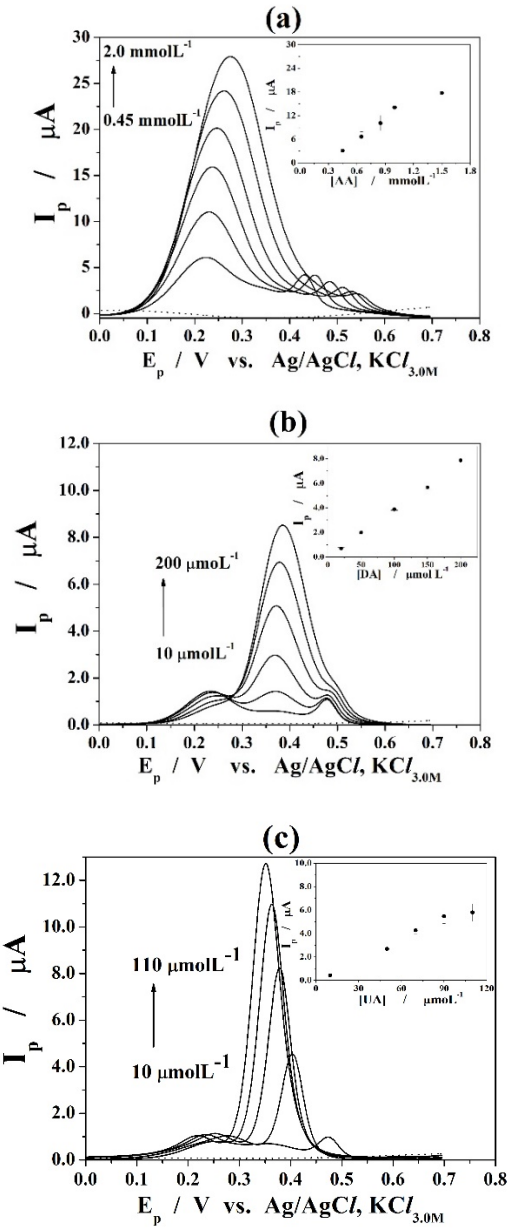


Figure 3. Differential pulse voltammograms were recorded over CNTPE in 50 mM phosphate buffer (pH = 4.0) with increasing additions of AA for 50 µM DA + 50 µM UA (a), DA for 10 µM UA + 70 µmol·L^{-1} AA (b), and UA for 40 µM AA + 10 µM DA (c). Experimental: $\nu = 5.0$ mV s^{-1}, $A_p = 20$ mV and $\Delta E_i = 10$ mV. Equations of the linear lines inserted in the figure, 6(a): I_p (µA) = –5.74 + 20.3 (± 0.8) µM [AA], $R^2 = 0.9953$; 6(b): I_p (µA) = –0.062 + 39.2 (± 0.00) *n*M [DA], $R^2 = 0.9986$; 6(c): I_p (µA) = -0.159 + 58.8 (± 0.00) *n*M [UA], $R^2 = 0.9947$. Source: the authors.

The linear ranges for the simultaneous determination of AA, DA, and UA by DPV were 0.45 – 1.0 mM, 50 – 200 µM and 10 – 90 µM, respectively (Fig. 3). The limits of detection (LOD) of the proposed method for determining AA, DA,

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and UA were 7.97 mM, 8.57 μM and 5.96 μM, respectively. The relative standard deviation of 10 successive scans was 4.6, 2.8, and 1.6% for 0.45 mM of AA, 50 μM of DA, and 50 μM of UA.

3.2. Discussion

Figure 2 presents peaks corresponding to AA and AU have potentials of 225 mV and 500 mV, respectively. The peak corresponding to DA presented a redox couple, which commonly only appears in this analyte (Lin et al., 2008).

The anodic and cathodic peak potentials for DA are 400 mV and 350 mV, respectively. The oxidation mechanism of AA, UA, and DA is a process that involves two electrons and 2 protons, and it agrees with the mechanism presented by Zhao et al. (2005). According to Lin et al. (2008), electrochemical detection of DA in the presence of high levels of AA on carbon-based electrodes becomes difficult due to the catalytic oxidation of AA by DA. But, as shown in Figure 3, the CNTPE achieved a good voltammetric response in the ternary mixture of these analytes.

During the additions of the standard to the ternary mixture (Fig. 3), it was observed that the potentials of AA and DA were shifted to more positive values, while UA behaved differently, as the potential was shifted to more negative values. It is unknown whether this new electrode surface causes this behavior or is due to another event, as this behavior has not yet been reported in the literature.

For the three molecules, AA, UA, and DA, it is observed that the oxidation peak currents increased with increasing concentration. No change in DA and UA currents was observed after increasing the concentration of AA; however, during the increasing addition of UA, it was observed that its potential was shifted to more negative values, leading UA to approach the oxidation potential of DA, causing possible interference in the quantitative determination of UA. In this case, UA needs to improve the conditions for analysis.

4. CONCLUSIONS

This work presents the advantages of CNTPE without chemical modification for the simultaneous determination of species of biological interest: ascorbic acid (AA), uric acid (UA), and dopamine (DA), as it showed good electrocatalytic activity for the oxidation of these species. Due to the chemical stability of carbon nanotubes, this electrode surface can be used in electroanalysis as an electron transfer mediator. Optimizing the voltammetric working conditions indicated that the electrode's electrochemical behavior strongly depends on the pH of the solution.

The CNTPE allowed the separation of the oxidation peaks of the ternary mixture of AA, UA, and DA by cyclic voltammetry. The limits of detection of the proposed method for determining AA, DA, and UA were 7.97 mM, 8.57 μM and 5.96 μM, respectively. Therefore, it showed quantitative application when associated with DPV, as it allows the simultaneous determination of these biological compounds in an aqueous solution with good sensitivity and selectivity.

5. DECLARATIONS

5.1. Acknowledgements

To funding agencies: CNPq for granting research grants. Hélcio Silva dos Santos and Murilo Sérgio da Silva Julião are grateful for the financial support provided by PQ/CNPq (Grant#: 306008/2022-0) and FUNCAP (Grant#: BP5-0197-00087.01.00122), respectively.

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Southern Science Conference, 2024.

Simultaneous Determination of Ascorbic Acid, Uric Acid, and Dopamine on Carbon Nanotube Paste Electrode

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November/2024

INTRODUCTION

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- Ascorbic acid (AA), uric acid (UA), and dopamine (DA) are crucial in metabolism.
- They are present in biological fluids, such as blood and urine.
- Problem: close oxidation potentials on conventional electrodes.
- This leads to signal overlap, making simultaneous detection difficult.

INTRODUCTION

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- Traditional methods are expensive and slow.
- Voltammetry is a faster alternative.
- The carbon nanotube paste electrode (CNTPE) has a high surface area.
- It will allow the separation of AA, UA, and DA oxidation peaks.
- It will enable simultaneous and accurate detection of these molecules.

AIM/OBJECTIVE

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- To develop an electrochemical method to simultaneously determine the concentrations of AA, UA, and DA in natural water samples using a carbon nanotube paste electrode (CNTPE).

METHODOLOGY

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All voltammetric measurements were recorded on a μAUTOLAB potentiostat/galvanostat (Metrohm) connected to a three-electrode electrochemical cell: working, reference (Ag/AgC*l*, KC*l* 3.0M), and auxiliary (platinum).

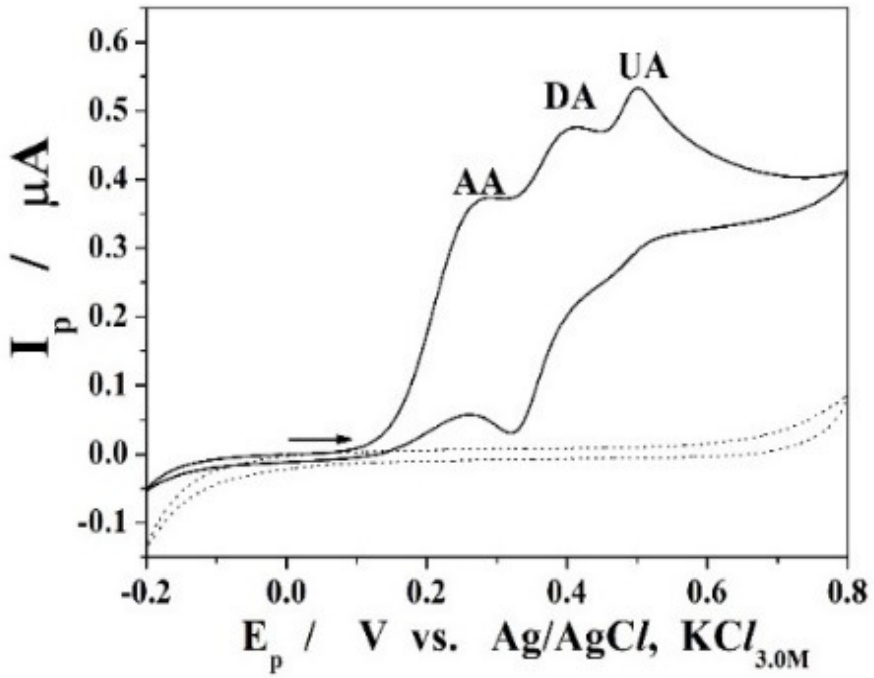
- Preparation of the working electrode: a brass wire was inserted into a Teflon cylinder, leaving space for the carbon nanotube paste and mineral oil.
- Techniques used: cyclic voltammetry (CV) and differential pulse voltammetry (DPV).
- Experimental conditions:

  supporting electrolyte: 50 mM phosphate buffer (pH = 4.0).

  scan rate: 10 mVs^{-1}.

RESULTS AND DISCUSSION

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Cyclic voltammetry (CV) separated oxidation peaks for AA, DA, and UA.
Peaks at 200 mV (AA), 380 mV (DA), and 470 mV (UA).

Figure 1. Cyclic voltammograms were recorded on CNTPE in 50 mM phosphate buffer (pH = 4.0) and mixture: 70 µM AA + UA 10 µM + DA 20 µM. Experimental: $E_i = E_f = 0.0$ V; $E_{\lambda 1} = -0.20$ V; $E_{\lambda 2} = 0.80$ V, and $\nu = 10$ mV.s^{-1}. Source: the authors.

RESULTS AND DISCUSSION

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- Differential pulse voltammetry (DPV) showed better sensitivity.
- Linear detection ranges:

AA: 0.45 – 1.0 mM
DA: 50 – 200 µM
UA: 10 – 90 µM

- Detection limits:

AA: 7.97 mM
DA: 8.57 µM
UA: 5.96 µM

- Relative standard deviations (RSD):

AA: 4.6%
DA: 2.8%
UA: 1.6%

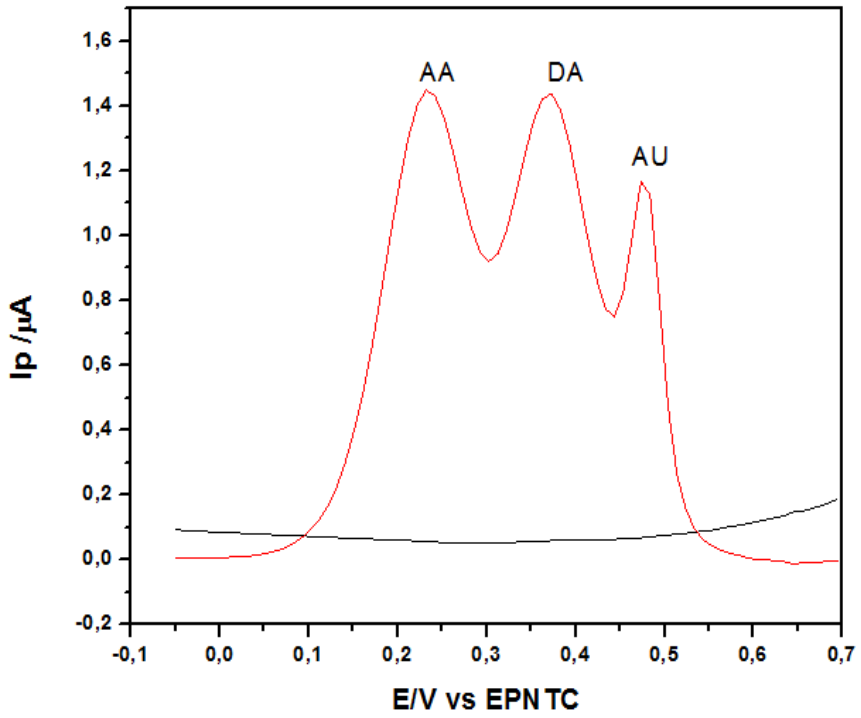


Figure 2. Differential pulse voltammograms were recorded over CNTPE in 50 mM phosphate buffer (pH = 4.0) containing 70 µM AA, 10 µM UA, and 20 µM DA. Experimental: ν = 5.0 mV·s^{-1}, A_p = 20 mV, and ΔE_i = 10 mV. Source: the authors.

RESULTS AND DISCUSSION

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- CNTPE efficiently separates oxidation peaks for AA, DA, and UA.
- Allows simultaneous detection of biologically important molecules.
- Highly sensitive and cost-effective method.
- Comparable or superior to traditional methods in terms of speed and selectivity.

The method enabled the simultaneous detection of AA, DA, and UA with high sensitivity, proving to be promising for biomedical and environmental applications.

RESULTS AND DISCUSSION

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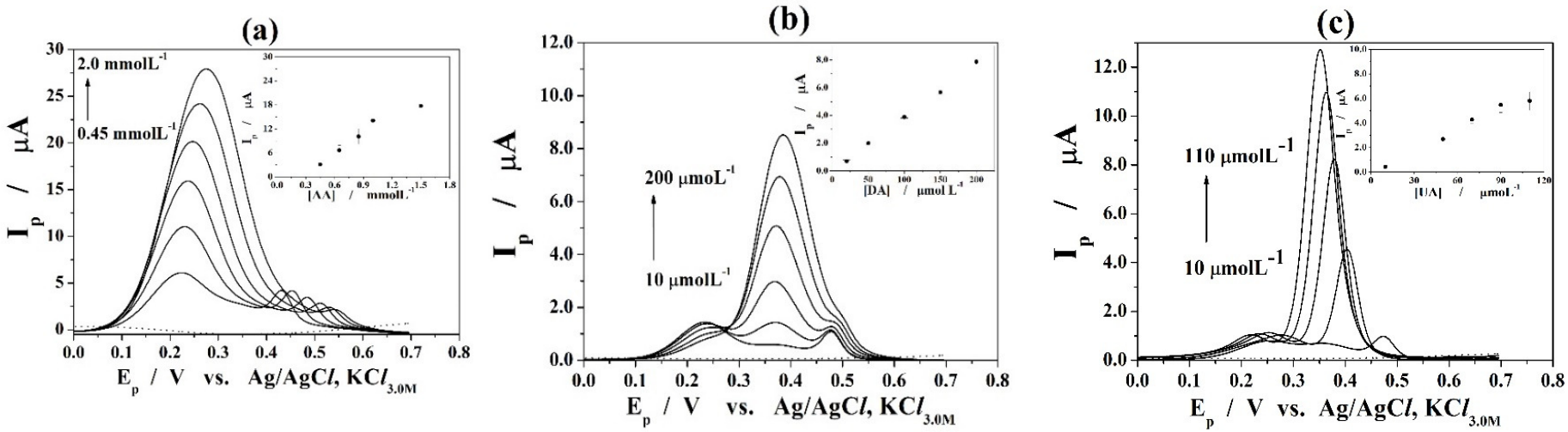


Figure 3. Differential pulse voltammograms were recorded over CNTPE in 50 mM phosphate buffer (pH = 4.0) with increasing additions of AA for 50 µM DA + 50 µM UA (a), DA for 10 µM UA + 70 µmol·L^{-1} AA (b), and UA for 40 µM AA + 10 µM DA (c). Experimental: ν = 5.0 mV s^{-1}, A_p = 20 mV and ΔE_i = 10 mV. Equations of the linear lines inserted in the figure, 6(a): I_p (µA) = –5.74 + 20.3 (± 0.8) µM [AA], R^2 = 0.9953; 6(b): I_p (µA) = –0.062 + 39.2 (± 0.00) *n*M [DA], R^2 = 0.9986; 6(c): I_p (µA) = -0.159 + 58.8 (± 0.00) *n*M [UA], R^2 = 0.9947. Source: the authors.

CONCLUSIONS

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The unmodified CNTPE exhibited excellent electrocatalytic activity, successfully separating the oxidation peaks of the three analytes. DPV allowed for accurate quantification of AA, DA, and UA in aqueous solutions, demonstrating good sensitivity and selectivity.

This method is an effective alternative for real-time electrochemical analysis.

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- Murilo Sergio da Silva Julião acknowledges financial support from the BPI/ FUNCAP (Grant#: BP5-0197-00087.01.00/22).

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EFFECTS OF PHYSIOTHERAPY ON THE FUNCTIONALITY OF PATIENTS WITH MULTIPLE SCLEROSIS

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ABSTRACT

Multiple sclerosis is a neurodegenerative disease that affects about 20.5 million people worldwide. This disease causes changes in the patient's functionality with symptoms such as fatigue and strength decrease muscle. Consequently, the progression of this disease requires a physiotherapeutic approach, considering its capacity to mitigate symptoms and functional limitation. Therefore, this study's aim is to describe the effects of physiotherapy on the functionality of patients with multiple sclerosis. This study consists of an integrative review, in which were used the Physiotherapy Evidence Database (PEDro), Biblioteca Virtual em Saúde (BVS), and PubMed databases in October 2024. The search descriptors used were: "Multiple Sclerosis", "Physical Therapy," and "Functional Status". The research restriction period of publication was 5 years (2019 to 2024). There has been an emphasis on treatments based on physical training, such as strength training for the upper limbs and respiratory muscle exercises, which led to significant improvements in cognitive and physical functions, as well as mitigation of the disease's main symptoms. Thus, other treatments had significant effects, such as Motor Neuron Activation Therapy, which led to an increase in brain activity and improved gait and functionality. In contrast, whole-body cryotherapy has shown to be beneficial for mental and physical health, reducing depressive symptoms and fatigue. For those reasons, physiotherapy presents a promising role in improving functionality in patients suffering from multiple sclerosis.

Keywords: *Neuroinflammatory diseases, Functional status, Therapy, Physical Exercise, Rehabilitation.*

1. INTRODUÇÃO

A esclerose múltipla (EM) consiste em uma doença neurodegenerativa crônica, progressiva, desmielinizante e autoimune, causando múltiplas lesões no Sistema Nervoso Central (SNC) devido à destruição da bainha de mielina dos neurônios (Almeida *et al*., 2022). Em consequência da doença, ocorre redução da velocidade de condução nervosa alterando a funcionalidade do indivíduo, causando sintomas como fadiga, prejuízos nos movimentos e na sensibilidade, fraqueza muscular, espasticidade e redução de equilíbrio (Schiewe *et al*., 2016).

De acordo com o ministério da saúde, o público-alvo afetado por essa doença são adultos na faixa etária de 20-50 anos de idade; no Brasil, a taxa de prevalência é de aproximadamente 8,69 por 100.000 habitantes (Ministério da Saúde, 2022).

Diante das dificuldades impostas pela EM e o comprometimento progressivo dos movimentos, os indivíduos têm uma perspectiva de incapacidade em lidar com a doença, adquirindo o sentimento de baixa autoestima, impotência, desamparo, confusão e solidão. Portanto, deve-se cuidar de todos os aspectos que englobam a saúde do indivíduo, manter equilíbrio na saúde física e psicológica, buscando melhorar a qualidade de vida do paciente (Pawik; Kowalska; Rymaszewska, 2019).

No tratamento da EM, são utilizados recursos farmacológicos com a finalidade de atenuar o processo inflamatório da patologia, porém intervenções fisioterapêuticas também têm se apresentado bastante relevantes no manejo da doença, minimizando as limitações e

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maximizando a capacidade funcional, promovendo uma qualidade de movimento, habilidades motoras, manutenção cognitiva e de força, coordenação, padrão de marcha e estabilidade postural. Ademais, a fisioterapia pode promover, impedir e retardar complicações secundárias da EM (Martins; Silva, 2022).

Tendo em vista que a EM afeta significativamente a funcionalidade, este estudo busca descrever os efeitos de tratamentos fisioterapêuticos, abordando diferentes técnicas e exercícios visando à melhora da qualidade de vida, incluindo impactos físicos, emocionais e sociais de pacientes com EM. A revisão realizada apresenta as comprovações existentes na íntegra, avaliando a aplicabilidade dessas intervenções.

2. MATERIAIS E MÉTODOS:

O estudo consiste em uma revisão integrativa da literatura, na qual foram utilizadas as bases de dados das plataformas Physiotherapy Evidence Database (PEDro), Biblioteca Virtual de Saúde (BVS) e PubMed em outubro de 2024; utilizando, respectivamente, os descritores: “Multiple Sclerosis”, “Physical Therapy” e “Fuctional Status”. A busca foi realizada com o período de restrição de 5 anos (2019 a 2024). Foram desclassificados artigos indisponíveis na íntegra, indexações duplicadas, estudos pediátricos, revisões sistemáticas e de literatura, teses e dissertações, relatos de casos e artigos em que não houve participação da fisioterapia. O escopo da pesquisa foi delimitado à luz da seguinte pergunta norteadora: “Como a atuação do fisioterapeuta contribui para a funcionalidade de pacientes portadores de esclerose múltipla?”. A triagem foi realizada por meio do fluxograma de Principais Itens para Relatar Revisões Sistemáticas e Meta-análises PRISMA, conforme demonstrado na figura 1.

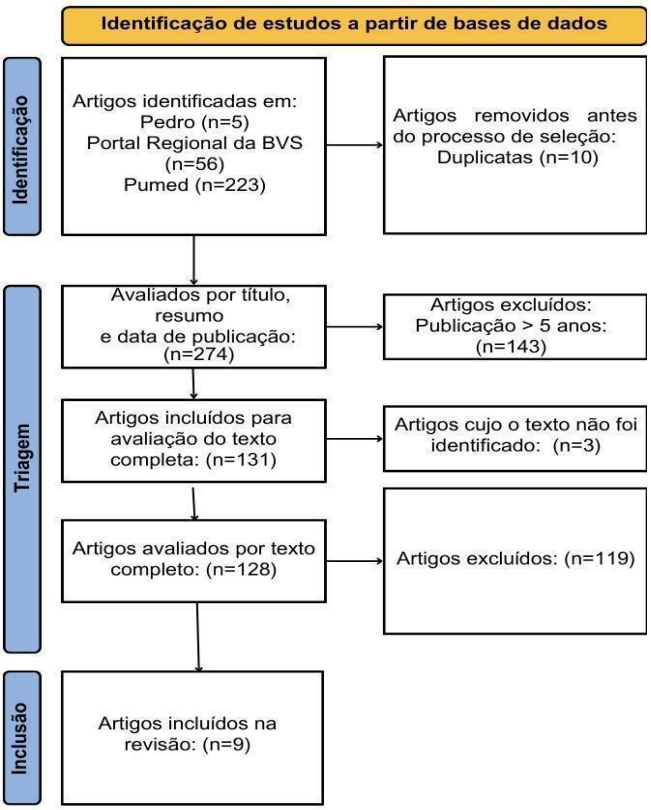


***Figura 1**. Fluxograma de triagem PRISMA.*

3. RESULTADOS E DISCUSSÕES

3.1. RESULTADOS:

Os estudos analisados demonstraram benefícios dos tratamentos fisioterapêuticos em portadores de EM, com melhorias funcionais e no bem-estar físico e psicológico.

O uso de exoesqueleto foi testado em 11 pessoas para redução de riscos de quedas, mostrando-se um recurso promissor (Sakel *et al*., 2022). Em outro estudo, exercícios de membros superiores e respiratórios foram avaliados através de testes de preensão palmar e escala EVA (Grubic Kezele *et al*. 2020).

A fisioterapia na síndrome da dor miofascial foi estudada comparando reflexoterapia com alongamento versus massagem terapêutica (Zinovyi M. Ostapyak *et al*., 2020). O treinamento combinado de força e exercício aeróbico mostrou melhorias no equilíbrio e redução da fadiga (Grazioli *et al*., 2019).

A crioterapia corporal com exercícios de resistência foi avaliada em três grupos (Pawik, Kowalska, Rymaszewska 2019), enquanto a estimulação magnética cervical foi testada para controle postural (Fawaz *et al*., 2022). A locomoção reflexa foi estudada com ressonância magnética funcional (Prochazkova *et al*., 2021).

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O programa Tai-Geiko foi avaliado para aspectos físicos e funcionais (Ultramari *et al*., 2020), e um estudo comparou yoga Iyengar com exercícios fisioterapêuticos em 12 sessões (Lysogorskaia *et al*., 2023).

Tabela 1. Resultados dos artigos coletados.

Autor	Tratamento usado	Resultado encontrado
Mohamed Sakel *et al*., 2022	Exoesqueleto	Melhora do equilíbrio, mobilidade articular, espasticidade e qualidade de vida.
Grubic Kezele *et al*., 2020	Exercícios respiratórios e de membros superiores	Melhora da dor física, independência funcional e pressão manual.
Zinovyi M Ostapyak *et al*., 2020	Reflexoterapia com alongamento muscular	Redução da espasticidade e da dor muscular.
Grazioli, Elisa *et al*., 2019	Treinamento de força nos membros superiores e inferiores e aeróbico	Melhora da marcha e atua na redução da depressão, fadiga e gravidade da doença.
Malwina Pawik, Joanna Kowalska, Joanna Rymaszewska. 2019	Crioterapia combinada com exercício de resistência	Reduziu os sintomas de depressão e melhorou o estado funcional e fadiga dos pacientes.
Fawaz, Shereen *et al*., 2022	Estimulação magnética cervical	Ajuda na melhora do equilíbrio e da deambulação funcional, diminuindo o risco de quedas.
Prochazkova, Marie *et al*., 2021	Locomoção reflexa Vojta (VRL) e terapia de ativação do programa motor (MPAT)	Aumento da atividade cerebral podendo envolver processos conectados com a ativação do movimento.
Ultramari, Viviane *et al*., 2020	Técnica de exercício Tai-Geiko	Melhoria de 12 variáveis em comparação a 3 do GC.
Lysogorskaia, Elena *et al*., 2023	3 grupos designados aleatoriamente para ioga, fisioterapia ou nenhum exercício	Melhora funcional física, atividade de vida, saúde mental e social em favor do grupo de ioga.

3.2. Discussões:

A análise dos resultados demonstrou o impacto positivo dos tratamentos fisioterapêuticos na funcionalidade dos portadores de EM. Os estudos sobre exoesqueleto (Sakel *et al*., 2022) e treinamentos para membros inferiores (Grazioli *et al*., 2019) reduziram o risco de quedas e melhoraram a deambulação.

O programa de exercícios combinados para membros superiores e respiração aumentou a independência funcional através da diminuição de citocinas pró-inflamatórias e aumento do fator neurotrófico cerebral (Tanja Grubić Kezele *et al*., 2019).

Para pacientes com síndrome miofascial na EM, a integração do alongamento e reflexoterapia melhorou o tônus muscular e bem-estar físico (Zinovyi M. Ostapyak *et al*., 2020). Os efeitos criogênicos contribuíram para redução da sobrecarga emocional (Tanno & Marcondes, 2002) e diminuição da dor (Rocha *et al*., 2007).

A estimulação magnética cervical usando Neurosoft melhorou locomoção, propriocepção e controle postural (Shereen I Fawaz *et al*., 2022). As terapias de locomoção reflexa demonstraram expansão cerebral e melhoria nas funções cognitivas (Prochazkova *et al*., 2021).

O Tai-Geiko beneficiou a velocidade de deslocamento e equilíbrio através de exercícios isométricos e aeróbicos (Ultramari *et al*., 2020), fatores importantes para atividades diárias (Farias; Albuquerque; Rech, 2012).

Quanto ao estudo comparativo entre yoga e fisioterapia, não houve diferença estatística significativa, porém a pesquisa apresentou limitações na amostragem que sugerem necessidade de novos estudos (Elena Lysogorskaia *et al*., 2023).

4. CONCLUSÕES:

Com este estudo, evidencia-se a perspectiva promissora dos efeitos da fisioterapia na funcionalidade de pacientes portadores de EM. De acordo com os achados dos artigos, verifica-se um grande potencial de tais terapias e protocolos de exercícios usados pelos fisioterapeutas, como o treinamento de força e a reflexoterapia, que contribuem significativamente para a melhora do funcionamento físico e da qualidade de vida.

Para mais, pode-se inferir a importância da atuação da fisioterapia, haja vista a sintomatologia presente em indivíduos com EM, como a perda de equilíbrio e dificuldades na deambulação. Dessa maneira, novas pesquisas nesse âmbito são

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essenciais ao desenvolvimento de novos protocolos fisioterapêuticos, a fim de minimizar a progressão desta patologia.

5. DECLARAÇÕES

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EFFECTS OF PHYSIOTHERAPY ON THE FUNCTIONALITY OF PATIENTS WITH MULTIPLE SCLEROSIS

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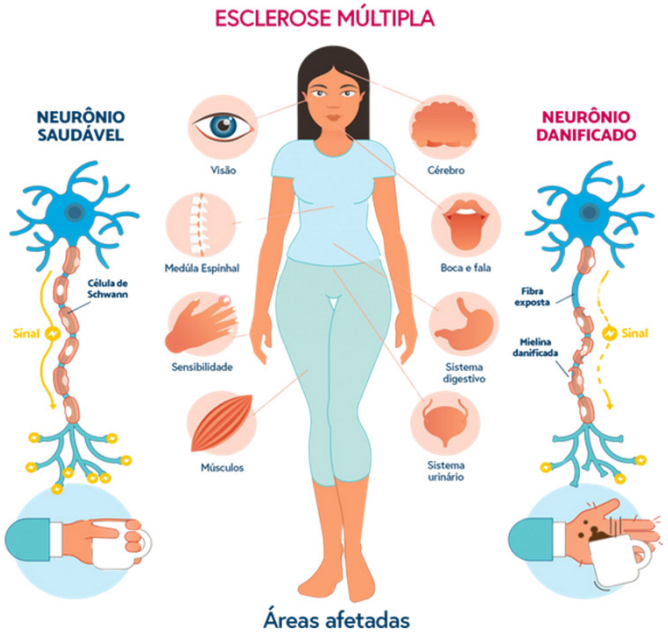
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November/2024

INTRODUCTION

- A Esclerose múltipla (EM) é uma doença neurodegenerativa, autoimune e desmielinizante que acomete cerca de 20,5 milhões de pessoas no mundo.
- Ocorre uma redução da velocidade de condução nervosa alterando a funcionalidade do indivíduo.
- Causa sintomas como fadiga, prejuízos nos movimentos e na sensibilidade, fraqueza muscular, espasticidade e redução de equilíbrio.
- No tratamento são utilizados recursos farmacológicos, porém intervenções fisioterapêuticas têm se apresentado bastante relevantes.



AIM/OBJETIVE/PURPOSE

- Descrever a partir da literatura os efeitos de tratamentos fisioterapêuticos para a esclerose múltipla.



METHODOLOGY

- O estudo trata de uma revisão integrativa da literatura, na qual foram utilizadas as bases de dados das plataformas Physiotherapy Evidence Database (PEDro), Biblioteca Virtual de Saúde (BVS) e PubMed em outubro de 2024.
- Os descritores usados foram: “Multiple Sclerosis”, “Physical Therapy ” e “Fuctional Status”.
- A busca foi realizada com o período de restrição de 5 anos (2019 a 2024).
- Foram desclassificados artigos indisponíveis na íntegra, indexações duplicadas, estudos com pacientes pediátricos, revisões de literatura, teses e dissertações, relatos de casos e artigos em que não houve participação da fisioterapia.

Artigos Identificados	**284**
Artigos Excluídos	**275**
Artigos Incluídos	**9**

RESULTS AND DISCUSSION



Exoesqueleto
(Mohamed, Sakel et al., 2022)



Exercícios respiratórios e de membros superiores
(Grubic, Kezele et al., 2020)



Reflexoterapia com alongamento muscular
(Zinovyi, M, Ostapyak et al.,2020)



Treinamento de força nos membros superiores e inferiores aeróbicos
(Grazioli, Elisa et al.,2019)



Crioterapia combinada com exercício de resistência
(Malwina Pawik, Joana et al.,2019)

RESULTS AND DISCUSSION



Estimulação magnética cervical
(Fawaz, Shereen et al.,2022)



Locomoção reflexa Vojta e terapia de ativação do programa motor
(Prochazkova, Marie et al.,2021)



Técnica de exercício Tai-Geiko
(Ultramari, Viviane et al.,2020)



Ioga VS fisioterapia
(Lysogorskaia, Elena et al.,2023)

CONCLUSIONS

- Evidencia-se a perspectiva promissora dos efeitos da fisioterapia na funcionalidade de pacientes portadores de EM.
- Tais terapias e protocolos de exercícios usados pelos fisioterapeutas, como o treinamento de força e a reflexoterapia, contribuíram significativamente para a função física, cognitiva e funcional dessas pessoas.
- Portanto, o incentivo a novos estudos para o desenvolvimento de intervenções fisioterapêuticas deve ser reforçado, a fim de minimizar a progressão desta patologia.



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OPTIMIZATION OF THE CALCIUM SILICATE HYDRATED COMPOUNDS SYNTHESIS FROM THE RECYCLING OF MATERIAL DERIVED FROM COAL INDUSTRY WASTE

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ABSTRACT

The intensification of society's consumption and population growth are the main aspects that most contribute to negative impacts on living beings and environmental management due to the generation of large quantities of waste generated daily by industrial production processes. As a result, the valorization of these industrial by-products has been highlighted with the aim of obtaining value-added materials. The concepts of reuse and recycling are presented as a new production model aiming at more sustainable processes.**:** In the present work, the optimization of the synthesis of calcium silicate hydrated compounds was carried out from sulfated coal ash generated in the flue gas desulfurization process in a thermoelectric plant using the two-stage method (alkaline fusion followed by hydrothermal treatment). The studied parameters that influenced the synthesis were fusion time, agitation time, volume of water for the hydrothermal treatment of the samples, and two types of agitators (rod with blade-type propeller and shaking table). XRF and XRD characterized the ash and products. According to the characterization results, the highest crystallinity of calcium silicate hydrated compounds was identified in the product synthesized under the following conditions: fusion time of 3 h; volume of water for hydrothermal treatment of 100 mL; agitation time of 2 h agitator equipped with rod and blade-type propeller.**:** It can be concluded that sulfated ash is viable as a starting material for the formation of hydrated calcium silicate compounds, following the principles of environmental sustainability and the objectives of the circular economy.

Keywords: *FGD ash; C-S-H compounds; Industrial waste; Circular economy; Sustainability*.

1. INTRODUCTION

Production processes significantly impact the environment. The Circular Economy proposes sustainable closed-loop processes to improve resource use and waste reuse (Unep, 2024; Kanwal et al., 2023).

Coal industries generate large amounts of coal ash. In Brazil, flue gas desulfurization in thermoelectric plants reduces NOx emissions by 70-80%, operating at 750-900°C. This process generates sulfated ash or FGD ash (Bibiano, 2021), which contains high sulfur and calcium levels that can harm ecosystems if improperly disposed of (Grosche, 2019).

The cement industry also contributes significantly to greenhouse gas emissions. Portland cement production emits approximately one ton of CO2 per ton of cement, representing 7% of global CO2 emissions (Arachchige et al., 2019; IEA, 2018).

Calcium silicates hydrated (C-S-H) compounds comprise 75% of hydrated Portland cement and show high cation immobilization potential (Tang et al., 2021). Tobermorite (TOB), structurally similar to C-S-H, can be obtained through alkaline hydrothermal treatment and may improve cement matrix properties (Kremleva et al., 2020).

TOB synthesis depends on various parameters, including Ca/Si ratio, temperature, and pH (Majdinasab and Yuan, 2020). Studies have explored TOB as a cement additive (Land and Stephan, 2015) and contaminant removal agent (Berg et al., 2006), using various sources like newspaper ash (Coleman and Brassington, 2003) and quartz sand (Galvánková et al., 2018).

This work aimed to obtain C-S-H

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compounds from sulfated coal ash through alkaline fusion and hydrothermal treatment as an alternative for supplementary cementitious material production.

2. MATERIALS AND METHODS

2.1. Materials

The Porto provided the sample of FGD ash do Pecém coal power plant located in São Gonçalo do Amarante City, State of Ceará, Brazil. Sodium hydroxide (Synth, P.A. 100 %), shaking table (Quimis - modelo Q-225M), agitator equipped with rod and blade-type propeller, oven and muffle (Fanem) and quantitative filter paper (Nalgom 3400, diâmetro = 150 mm) were used. X-ray fluorescence (Philips - Malvern Panalytical, Venus-Zetium model) and X-ray diffraction (Rigaku multiflex diffractometer with Cu anode using Co Kα radiation at 40 kV and 20 mA over the range (2 θ) of 5–60 ° with a scan time of 0.5 °/min) were performed to characterize the prepared materials.

2.2. Methods

The characterization of FGD ash was the first step defined in this study, with the aim of evaluating the chemical composition of the precursor material to see if it is favorable for the development of C-S-H compounds. Therefore, the characterization of the FGD ash and the products obtained were characterized by XRF and XRD.

For the synthesis of the compounds, the two-step method was evaluated, which consists of first fusing the ash mass with solid NaOH mass and then subjecting the fused mass to hydrothermal synthesis. First, the NaOH mass was ground and homogenized with the ash mass (ash:NaOH = 1/1.2). After grinding, the sample was fused at 600 °C in a muffle furnace. After the fusion time, the sample was cooled to room temperature and then ground again until a fine material was obtained. Right after, the volume of bidistilled water was added to the sample and agitated in two types of agitators: one equipped with a rod and blade-type propeller and a shaking table. After agitation, the sample was heated in an oven for 24 h at 100 °C. After the heat treatment, the suspension was filtered with quantitative filter paper, washed with bidistilled water, and then dried in an oven for 12 h at 100 °C.

Table 1 shows the samples and their respective synthesis parameters.

The products obtained were named as: SPF-1, SPF-2, SPF-3, SPF-4, SPF-5, and SPF-6. The arbitrary criterion used to evaluate the synthesis results was the comparison of the relative intensity of the main TOB peak (2 Θ ~ 8 °) present in the products obtained.

Table 1. Parameters of the synthesis of CSH compounds

Sample	T_{Fusion}/h	V_{H2O}/mL	t_{Agit}/h
1^1	1	100	18
2^1	3	100	18
3^2	1	100	2
4^2	3	100	2
5^2	1	200	6
6^2	1	100	6

(*) 1: table; 2: rod and blade-type propeller

3. RESULTS AND DISCUSSION:

3.1. Results

3.1.1. Characterization of FGD ash

According to the XRF results (in mass %), the main chemical constituents of FGD ash are SiO_2 (31.4); CaO (22.1); Al_2O_3 (12.4); SO_3 (11.9) and Fe_2O_3 (6.22). From the results of the XRD analysis (not shown), it was confirmed that the mineralogical content of the FGD ash is mainly calcite and quartz, with a smaller fraction of mullite and magnetite.

3.1.2. Synthesis of C-S-H compounds

XRD analyzed the results of the synthesis of C-S-H compounds using the two-step method, which is shown in Figure 1.

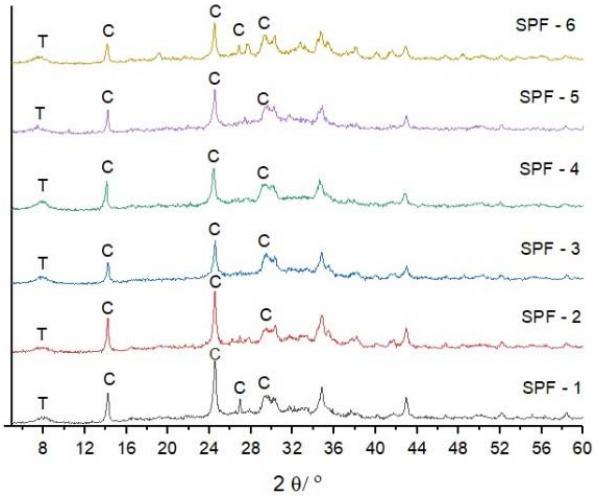


Figure 1. Diffractograms of the C-S-H compounds (T = Tobermorite;C = calcium silicate hydrated compound)

3.2. Discussion

3.2.1. Characterization of FGD ash

It was found that calcium and silicon, which

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are the main elements for the formation of C-S-H compounds, are present in larger quantities (Tang *et al*., 2021). It is also possible to observe the presence of a high content of SO_3 (11.9) originating from the desulfurization process.

3.2.2. Synthesis of C-S-H compounds

From the analysis, it is possible to observe that the C-S-H and TOB phases were formed in all synthesized products. During the process of formation of C-S-H gels, there is an intermediate and unstable phase with free calcium and silicon ions, and it is in this phase that TOB is formed (Smalakys, 2021).

Figure 2 shows the arbitrary comparison of the relative intensities in the 8° region at 2 Θ obtained from the products.

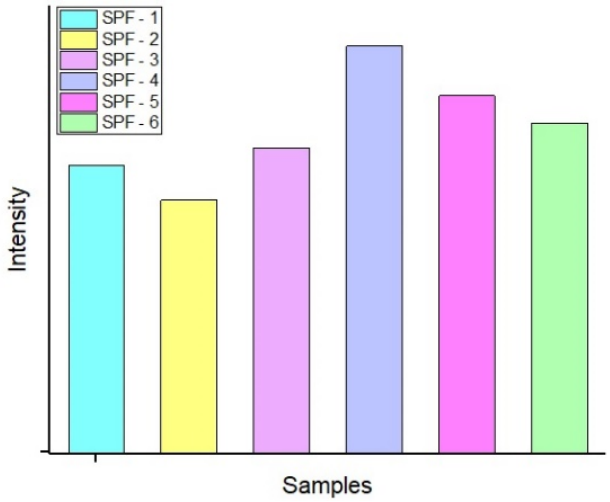


Figure 2. Comparison of the relative intensities of the samples in the region of 2Θ = 8º.

From the comparison of the relative intensities of the samples, it was possible to define that the SCF-4 sample has the highest crystallinity of the product, for which the following parameters were used: melting time – 3 h; volume of water for TH – 100 mL; stirring time – 2 h; and agitator equipped with rod and blade-type propeller.

The 3 stages of synthesis of CSH compounds in this study consist of: 1 - fusion, is the stage in which the compounds containing Si^{4+} and Ca^{2+} present in the FGD ash dissolve, forming the molten C-S-H compound, which is soluble in water; 2 - through contact of the molten sample with water under agitation, the condensation of silicate and calcium ions occurs in an alkaline solution to form CSH and TOB gel; and 3 - TH in an oven, which is the stage in which the gel crystallizes, producing crystalline C-S-H compounds.

According to the results, a longer fusion time provided a greater formation of TOB and C-S-H compounds. It can also be concluded that the formation of C-S-H compounds and TOB decreases with the increase in the value of the water-to-solid ratio. This fact was observed in the literature (Galvánková *et al*., 2018; Kikuma et al., 2011).

Agitation in water helps dissolve the molten compounds, form the initial gel formation, and maintain a homogeneous gel. The use of a rod instead of a stirring table facilitates the breaking of the $CaSO_2$/$CaSO_3$ and Si-O bonds in the ash. Consequently, this results in a faster dissolution rate of these compounds in the alkaline solution during aging with water. The complete dissolution of the C-S-H compounds and the formation of a homogeneous gel make the raw material available for the growth of TOB crystals. Since the agitation is efficient, the TOB formed in the last stage is purer, more crystalline, and has a higher yield (Rosa, 2024).

4. CONCLUSIONS:

This study showed that industrial waste, sulfated coal ash from coal-fired power plants, is an efficient material for obtaining calcium silicate hydrated compounds through alkaline fusion followed by hydrothermal treatment. According to the characterization of the materials and the optimization of the synthesis process, the greatest crystallinity of the products was observed under the following conditions: fusion time of 3 h; volume of water in the agitation of 100 mL; agitation time of 2 h; and agitator equipped with rod and blade-type propeller. Therefore, this study demonstrates the possibility of managing waste from the coal industry following the principles of the circular economy and Sustainable Development Goal (SDG) number 12, specifically in item 12.5: “By 2030, substantially reduce waste generation through prevention, reduction, recycling and reuse”.

5. DECLARATIONS

5.1. Acknowledgements

The authors thank the National Council for Scientific and Technological Development (CNPq), Brazil for the financial support and Porto do Pecém Coal Power Plant for supplying the FGD ash samples.

5.2. Open Access

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Southern Science Conference, 2024.

OPTIMIZATION OF THE CALCIUM SILICATE HYDRATED COMPOUNDS SYNTHESIS FROM THE RECYCLING OF MATERIAL DERIVED FROM COAL INDUSTRY WASTE

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November/2024

INTRODUCTION





INDUSTRIAL WASTES

- **COAL INDUSTRY**



- **CEMENT INDUSTRY**



INTRODUCTION

INDUSTRIAL WASTES

- Responsible for a **large amount of coal ash**;
- Flue gas desulfurization (FGD) process is a technology in thermoelectric plants, and its main characteristic (Bibiano, 2021; Grosche, 2019):



- **COAL INDUSTRY**

✓ Combustion of fuel with **low NO_x emissions** (reduction between **70 and 80 %**), since combustion **temperatures** are typically **between 750 °C and 900 °C**;

✓ The **capture of sulfur** by feeding compounds that react with SO_x within the flue, at the time of its generation;

✓ The **residue generated** in this process are called **sulfated ash or FGD ash**;

✓ **FGD ash** has a **high content of sulfur and calcium**;

✓ **The negative impacts on human health and the environment**.

INTRODUCTION

INDUSTRIAL WASTES

- Sector responsible for **high levels of greenhouse gas emissions**;
- Portland cement has been the most widely used product in the world in recent decades, its production is basically from **calcium oxide and silica**, which can be extracted from different sources such.



- **CEMENT INDUSTRY**

- During the cement production process, approximately **one ton of CO_2 is emitted for each ton of cement produced, representing around 7 % of the CO_2 emitted worldwide** (Arachchige *et al.*, 2019).

INTRODUCTION

INDUSTRIAL WASTES

C-S-H COMPOUNDS

- The **main compounds** present in cement are **calcium silicates hydrated (C-S-H);**
- They **represent about 75 % by mass** of the final hydrated product present in Portland cement, and are the low crystalline phases with variable stoichiometry;
- Among its **main characteristics**, its potential to control the release of radionuclides stands out due to its long-term stability and its **high potential for cation immobilization** (Tang *et al*., 2021).

INTRODUCTION

INDUSTRIAL WASTES

TOBERMORITE

- Tobermorite is a compound that **has a similar structure to that of the C-S-H compounds** found in hydrated cement, and **can be considered as a structural model of cement** (this being one of the main interests in studying it) (Kremleva *et al*., 2020);
- It **can be obtained** by **alkaline hydrothermal treatment** from systems containing **CaO-SiO_2-H_2O;**
- Several **synthesis parameters** that directly influence the production of TOB and C-S-H compounds, including: Ca/Si ratio, temperature, reaction time, pH, partial substitution of aluminum by silicon and precursors, etc (Majdinasab and Yuan, 2020).

BACKGROUND

- Therefore, as the **production processes are responsible for a large part of the negative impacts on the environment**. As an alternative, the **Circular Economy** proposes a sustainable closed-loop process, improving the use of resources and collaborating in the reuse of this waste (Unep, 2024).

AIM

The **objective of this work** was to **obtain C-S-H compounds from sulfated coal ash by means of alkaline fusion followed by hydrothermal treatment**. This approach is an alternative to produce value-added material that can be used as a supplementary cementitious material, in addition to minimizing the impact that this residue causes on the environment due to inadequate disposal.

METHODOLOGY

MATERIALS

For synthesis:

- The sample of **FGD ash was provided by the Porto do Pecém coal power plant** located in São Gonçalo do Amarante City, State of Ceará, Brazil;
- Sodium hydroxide (Synth, P.A. 100 %)
- Shaking table (Quimis - modelo Q-225M);
- Agitator equipped with rod and blade-type propeller
- Oven and muffle (Fanem)
- Quantitative filter paper (Nalgom 3400, diâmetro = 150 mm) were used.

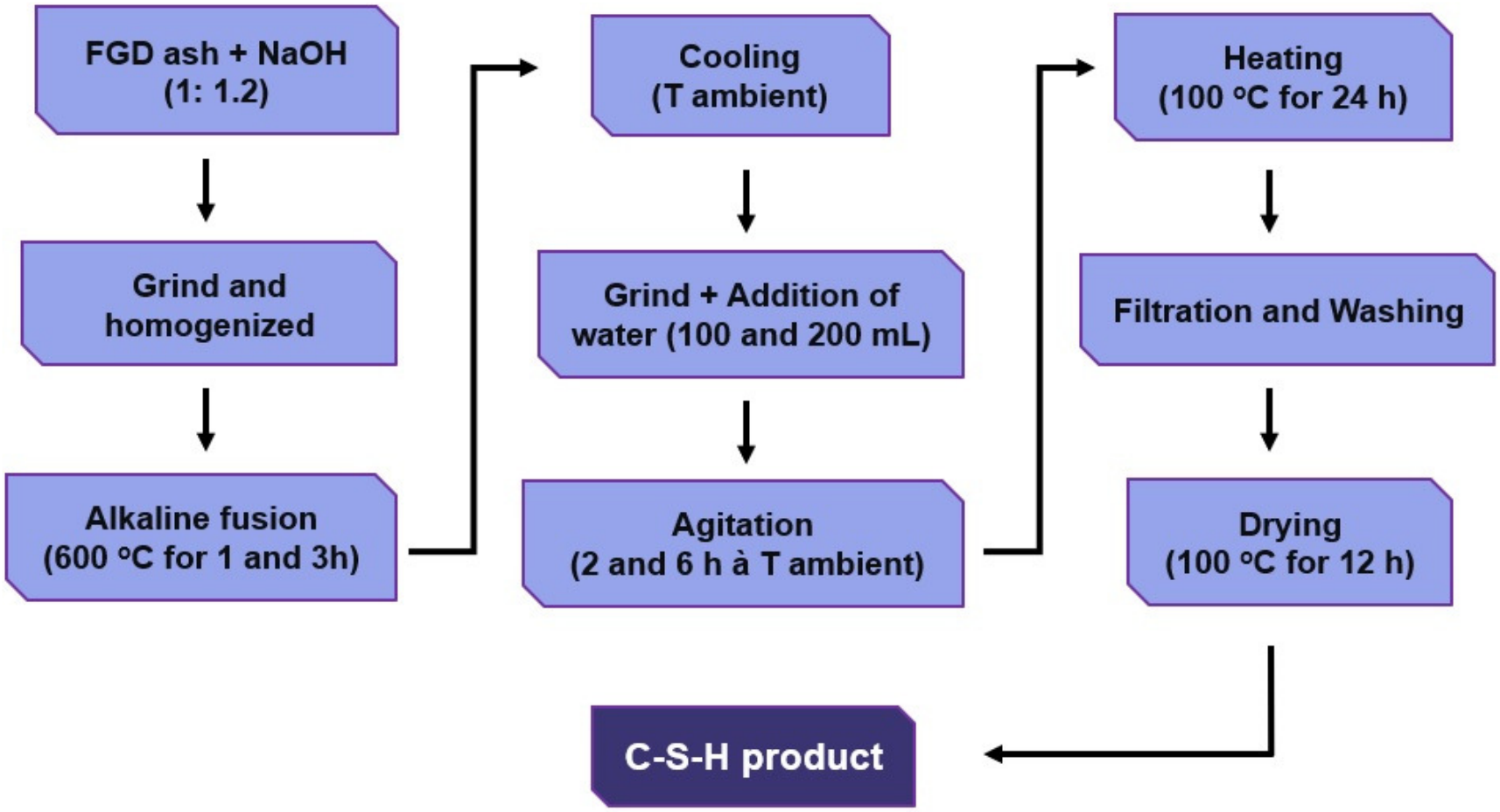
For characterize the materials

- **X-ray fluorescence** (Philips - Malvern Panalytical, Venus-Zetium model)
- **X-ray diffraction** (Rigaku multiflex diffractometer with Cu anode using Co Kα radiation at 40 kV and 20 mA over the range (2 θ) of 5–60 ° with a scan time of 0.5 °/min) were performed.

METHODOLOGY

METHODS

- The **characterization of FGD ash** was **the first step** defined in this study;
- **For the synthesis** of the compounds:



METHODOLOGY

METHODS

- The Table 1 shows the samples and their respective synthesis parameters.

Sample	T_{Fusion}/h	V_{H2O}/mL	t_{Agit}/h
1^1	1	100	18
2^1	3	100	18
3^2	1	100	2
4^2	3	100	2
5^2	1	200	6
6^2	1	100	6

(*) 1: table; 2: rod and blade-type propeller

- The products obtained were named as: **SPF-1, SPF-2, SPF-3, SPF-4, SPF-5 and SPF-6**;
- The **arbitrary criterion used to evaluate the synthesis results was the comparison of the relative intensity of the main tobermorite peak (2 Θ ~ 8 °) present in the products obtained**.

RESULTS AND DISCUSSION

RESULTS

Characterization of FGD ash

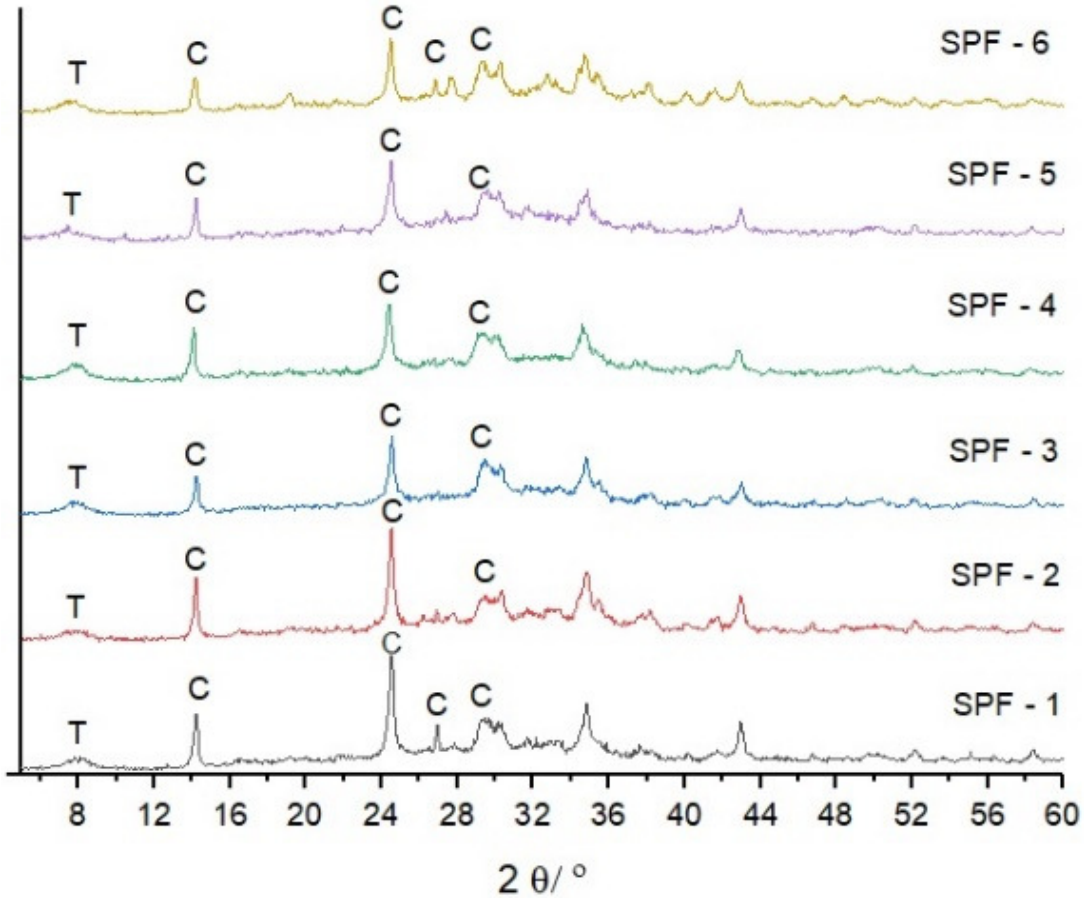
- **XRF results** (in mass %), the main chemical constituents of FGD ash are: **SiO_2 (31.4); CaO (22.1); Al_2O_3 (12.4); SO_3 (11.9) and Fe_2O_3 (6.22)**.
- **XRD analysis** (not shown), it was **confirmed that the mineralogical content of the FGD ash is mainly calcite and quartz**, with a smaller fraction of mullite and magnetite;
- It was **found that calcium and silicon**, which are the **main elements for the formation of C-S-H compounds**, are present in larger quantities (Tang *et al.*, 2021).
- Presence of **high content of SO_3 (11.9)** originating from the **desulfurization process.**

RESULTS AND DISCUSSION

RESULTS

Synthesis of C-S-H compounds

- **C-S-H and TOB phases were formed** in all synthesized products;



- ***Figure 1***. Diffractograms of the C-S-H compounds (T = Tobermorite; C = calcium silicate hydrated compound)

RESULTS AND DISCUSSION

RESULTS

Synthesis of C-S-H compounds

- Define that the **SCF-4 sample** has the **highest crystallinity** of the product, for which the following parameters were used: **melting time – 3 h; volume of water for TH – 100 mL; stirring time – 2 h; and agitator equipped with rod and blade-type propeller.**

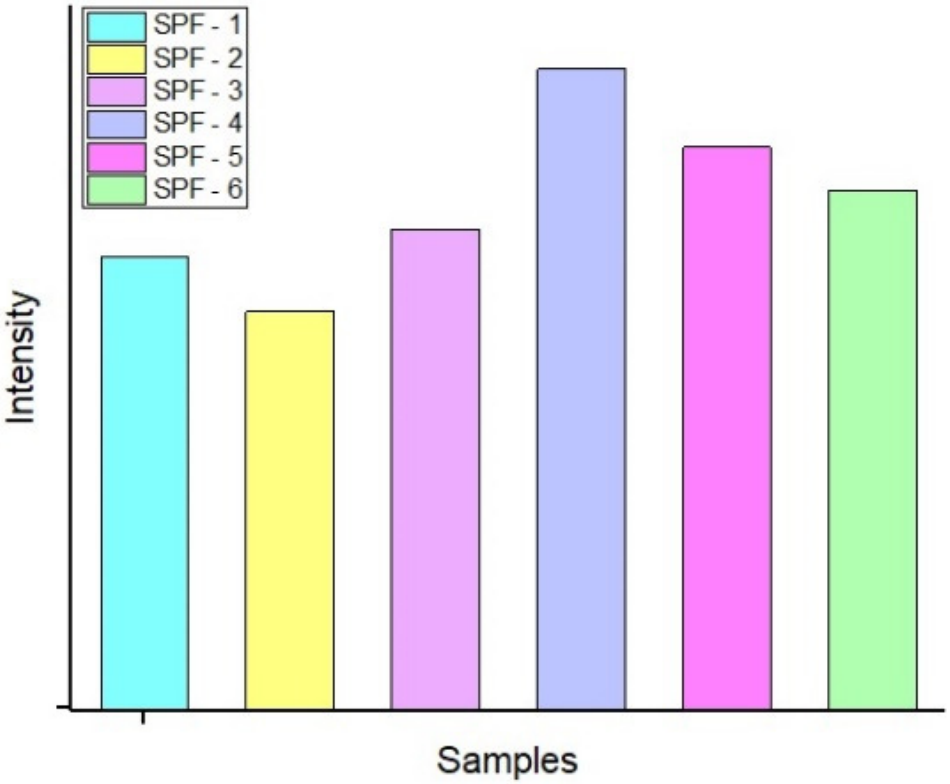


Figure 2. Comparison of the relative intensities of the samples in the region of 2Θ = 8°.

RESULTS AND DISCUSSION

RESULTS

Synthesis of C-S-H compounds

- A **longer fusion time** provided a **greater formation of TOB and C-S-H compounds**. It can also be concluded that **the formation of C-S-H compounds and TOB decreases with the increase in the value of the water-to-solid ratio** (Galvánková et al., 2018).
- The use of a **rod instead of a stirring table facilitates the breaking of the $CaSO_2$/$CaSO_3$ and Si-O bonds in the ash**. Since the agitation is efficient, the TOB formed in the last stage is more crystalline, purer and with a higher yield (Rosa, 2024).

CONCLUSIONS

- This study showed that **industrial waste**, **sulphated coal ash from coal-fired power plants, is an efficient material for obtaining calcium silicate hydrated** compounds through **alkaline fusion followed by hydrothermal treatment**;
- According to the **characterization** of the materials and the **optimization of the synthesis** process, the greatest crystallinity of the products was observed under the following conditions: **fusion time of 3 h; volume of water in the agitation of 100 mL; agitation time of 2 h; and agitator equipped with rod and blade-type propeller**;
- Therefore, this **study demonstrates the possibility of managing waste** from the coal industry following the **principles of the circular economy** and **Sustainable Development Goal (SDG) number 12**, specifically in item 12.5: "By 2030, substantially reduce waste generation through prevention, reduction, recycling and reuse".

ACKNOWLEDGEMENTS

- The authors thank the National Council for Scientific and Technological Development (**CNPq**), Brazil for the financial support and **Porto do Pecém Coal Power Plant** for supplying the FGD ash samples.

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ECOSYSTEM SERVICES, ENERGETIC EMERGY ANALYSIS AND ECOSYSTEM EQUILIBRIUM

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ABSTRACT

Ecosystems are complex systems characterized by intense interactions and material exchanges, driven by high energy flows. Understanding how these networks function, including their inputs and outputs, is essential for more effective protection of natural ecosystems and for applying the concept of sustainability to human activities. Ecosystems, as bounded systems, are defined by their energy exchanges with external systems and their internal dynamics. This review explores the relationship between ecosystem services and energy flows, focusing on how the quality and quantity of inputs influence system development. Emergy, a tool to assess the convergence of matter and energy within systems, is measured in solar emergy joules (seJ) and represents the work performed by nature to provide services. On the other hand, the ecosystem services approach, increasingly used in environmental policies, quantifies ecosystem outputs through an anthropocentric perspective. The analysis reveals that various methodologies, including eco-exergy and emergy analysis, offer complementary ways to characterize the state and function of ecosystems. These approaches provide valuable insights by integrating both the internal organization of ecosystems and the value of services they provide to humans, contributing to a more comprehensive understanding of ecosystem dynamics and their role in supporting human well-being.

Keywords: *energy emergency, ecosystem services, sustainability*

1. INTRODUÇÃO

Os ecossistemas são sistemas complexos com intensas interações e troca de materiais, envolvendo fluxos elevados de energia. Compreender como essa rede opera, incluindo seus insumos e produtos, pode resultar em uma proteção mais eficaz dos ecossistemas naturais e em uma aplicação mais eficiente do conceito de sustentabilidade nas atividades humanas. Odum (1996) sugere que a biodiversidade (ou seja, a variedade genética da flora e fauna de uma determinada região) e a emergência (ou seja, a energia disponível acumulada utilizada para produzir um componente de um sistema observado) estão inter-relacionados e que, à medida que o fluxo de emergência renovável capturado por um sistema aumenta, a biodiversidade aumenta proporcionalmente. Em 1998 Odum sugere que um sistema se auto-organizará para melhor tirar proveito da emergência da assinatura de energia disponível, maximizando o fluxo de energia através do sistema ao longo do tempo. Um ecossistema, enquanto sistema delimitado, é definido por seu funcionamento e pela troca de energia com sistemas externos. Conforme descrito por Federico M. Puselli (2011), “os sistemas ecológicos são termodinamicamente abertos, hierárquicos, auto-organizados e auto-regulados”.

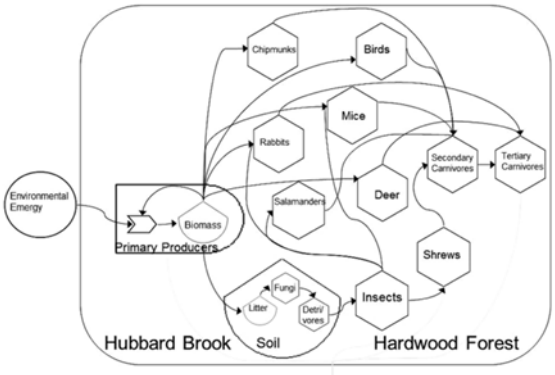


Figura 1 - Diagrama da linguagem dos sistemas energéticos da floresta experimental de Hubbard Brook, adaptado de Gosz et al. (1978). (Fonte: “Relationships between renewable emergy storage or flow and biodiversity: a modeling investigation.”)

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A manutenção de um ecossistema é regulada pelas entradas e saídas de energia, que são determinadas pelas fronteiras do sistema e pela dinâmica interna que sustenta seu funcionamento. As entradas (inputs) de um ecossistema referem-se a todos os fluxos de energia e matéria que ingressam no sistema a partir do ambiente externo. Por outro lado, as saídas (outputs) são os fluxos de energia e matéria que deixam o sistema e retornam ao ambiente.

2. MATERIAIS E MÉTODOS

Foi realizada a leitura de três artigos, o artigo; "Ecosystem services as a counterpart of emergy flows to ecosystems" (Serviços ecossistêmicos como contrapartida dos fluxos de emergia para os ecossistemas), publicado pelos autores Federico M. Pulselli, Luca Coscieme e Simone Bastianoni, do Departamento de Química da Universidade de Siena na Itália em 2011, o artigo; "Relationships between the Storage or Flow of Renewable Emergy and Biodiversity: A Modeling Investigation" (Relações entre armazenamento ou fluxo de emergia renovável e biodiversidade: uma investigação de modelagem), publicado por Elliott T. Campbell e David R. Tilley, Universidade de Maryland, College Park, EUA em 2016, e por fim o artigo “Emergy, transformity and ecosystem health.” (Emergência, transformidade e saúde dos ecossistemas), publicado em 2004 nos Estados Unidos, Nova Iorque.

3. RESULTADOS E DISCUSSÃO:

Após levantamento da literatura, três artigos foram utilizados como base para o presente trabalho, eles destacam que a qualidade e quantidade dos fatores de produção são fundamentais para o desenvolvimento de um sistema. A abordagem do “lado do doador” analisa os inputs dos ecossistemas, e a emergia é uma ferramenta que permite avaliar a convergência de matéria e energia para o sistema em uma base comum. Segundo Odum et al. (2000), emergia é definida como “a disponibilidade de energia de um tipo que é utilizada em transformações diretas e indiretas para fazer um produto ou serviço”. A emergia representa o trabalho realizado pela natureza para fornecer um fluxo ou um serviço, calculado com base na energia solar processada e armazenada ao longo do tempo. A unidade de medida da emergia solar é o solar emergy joule (seJ) (Odum, 1996, 2000).

Por outro lado, a abordagem dos serviços ecossistêmicos, que adota uma perspectiva antropocêntrica, vem sendo cada vez mais aplicada nas políticas ambientais. Essa abordagem considera os outputs do ecossistema em termos das funções que ele desempenha e dos serviços que fornece aos humanos, e a quantificação desses valores é realizada através de metodologias econômicas ambientais.

Entender o processo de emergia enérgica e suas conexões entre os componentes naturais (sistemas) alinham ações mais sólidas no sentido de preservação e conservação dos recursos naturais.

4. CONCLUSÃO:

Diversas abordagens buscam caracterizar o estado de um sistema, com base na descrição da organização interna da rede, na complexidade do sistema ou no estudo do ciclo de energia e matéria ao longo do tempo. A emergia enérgica ou simplesmente emergia é um conceito que analisa as saídas e entradas de energia em um sistema/componente natural com foco principal da energia solar absorvida, redirecionada ou consumida. Com relação a entrada e saída de energia de um componente natural é possível quantificar essa energia que é utilizada em seus processos internos e o excedente, esse excedente é calculado e apresentado como a prestação de serviços ecossistêmico desempenhado por determinado componente natural, por exceder a energia necessária para sua autorregularão e funcionamento.

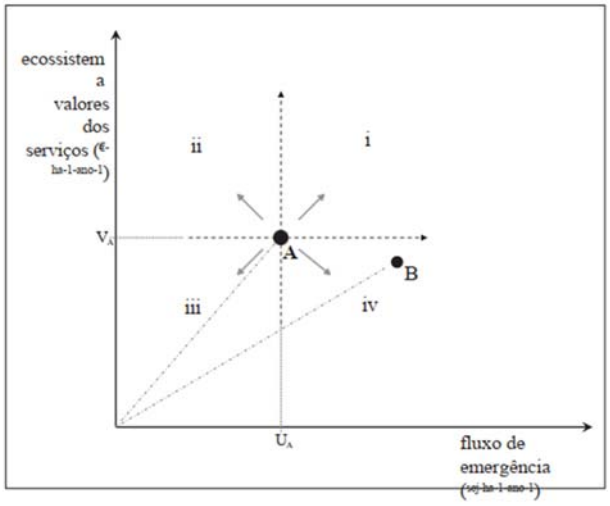


Figura 2 - Dinâmica do ecossistema representada pela alteração do fluxo de emergia e do valor dos serviços do ecossistema. (Fonte: Emergy, transformity and ecosystem health).

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Essa energia excedente incorpora em outros componentes naturais ao longo das relações intrínsecas entre ecossistemas, espécies flora e espécies de fauna.

Uma importante política ambiental foi consolidada com base nas informações disponíveis através dos estudos da emergia enérgica dos ecossistemas, o PSA (Pagamento por serviços ambientais) remunera financeiramente quem permite em sua propriedade a permanência de componentes naturais. Até o momento o PSA focou (devido a importância da discussão da segurança hídrica global) em nascentes e em sua faixa marginal de proteção. Mas já existe dentro dos comitês de bacias hidrográficas em seus grupos de trabalho uma pressão, para que seja incorporada ao PSA ações como a demarcação de Unidade de Conservação da Natureza, áreas com RAD (Recuperação de área de degradada) e ações de mitigação de combate a incêndio em propriedades rurais.

O conceito da emergia desenvolvido por Howard T. Odum trouxe uma visão mais exata e mais tangível das relações dos ecossistemas e os seres vivos, aumentando o interesse na preservação e conservação desses componentes e assegurando mais uma frente para mitigação dos impactos gerados pela destruição desses componentes, como a insegurança hídrica e a emergência climática.

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Southern Science Conference, 2024.

Os Serviços Ecossistêmicos e a Análise da Emergia Enérgica e o Equilíbrio dos Ecossistemas

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INTRODUCTION

- **Ecossistemas como sistemas complexos**: Interações intensas e troca de materiais com altos fluxos de energia.

- **Objetivo**: Proteger ecossistemas naturais e aplicar o conceito de sustentabilidade.

- **Relação entre biodiversidade e emergia**: Fluxo de emergia está relacionado ao aumento da biodiversidade.

BACKGROUND

Emergia: Medida em *solar emergy joules* (seJ); avalia a convergência de energia e matéria dentro de sistemas naturais.

Serviços Ecossistêmicos: Abordagem antropocêntrica, quantificando as saídas do ecossistema em termos dos serviços fornecidos aos seres humanos.

AIM

Emergia: Convergência de matéria e energia avaliada em termos de serviços fornecidos pela natureza.

Serviços Ecossistêmicos: Considera as funções desempenhadas pelos ecossistemas e seus benefícios aos seres humanos.

METHODOLOGY

Revisão de três artigos principais:

1. "Serviços ecossistêmicos como contrapartida dos fluxos de emergia para os ecossistemas" (Pulselli et al., 2011).
2. "Relações entre armazenamento/fluxo de emergia renovável e biodiversidade" (Campbell & Tilley, 2016).
3. "Emergia, transformidade e saúde dos ecossistemas" (Brown & Ulgiati, 2004).

RESULTS AND DISCUSSION

Emergia: Convergência de matéria e energia avaliada em termos de serviços fornecidos pela natureza.

Serviços Ecossistêmicos: Considera as funções desempenhadas pelos ecossistemas e seus benefícios aos seres humanos.

CONCLUSIONS

Importância da emergia: Ferramenta crucial para quantificar energia e serviços ecossistêmicos.

Políticas Ambientais: Base para o PSA (Pagamento por Serviços Ambientais), que remunera a preservação de componentes naturais.

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PLANT EXTRACTS AND ESSENTIAL OILS: EVALUATION OF PROFILES AS A STRATEGY IN TEACHING CHEMISTRY

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ABSTRACT

This study examines the application of thin-layer chromatography as an effective analytical technique for identifying terpenoids in essential oils and plant extracts from Rosemary (*Rosmarinus officinalis*) and Peppermint (*Mentha piperita*). The methodology involved preparing and analyzing samples on chromatographic plates, utilizing UV light revelation and the vanillin-sulfuric acid technique, which enabled clear identification of the compounds present. The results demonstrated significant correspondences between the chemical profiles of the extracts and essential oils, highlighting menthol as a predominant terpenoid in peppermint. In addition to its analytical applications, thin-layer chromatography was integrated into chemistry education, fostering a connection between theory and practice. This integration stimulated students' curiosity and critical thinking, allowing them to become active participants in their learning process. The practical experience offered valuable opportunities for students to directly observe chemical interactions and understand the relevance of chemical compounds in everyday contexts, reinforcing the notion that chemistry is embedded in their daily lives. The pedagogical approach employed in this study enriched students' understanding of fundamental chemical concepts while preparing them to effectively apply scientific knowledge in various situations. Therefore, incorporating analytical techniques like thin-layer chromatography into the educational curriculum is essential for promoting dynamic and meaningful learning. This strategy contributes to a more robust academic formation, equipping students to face real-world challenges and develop critical skills necessary in a complex world. In summary, this study highlights the importance of active and practical methodologies in chemistry education, demonstrating how analytical techniques can enhance scientific comprehension while deeply engaging students in the learning process. thin-layer chromatography serves as a model for future educational practices, expanding the application of scientific knowledge in students' everyday lives.

Keywords: *Thin-layer chromatography, Essential oils, Terpenoids, Chemistry education.*

1. INTRODUÇÃO

A cromatografia em camada delgada é uma técnica usada para separação de misturas, que pode ser executada em placas de vidro, plástico ou alumínio, revestida com uma fase estacionária adsorvente, como sílica, óxido de alumínio ou celulose (Bele e Khale, 2011). É amplamente utilizada na análise de alimentos, composição química e detecção de diversas classes de metabólitos secundários (Cabezudo et al., 2022). É uma técnica de adsorção líquido-sólido, em que a separação ocorre por meio da migração diferencial em uma camada de adsorvente (fase estacionaria) por meio de um solvente (fase móvel) (Amorim, 2019). A separação pode ocorrer tanto por partição ou troca iônica, guiada pela diferença da afinidade dos componentes da mistura pela fase estacionária. É uma técnica econômica, costumeiramente são utilizadas amostras em microgramas. A revelação dos componentes eluidos pode ser realizada de forma física (luz UV), química (reagentes específicos) e em alguns casos biológica (borrifação de esporos).

É uma tecnica importante e de fundamental conhecimento em cursos de química, disciplinas ou áreas afins, como é o caso da disciplina métodos analíticos, presente no curso de Ciências Biológicas da Universidade Estadual de Montes Claros.

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Situações e ações que busquem relacionar o cotidiano com transposições didáticas durante o processo de ensino-aprendizagem é uma ferramenta essencial para o desenvolvimento didático em sala de aula (Souza e Ibiapina, 2023). Junto a isso, a realização de experimentos é um elemento incentivador, no qual os alunos sintam-se parte ativa do processo, possibilitando que o papel do professor seja mais flexível, interangindo em momentos chave (Machado, 2015).

Em contexto de abordagem demonstrativa investigativa, o professor expões fenômenos simples, e a partis deles introduz novas abordagens e aspectos que estão relacionados a ideia inicial, ou seja o fenômeno estudado (Chaves et al., 2024). No caso do presente estudo, o foco foi voltado para a presença de metabólitos secundários, mais especificamente terpenoides, em plantas medicinais e em óleos essenciais das mesmas.

Desta forma o objetivo do trabalho foi realizar a cromatografia em camada delgada de amostras de óleos essenciais e de extratos vegetais das plantas na busca por correpondência do perfil químico.

2. MATERIAL E MÉTODOS

2.1. Preparo da Placa Cromatografica

A placa cromatográfica foi cortada no tamanho 7cm de altura por 5 cm de largura. Foi feita duas marcação, a primeira de 0,5 cm no limite inferior e a segunda de 0,5 cm no limite superior da placa. Foi a eluição da placa em metanol até atingir a marcação da borda superior, posteriormente foi verificado em luz UV 254nm se a placa possuia alguma mancha. Validado o material, foi reservado.

2.2. Coleta do Material Vegetal

Folhas de Alecrim (AL) (*Rosmarinus officinalis*) e Hortelã-Pimenta (HP) (*Mentha piperita*) foram coletados na Farma Verde, farmácia viva do município de Montes Claros. As folhas foram coletadas as 7:00h da manhã, cada espécie foi acondicionadas em caixa de isopor, e posteriormente levadas ao freezer do Laboratório de Produtos Naturais da Universidade Estadual de Montes Claros, até o momento do uso.

2.3. Preparo do Extrato Vegetal

Foram macerados 2 gramas de folhas em 5 mL de etanol 70% com auxílio do graal e pistilo por 5 minutos. Os macerados EAL e EHP foram colocados em béqueres e levados ao banho ultrassonico em temperatura ambiente por 15 minutos, o bequer foi selado com plástico filme para evitar evaporação dos oleos. Após, recolha o sobrenadante, coloque em microtúbulos e centrifugue por 2 minutos a 5000 rotações por minuto, reserve.

2.4. Preparo dos Óleos Essenciais

Óleos essenciais de AL (WNF, São Paulo) e HP (Laszlo,Minas Gerais) foram adquiridos pela internet em lojas especializadas. Os óleos foram diluídos na proporção de 1:1 para óleo essencial e etanol, em microtúbulos previamente identificados.

2.5. Aplicação das Amostras na Placa

Com as placa cromatográficas já prontas para a análise, foi feito quatro marcações, intercalando óleo essencial e extrao vegetal correspondentes, com auxílio do capila. Após depositadas as amostras, secou-se a placa por 5 minutos em temperatura ambiente.

2.6. Eluição e Revelação

Com a cuba preparada com béquer, a placa foi levada para ser eluida com a fase móvel tolueno-acetato de etila (97:3) já posicionada na capela de exaustão, a placa foi eluida até a marcação próxima do limite superior, esperou-se secar e os resultados foram avaliados em luz UV-254nm. Para a revelação química foi feita a borrifação da placa com vanilina sulfúrica a 1%, esperou-se secar, e a placa foi aquecida até a revelação de machas (Wagner e Bladt, 1996).

3. RESULTADOS E DISCUSSÃO

Foram observados em luz UV-254nm quatro manchas para o óleo essencial de HP e uma para o EHP, já para o AL foram observadas três manchas e para o EAL foram observadas duas (Figura 1).

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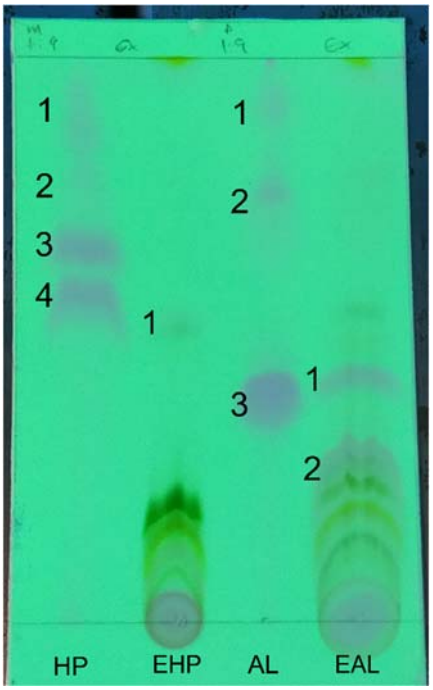


Figure 1. *Observação das amostras em luz UV-254nm*

Como pode ser obervado na figura 1, houve correspondência nos pontos 4 do HP e o 1 do EHP, possivelmente relacionado ao mentol, terpenoide em maior concentração na folha, e no óleo essencial (45-55%, Lazslo). Já na amostra AL e EAL não houveram correspondências diretas, mas sim três bandas próximas a AL 3 e a EAL 1 e 2.

Após a borrifação do revelador químico vanilina slfurica foram observada duas correspondências para o HP e EHP, e três para AL e EAL (Figura 2).

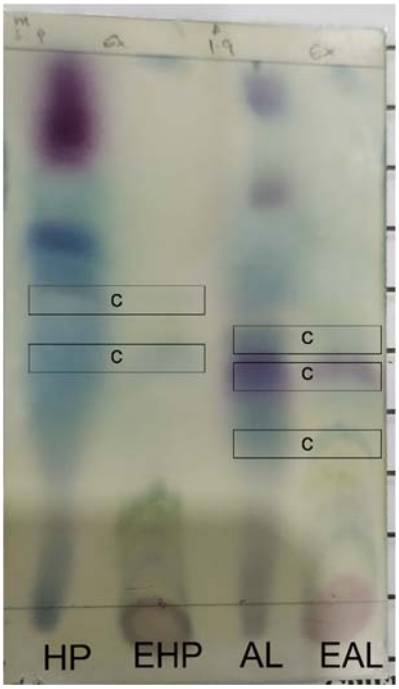


Figure 2. *Correspondencia entre os óleos essenciais e os extratos.*

Na figura 2, pode-se observar pontos de correspondência entre as amotras, as mesmas observadas para os extratos, mais intensas. Para o HP e EHP maior corrspondencia para um tom azul, que acreditamos ser o mentol e um segundo tom azul que pode indicar a presença de isomentona, e para AL e EAL tons em azul claro e roxo que podem indicar a presença de ácido rosimarinico ou cânfora, cineol e borneol .

É possível observar grandes diferenças entre as amostras de óleos essenciais e extratos vegetais, isso se dá devido a forma extrativa e o solvente utilizado. Isso é, o uso do etanol, solvente verde, de fácil manuseio e alta polaridade, o que justifica a presença de manchas somente até a metade da placa, provavelmente relacionado aos tipos de substancias estraídas. Como as citadas acima, com grupos funcionais álcool e cetona.

A composição química dos óleos essências, geralmente, é predominantemente constituída por terpenos e terpenóides, sendo os mais comuns nessa matriz os monoterpenos, responsáveis pela volatilidade e aromaticidade (Cox-Gerorgian et al., 2019). Trabalhos que envolvem o uso de óleos essenciais como elementos do ensino de química são bastante variados, podem assumir um papel mais analítico com ensaios mais completos como o uso da cromatografia gasosa (Barbosa de Paula et al., 2023). Ou de forma mais lúdica como a produção de aromatizadores de ambiente (Pinto et al., 2024).

A atividade proposta neste trabalho possuí a proposta da interatividade entre os alunos envolvidos na aula prática, desenvolvendo a curiosidade e o senso crítico. Com uma nova abordagem, pespectivas e olhares sobre o conhecimento construído durante a formação acadêmica. Isso proporciona a interatividade e a autonomia do aluno (Freire, 1996). Contribuindo para a formação de profissionais com capacidade de lidar com elementos do cotidiano de forma aprofundada e direcionada a contruir e contribuir em ambientes nos a química de produtos naturais e os métodos analíticos estão em discussão. O que os prepara para situações no qual o conhecimento ciêntifico é fundamental para a discussão.

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4. CONCLUSÕES

A cromatografia em camada delgada provou ser uma ferramenta valiosa para a aprendizagem em química, permitindo que os alunos realizassem análises práticas de terpenóides em óleos essenciais e extratos vegetais. Essa abordagem facilitou a conexão entre teoria e prática, estimulando a curiosidade e o pensamento crítico. Ao se envolverem diretamente com os experimentos, os alunos se envolveram como protagonistas do processo de aprendizagem, promovendo um ambiente interativo e engajado que incentivou a autonomia e a investigação. Assim, a integração de técnicas analíticas no ensino de química é essencial para enriquecer a formação dos estudantes, transformando o aprendizado em uma experiência dinâmica e relevante.

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PLANT EXTRACTS AND ESSENTIAL OILS: EVALUATION OF PROFILES AS A STRATEGY IN TEACHING CHEMISTRY

EXTRATOS VEGETAIS E ÓLEOS ESSENCIAIS: AVALIAÇÃO DE PERFIS COMO ESTRATÉGIA NO ENSINO DE QUÍMICA

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Novembro/2024

INTRODUCÃO

- Cromatografia em Camada Delgada;
- Elementos cotidianos e transposições didáticas no processo de ensino-aprendizagem;
- Abordagens demonstrativas investigativas;
- O fenômeno abordado e possibilidades de aprofundamento durante o processo de aprendizagem;

OBJETIVO

O objetivo do trabalho foi realizar a cromatografia em camada delgada de amostras de óleos essenciais e de extratos vegetais das plantas na busca por correspondência do perfil químico

METODOLOGIA

- Preparo da placa cromatográfica;
- Coleta do material vegetal;
- Preparo do material vegetal;
- Preparo dos óleos essenciais;
- Aplicação das Amostras na Placa;
- Eluição e revelação;

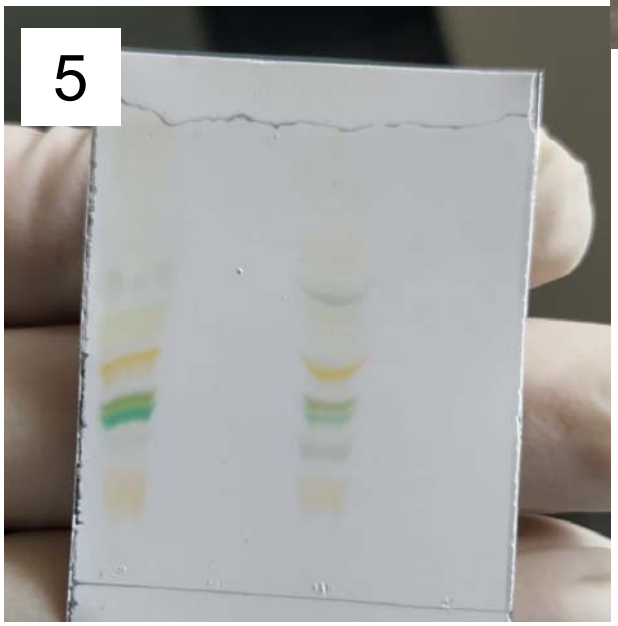
METODOLOGIA









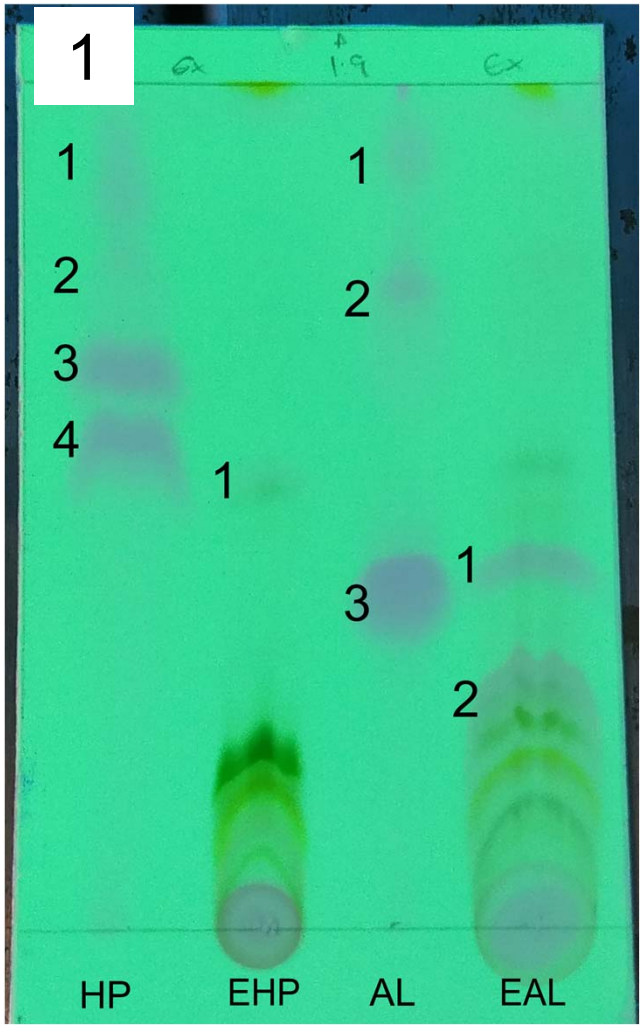


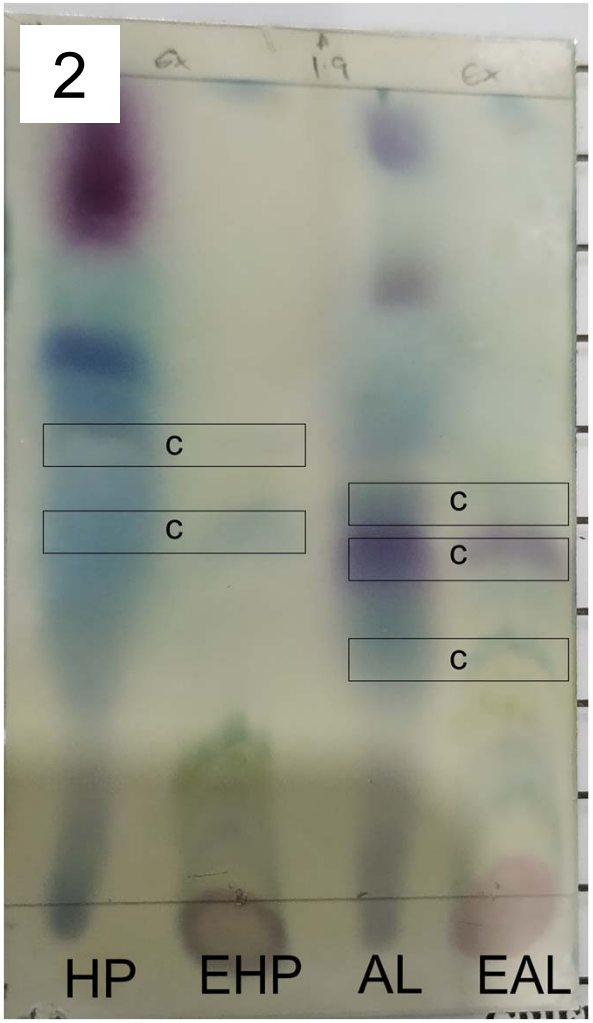
RESULTADOS E DISCUSSÃO

- Foram observados em luz UV-254nm quatro manchas para o óleo essencial de Hortelã-Pimenta (HP) e uma para o Extrato de Hortelã-Pimenta (EHP), já para o óleo essencial de Alecrim (AL) foram observadas três manchas e para o Extrato de Alecrim (EAL) foram observadas duas (Figura 1);

- Houve correspondência nos pontos 4 do HP e o 1 do EHP, possivelmente relacionado ao mentol, terpenoide em maior concentração na folha, e no óleo essencial (45-55%, Lazslo). Já na amostra AL e EAL não houveram correspondências diretas, mas sim três bandas próximas a AL 3 e a EAL 1 e 2 (Figura 2).

RESULTADOS E DISCUSSÃO





RESULTADOS E DISCUSSÃO

- Composição química dos óleos essenciais;
- Trabalhos com abordagens diversificadas;
- Interatividade e uso de elementos do cotidiano;
- Participação ativa dos alunos.

CONCLUSÕES

- A cromamatografia em camada delgada foi uma ferramenta efetiva;
- Conexão entre a teoria e a prática;
- Ambientação no processo de aprendizagem investigativa;
- Formação a partir de uma experiência dinâmica;

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ESSAY ON GLOBAL WARMING: SOLAR RAYS. FRIEND OR FOE?

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ABSTRACT

In this review, the documentary "An Inconvenient Truth", directed by Davis Guggenheim and presented by the former Vice President of the United States, Al Gore, has been analyzed, focusing on the mechanisms by which solar radiation and infrared radiation (IR) contribute to the Earth's energy dynamics, and how these phenomena impact global warming, terrestrial albedo, the greenhouse effect and the regulation of atmospheric temperature. Discussing also the information that the documentary inspires to provide with it, the analysis was opened through a literature search and the review of five keywords in order to highlight the role of science communication and its function in promoting and providing clear examples of how the phenomenon of climate change has manifested itself in recent years.

Keywords: *Greenhouse Effect, Global Warming, Atmospheric Temperature, Albedo, Infrared Radiation.*

1. INTRODUCTION

Global warming is a phenomenon that, year after year, gives much to talk about; successive investigations are carried out on the subject, and everything seems to indicate that the situation of life on earth is becoming more and more complicated at a global level, due to the gradual increase of the earth's temperatures in certain seasons of the year. In order to understand this issue in more depth, it is important to be clear about some important concepts and ideas.

The Earth's atmosphere is a thin layer of gases that surrounds our planet; to give an idea of the scales, the atmosphere is equivalent to wrapping a soccer with aluminum foil: the football represents the Earth, and the thickness of the foil is the thickness of the atmosphere. This thin layer of gases that surrounds the planet is very important since it contains the gases that are fundamental for the development of most of the life on the planet, in addition to the fact that the atmosphere represents an important medium in which a good part of the life on Earth resides (Caballero M. et al., 2007).

From the moment they leave the sun, UV rays take about 8 minutes to reach the Earth's surface and begin to heat it; part of the rays is absorbed by atmospheric components and another part strikes the Earth's crust, heating it in a short time. Part of these rays emitted from the sun and absorbed by the Earth's surface is radiated back into the atmosphere in the form of infrared radiation (albedo). Due to anthropogenic activity throughout contemporary times, atmospheric pollution is increasing, which has led to a thickening of the atmospheric layer due to the generation and release of greenhouse gases into the atmosphere. This phenomenon of atmospheric thickening generates a higher concentration of infrared radiation trapped in the Earth's atmosphere, producing a gradual and gradual increase of temperatures in the biosphere, generating an increasingly recurrent thermal, seasonal and biological imbalance.

The following figure (Figure 1), taken from the documentary "An Inconvenient Truth" (2006), shows an outline of what was explained in the previous paragraph:

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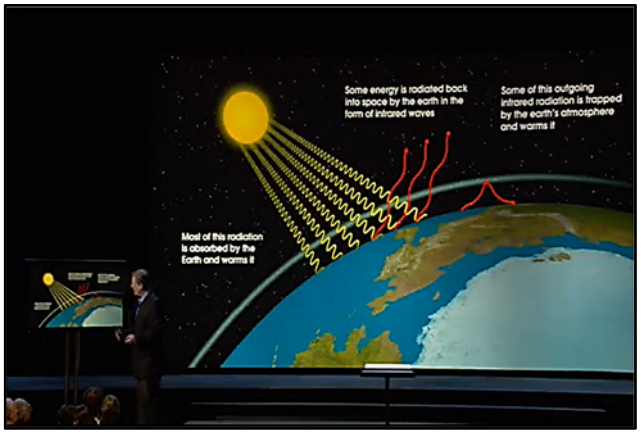


Figure 1. *Solar radiation that reaches the Earth from the sun is reflected and trapped by the atmosphere.*

Greenhouse gases are gaseous molecules that generate a phenomenon of thermal capture of solar radiation, which leads to an increase in atmospheric temperature. Among the direct greenhouse gases par excellence, Blanquicett C. et al. (2018)[2], find:

- Carbon dioxide (CO_2) is produced by the combustion of oil, natural gas, coal, and other fossil agents; it is responsible for 70% of the greenhouse effect.
- Methane (CH_4): produced by biomass burning, decomposition of organic waste, wetlands, livestock fecal matter, and rice crops; responsible for 20% of the greenhouse effect.
- Nitrous oxide (N_2O) is produced in industrial processes and is burned by biomass; it is responsible for 7% of the greenhouse effect.
- Water vapor: due to its capacity to retain heat emanating from the earth's surface.

This thermal capture is due to the fact that the molecular structure of each gas mentioned has the ability to vibrate so that these gases absorb energy in the form of heat. When the molecules of these gases absorb radiation, their chemical bonds vibrate (stretch and/or compress), generating this thermal capture and raising the average atmospheric temperature.

The objective of this work is to search for five words pertinent to the described topic in four search engines and in different time ranges in order to obtain the number of results returned by these engines and to analyze the relevance of this topic in relation to the selected period or time range.

2. MATERIALS AND METHODS

2.1 Methods

A bibliographic search was performed using different search engines, Google Search, Google Scholar, Google Trends, and scientific and social platforms such as Academia.edu. In each of these engines and/or platforms, the following keywords were searched:

- Greenhouse Effect
- Global Warming
- Atmospheric Temperature
- Albedo
- Infrared Radiation

For the analysis, the amount and/or percentage of appearance of each of the words (number of results) was searched in each of the platforms and engines, and a comparison was made according to the loading date in different periods. The Google Trends engine was also used to obtain information on the recurrence and distribution of searches in different regions around the world.

2.1.1. Google Search

The main page of Google (Google, 2024)[3] was accessed, and a search was performed for the different keywords for the periods of 1 week, 1 year, and 10 years ago, respectively. These data were compiled and tabulated for comparison in the Discussion and Results section.

2.1.2. Google Trends

We entered the Google Trends page (Google Trends, 2024)[4] and entered the keywords in the search engine, allowing us to observe the search interest at different periods, including in real-time, for different places, regions, countries, etc. For this case, we took the 5 years and its search distribution around the globe according to a graph by regions and another one of search frequency.

2.1.3. Google Scholar

The main page of Google Scholar (Scholar Google, 2024)5 was accessed, and the 5 keywords were searched for a period of 1, 5, and 10 years ago. These data were compiled and tabulated for comparison in the following results and discussion section.

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2.1.4. Academia.edu

We accessed the Academia.edu platform (Academia.edu, 2024)[6] and the main search engine for articles, entering the 5 keywords in English; given that the engine provides results of titles in articles and papers containing these words, the search was considered for the periods 1, 5 and 10 years ago. These data were compiled and tabulated for comparison in the following section of results and discussions.

3. RESULTS AND DISCUSSION:

With respect to the searches performed for the five words/phrases related to the subject matter covered, tables were constructed (Table 1), and graphs were displayed containing information on the search results for each search engine:

3.1. Google Search

The following table (Table 1) shows the results of the searches for the five key phrases or keywords in Google Search:

keywords	1 year	1 week	10 years
Greenhouse Effect	3.860.000	84.700	17.000.000
Global Warming	4.330.000	121.000	18.400.000
Atmospheric Temperature	1.860.000	50.300	10.200.000
Albedo	13.500.000	1.310.000	40.200.000
Infrared Radiation	61.700	3.360	165.000

Table 1. *Google search results for the five words range from one year to one week and one decade.*

It can be seen that the word with the highest search results was Albedo within all-time ranges. However, terms such as Greenhouse Effect, Global Warming and Infrared Radiation also generated many queries due to their direct relationship with rising temperatures and the interest in understanding the functioning of the climate system.

3.2. Google Trends

Five graphs (Figures 2-6) are presented below for each keyword or phrase chosen, showing the countries or regions that most searched for these phrases worldwide:

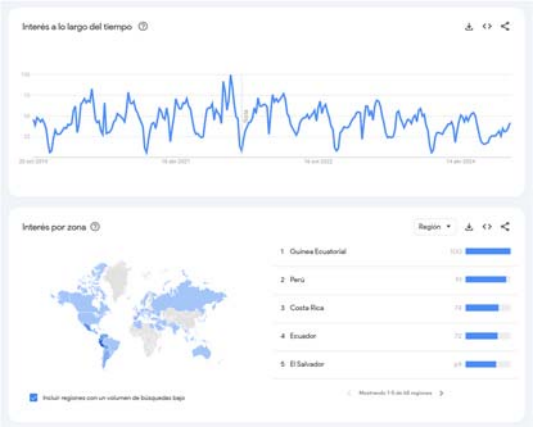


Figure 2. *Searches for "Greenhouse Effect".*

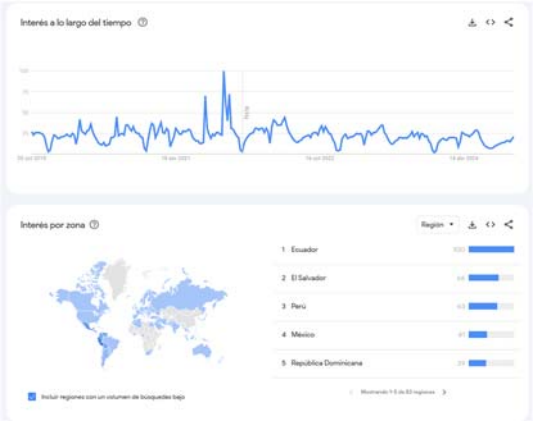


Figure 3. *Searches for "Global Warming".*

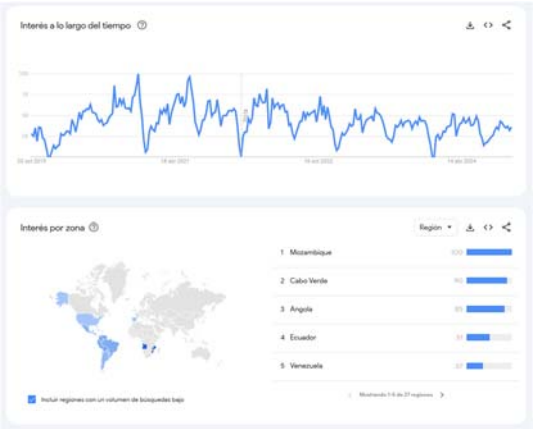


Figure 4. *Searches for "Atmospheric Temperature".*

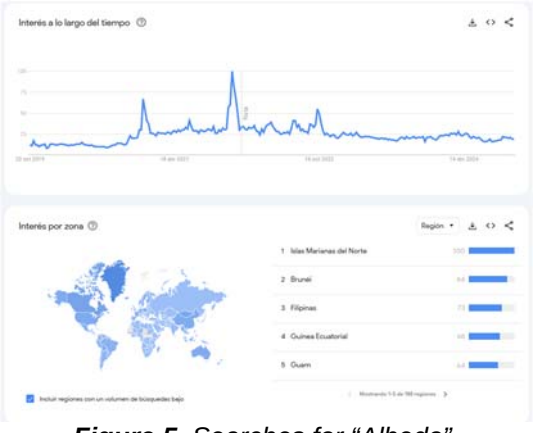


Figure 5. *Searches for "Albedo".*

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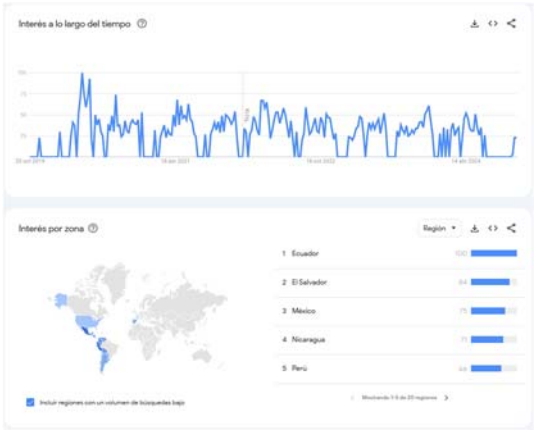


Figure 6. Searches for “Infrared Radiation”.

These graphs show that most of the words and phrases selected were mostly searched by countries with very extreme climatic conditions, as far as hot climates are concerned, countries located in the equatorial region of the globe, which gives rise to inferences about an indication of interest (or, why not, concern) regarding the environmental problems caused by the phenomenon of global warming and the greenhouse effect.

It is thought that these equatorial countries, with such extreme summer climates, need to act and combat global warming with greater impetus since the effects of this problem are felt more intensely in their territory, with more frequent heat waves, prolonged droughts, and greater vulnerability to extreme weather phenomena, which affects their agriculture, water availability and the quality of life of the local population.

3.3. Google Scholar

In this section, the results of the searches for the five phrases or keywords in Google Scholar are presented in the following table (Table 2):

Keywords	1 year	5 years	10 years
Greenhouse Effect	16.200	19.400	29.900
Global Warming	16.900	17.600	23.300
Atmospheric Temperature	13.100	16.500	26.800
Albedo	17.600	39.200	89.800
Infrared Radiation	5.840	15.800	16.000

Table 2. *Google Scholar search results for the five words range from one year to one lustrum and one decade.*

From the analysis of these results it can be seen that the word Albedo continues to stand out as the most searched word, especially in the long term, with almost 90,000 searches in the last 10 years. However, the Greenhouse Effect and Global Warming remain relevant in these results, reflecting not only a very close relationship between all these terms, but also the concern about understanding each climatic factor that takes place or interacts in this environmental issue.

3.4. Academia.edu

The following table (Table 3) shows the results of the searches for the five phrases chosen in the Academia.edu scientific platform:

Keywords	1 year	5 years	10 years
Greenhouse Effect	20	276	500
Global Warming	151	1.054	2.251
Atmospheric Temperature	13	146	386
Albedo	20	294	719
Infrared Radiation	7	125	332

Table 3. *Academia.edu search results for the five words range from one year to five years and a decade.*

With a lower number of search results in relation to the previous engines, this platform is dominated by search results for Global Warming in all selected time ranges. At the same time, although the terms Albedo and Greenhouse Effect were also in demand, the focus was especially on the impacts and understanding provided by scientific papers on global warming.

In addition, it was considered that the results referring to this platform have a greater incidence for the titles of specific articles and papers, giving sense to why greater results were obtained for Global Warming and, on the other hand, Alb edo, rather a subtopic that can be perfectly treated within research on this topic.

4. CONCLUSIONS:

In this work, by means of a simple methodology, it was possible to observe the trend

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and volume of information that contemplates the key aspects proposed in this work. Through the bibliographic analysis, it was noticeable that terms such as “Albedo” and “Global Warming” reflected greater public and scientific interest, in addition to representing a growing trend in search results during the last decade.

Given the analysis and understanding of this problem, it is often believed that the phenomena rooted in solar radiation (specifically, infrared radiation) are largely ignored since their interaction with the abundance of greenhouse gases (mostly anthropogenic) generates an increase in atmospheric temperature, which directly leads to global warming on a large scale. However, the importance of the sun’s rays as a vital source for the subsistence of terrestrial life has been disregarded.

This working group, in particular, considers that articles and reviews of this type represent a very important message regarding climate action and scientific dissemination. By proposing a methodology that is achievable, simple, yet efficient and popular in today’s society, we can make the evolution of this issue visible. As in the documentary under study, we emphasize the importance of statistical data, being, in essence, the fundamental tool to compare, contrast, and demonstrate the existence of phenomena that contribute to climate change.

5. DECLARATIONS

5.1. Acknowledgements

The authors MFF and JPS would like to thank the Department of Physical Chemistry (DFQ), the Faculty of Chemical Sciences (FCQ), the National University of Córdoba (UNC), and the professors of Environmental Physical Chemistry B (Belén Blanco and Walter Peláez) for the opportunity and help in the preparation of this work.

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Southern Science Conference, 2024.

ESSAY ON GLOBAL WARMING: SOLAR RAYS. FRIEND OR FOE?

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November/2024

INTRODUCTION

Global warming is an increasingly concerning phenomenon worldwide due to the gradual rise in Earth's temperatures. The atmosphere, a thin layer that envelops the Earth, plays a crucial role in regulating temperature through its interaction with solar radiation and infrared radiation. Solar rays that reach the Earth's surface are partly absorbed and then re-emitted as infrared radiation, a process influenced by albedo and greenhouse gases. However, pollution has increased the concentration of these gases, trapping more heat and contributing to the rise in atmospheric temperatures, which destabilizes the climate and life on Earth.

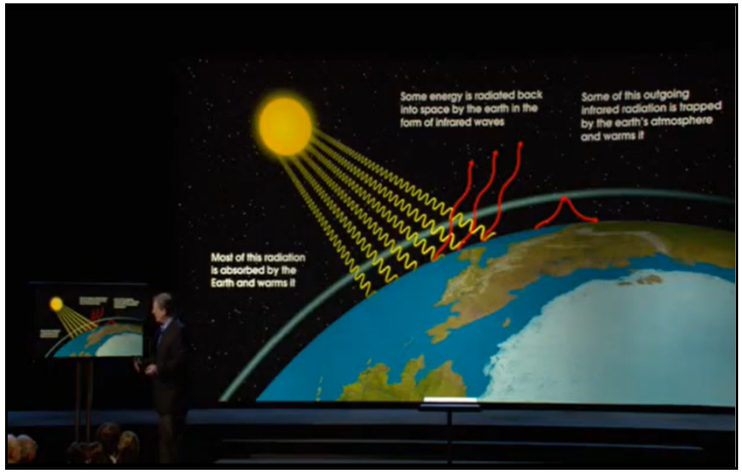


Image extracted from “An Inconvenient Truth” (2006).

AIM/OBJECTIVE/PURPOSE

To analyze the impact of solar and infrared radiation on Earth's energy dynamics, particularly focusing on global warming, the greenhouse effect, and atmospheric temperature regulation. Using bibliographic research on key terms, this study aims to highlight the role of scientific communication in raising awareness of climate change, as inspired by the documentary *An Inconvenient Truth*. The methodology emphasizes accessible approaches for examining the relevance and societal implications of climate phenomena.

METHODOLOGY

The methodology consisted of a literature search in various platforms such as Google Search, Google Scholar, Google Trends and Academia.edu, using five keywords:

- Greenhouse Effect.
- Global Warming
- Atmospheric Temperature
- Albedo
- Infrared Radiation

Search results were collected and compared for three time periods: 1 year, 5 years and 10 years. Google Trends allowed us to analyze the frequency and distribution of searches globally, while Google Scholar and Academia.edu provided more specialized scientific information. The data obtained were tabulated to analyze the relevance of each term in different temporal and geographical contexts.

RESULTS AND DISCUSSION

The ***Google Search*** results for the five key terms are shown in the table below. Over 1 year, 1 week, and 10-year time spans, **"Albedo"** had the highest number of searches, reflecting a strong interest in how Earth's reflective capacity impacts climate dynamics. However, terms such as **"Global Warming"** and **"Greenhouse Effect"** also generated substantial search volumes, indicating widespread public and scientific interest in understanding factors directly influencing temperature increases and the climate system's behavior.

	1 year	1 week	10 years
Greenhouse Effect	3.860.000	84.700	17.000.000
Global Warming	4.330.000	121.000	18.400.000
Atmospheric Temperature	1.860.000	50.300	10.200.000
Albedo	**13.500.000**	**1.310.000**	**40.200.000**
Infrared Radiation	61.700	3.360	165.000

RESULTS AND DISCUSSION

The search results from ***Google Scholar*** are summarized in the table below. Over 1, 5, and 10-year periods, **"Albedo"** consistently shows the highest search volumes, with nearly 90,000 results over 10 years, highlighting significant scientific interest in how Earth's reflectivity influences climate. Meanwhile, terms like **"Greenhouse Effect"** and **"Global Warming"** also retained strong relevance, reflecting ongoing scholarly focus on core processes affecting atmospheric warming.

	1 year	5 years	10 years
Greenhouse Effect	16.200	19.400	29.900
Global Warming	16.900	17.600	23.300
Atmospheric Temperature	13.100	16.500	26.800
Albedo	**17.600**	**39.200**	**89.800**
Infrared Radiation	5.840	15.800	16.000

RESULTS AND DISCUSSION

In Academia.edu, the analysis of the searches for the five key phrases showed **"Global Warming"** as the dominant term, particularly over longer timeframes. This reflects a strong academic drive to understand the broader impacts of global warming, as supported by numerous research articles and papers available on this topic. While **"Albedo"** and **"Greenhouse Effect"** also garnered substantial searches, these were often explored as subtopics within studies on climate change, suggesting that scholars are particularly interested in how specific mechanisms, like Earth's reflectivity and greenhouse gas concentrations, contribute to global temperature rise. Additionally, the platform's focus on article titles and research summaries likely influenced the prominence of **"Global Warming"**, as it remains a critical focal point in scientific research and communication.

	1 año	5 años	10 años
Efecto Invernadero	20	276	500
Calentamiento Global	151	1.054	2.251
Temperatura Atmosférica	13	146	386
Albedo	20	294	719
Radiación Infrarroja	7	125	332

RESULTS AND DISCUSSION

The ***Google Trends*** analysis for revealed notable geographical variations in search interest. These terms were most frequently searched in regions experiencing extreme climates, particularly in equatorial areas, indicating heightened concern or awareness in countries that are more directly impacted by climate issues. This suggests a correlation between climate-related challenges, such as frequent heatwaves and droughts, and public interest in climate science topics, highlighting a regional urgency in understanding and addressing global warming and its effects on local environments.



Greenhouse Effect



Atmospheric Temperature



Infrared Radiation



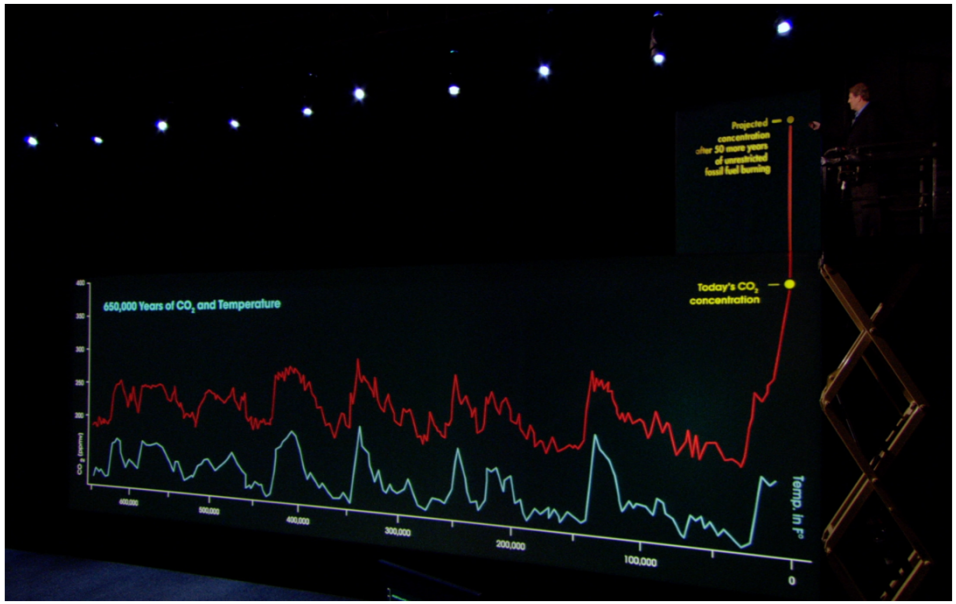
Global Warming



Albedo

CONCLUSIONS

This review, using a straightforward methodology, highlighted growing public and scientific interest in terms like "Albedo" and "Global Warming," showing a marked increase in search results over the past decade. The analysis underscores how solar radiation, especially infrared, interacts with greenhouse gases—mainly anthropogenic—to raise atmospheric temperatures, directly contributing to global warming. Yet, solar rays are vital for sustaining life on Earth. This study emphasizes the role of accessible and efficient methods, such as bibliographic reviews and statistical data, to promote climate awareness and scientific communication. Statistical evidence, as shown in the studied documentary, is essential to identifying and understanding climate change factors.



https://talkfilmsociety.com/articles/revisiting-an-inconvenient-truth

ACKNOWLEDGEMENTS

- Universidad Nacional de Córdoba (UNC).
- Facultad de Ciencias Químicas (FCQ)
- Departamento de Fisicoquímica (DFQ).
- Special thanks to prof. Walter Peláez & María Belén Blanco (Professors of Environmental Physical Chemistry B), for the opportunity and his help in preparing this work.
- Our families, for their unconditional love and support regarding our university careers.

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LACCASE-BASED ELECTROCHEMICAL BIOSENSOR AS AN ALTERNATIVE FOR POLYPHENOLS DETERMINATION IN QUINCE EXTRACTS

PICCOLI, María Belén[1,2]; BUSTAMANTE BRIZUELA, Alejandra Belén[3,4]; BARONI, María Verónica[3,4]; VICO, Raquel Viviana[2,3]; FERREYRA, Nancy Fabiana[1,2*]

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ABSTRACT

We developed a laccase biosensor by modifying glassy carbon electrodes with single-walled carbon nanotubes functionalized with diazonium salt. The biosensor provided fast, stable, and sensitive electroanalytical responses to different polyphenols and was successfully applied to determine the total content of polyphenols in quince extracts. The results obtained indicate that the biosensor is a new analytical tool that avoids the interferences of the Folin-Ciocalteu method and represents a simple alternative compared to chromatography.

Keywords: *laccase, electrochemistry, biosensor, polyphenols, quince extracts*.

1. INTRODUCTION

Quince is rich in bioactive compounds such as polyphenols, which have antioxidant and antimicrobial properties (Herrera-Rocha *et al*., 2022). During the production of quince paste, significant waste is generated, including peels, skins, and seeds. This agro-industrial waste can be used to extract polyphenols, but it is necessary to assess new environmentally friendly alternative methods of extraction that comply with the principles of green chemistry, avoiding or reducing the use of organic solvents. To evaluate the efficiency of these methods, the total content of polyphenols (TCP) should be quantified and compared in the resulting samples. TCP determination is commonly performed using the Folin-Ciocalteu (FC) assay. This method presents some disadvantages, as the use of non-eco-friendly reagents, prolonged processing time, low specificity, and multiple interferences (Bastola *et al*., 2017). As alternative for TCP quantification we propose an electrochemical biosensor based on the enzyme Laccase (Lac). This protein is capable of oxidizing a variety of substrates, including phenolic compounds, in the presence of molecular oxygen. To develop the biosensor, we used glassy carbon electrodes (GCE) modified with single-walled carbon nanotubes chemically functionalized to expose carboxylic groups (SWCNT-pBA).

Under optimized conditions, the developed biosensor provided fast, stable, and sensitive electroanalytical responses to different polyphenolic compounds. Taking advantage of the excellent response achieved, the biosensor was used to analyze the TCP of quince extracts obtained through different chemical and thermal treatments. The values were compared with those determined by the FC method. The results showed very good agreement between both methodologies and an adequate correlation with the chemical profiles of the samples analyzed by HPLC. Although the chemical identification of each phenolic compound can't be achived with the proposed biosensor, our results demonstrates that it is a relatively simple and adequate alternative for determining TCP in complex matrices and could be applied as analytical tool for food analysis.

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DOI: 10.48141/SSCON_42_2024.pdf

2. MATERIALS AND METHODS

2.1. Reagents

Single-walled carbon nanotubes (SWCNT) of chirality (7, 6), 4-aminobenzoic acid (pBA), anhydrous N, N-dimethylformamide, isopentyl nitrite (IPN) and Laccase from *Trametes versicolor* (oxygen oxidoreductase EC 1.10.3.2), were from Sigma-Aldrich. All reactives were of an analytical degree. Solutions were prepared with ultrapure water (18 MΩ cm). SWCNT were functionalized in-situ with diazonium salt derived from the 4-aminobenzoic acid (pBA) using IPN as it is represented in Figure 1 (Piccoli *et al*., 2021).

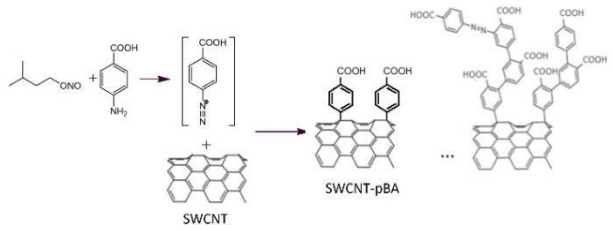


Figure 1. *Functionalization of SWCNT with the diazonium salt derived from 4-aminobenzoic acid.*

2.2. Equipment

FTIR spectra were recorded with a Thermo Scientific Nicolet iN10 infrared Microscope. Spectrophotometric analysis was carried out with a Shimadzu UV-2600 spectrophotometer. Cyclic voltammetry (CV) and chronoamperometry (CA) were performed with an Autolab PGSTAT128N and a Teq4 potentiostat, respectively. A GCE of 3 mm diameter (CHI104, CH Instruments), a Pt wire, and an Ag/AgCl, 3M NaCl electrode (RE-5B, BAS) were used as working, counter, and reference electrodes, respectively. All reported potentials are referred to this reference electrode. The experiments were performed at room temperature.

2.3. Surface modification and construction of the biosensor

The GCE was polished with 0.05 µm alumina powder for 2 minutes, followed by sonication in deionized water for 30 seconds, and then cycled between -0.30 V and 0.80 V at 0.10 V/s in 0.10 M phosphate buffer (pH 7.0). The electrodes were modified by drop-coating with 10 µL of 0.50 mg/mL SWCNT-pBA dispersion, prepared in a 50/50 % (V/V) ethanol/water solution. The solvent was allowed to evaporate at 60 ºC for 20 minutes. Lac was adsorbed onto the GCE/SWCNT-pBA from a 2 mg/mL solution for 60 minutes at 8 ºC. The resulting electrode is named GCE/SWCNT-pBA/Lac.

2.4. Preparation of quince extracts and determination of total polyphenol content

Samples of residues obtained during the industrial production of quince jam were analyzed. Polyphenols extraction was carried out using different methods: ultrasonic treatment in a 50:50 methanol/water solution with 0.1% v/v HCl (Sample I) or a hydrothermal “steam explosion” treatment with high-pressure saturated steam in an autoclave followed by rapid decompression using water (Sample II) or water with 2% w/v citric acid (Sample III). The TCP was determined using the FC method with GA as standard (Bastola *et al*., 2017).

2.5. Chronoamperometric measurements and statistical analysis of the response

The response of the biosensor to catechol (CAT), hydroquinone (HQ), resorcinol (RES), gallic acid (GA), was analysed by CA. The working potential (E_{ap}) for each phenolic compound was selected based on their voltammetric response at a pH of 5.0. The E_{ap} selected is 0.20 V for CAT, 0.00 V for HQ, 0.10 V for RES, and 0.00 V for GA. CA experiments were conducted under convective conditions achieved by magnetic stirring. The transient current was allowed to decay to a steady-state value before the addition of a specific amount of the polyphenol. The subsequent current generated was monitored over time to obtain calibration curves. The sensitivity (S) of the biosensor was determined from the slope of the linear portion of the calibration curve. The limits of detection (LOD) and quantification (LOQ) were calculated as 3.3 × SD/S and 10 × SD/S, respectively, where SD is the standard deviation of the background current. The TCP in quince extracts was determined using the standard addition method at 0.00V employing GA.

3. RESULTS AND DISCUSSION:

3.1. Characterization of SWCNT-pBA

Figure 2A shows the FTIR spectra of the nanotubes before and after chemical functionalization.

In the SWCNT-pBA spectrum, several signals can be identified: at 3332 cm^{-1} and 1316 cm^{-1}, the vO-H and vC-O from the carboxylic acid groups, respectively; at 3072 cm^{-1}, the vC-H from the aromatic groups; at 2920 and 2850 cm^{-1}, the asymmetric and symmetric vC-H sp^3 vibrations, respectively; at 1720 cm^{-1}, the vC=O of the

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carboxylic acid group; at 1655, 1525, and 1420 cm^{-1}, the C-C bond from aromatic compounds overlapped with the asymmetric and symmetric stretching vibrations of the carboxylate group; and a signal at 1370 cm^{-1} from δO-H. The SWCNT spectrum presents only a broad band around 3500 $cm^{-1,}$ probably due to adsorbed water or other impurities in the sample.

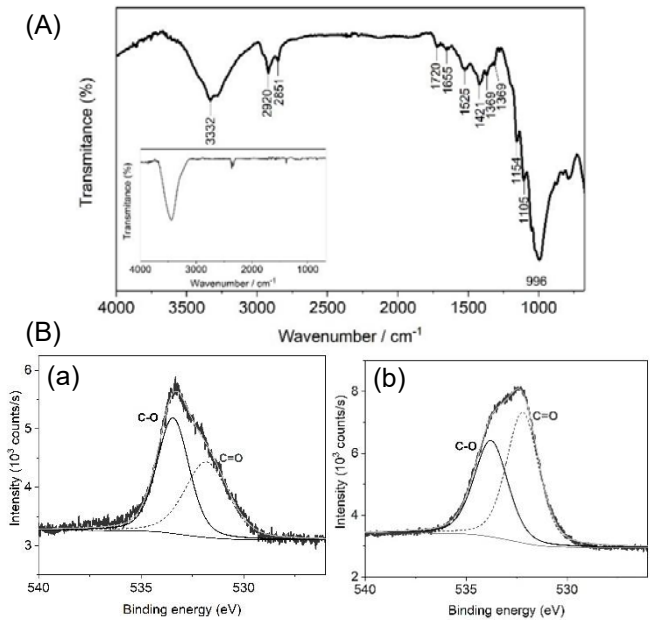


***Figure 2**. (A) FTIR spectra of SWCNT-pBA and SWCNT (inset). (B) High-resolution XPS spectra of O_{1s} for SWCNT (a) and SWCNT-pBA (b).*

Figure 2B shows the high-resolution XPS spectra of O1s for SWCNT and SWCNT-pBA. A clear increment in oxygen content is observed after the functionalization, being 6.17 % and 10.30 % for SWCNT and SWCNT-pBA, respectively. In addition, a change in the contributions assigned to the C-O and C=O bonds is observed. These results demonstrate the incorporation of carboxylic groups, among other oxygenated groups, onto the SWCNT surface as a result of the chemical functionalization. These functional groups impart a pH-dependent surface charge to the nanotubes, enabling the formation of stable colloidal dispersions. Moreover, the charges exposed on the GCE/SWCNT-pBA favor Lac immobilization, as the protein is positively charged at the working pH of 4.5.

3.2. Chronoamperometric response of phenolic compounds on GCE/SWCNT-pB/Lac

Lac can catalyze the oxidation of *o*-, *m*-, and *p*-benzenediols and phenol to *o*-, *m*-, *p*-quinones or radical species in the presence of molecular oxygen according to the following global reaction:

$$AH_2 + 1/2\ O_2 \ \ laccase \rightarrow A + H_2O$$

where AH_2 and A are the reduced and oxidized species of the phenolic compounds, respectively. The product of the enzymatic reaction, A, is reduced at the working electrode at the appropriate potentials, E_{ap} (Villalba-Rodríguez *et al*., 2022). Figure 3 shows the CA response of the biosensor towards GA and the calibration curve (inset). GA is widely used as a standard in the determination of TPC using the FC method, so it is interesting to compare the biosensor's response using the same compound. From the calibration curves, the sensitivity of the electrode towards CAT, RES, HQ, and GA was determined; Table 1 summarises the corresponding analytical parameters. Additionally, the biosensor retains 97% and 60% of the initial response after 5 consecutive uses or 11 days of storage in buffer solution, respectively.

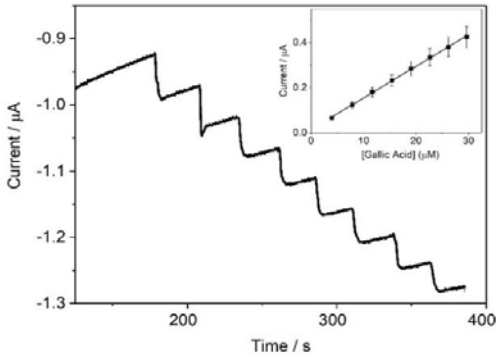


***Figure 3**. CA response and calibration curve (inset) of GA. Supporting electrolyte: acetate buffer 0.10 M pH 5.0. Eap: 0.00 V.*

***Table 1**. Analytical parameters of the biosensor*

Substrate	Sensitivity (μA m**M**$^{-1}$)	LOD/LQO (μ**M**)
CAT	(17.8±0.7)	0.6/2
HQ	(7±1).10	0.2/0.5
RES	(0.150±0.007)	140/400
GA	(13.4±0.8)	1/3

3.3. Determination of TPC in quince extracts

The extract obtained from residues from the industrial production of quince jam was analyzed using the standard addition of GA. Figure 4 shows the calibration plot of the samples obtained with the different extraction methods, while the inset shows the voltammetric profile. A TCP of (238 ± 34), (258 ± 1), and (255 ± 51) µg of GA/mL was determined for samples (I), (II), and (III), respectively, indicating that the three extraction methods allow for obtaining similar

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amounts of polyphenolic compounds. These results were confirmed by UHPLC-MS/MS (Fig. 4B). In contrast, the FC method yields results of (193 ± 23), (253 ± 17), and (408 ± 24) µg of GA/mL for the respective samples, evidencing the interference of citric acid in the assay (Mello *et al.*, 2003).

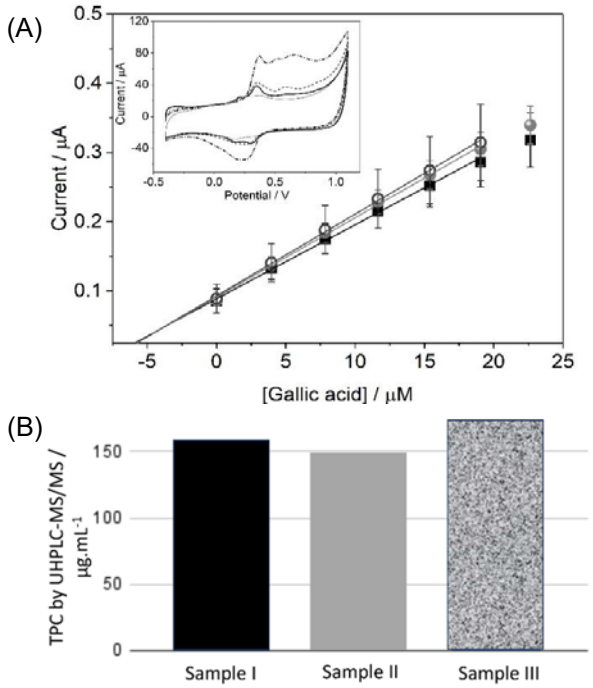


***Figure 4**. Analysis of the TPC of samples I (●), II (■), and III (○) by using: A) Lac biosensor measuring at 0.00 V in acetate buffer 0.10 M pH 5.0 and B) UHPLC-MS/MS. Inset in fig. A shows the voltammetric profile of supporting electrolyte (—) and samples I (—•—), II (—) and III. (---).*

In addition, the inset in Fig. 4A suggests the presence of a higher proportion of flavonoid compounds in the sample (I). Complementary analysis by HPLC indicated that the proportion of hydroxycinnamic acids (chlorogenic, cryptochlorogenic, and neochlorogenic acid) was similar for the three samples, but the profile of the flavonols (kaempferol, quercetin, rutin and its derivatives) and flavanols (catechin and derivatives) was variable, being more abundant in sample I, not shown. The oxidation of flavonols and flavanols has been reported at carbon electrodes at a higher potential than polyphenols, so the strong signal observed at a potential mayor than 0.5 V in the voltammogram of the sample I could be associated with the presence of these compounds in the extract.

4. CONCLUSIONS:

The modification of GCW with SWCNT-pBA increased the electroactive area, enhanced the electrochemical response to polyphenols, and promoted the adsorption of laccase. These properties contributed to increasing the biosensor's sensitivity. Under optimized conditions, the developed biosensor provided fast, stable, and sensitive electroanalytical responses to different polyphenolic compounds. The biosensor was successfully applied to quantify the TPC, and the results presented a good agreement with the results obtained from the traditional chromatographic methods, avoiding the interference observed with the Folin-Ciocalteu method.

5. DECLARATIONS

5.1. Acknowledgements

The authors thank SECyT-UNC, and ANPCYT [PICT-2020-2524] for their financial support. M. B. Piccoli, thanks CONICET for the fellowship.

5.2. Open Access

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Southern Science Conference, 2024.

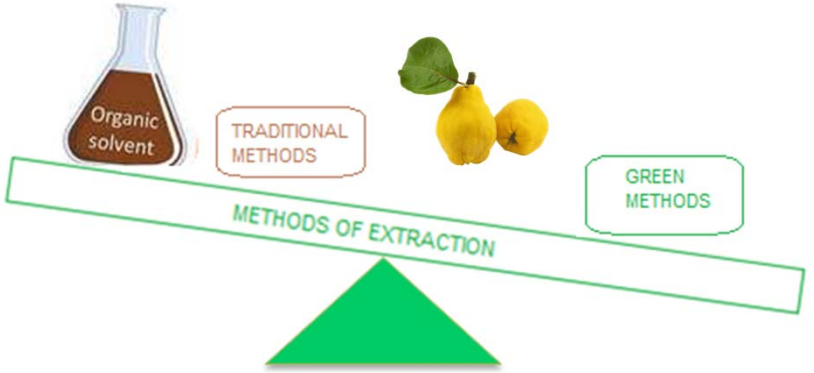
LACCASE-BASED ELECTROCHEMICAL BIOSENSOR AS AN ALTERNATIVE FOR POLYPHENOLS DETERMINATION IN QUINCE EXTRACTS

María Belén Piccoli
Universidad Nacional de Córdoba, Facultad de Ciencias Químicas, Departamento de Fisicoquímica. Instituto de Investigaciones en Fisicoquímica de Córdoba (INFIQC), CONICET. Argentina
Alejandra Belén Bustamante Brizuela
Universidad Nacional de Córdoba, Facultad de Ciencias Químicas, Departamento de Química Orgánica. Insituto de Ciencia y Tecnología de los alimentos (ICyTAC), CONICET. Argentina.
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Universidad Nacional de Córdoba, Facultad de Ciencias Químicas, Departamento de Química Orgánica. Insituto de Ciencia y Tecnología de los alimentos (ICyTAC), CONICET. Argentina.
Raquel Viviana Vico
Universidad Nacional de Córdoba, Facultad de Ciencias Químicas, Departamento de Química Orgánica. Instituto de Investigaciones en Fisicoquímica de Córdoba (INFIQC), CONICET. Argentina
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November/2024

INTRODUCTION

- Quince is rich in bioactive compounds, such as polyphenols, which have antioxidant and antimicrobial properties.
- The agro-industrial waste generated during the production of quince paste can be used to extract polyphenols, making it important to find environmentally friendly methods for their extraction.



Methods for determining Total Polyphenolic Content (TPC)

Folin-Ciocalteu assay

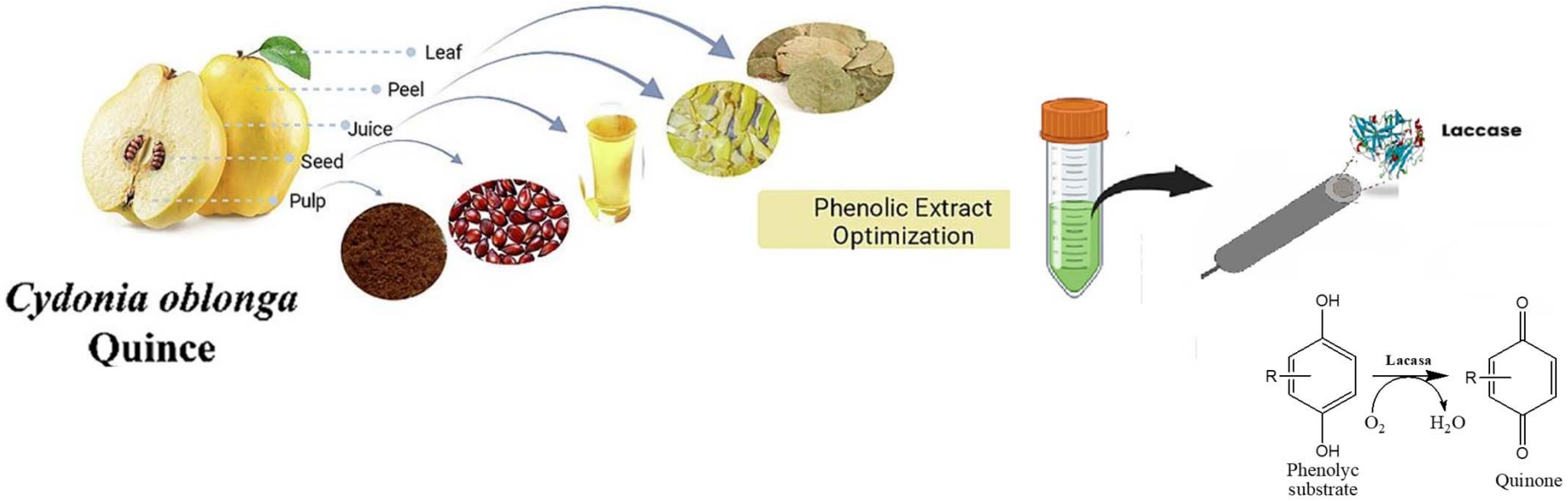
- ✓ Simple
- ✓ Economical
- X Use of non-ecofriendly reagents
- X Low specificity

Chromatography (as HPLC)

- ✓ High sensitivity
- ✓ Identification of polyphenols
- X Specific equipment
- X Expensive
- X Use high amount of organic solvents

PURPOSE

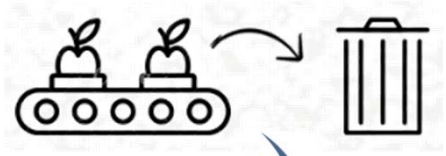
We propose an **electrochemical biosensor** based on the enzyme **laccase** as an alternative to **TCP quantification** to evaluate the efficiency of eco-friendly extraction methods of polyphenols in quince extracts.



METHODOLOGY

Preparation of quince extracts

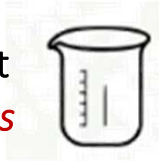
Waste from industrial production of quince paste



Treatment of polyphenols extract



Ultrasonic treatment
With organic solvents



Methanol + H_2O (50:50) + HCl (0,1%V/V)

Hydrothermal treatment "steam explosión"
Without organic solvents



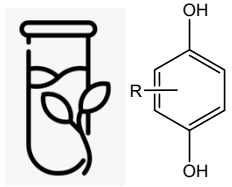
High pressure saturated steam followed by rapid decompression

(T = 121 ºC; t = 15 min; P = 0.1 MPa)

H_2O

H_2O + citric acid 2% W/V

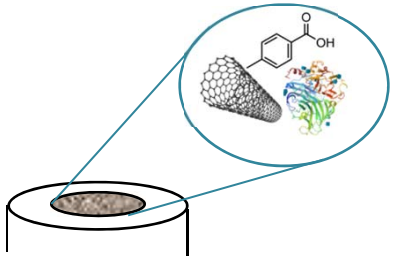
Determination of TPC



Folin-Ciocalteu (FC) assay

UHPLC-MS/MS triple quadrupole

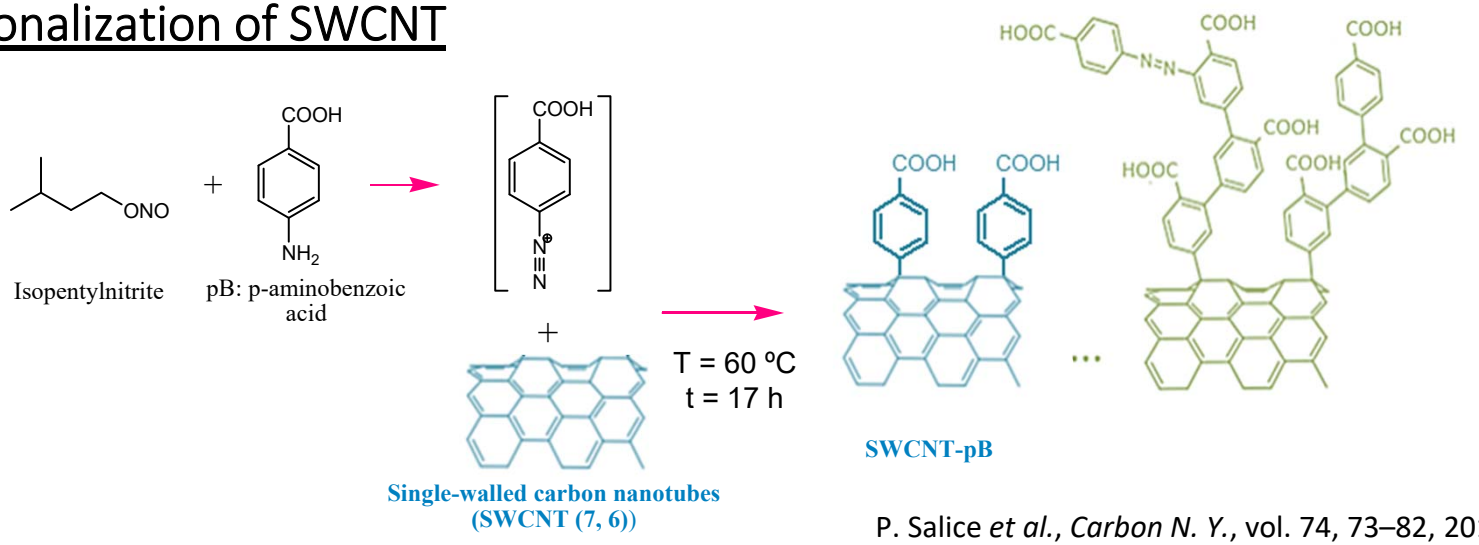
Laccase-based electrochemical biosensor



GCE/SWCNT-pB/Lac

METHODOLOGY

Functionalization of SWCNT



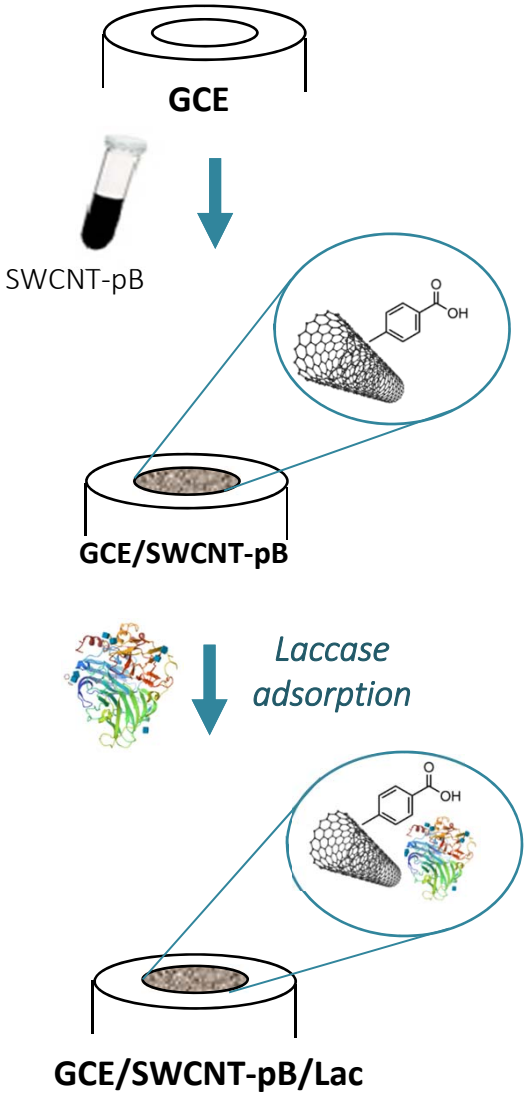
P. Salice *et al.*, *Carbon N. Y.*, vol. 74, 73–82, 2014.

Preparation of dispersions of SWCNT-pB

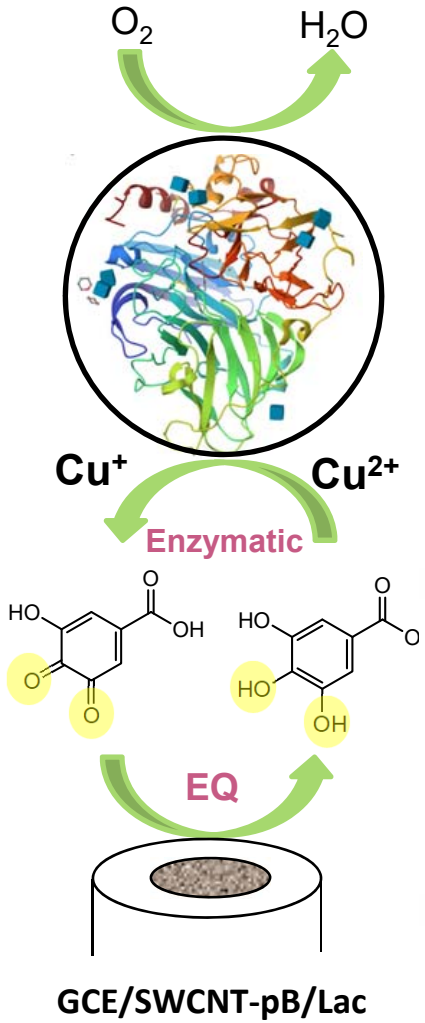


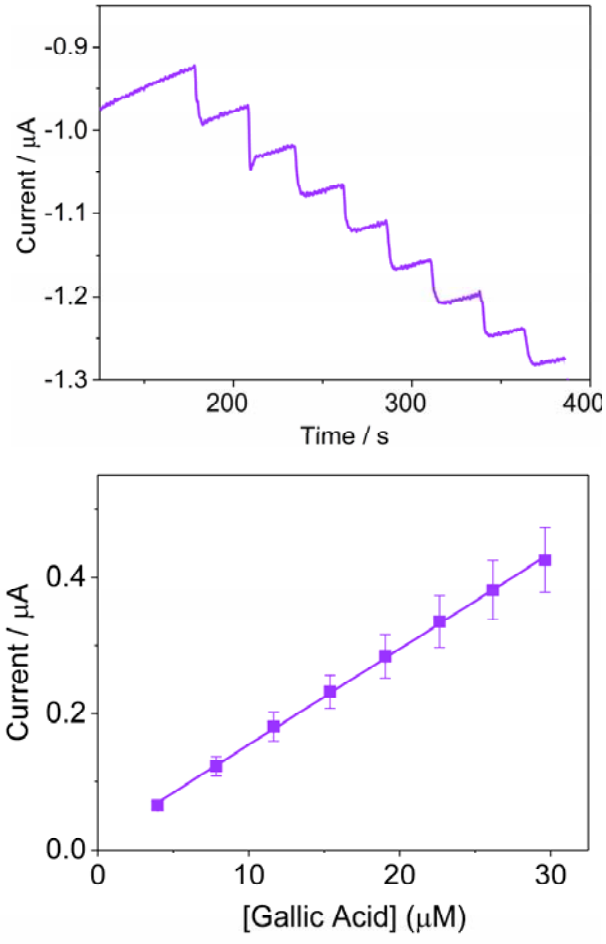
METHODOLOGY

Construction of biosensor



Quantification of TPC

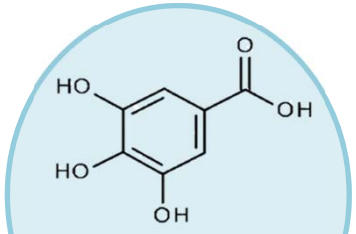




Supporting electrolyte: acetate buffer 0.10 M pH 5.0. Eap: 0.00 V.

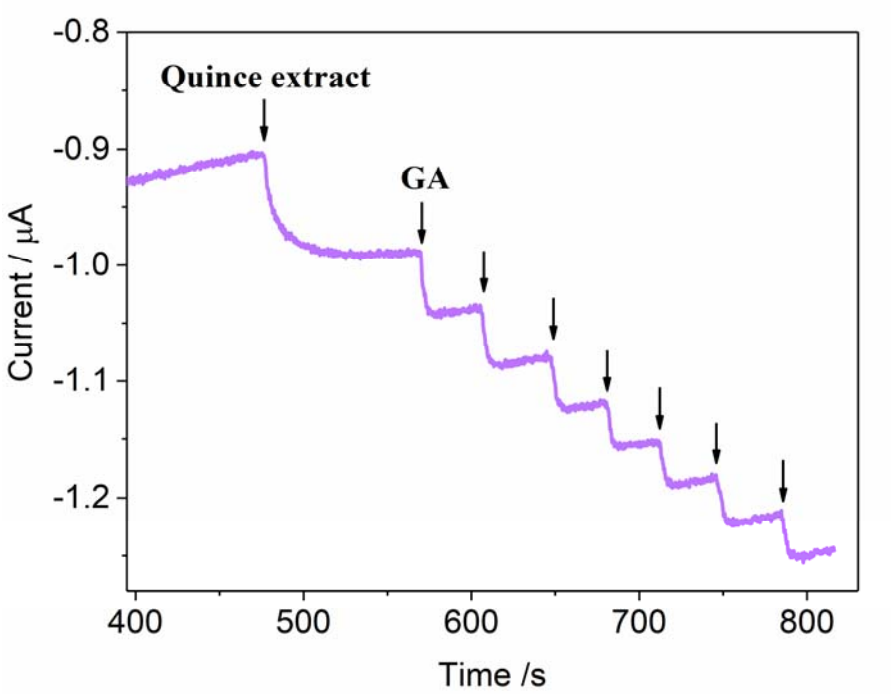
RESULTS AND DISCUSSION

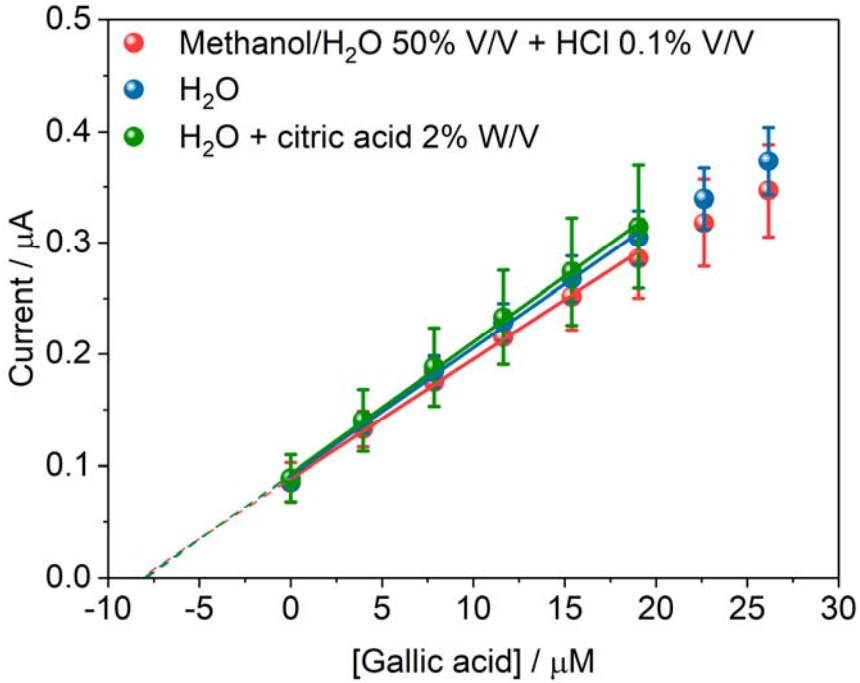
Determination of TPC in quince extracts



Gallic acid (GA)

Solvent	TPC (µg eq GA/mL)
Methanol/H_2O 50% V/V + HCl 0.1% V/V	(238±34)
H_2O	(258±1)
H_2O + citric acid 2% W/V	(255±51)



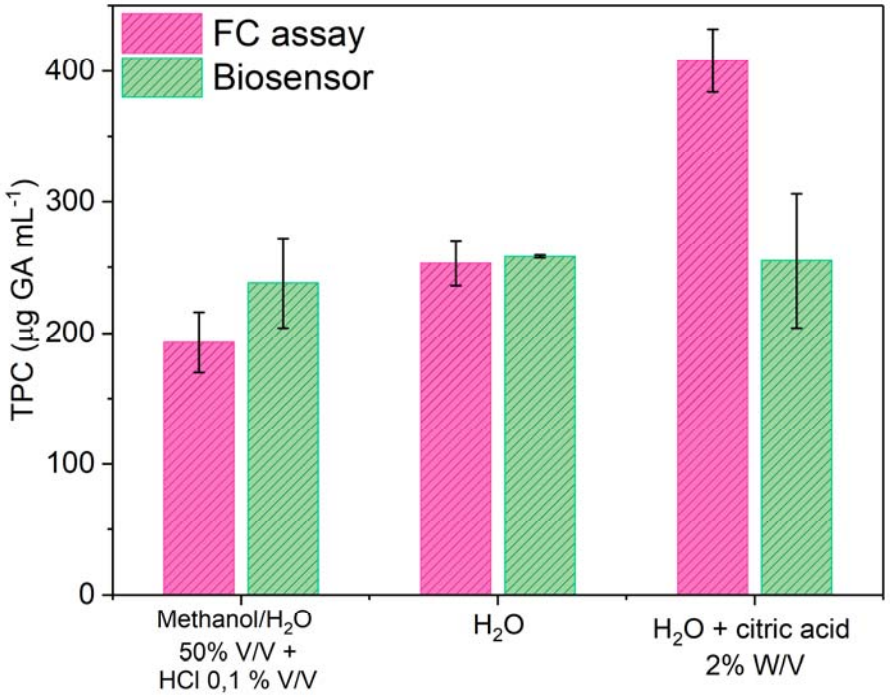


Supporting electrolyte: acetate buffer 0.10 M pH 5.0. Eap: 0.00 V.

RESULTS AND DISCUSSION

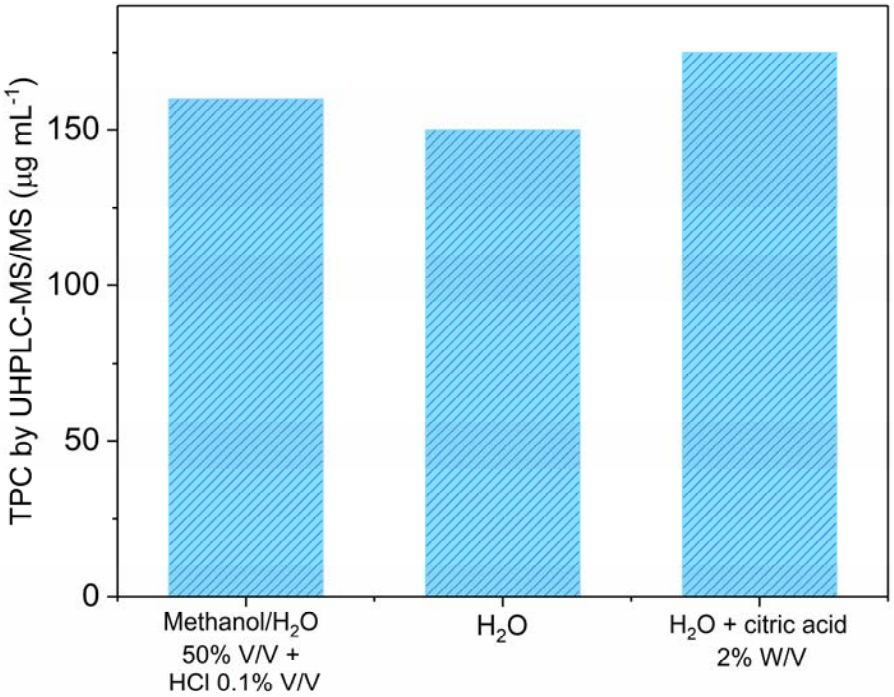
Determination of TPC in quince extracts

FC assay and biosensor



Classical extraction methods would have similar yields to hydrothermal methods.

UHPLC-MS/MS



TPC determined with Laccase Biosensor is in agreement with results obtained with UHPLC-MS/MS.

CONCLUSIONS

- An eco-sustainable extraction of polyphenols from industrial quince residue was achieved.
- The enzymatic biosensor is a relatively simple and less expensive methodology for the quantification of total polyphenol content in quince extracts.
- The biosensor is specific for TPC.
- The results are in agreement with those obtained by UHPLC-MS/MS.





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II SOUTHERN SCIENCE CONFERENCE
2024 - VIRTUAL CONFERENCE AND IN PERSON EDITION

INFLUENCE OF COGNITIVE REFLECTION AND METACOGNITIVE SKILLS (CALIBRATION) ON CONVERGENT SCIENTIFIC CREATIVITY

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ABSTRACT

Background: The demand for scientific creativity has become essential for societal progress, enabling the generation of innovative ideas to address current and future challenges. Aims: The study evaluates the convergent scientific creative competence of secondary education students and analyze how grade level, gender, cognitive reflection, and metacognitive skills (calibration) affect it. Methods: To carry out this study, several specific tests were used. To measure cognitive reflection, a test based on the “Cognitive Reflection Test-Developmental (CRT-D)” with nine questions by Young & Shtulman (2020) was employed. Additionally, to assess convergent scientific creativity and metacognitive calibration, a test based on the work of Yang et al. (2019) was utilized. A statistical analysis was then conducted to examine the relationships between these variables. Results: Students' convergent scientific creative competence is generally low. Additionally, there is no significant influence of gender or academic level on this competence. Regression analysis shows that calibration is the only significant predictor variable. Mediation analysis reveals that calibration acts as a mediator between cognitive reflection and convergent scientific creativity.. Discussion: These findings highlight the crucial role of both cognitive reflection and accurate self-assessment in enhancing students' convergent scientific creativity. The lack of gender or academic level influence suggests that educational strategies should focus on developing metacognitive skills across all demographics. Conclusions: Students' convergent scientific creativity is generally low and is not influenced by academic level or gender. It is primarily predicted by calibration, with cognitive reflection playing a mediating role.

Keywords: *Scientific creativity, cognitive reflection, calibration, grade level, secondary school* .

1. INTRODUCTION

In today's fast-evolving world, marked by rapid social, scientific, and technological changes, adaptability is more crucial than ever. The continuous development of society and technology demands innovative problem-solving skills, which has led to a growing emphasis on promoting scientific thinking, analytical capacity, and creativity among students. Scientific creativity, in particular, has become essential for addressing current and future challenges, as it fosters the generation of original and innovative ideas necessary for societal progress.

In the educational sphere, creativity is traditionally associated with originality and innovation. Scholars like Vygotsky (2004) have underscored the importance of fostering creativity in students to prepare them for an uncertain future, especially in the digital age, where uncertainty is felt more acutely (Craft, 2011). This concern is echoed by researchers such as Bronson and Merryman (2010), who highlight a "creativity crisis" in schools, calling for an educational shift toward fostering creative skills.

Alongside creativity, cognitive reflection and metacognitive skills play a significant role in the learning process, particularly during adolescence, a critical phase for identity and autonomy development. Cognitive reflection enables students to analyze and evaluate their experiences and knowledge, thus enhancing understanding and learning. Metacognitive skills, on the other hand, help students plan, monitor, and assess their learning processes, leading to deeper, self-regulated learning.

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In this context, this study aims to evaluate the convergent scientific creativity of secondary school students and to analyze the impact of factors such as educational level, gender, cognitive reflection, and metacognitive skills on this competence. Specifically, the research is based on tests that assess cognitive reflection, such as the "CRT-D" test by Young and Shtulman (2020), and tests that measure convergent scientific creativity and metacognitive calibration, following Yang et al. (2019). The study involves 153 students from a secondary school in Valencia, including those in 3rd and 4th year of secondary education and the first year of baccalaureate.

This research contributes to understanding how cognitive and metacognitive abilities intersect with creativity in scientific contexts, providing insights into how these factors influence students' ability to solve complex scientific problems and adapt to the demands of an increasingly unpredictable world.

2. MATERIALS AND METHODS

For this study, a quantitative and cross-sectional research design was used. The dependent variable was convergent scientific creativity, while the independent variables were metacognitive skills (evaluated in the form of calibration), cognitive reflection, academic training (or academic level), and gender.

2.1. Participants

A total of 153 secondary school students from a public high school in Valencia participated in the study. All students were enrolled in physics and chemistry classes at different levels: 9th grade (25 boys and 18 girls), 10th grade (33 boys and 21 girls), and 11th grade (28 boys and 28 girls). The study ensured a balanced distribution across grades to allow for fair comparisons and more reliable results.

2.2. Instruments

This study utilized three tests to evaluate scientific creativity among secondary school students: two tests focused on convergent scientific creativity and metacognitive skills, and one assessing cognitive reflection.

To measure convergent scientific creativity and metacognitive skills, we adapted two tests from Yang et al. (2019). The tests selected for this study included:

- **Test 1**: "Observe the drawing and provided objects carefully. Develop a strategy to remove water from a tank. The dog is thirsty, but it can't reach the tank, and the caretaker is not tall enough. You have a 60 cm chair, a 250 cm water tube, some stones, an aquarium with 1 liter of water, and rubber bands."
- **Test 2**: "Compare and describe the differences between (a) using an insulated 'thermos' and (b) a steel container filled with hot milk, sealed, and stored in the refrigerator. Explain what will happen in both containers."

To gauge metacognitive skills, both tests included the statement: "My confidence in the quality of my response is," with options scoring 1 for "fairly high" and 0 for "fairly low."

Responses were evaluated using a rubric outlined in Table 1.

For cognitive reflection, we employed the “Cognitive Reflection Test - Developmental (CRT-D)” by Young and Shtulman (2020). This test, shown in Table 2, consists of nine items designed to measure students’ ability to reflect on their intuitive responses and arrive at correct analytical answers. Each question has a commonly incorrect intuitive response; scoring is based on the number of correct responses, with a maximum score of 8 points. For example, an intuitive response to "What do cows drink?" is "milk," while the correct answer is "water."

2.3. Data Collection

The tests were administered during a single class session of the Physics and Chemistry course, with each scientific creativity test allocated 20 minutes and the cognitive reflection test 5 minutes. After grading, the results were recorded in an Excel spreadsheet for statistical analysis to explore relationships among the studied variables.

3. RESULTS AND DISCUSSION

The study analyzed convergent scientific creativity, cognitive reflection, and calibration across three educational levels and by gender.

The overall average score for convergent scientific creativity were low across all academic levels, with an average of 1.56 out of 6. No significant differences were found in academic level or gender. This indicates that students generally underperform in this domain, suggesting that educational curricula may need to place more

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emphasis on fostering creative and scientific thinking. This aligns with prior research showing a need for structured opportunities to develop creativity in academic contexts (Sternberg et al., 2020).

In terms of calibration, measured as the difference between actual performance and self-estimation, showed moderate accuracy across students, with no significant gender differences, though girls tended to overestimate slightly compared to boys.

The cognitive reflection test, with an average score of 6.69 out of 8, revealed higher scores for 4th-year students and lower scores for 3rd-year students. Gender differences were minimal, except in the 3rd-year, where girls scored slightly lower than boys. This result aligns with literature suggesting that cognitive reflection develops alongside academic and cognitive maturity (Gómez-Veiga et al., 2018; Guerin et al., 2021).

The results were analyzed with a correlation matrix. The results showed a positive correlation between convergent scientific creativity and cognitive reflection ($r = 0.242$, $p < .01$). A strong correlation between calibration and convergent scientific creativity ($r = 0.846$, $p < .001$) and a significant correlation between cognitive reflection and calibration ($r = 0.191$, $p < .05$). These results suggest that cognitive reflection and calibration are important factors that may influence students' convergent scientific creativity. The strong correlation between calibration and convergent scientific creativity highlights the importance of students' ability to accurately assess their own performance.

After that, a backward stepwise multiple regression analysis was conducted. It revealed that calibration was the strongest predictor of convergent scientific creativity, explaining 71.3% of the variance (adjusted $R^2 = 0.713$). While cognitive reflection did not directly predict creativity, it had a significant indirect effect mediated by calibration ($z = 2.375$, $p = .018$) .

4. CONCLUSIONS

The study presents several key findings:

- Low levels of convergent scientific creativity among students suggest a need for curricular improvements to promote creative and scientific thinking.
- Grade level and gender do not significantly influence convergent scientific creativity, implying that other factors may play a more critical role.
- Calibration is the primary predictor of convergent scientific creativity, with cognitive reflection having an indirect effect through calibration.

These results highlight the importance of fostering accurate self-assessment and cognitive reflection to enhance students' creativity in scientific contexts. Educators should focus on developing these skills to improve creative performance, given the overall low levels of scientific creativity observed.

5. DECLARATIONS

5.1. Open Access

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Table 1. *Rubric to assess convergent scientific creativity . Source: the author*

Test	Score	Criterion
Test 1	0	No answer provided or the answer is completely incorrect in terms of scientific explanation.
	1	The answer includes a small part of option 3 (missing tools and/or the scientific basis is flawed/partially incorrect) or simply uses the stones to raise the water level in the tank.
	2	The answer includes a large part of option 3 but is missing some aspects, especially in the scientific explanation.
	3	The answer is complete, uses the appropriate tools, and correctly explains how to extract the water based on scientific criteria: air extraction from the tube and water exiting from the other end due to pressure differences.
Test 2	0	No answer provided or the answer is completely incorrect in terms of scientific explanation.
	1	The answer includes a small part of option 3, but the scientific foundation is flawed/partially incorrect.
	2	The answer includes a large part of option 3 but is missing some aspects, especially in the scientific explanation.
	3	In the case of the thermos, since there is a "vacuum" chamber and even though the inner part is made of steel, the transfer of energy in the form of heat is greatly hindered by the absence of material particles that could participate in the heat transfer process. Additionally, the external part is also not made of steel (it is usually made of a material with lower thermal conductivity). Therefore, if both containers are kept in the refrigerator for the same amount of time, the temperature difference of the milk between the two containers will be significant: the milk in the thermos will have cooled down less.

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Table 2. *Test to assess cognitive reflection test and correction criteria.*

Number	Question	Correct	Incorrect
1	If you are participating in a race and pass the person in second place, what position are you in?	Second	First
2	Emilia's father has three daughters. The first two are named Monday and Tuesday, what is the name of the third daughter?	Emilia	Wednesday
3	A farmer has five sheep, all but three run away. How many are left?	3	2
4	If there are three apples and you take two, how many do you have?	2	1
5	What do cows drink?	Water	Milk
6	What weighs more: a pound of rocks or a pound of feathers?	Equal	Rocks
7	What hatches from a butterfly's egg?	Caterpillar	Butterfly Baby
8	Jorge is playing the game "the four corners" with three of his friends: January, March, and April. Who is the 4th player?	Jorge	February

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Southern Science Conference, 2024.

INFLUENCE OF COGNITIVE REFLECTION AND METACOGNITIVE SKILLS (CALIBRATION) ON CONVERGENT SCIENTIFIC CREATIVITY

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October/2024

INTRODUCTION

- We live in an era of constant social, scientific, and technological changes.
- Scientific creativity is essential for facing challenges and promoting ideas.



Scientific creativity

The ability to generate scientific ideas or products that are both original and useful within a scientific context.

(Boden,2004)



Cognitive reflection

The ability of individuals to analyze and evaluate their intuitive responses to reach more reasoned and accurate solutions.



Metacognitive skills

Skills that enable students to plan, monitor, and evaluate their own learning process. Fundamental for self-regulated learning and improving academic performance.

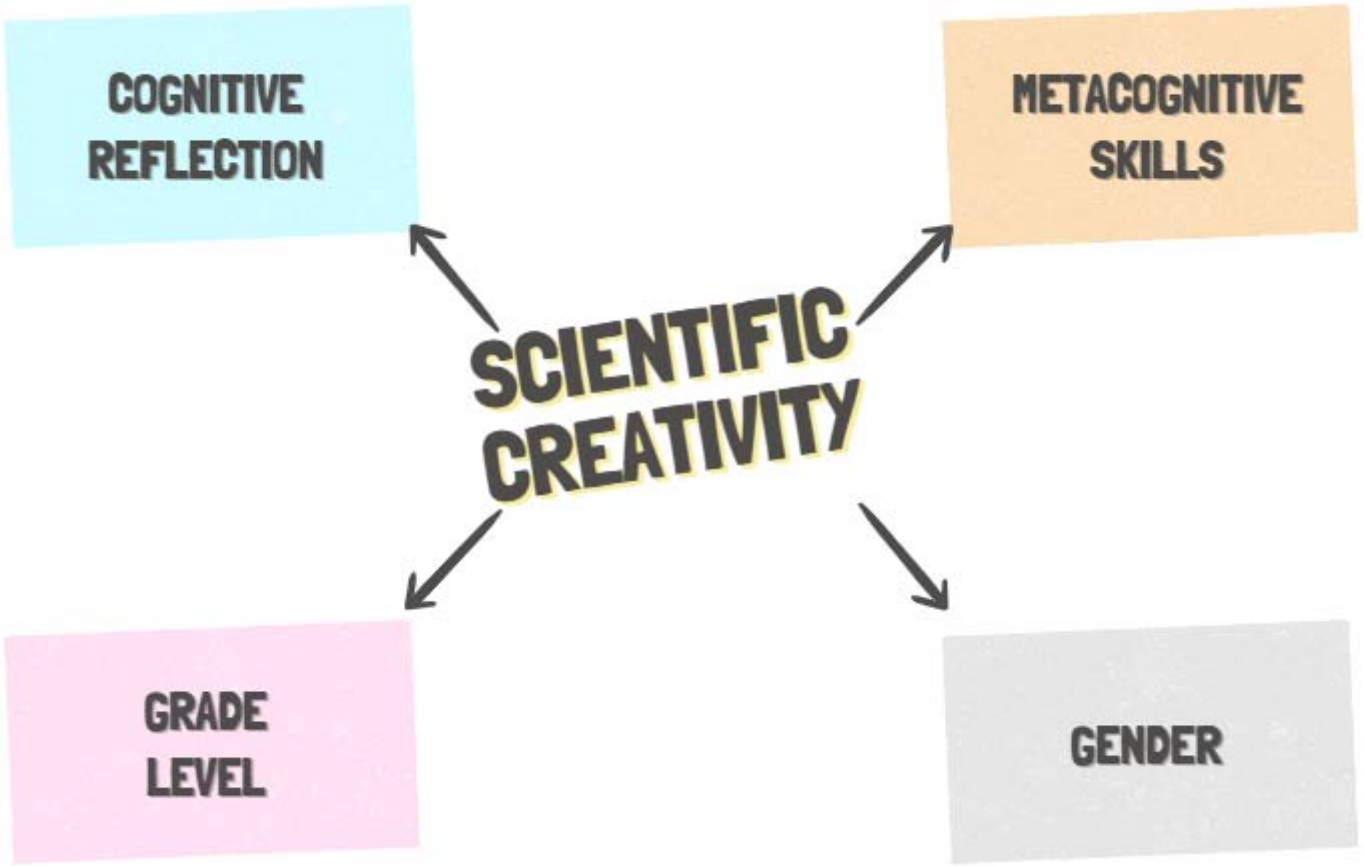
(Schraw & Dennison, 1994)

OBJECTIVES

- **Objective 1:** Determine the level of convergent scientific creativity across different grade levels in secondary education.

- **Objective 2:** Analyze the effects of grade level, gender, cognitive reflection, and metacognitive skills (in the form of calibration) on convergent scientific creativity.

OBJECTIVES



(Shtulman i McCallum,2014)
(Bae i Kwon, 2021)

METHODOLOGY

Research Design: Quantitative and cross-sectional study.

PARTICIPANTS

- 153 secondary education students
- Public school in the city of Valencia (Spain)
- All students were taking the Physics and Chemistry subject
- Different levels: 9^{th}, 10^{th}, and 11^{th} grades

METHODOLOGY

Research Design: Quantitative and cross-sectional study.

INSTRUMENTS

- Test 1
- Test 2

→ Convergent Scientific Creativity + Calibration task

- Open-ended response problem to assess scientific creativity
- Level of confidence with the answer

Yang et al. (2019)

- Test 3

→ Cognitive Reflection Evaluation

- 8 rapid questions

Young & Shtulman (2020)

	Intuitive answer	Correct answer
• What do cows drink?	Milk ✗	Water ✓

METHODOLOGY

Research Design: Quantitative and cross-sectional study.

DATA COLLECTION

- Class session: Physics and Chemistry subject
  - Scientific creativity test + Calibration task: 20 minutes
  - Cognitive reflection test: 5 minutes

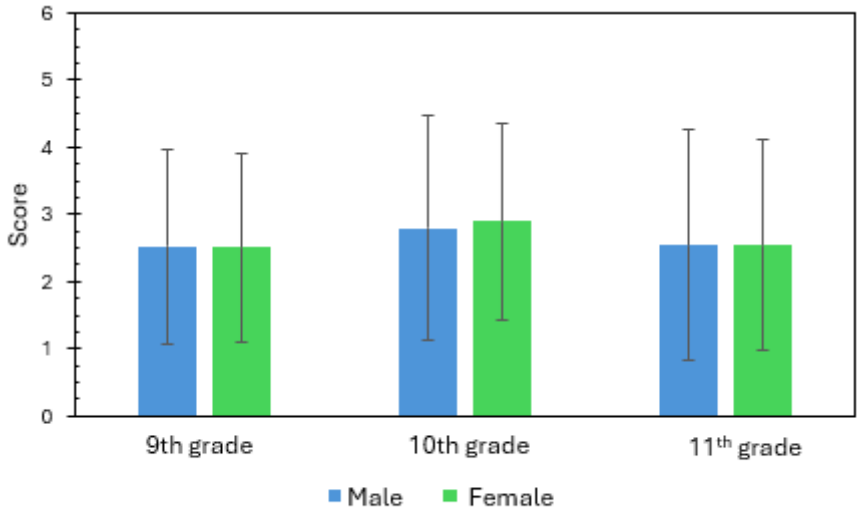
- Assessment rubric for the scientific creativity test

- Statistical Analysis: Excel Spreadsheet

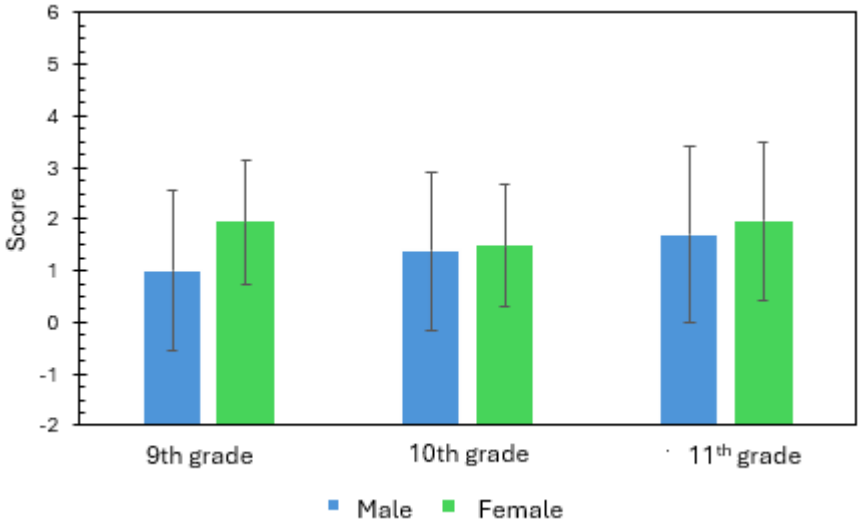
- Data includes:
  - Grade level
  - Gender
  - Creativity test results
  - Calibration (Metacognitive skills)

RESULTS AND DISCUSSION

Convergent Scientific Creativity



Calibration



RESULTS AND DISCUSSION

Correlation matrix

	Convergent scientific creativity	Academic Level	Gender	Cognitive reflection	Calibration
Convergent scientific creativity	1	0.0130	-0.0150	0.2419**	0.8456***
Academic Level		1	0.0709	0.2624**	0.1203
Gender			1	-0.1436	0.1696
Cognitive reflection				1	0.1908*
Calibration					1

- Positive correlation between convergent scientific creativity and cognitive ($r = 0.242$, $p < .01$).
- Strong correlation between calibration and convergent scientific creativity ($r = 0.846$, $p < .001$)
- Significant correlation between cognitive reflection and calibration ($r = 0.191$, $p < .05$).

These results suggest that cognitive reflection and calibration are important factors that may influence students' convergent scientific creativity.

RESULTS AND DISCUSSION

Multiple Linear Regression Analysis, Backward stepwise: $F(1,151)=378.98$, $p<.001$

- Iteration 1

	Coeff (B)	SE	t-stat	Lower t0.025 (150)	Upper t0.975 (150)	Stand coeff (β)	p-value	VIF
Intercept	0.7312	0.3164	2.3109	0.1060	1.3564	0	0.0222	
Cognitive Reflection	0.0897	0.0471	1.9063	-0.0033	0.1827	0.0836	0.0585	1.0378
Calibration	0.8466	0.0448	18.9122	0.7581	0.9350	0.8297	2e-16	1.0378

- Iteration 2

	Coeff B	SE	t-stat	Lower t0.025 (150)	Upper t0.975 (150)	Stand coeff (β)	p-value	VIF
Intercept	1.3057	0.0973	13.4223	1.1135	1.4979	0	<0.001	-
Calibration	0.8629	0.0443	19.4675	0.7753	0.9504	0.8456	0	1

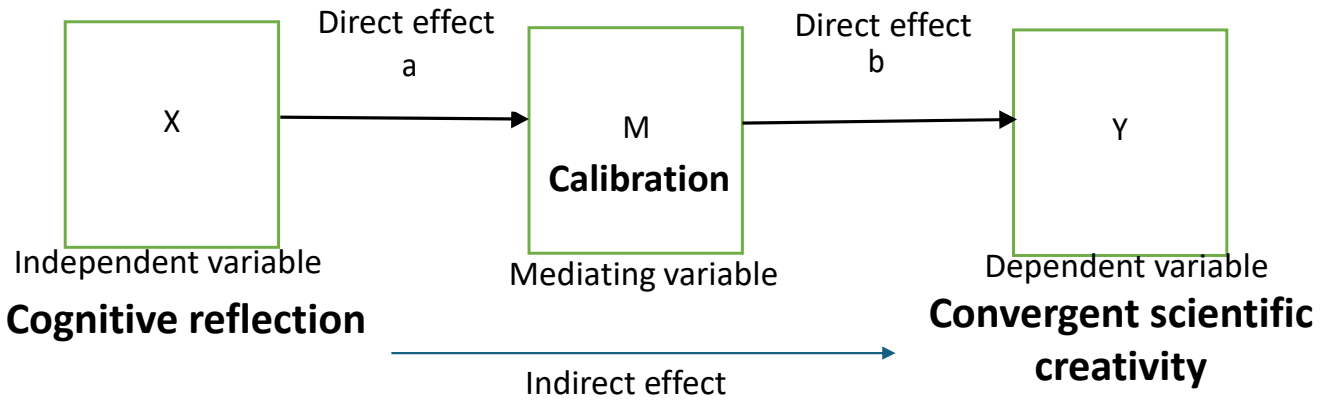
Regression analysis shows that calibration is a strong predictor of convergent scientific creativity, explaining 71.3% of its variance ($R^2=.713$)

RESULTS AND DISCUSSION

- **Correlation matrix**: The cognitive reflection correlates positively and significantly with convergent scientific creativity and with calibration.

- **Multiple linear regression analysis:** The cognitive reflection does not appear as a significant predictor variable of convergent scientific creativity.

Calibration as a mediator between cognitive reflection and convergent scientific creativity, Sobel test: z=2.375, p=.018



CONCLUSIONS

- C1: The level of convergent scientific creativity among secondary students is generally low.

- C2: Convergent scientific creativity is not influenced by grade level or gender.

- C3: Convergent scientific creativity can be primarily predicted by calibration, with cognitive reflection having an indirect effect.

LIMITATIONS

- Small Sample Size: The sample includes only three academic levels, limiting generalizability.
- Self-Perception Bias: The test for cognitive reflection and calibration relies on participants' self-assessment, potentially introducing bias.
- Complex Wording: The test's wording may have been misinterpreted by some participants, especially those from lower grade levels.
- Specific Context: Conclusions are only applicable to the students in this study and the specific instruments used.

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THE ROLE OF PROGESTERONE METABOLITES ON THE PROLIFERATIVE-APOPTOTIC BALANCE OF HUMAN OVARIAN CARCINOMA-DERIVED CELL LINES

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ABSTRACT

Ovarian cancer is the most lethal gynecologic malignancy and the fifth leading cause of cancer death in women. Progesterone can have different effects depending on the hormonal conditions or the physiological environment in which it is administered. Its effect varies depending on the hormonal concentrations present in the body, since these can modify the body's response to the drug , particularly in cancer. P4 is metabolized into two groups: the 5α-pregnans, including allopregnanolone (ALLO), and the 4-pregnans, such as 3α-dihydroprogesterone (3αHP) and 20α-dihydroprogesterone (20αHP). Previous studies in the breast suggest that 5α-pregnans promote tumor growth, whereas 4-pregnans have antitumorigenic effects. This study aimed to evaluate the effects of these metabolites on the proliferation-apoptosis balance in the human ovarian cancer cell lines IGROV-1 and SKOV-3. Both cell lines were cultured and treated with increasing concentrations of ALLO, 3αHP, and 20αHP. Proliferation was measured by MTT assay, and apoptosis was assessed by immunocytochemistry and flow cytometry. ALLO significantly increased cell proliferation in the IGROV-1 cell line, whereas no effect was observed in SKOV-3. In contrast, 3αHP and 20αHP decreased cell proliferation in both cell lines. In addition, 20αHP increased the expression of cleaved caspase-3 in IGROV-1, indicating an apoptotic effect. Flow cytometry showed that 4-pregnane derivatives increased apoptotic effect. This study provides new insights into the role of P4 derivatives in ovarian epithelial carcinoma-derived cells. It lays the groundwork for future research on signaling pathways and molecular mechanisms to elucidate the physiological role of these molecules in contributing to the development of new diagnostic and therapeutic approaches.

Keywords: *ovarian cancer, progesterone, metabolites, proliferation, apoptosis.*

1. INTRODUCTION

Ovarian cancer (OC) is the fifth leading cause of cancer death in women. It is detected in advanced stages being the most lethal form of gynecological neoplasia (Siegel *et al.,* 2023). The role of progesterone (P4) in OC is controversial (Lima *et al*., 2020; Kim *et al*., 2020; Tsilidis *et al*., 2011). P4 can be converted into two groups of metabolites: into 5α-pregnane derivatives, a group to which allopregnanolone (3α-hydroxy-5α-pregnane-20-one, ALLO) belongs, and into 4-pregnane derivatives, a group in which 3α-dihydroprogesterone derivatives; 3αHP and 20α-dihydroprogesterone (20αHP) are found. Wiebe (2005) in breast cancer showed that the 5α-pregnane derivatives are pro-tumorigenic, whereas the 4-pregnanes could have anti-tumorigenic effects.

Under physiological conditions, there is a balance between the processes of cell proliferation and apoptosis. When this balance is disturbed, tumor growth or remission may be favored. 4-pregnans are able to inhibit cell proliferation and tumor growth, increasing apoptosis, while 5α-pregnan-3,20-dione (DHP), a metabolite of 5α-pregnan, shows an opposite effect (Wiebe, 2005; Wiebe *et al.,* 2015).

Recently, we have shown that ALLO increases proliferation and clonogenic capacity in cell lines derived from OC (Pelegrina *et al*., 2020). However, the role of these metabolites and their mechanisms of action in OC is still unknown.

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Considering the background it is relevant to explore the effects of these metabolites to understand the biology of OC and improve therapeutic strategies. Our aim is to evaluate the action of P4 metabolites (ALLO, 20αHP and 3αHP) on the proliferation-apoptosis balance of epithelial ovarian carcinoma-derived cell lines.

2. MATERIALS AND METHODS

2.1. Cell Culture and treatment

Human ovarian carcinoma cell lines IGROV-1 and SKOV-3 (ATCC; Manassas, USA) were maintained in RPMI medium supplemented with 2 mM L-glutamine, 80 µg/ml gentamicin, 50 UI/ml penicillin and 10% FBS at 37°C in a humidified 5% CO_2 air. Cells were treated with increasing concentrations of ALLO, 3αHP and 20αHP (10^{-11} to 10^{-5} M) for 72 h. The treatment was replaced every 24 hours. Cells without treatment served as a control group.

2.2. MTT assay:

Proliferation was measured using the 3-(4,5-Dimethylthiazol-2-yl)-2,5 diphenyltetrazolium bromide (MTT) colorimetric assay. Cells were seeded in 96-well microplates (5000 per well). After treatment, MTT solution (5 mg/mL) was added to each well and incubated for 4 h at 37°C. The production of formazan was evaluated by measuring the absorbance at 570 nm with an ELISA reader (Bio-Rad Laboratories, Inc. Oakland, CA, USA).

2.1. Immunocytochemistry

After treatment, cells were fixed in 4% formaldehyde for 15 min and permeabilized with 0.5% Triton X-100 for 5 min, (Cuello-Carrión *et al.,* 2015). They were incubated overnight at 4 °C with a rabbit polyclonal antibody against caspase 3 (Abcam; 1:400). A Dako EnVision System kit was used for detection, and nuclei were counterstained with hematoxylin and eosin. Slides were examined using a Nikon Eclipse E200 microscope, with nonspecific IgG1 and preimmune serum as negative controls (Pelegrina *et al*., 2020).

2.1. Flow cytometry

Cells were treated and stained with an Annexin V-FITC/PI Apoptosis kit to assess apoptosis. After incubation, the samples were tested using a flow cytometer (BD FACSAria III Cell Sorter). Results analyzed using FlowJo software.

3. RESULTS AND DISCUSSION:

The search for effective cancer treatments is a critical public health issue, especially given the rising incidence (Siegel et al., 2023; Sung et al., 2021). Ovarian cancer is a particularly complex , with 70% of cases diagnosed at advanced stages due to the tissue's nature and endocrine function. Hormones like P4 and its metabolites may influence ovarian cancer progression, highlighting their significance (Anbarasy et al., 2023; Ahmed et al., 2022).

Cell proliferation is a key process in cancer progression, where tumor cells divide uncontrollably. In a breast cancer study, 4-pregnenes inhibited cell proliferation and tumor growth, whereas DHP (a 5-pregnane metabolite) stimulated them (Wiebe et al., 2013). In this work, the action of ALLO, 3αHP, and 20αHP on the proliferation of human ovarian cancer cell lines, IGROV-1 and SKOV-3. In IGROV-1 cell line , ALLO induced an increase in proliferation. The maximum effect of ALLO was at concentrations of 10^{-5} M ($p < 0.001$) and 10^{-11} M ($p < 0.001$) respectively. ALLO did not cause changes in proliferation in SKOV-3. Cell proliferation was decreased after treatment with 3αHP in both cell lines at the concentration of 10^{-10}M ($p<0.0001$). After treatment with 20αHP, proliferation decreased in the IGROV-1 cell line ($p<0.0001$) within the range of 10^{-7} to 10^{-5} M ($p<0.0001$. In the SKOV-3 cell line, 20αHP induced a decrease in proliferation in a range of 10^{-8} to 10^{-5} M.

Under physiological conditions, there is a balance between cell proliferation and apoptosis. In breast cancer, 3αHP induced an increase in apoptosis in contrast, a 5α-pregnane derivative had the opposite effect (Wiebe *et al*., 2009). ALLO had no effect on apoptosis in ovarian tumor lines (Pelegrina *et al.,* 2020). However, in this work, it was observed that only 20αHP increased cleaved caspase 3 expression in the IGROV-1 cell line, for all concentrations studied. The SKOV-3 cell line was not affected by the action of these derivatives. To further the understanding of the biological behavior of these lines after treatments with P4 metabolites, apoptosis was further evaluated by cytometry. Preliminary results showed that 4-pregnane derivatives increase early apoptosis, whereas ALLO had no effect.

4. CONCLUSIONS:

These findings show the first evidence that steroids can modulate the carcinogenesis of cells derived from human ovarian epithelial epithelial tumors. The 5a-pregnane derivatives and the 4-

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pregnenes showed opposite actions, suggesting pro-tumor and anti-tumor effects, respectively.

This study provides new insights into the role of P4 derivatives in ovarian epithelial carcinoma-derived cells and lays the groundwork for future research on signaling pathways and molecular mechanisms to elucidate the observed effects and contribute to the development of new diagnostic and therapeutic approaches.

5. DECLARATIONS

5.1. Open Access

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Southern Science Conference, 2024.

THE ROLE OF PROGESTERONE METABOLITES ON THE PROLIFERATIVE-APOPTOTIC BALANCE OF HUMAN OVARIAN CARCINOMA-DERIVED CELL LINES

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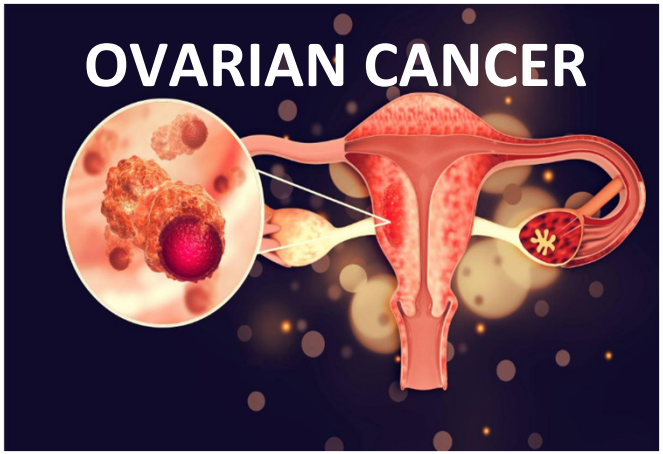
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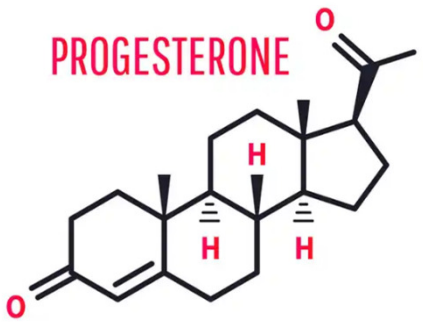
INTRODUCTION

Is the 5th leading cause of cancer-related death among women.

It is detected in advanced stages being the most lethal form of gynecological neoplasia.

It is known that cancer progression can be affected by hormones produced in the body.





There are controversial data on the effect of P4 on CaO (both epidemiological and *in vitro*)

P4 is converted to two groups of metabolites:

5α-pregnans
Allopregnanolone (ALLO)

4-pregnens
3α-dihydroprogesterone (3αHP)
20α-dihydroprogesterone (20αHP)

PRO-TUMORAL EFFECTS

ANTI-TUMOR EFFECTS

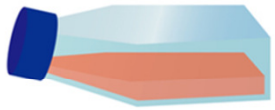
In breast cancer

AIM/OBJETIVE/PURPOSE

Our aim was to evaluate the action of P4 metabolites (ALLO, 3αHP and 20αHP) on the proliferation-apoptosis balance of epithelial ovarian carcinoma-derived cell lines.

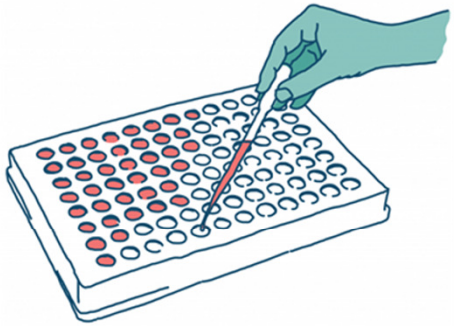
METHODOLOGY

EXPERIMENTAL DESIGN



Culture of cell lines derived from human ovarian epithelial carcinoma

- IGROV-1
- SKOV-3



Treatment for 72h to concentrations

10^{-5} a 10^{-11} M

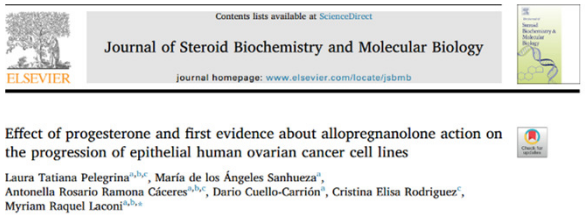
ALLO
20αHP
3αHP

- Cell Proliferation Assay
- Immunocytochemistry
- Flow cytometry

Statistical analysis
All experiments were repeated for at least three times, and the data were analyzed using GraphPad Prism 8.0 and displayed as mean ± SEM. The differences are evaluated using one-way analysis of variance (ANOVA) followed by Tukey's post hoc test. Differences were considered as statistically significant when $p<0.05$.

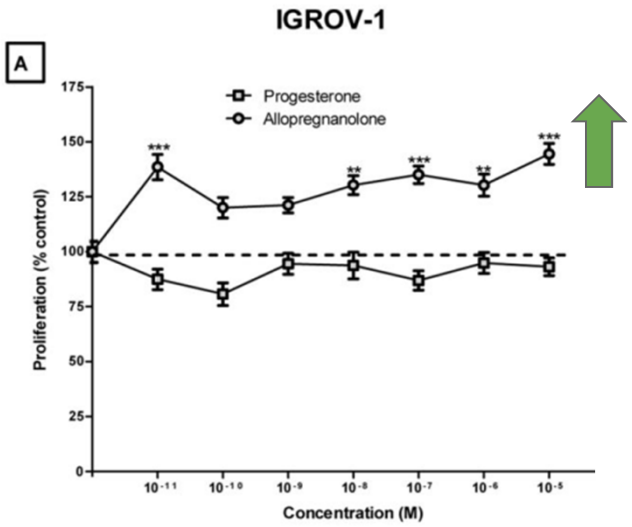
RESULTS AND DISCUSSION

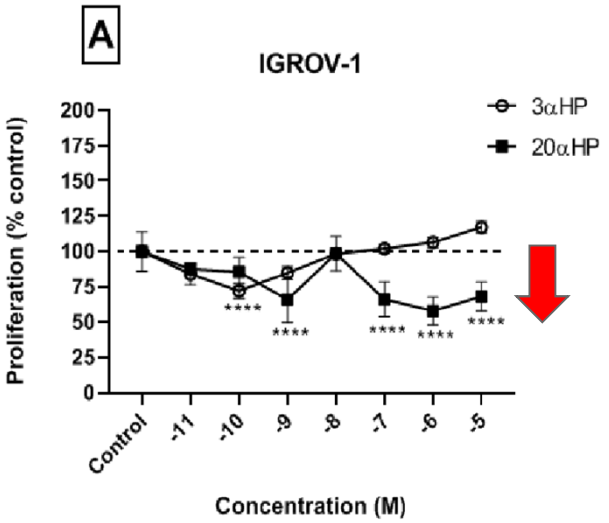
Action of ALLO, 3αHP and 20αHP on the cell proliferation of IGROV-1 and SKOV-3.

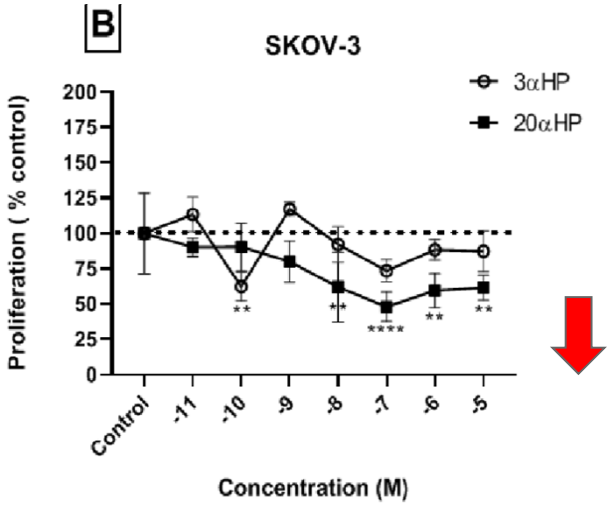

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Effect of progesterone and first evidence about allopregnanolone action on the progression of epithelial human ovarian cancer cell lines

Laura Tatiana Pelegrina[a,b,c], María de los Ángeles Sanhueza[a], Antonella Rosario Ramona Cáceres[a,b,c], Dario Cuello-Carrión[a], Cristina Elisa Rodriguez[c], Myriam Raquel Laconi[a,b,*]

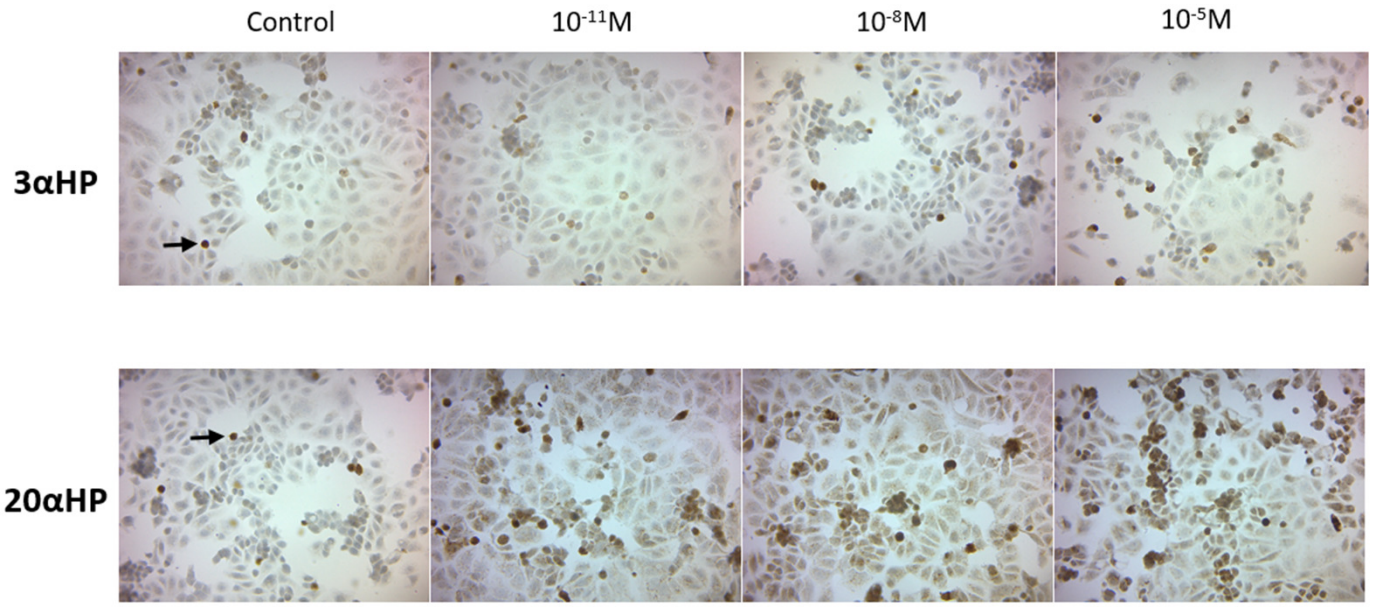


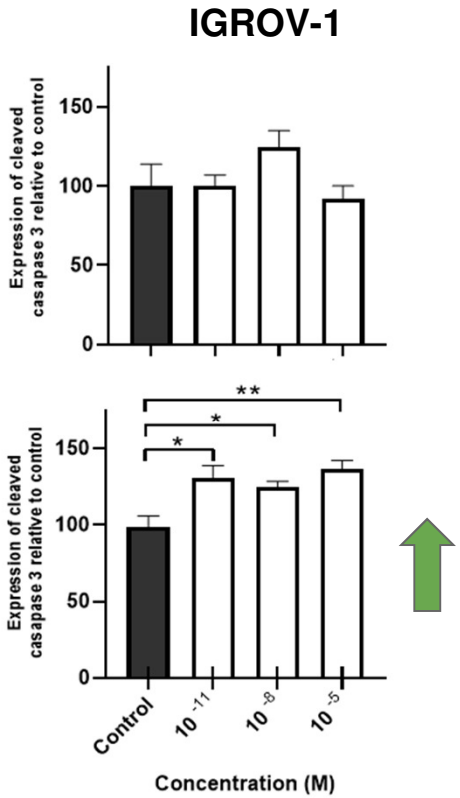




RESULTS AND DISCUSSION

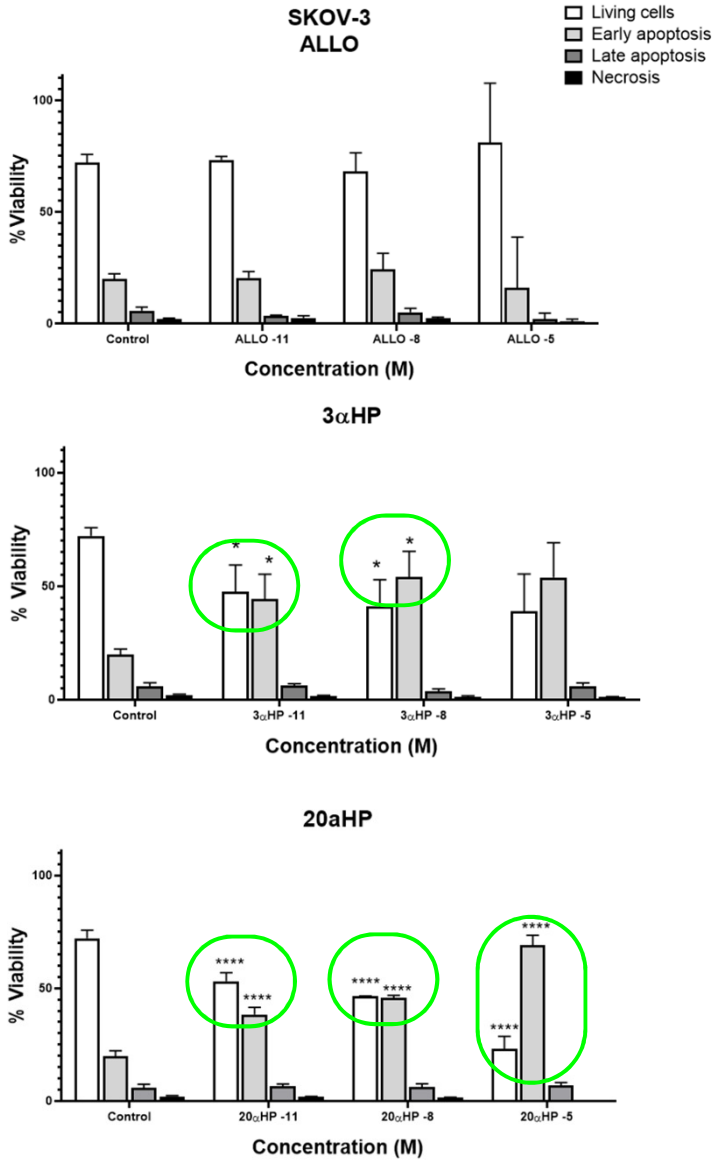
Action of ALLO, 3αHP and 20αHP on the apoptosis of IGROV-1 and SKOV-3.

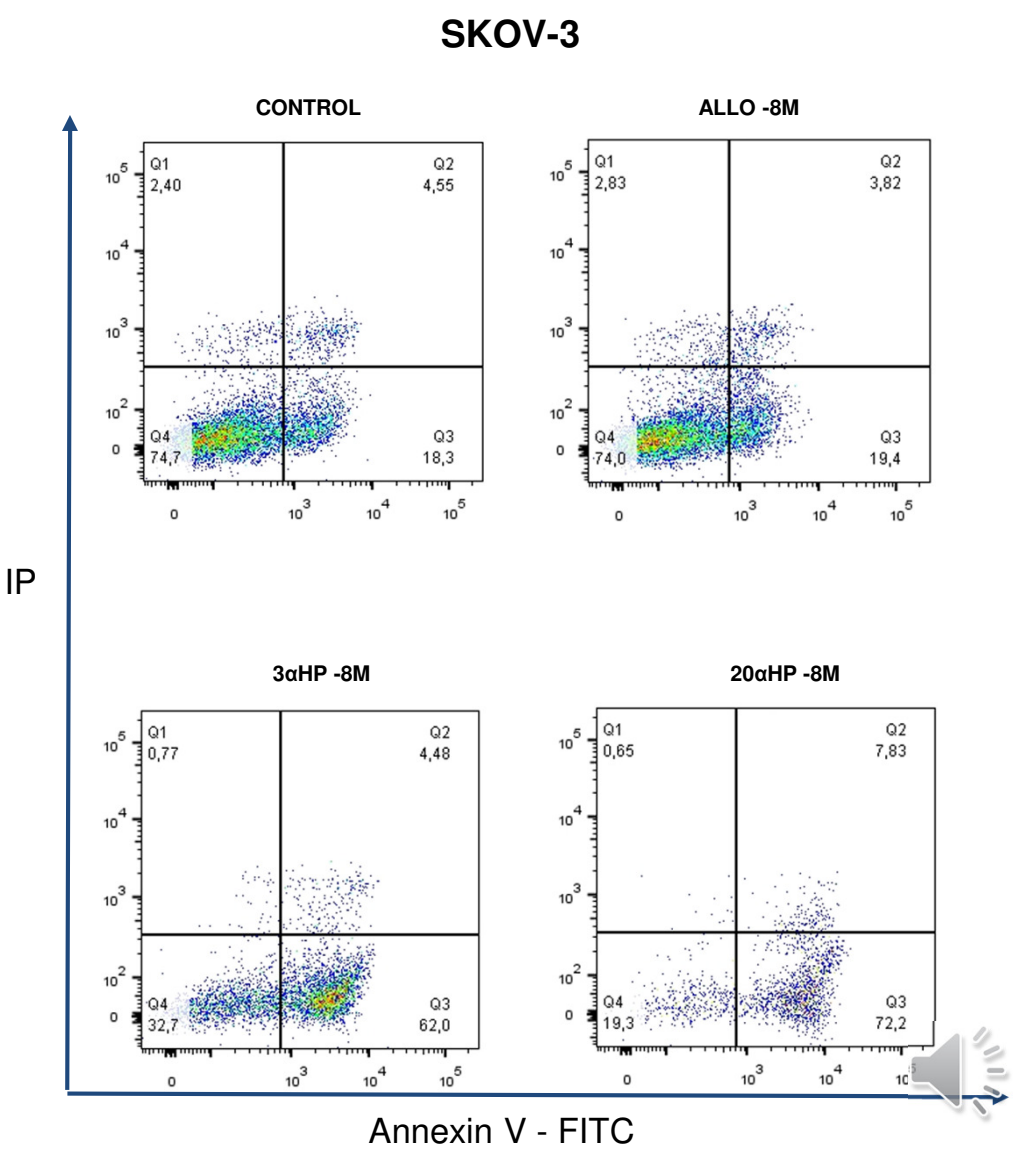




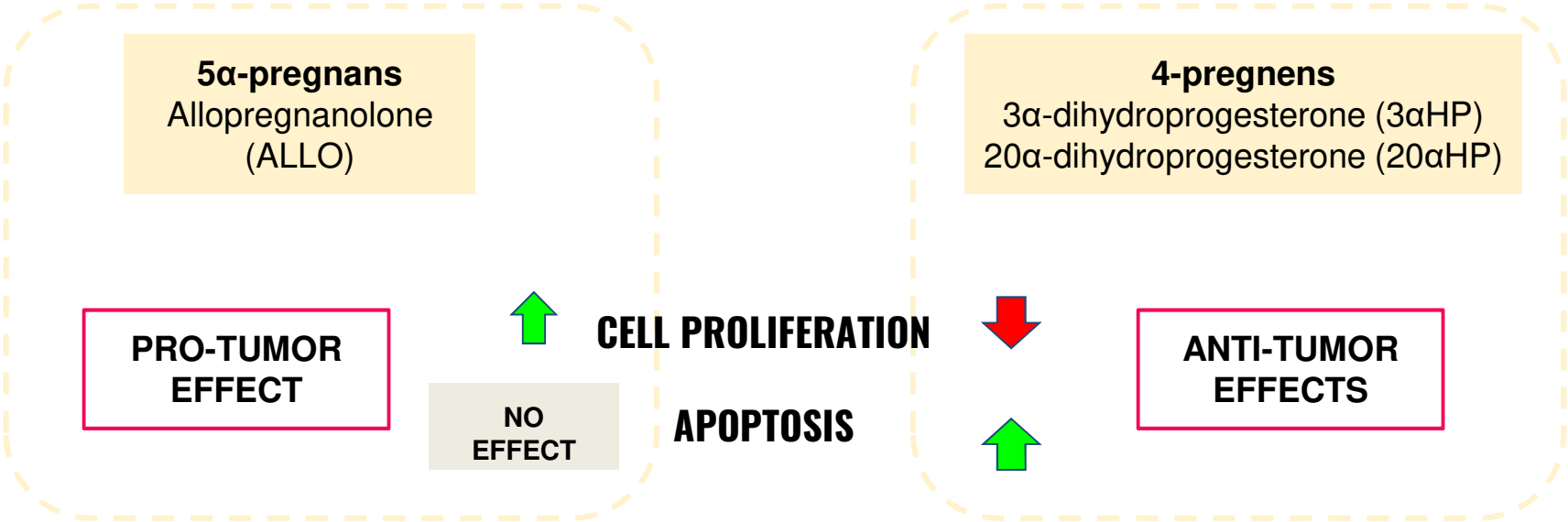
RESULTS AND DISCUSSION

Action of ALLO, 3αHP and 20αHP on the apoptosis of IGROV-1 and SKOV-3.





CONCLUSIONS



The 5a-pregnane and the 4-pregnenes derivatives showed opposite actions, suggesting pro-tumor and anti-tumor effects, respectively.

These are the first evidence that steroids can modulate the carcinogenesis of cells derived from human ovarian epithelial tumors.

Understanding how these steroids work could have important future implications for both diagnosis and treatment of patients.

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EXPEDITIOUS SYNTHESIS OF RHODANINE DERIVATIVES THROUGH MICROWAVE IRRADIATION

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ABSTRACT

In this study, we present an efficient and environmentally friendly method for the synthesis of 5-benzylidene and 5-cinnamylidene rhodanine derivatives, utilizing microwave irradiation as a green synthetic approach. This methodology provides several advantages, including short reaction times, high atom economy, and minimal environmental impact. The yields of the synthesized compounds ranged from 61% to 92%, with purities exceeding 95%. The use of microwave technology under mild conditions underscores the advantages of this approach for sustainable organic synthesis.

Keywords: *heterocycles, thioxothiazolidinones, water, eco-friendly methodology*

1. INTRODUCTION

To a large extent, our research group has devoted significant effort to the study and in-depth understanding of the synthesis, reactivity, and physicochemical properties of various heterocycles.[1-5] We have recently explored the antioxidant properties and antibiotic modulatory activity of a family of aryliden imidazolidinone derivatives **1a-e** and **2a-e** (Figure 1). When the whole set of compounds was screened for antibiotic activity in the fluoroquinolone-resistant *S. aureus* strain (SA-1199B), only the fluorine derivatives **1c** and **2c** demonstrated a slight activity on their own. An even more significant finding was that the combination of **1c** or **2c** with norfloxacin significantly increases its activity, producing a 6.4 and 4-fold decrease, respectively, of the norfloxacin minimum inhibitory concentration (MIC). Similar results were obtained for the same strain coupling **1c** and **2c** with ciprofloxacin. Further tests were made suggesting that the modulating effect of the fluorobenzylidene imidazolidinones involves inhibition of the NorA efflux pump.[6]

It is also important to highlight that we have already made significant progress in studying the physicochemical properties of the family depicted in Figure 1. Our findings indicate that the most thermodynamically stable form is the Z configuration, which undergoes isomerization to *E* isomer when exposed to UV light.[4]

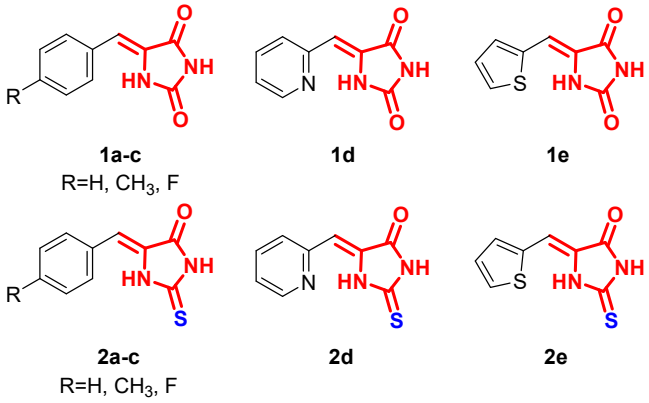


Figure 1. *Previously synthesized and screened imidazolidinone derivatives.*

It is also important to highlight that we have already made significant progress in studying the physicochemical properties of the family depicted in Figure 1. Our findings indicate that the most thermodynamically stable form is the Z

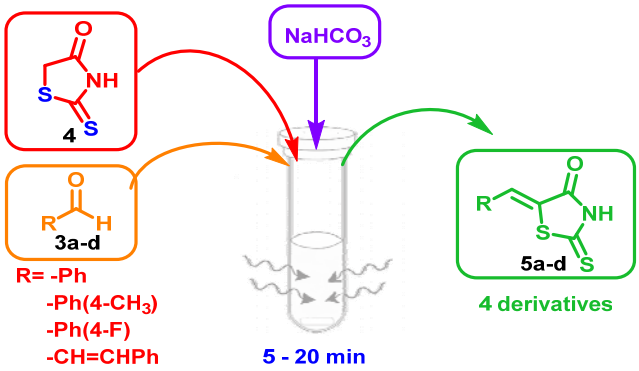
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DOI: 10.48141/SSCON_45_2024.pdf

configuration, which undergoes isomerization to *E* isomer when exposed to UV light.[7] A comprehensive and detailed study of the photochemical isomerization of (*Z*)-5-benzylidene-2-thioxoimidazolidin-4-one **2a** showed that it isomerize from their *Z* to the *E* form under 365 nm light irradiation, with the *E*→*Z* reversal process being thermal. The discovery of *Z*→*E* photoisomerization in (hetero)arylidene thioxoimidazolidinones **2a-e** was the starting point for recognizing that *E* isomers (after UV irradiation of the *Z* isomers) are active against Gram-positive *S. aureus* (ATCC 25923) and Gram-negative *E. coli* (ATCC 25922).[7] It is noteworthy that the oxygenated counterparts **1a-e** did not show photoactivity against the tested strains, revealing the key role of sulfur in the biological activity. As a step forward in the search for photophysical properties that support the application of thioxoimidazolidinones it was found that they can interact favorably with double-stranded DNA (dsDNA), enhancing the system fluorescence.[8] Hence, these compounds could be effectively used in biological imaging and labeling in the fields of biochemistry and molecular biology.

On another note, likewise, the mentioned thioxoimidazolidinones, 5-substituted rhodanine derivatives containing a double bond, have attracted significant attention in the fields of organic chemistry and materials science due to their unique optical and electrical properties. The double bond isomerizing system allows the precise control of photoswitch geometry. These derivatives can undergo predictable changes in their geometry under visible light irradiation of different colors. As a consequence, the 5-substituted rhodanines are highly regarded frameworks in various research areas, such as fluorophore design, ion sensing, dyes, and medicinal and biological chemistry.[8-11]

With the objective of furthering the biological and physicochemical exploration of related compounds we are focusing in the synthesis of 5-benzylidene or 5-cinnamylidene rhodanine derivatives. Several general procedures have been reported for the synthesis of rhodanine derivatives, where rhodanine or oxo-rhodanine (thiazolidine-2,4-dione) react with the corresponding aldehyde under Knoevenagel reaction. For instance, it was recently reported the obtention of 5-(hetero)aryliden rhodanines by neat heating at 110 °C or in methanol at 70 °C using urea as a catalyst (10% mol).[12]

Aside from that, this work proposes an expeditious, efficient, and environmentally friendly synthesis using microwave (MW) irradiation as an alternative and eco-friendly methodology, allowing for faster production of these derivatives in a benign solvent and with very good reaction yields (Scheme 1).



Scheme 2. *Proposed expeditious preparation of 5-benzylidene and 5-cinnamylidene rhodanines.*

2. MATERIALS AND METHODS

All the reagents were commercially available. The reactions were carried out using an Anton Paar Monowave 300 microwave system in a closed pressurized setup. In a typical reaction, the reagents were placed in a 10 mL borosilicate glass vial in the following order: 2 mmoles of rhodanine, saturated sodium bicarbonate solution, and 3 mmoles of aldehyde. Before starting the microwave synthesis, it is crucial to observe the insoluble and uncolored aspects. The microwave method involved the following steps: 1) Heat to 30 °C and stir for 30 seconds, 2) Heat to the target temperature and maintain it for the specified time, and 3) Cool down to 50°C. The progress of the reaction was monitored using thin-layer chromatography (TLC) on silica gel, with ethyl acetate and chloroform (7:3) as the mobile phase. Once the experiment was completed, a yellow solid was observed. The whole crude was transferred to an erlenmeyer flask, adding 15 mL of distilled water, forming a suspension. The soluble portion was at pH 10, so it was neutralized by dripping 0.10 M HCl solution until reaching pH 7, as measured with pH paper. The flask was left to rest in the refrigerator to increase precipitation. The solid was then filtered off and washed with cold distilled water. In most cases, the dried solid was found to be of high purity. To increase the product recovery, the mother liquors were single-extracted with 15 mL of ethyl acetate. Dried with anhydrous Na_2SO_4 and evaporated to dryness. This second solid was eventually purified by column chromatography.

All compounds were characterized using spectroscopic techniques. NMR spectra were recorded in acetone-d_6 on a Bruker Avance II 400

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MHz spectrometer (BBI probe, z gradient) (^{1}H at 400.16 MHz, ^{13}C at 100.56 MHz and ^{19}F at 376.53 MHz) at 22 °C. Chemical shifts are reported in parts per million (ppm) downfield from TMS. Gas chromatography/mass spectrometry (GC/MS) analyses were performed on a Shimadzu GCMS-QP 5050 spectrometer equipped with a VF column (30 m × 0.25 mm × 5 µm) using helium as eluent at a flow rate of 1.1 mL min^{-1}. The injector and ion source temperature were 280 °C selecting the electron impact mode (EI) at 70 eV. All acquired data is in agreement with the proposed structures.

3. RESULTS AND DISCUSSION:

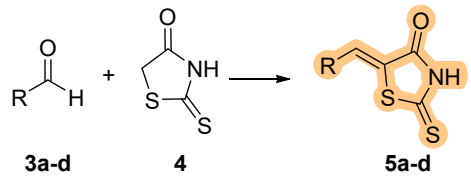
The synthesis of the target compound family was carried out using the same initial conditions previously reported for thioxoimidazolidinone derivatives **2a-e**.[7] These parameters were 90°C under microwave irradiation for 10 minutes using only 1 mL of saturated bicarbonate solution. The yields obtained (Table 1) were regarded as good to very good, ranging from 61% to 92%, with the synthesis methodology standing out for its speed, high atom economy, low environmental impact, and high purity of the solids obtained (>95%). The highest yield in the series was obtained when 4-methylbenzaldehyde was used, which correlates with the higher reactivity of this aldehyde due to its electron-donating effect and the lower water solubility of the corresponding product, facilitating its separation from the reaction medium. The cinnamaldehyde derivative presented purification difficulties because, even after thorough washing with water, the starting aldehyde remained stuck to the obtained crystals. This issue arises from the aldehyde being immiscible with water.

Considering the lower yields observed for the fluorinated derivative **5c**, some variations in conditions, such as temperature, time, and solvent volume, were made in order to improve the yields. The results shown in Table 2 indicate that the amount of **5b** increased to the same extent both when the temperature was raised to 110°C and when the reaction time was doubled. It is interesting to note that using lower temperatures facilitates the washing process of the resulting solid, making it the most favorable condition for this set of experiments. Further exploration at higher temperatures and extended reaction times would be required to determine which variable is best to modify definitively.

The characterization analyses of the compounds confirmed the proposed structures. Through the ^{1}H NMR experiments, characteristic signals of the products were confirmed, such as the vinyl hydrogen signal, which appears in the benzylidene derivatives **5a-c** around 7.6 ppm, while the corresponding imidazolidinone analogs **2a-c** exhibited that hydrogen at approximately 6.6 ppm.

For further reference, the ^{1}H and ^{13}C NMR chemical shifts for derivative **5b** are provided in Figure 2. On the other hand, the mass spectra confirmed that all the obtained products exhibit their molecular ion, thereby demonstrating their high stability under electron impact conditions.

Table 1. *Product yields under initial conditions*



3a-d 4 5a-d

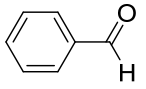
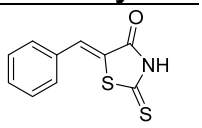
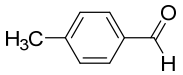
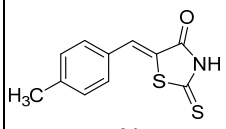
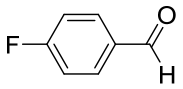
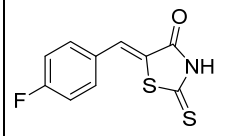
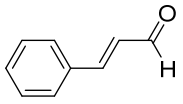
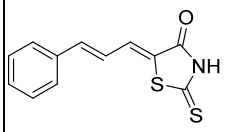
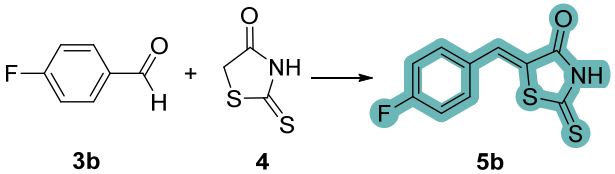
3	Conditions	Product - isolated yield
a 	10 min, 90°C, 1mL sat. $NaHCO_3$	 72%
b 		 92%
c 		 61%
d 		 72%

Table 2. *Optimization of **5b** reaction conditions.*



3b 4 5b

T (°C)	Time (min)	sat. NaHCO3 volume (mL)	5b yield (%)
110	10	1	79
90	20	1	81

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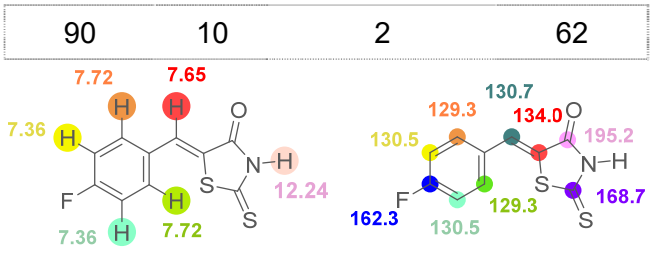


Figure 2. ^{1}H and ^{13}C NMR chemical shifts (ppm) for derivative **5b**.

4. CONCLUSIONS:

We have developed a fast and eco-friendly method for synthesizing 5-benzylidene and 5-cinnamylidene rhodanine derivatives using microwave irradiation. This technique stands out due to its use of water as the solvent, a short reaction time, high atom economy, and a minimal environmental footprint. The obtained yields ranged from 61% to 92%, with product purities surpassing 95%. This methodology offers an efficient and practical alternative to conventional heating techniques, with the added benefit of substantially lowering energy consumption and eliminating the use of hazardous organic solvents, fully aligning with sustainable synthesis practices.

The prepared rhodanines present unique structural features which make them particularly attractive for applications in fields such as medicinal chemistry, where they may serve as potential therapeutic agents, and materials science, where their photophysical properties could be harnessed for the development of new materials. This study not only provides a robust approach to synthesizing rhodanine derivatives but also lays the groundwork for future exploration of their biological and physicochemical properties.

Finally, the alignment of this method with the principles of green chemistry, through the minimization of hazardous solvents and energy-efficient processes, further reinforces its value as a sustainable approach to organic synthesis. Future studies could explore the broader applicability of this methodology and its impact on enhancing the environmental sustainability of industrial-scale synthesis.

5. DECLARATIONS

5.1. Acknowledgements

L. A. M. thanks to the Consejo Interuniversitario Nacional for the EVC-CIN fellowship. This work was supported by Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET-11220200101308CO), Fondo para la Investigación Científica y Tecnológica (FONCYT-PICT-2020-SERIE-A-01862) and Secretaría deCiencia y Tecnología (SeCyT-UNC-Nº258/23).

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J., *Bioorganic & Medicinal Chemistry Letters*. **2021**, *31*, 127670.
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Southern Science Conference, 2024.

EXPEDITIOUS SYNTHESIS OF RHODANINE DERIVATIVES THROUGH MICROWAVE IRRADIATION

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Noelia Marcela Ceballos

Walter José Peláez

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November/2024

unc Universidad Nacional de Córdoba

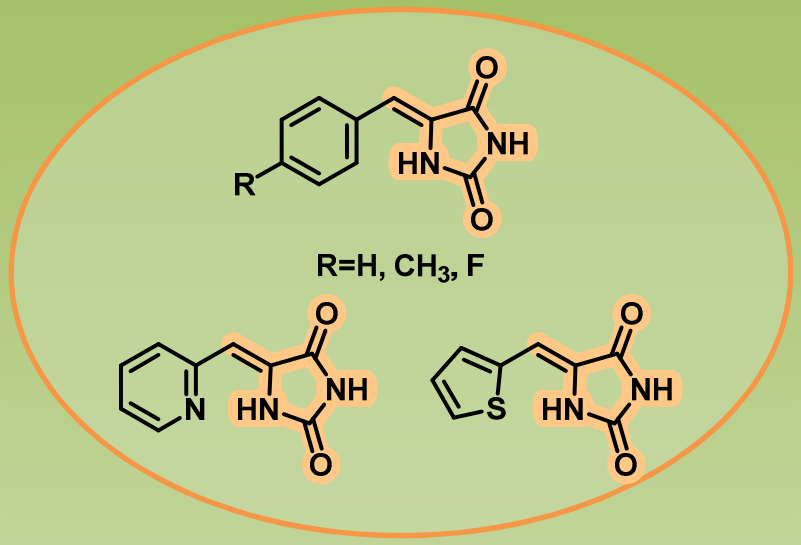
CONICET

FCQ Facultad de Ciencias Químicas

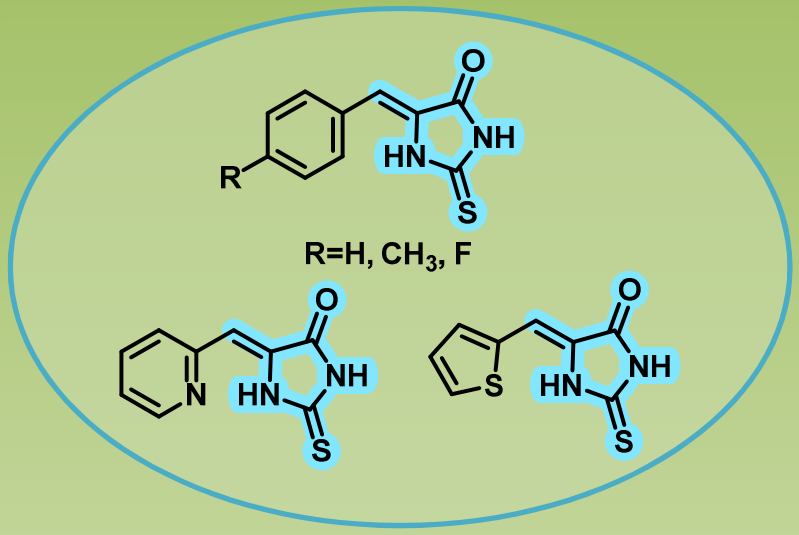
DFQ Departamento de Fisicoquímica

INFIQC2024 INSTITUTO DE INVESTIGACIONES EN FISICOQUÍMICA DE CÓRDOBA

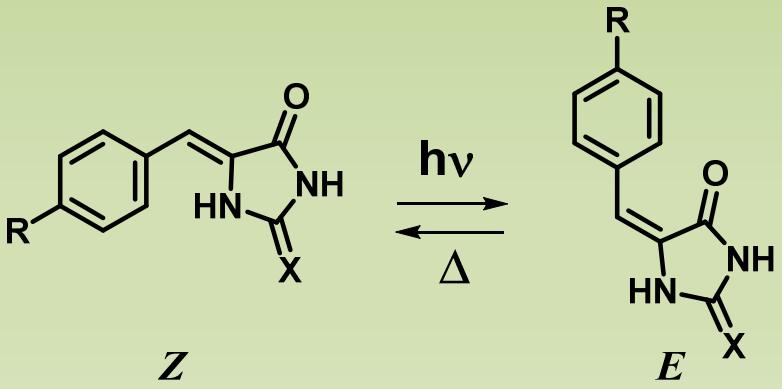
INTRODUCTION



imidazolidindiones



tioxoimidazolidinones



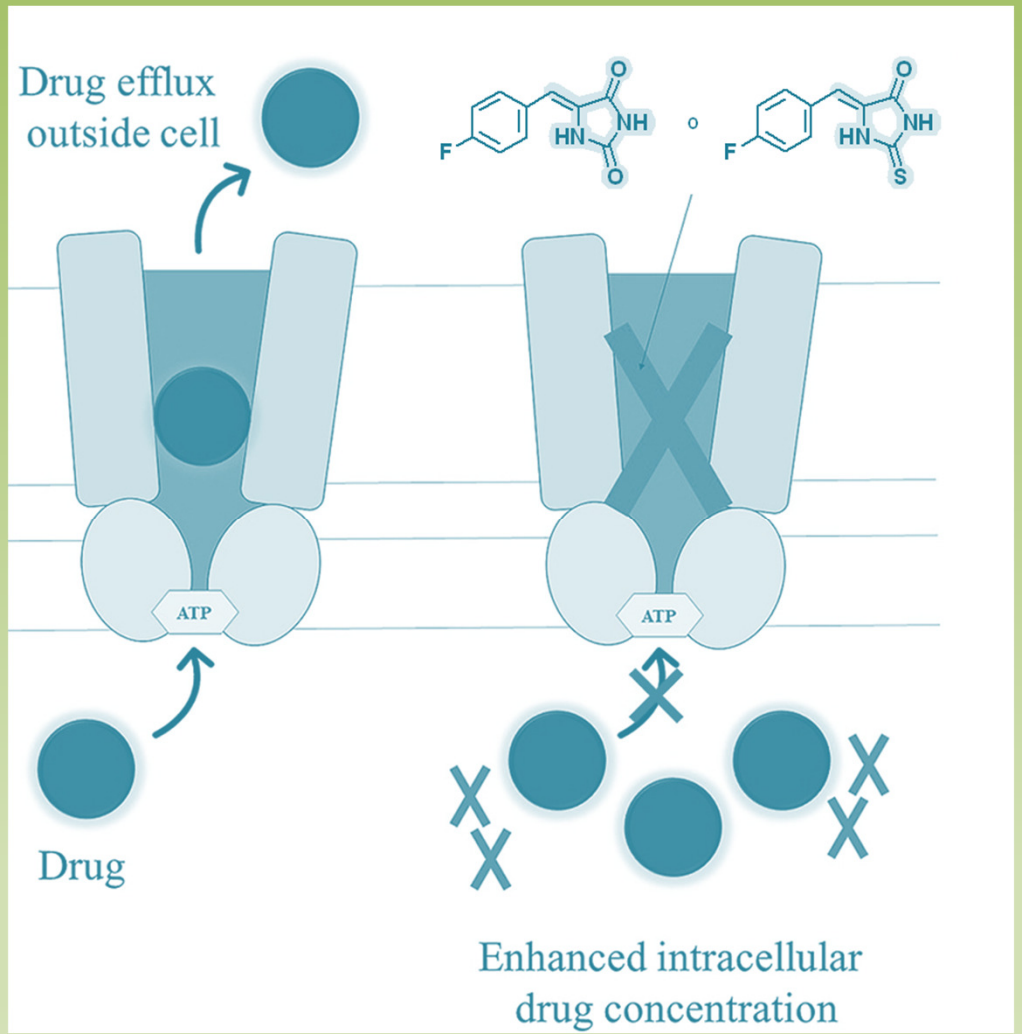
Thermodynamically stable form is in Z configuration

Undergoes isomerization to E isomer when exposed to UV light

E→Z reversal is a thermal process

Faillace, M. S., Alves Borges Leal, A. L., Araújo de Oliveira Alcântara, F., Ferreira, J. H. L., de Siqueira-Júnior, J. P., Sampaio Nogueira, C. E., Barreto, H. M., Peláez, W. J., *Bioorganic & Medicinal Chemistry Letters*. **2021**, *31*, 127670.

INTRODUCTION



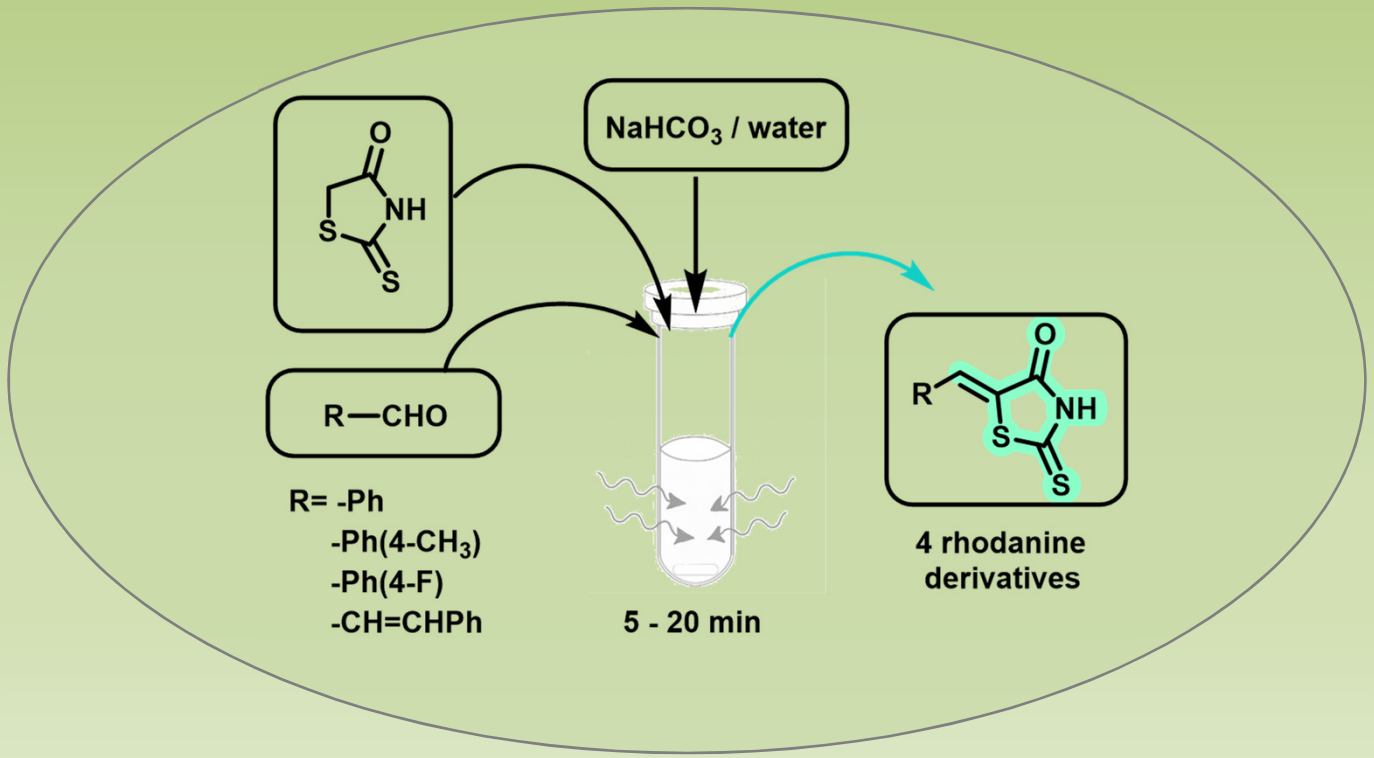
Fluorinated derivatives produce 6.4 and 4 fold decrease respectively, of the norfloxacin minimum inhibitory concentration (MIC) for the fluoroquinolone-resistant S. aureus strain.

Adapted from Gaikwad, V. L. *et al.*, *IJDDT*. **2024**, *94*, 105475.
Faillace, M. S., Silva, A. P., Alves Borges Leal, A. L., Muratori da Costa, L., Barreto, H. M., Peláez, W. J., *ChemMedChem*. **2020**, *15*, 851.

OBJECTIVES

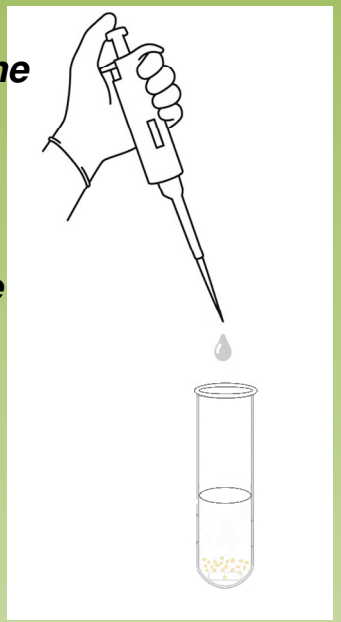
Prepare 5-benzylidene and 5-cinnamylidene rhodanines which are structurally closely related to the previous studied heterocycles.

Obtain the target compounds by an expeditious, efficient, and environmentally friendly synthesis using microwave (MW) irradiation as an alternative and eco-friendly methodology.



METHODOLOGY

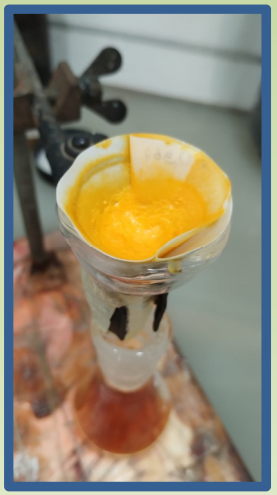
1. *2 mmoles rhodanine*
2. *1mL $NaHCO_3$ saturated solution*
3. *3 mmoles aldehyde*

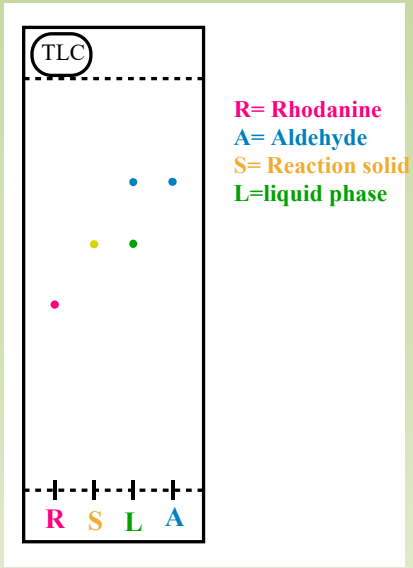






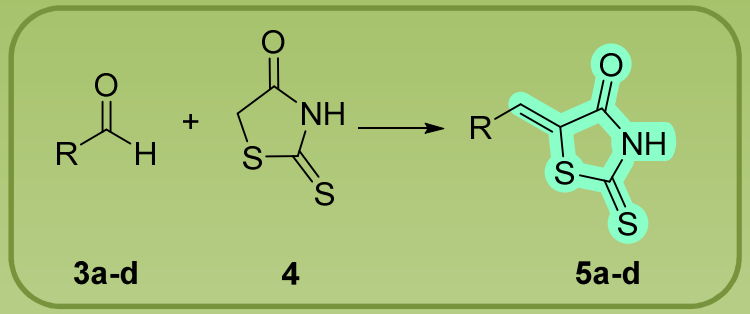
Neutralization to pH=7 using diluted HCl

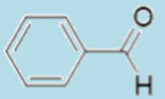
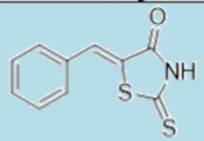
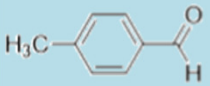
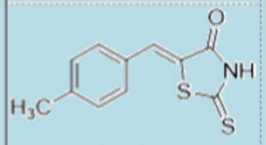
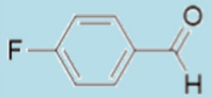
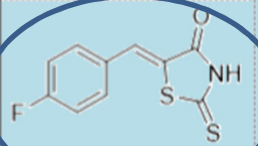
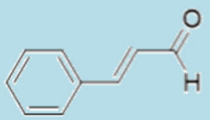
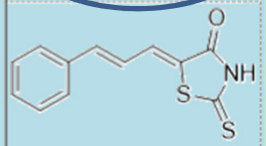


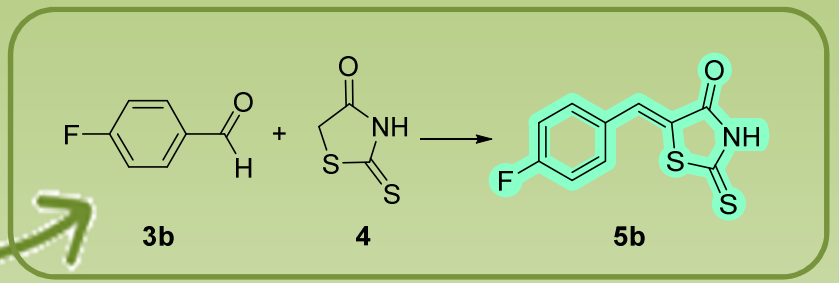


Column chromatography or recrystallization if needed

RESULTS AND DISCUSSION



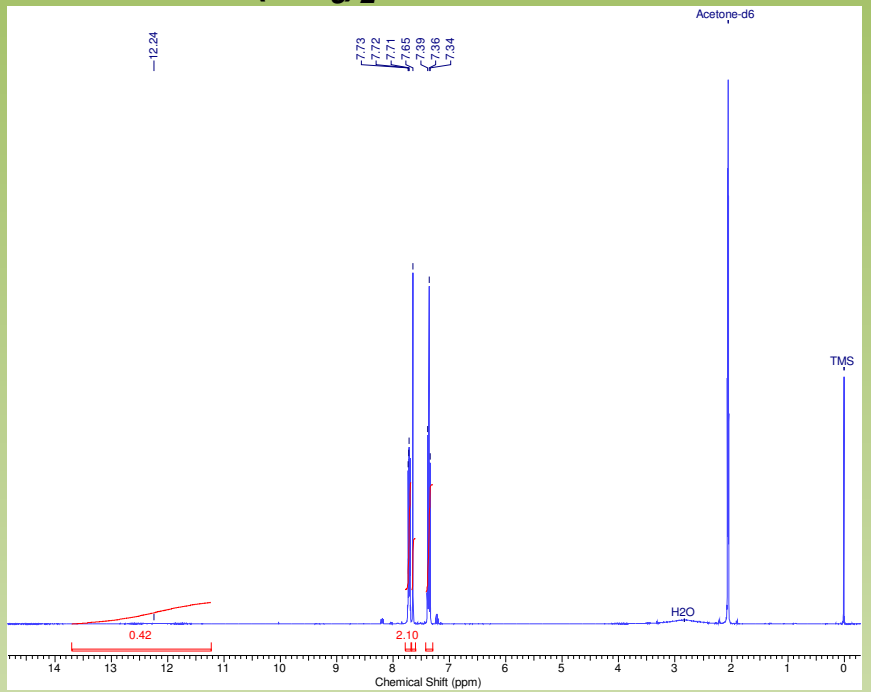
3	Conditions	Product - isolated yield
a 	10 min, 90°C, 1mL sat. $NaHCO_3$ ☑	 72%
b 		 92%
c 		 61%
d 		 72%



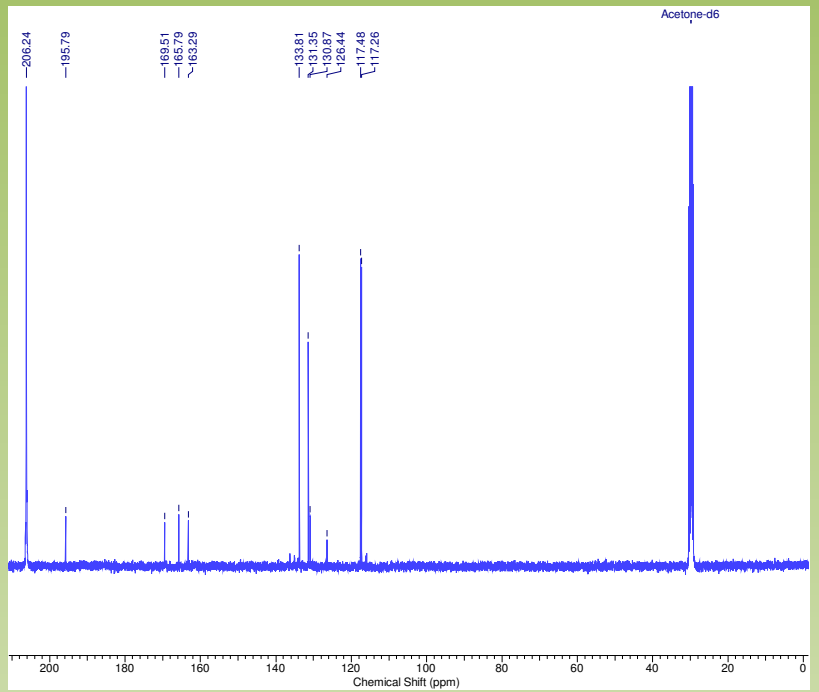
T (°C)	Time (min)	sat. NaHCO3 volume (mL)	5b yield (%)
110	10	1	79
90	20	1	81
90	10	2	62

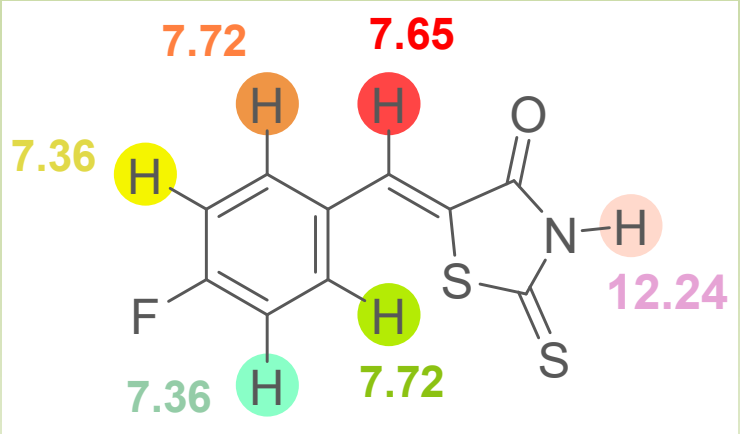
CHARACTERIZATION

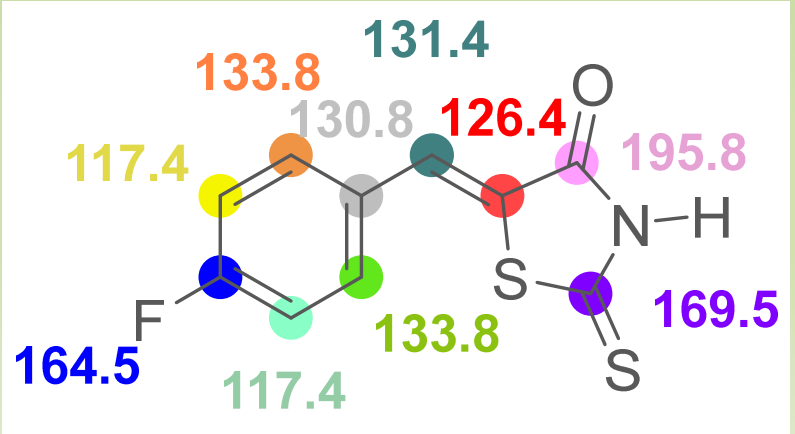
^{1}H-NMR -5b $(CD_3)_2CO$



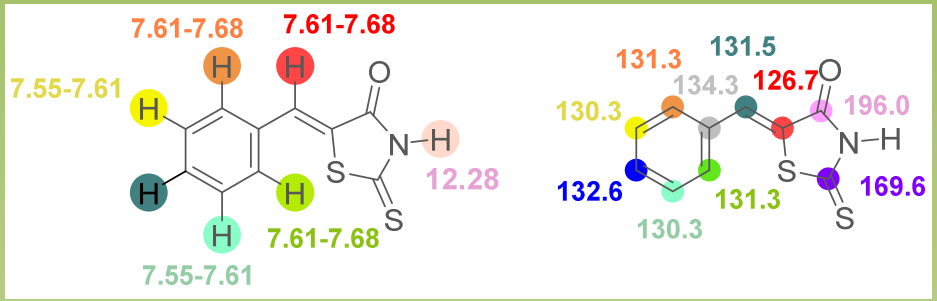
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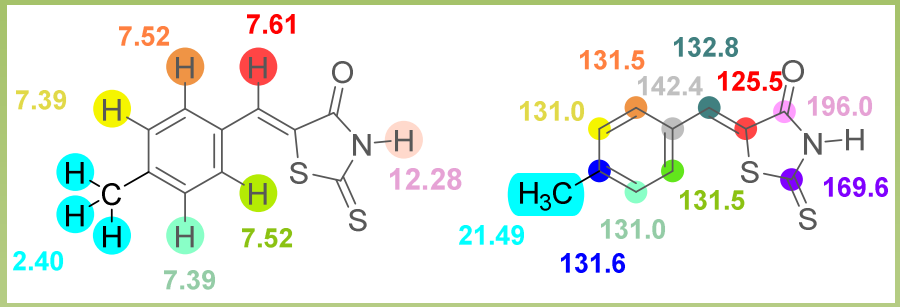


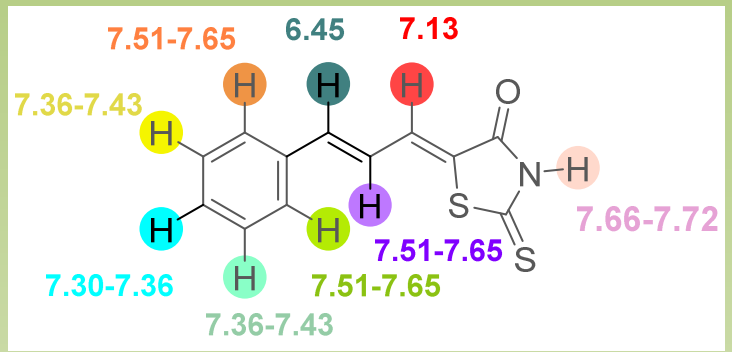


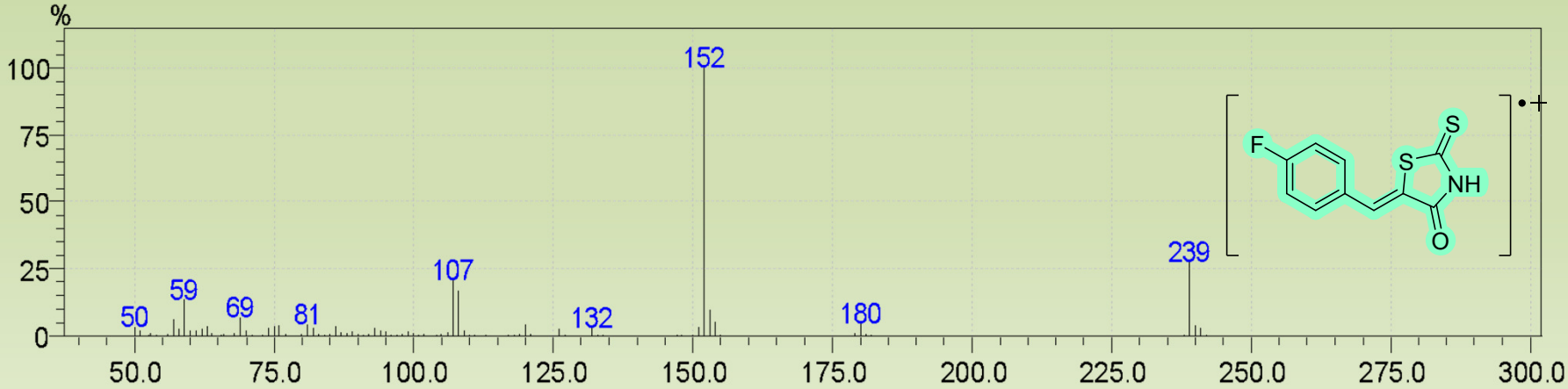


CHARACTERIZATION









CONCLUSIONS

- Fast and eco-friendly method for synthesizing 5-benzylidene and 5-cinnamylidene rhodanine derivatives using microwave irradiation. This technique stands out due to its use of water as the solvent, a short reaction time, high atom economy, and a minimal environmental footprint.

- The obtained yields ranged from 61% to 92%, with high product purities.

- The prepared rhodanines present unique structural features which make them particularly attractive for applications in fields such as medicinal chemistry or materials science.

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MACROALGAE AS MARINE MICRODEBRIS TRAPS: A CASE STUDY IN THE BAHÍA BLANCA ESTUARY

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ABSTRACT

Marine microdebris (MDs), including microplastics (MPs) and antifouling and/or anticorrosive paint particles (APPs) could have significant implications within coastal ecosystems of Argentina, particularly producers primary as macroalgae. In this study, we aimed to determine the abundance of MDs, including MPs APPs, among others, in seven different species of macroalgae (*P. morrowii, C. diaphanum, Bangia sp., Gelidium spp., Ulva spp., P. nakamurae, and B. minima*) and in surface waters from the Bahia Blanca Estuary (BBE). Fiber MPs were the most common type of MDs found in surface waters. In macroalgae, high concentrations of MPs were observed in brown algae (*P. nakamurae*), followed by red algae (*Gelidium spp. and Bangia sp.*). Green algae *B. minima* exhibited high concentrations of APPs. Additionally, other types of MDs, such as black soot particles, metallic microspheres, and fragments, were also identified in green algae *Ulva spp.* The most predominant colors of MDs found in macroalgae were black, white, and transparent. The size ranges of the MDs were primarily 0.5–2.5 mm and <0.5 mm in both surface waters and macroalgae samples. This study provided a baseline for MDs abundance, indicating the bioaccumulation of these emerging pollutants in the primary producers of the coastal trophic chain of BBE.

Keywords: *Microplastics, Paint particles; Macroalgae; Microdebris; Pellets; Mesoplastics*

1. INTRODUCTION

Recently, the presence of marine microdebris (MDs, debris ranging from 0.1 µm to <5 mm) has been reported in coastal aquatic environments worldwide (Kroon *et al*., 2018; Chan *et al*., 2019; Forero-López *et al*., 2024a and b). MDs are synthetic and semisynthetic particles that are persistent, manufactured, or processed solid material discarded or abandoned (Kroon *et al*., 2018; Forero-López *et al*., 2024a). These micromaterials have been modified, or used by humans, such as microplastics (MPs), antifouling or anticorrosive paint particles (APPs), metallic microparticles (Mmps), black particles, among others (Kroon *et al*., 2018; Turner and Keener, 2023).

Among MDs, plastic debris has attracted global attention, while other types, such as APPs, and glass microbeads, among others, have been ignored or underestimated due to their nature (Turner, 2021; Turner and Keener, 2023; Forero-López *et al*., 2024b). Based on size, plastic debris can be classified into mega-plastics (MegPs, >1 m diameter), macroplastics (MacroPs, between 2.5 cm and 1 m), mesoplastics (MesPs, between 5 mm and 2.5 cm), microplastics (MPs, between 0.1 µm and 5 mm) and nanoplastics (PNPs, <0.1 µm) (GESAMP, 2019); being the last two

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classifications cataloged as primary and/or secondary. Primary MPs/PNPs are manufactured in micro/nano size, while secondary ones are derived from the fragmentation of larger plastic debris as a result of aging in the environment opacity, density, and the presence of multiple layers, making them more intricate than typical MPs (Turner *et al*., 2021; Forero-López *et al*., 2024b). Furthermore, these anthropogenic particles can be accidentally ingested by various organisms, including aquatic species. Often confused with food, MPs, and APPs can have severe health consequences for these organisms, including intestinal blockages, entanglement, and death (Jovanovic, 2017; Kurtela & Antolović, 2019).

On the other hand, macroalgae are photosynthetic organisms that inhabit in aquatic environments and are part of the primary trophic chain. They are taxonomically categorized into three distinct groups based on the color of the thallus (e.g., Chlorophyta, green algae; Rhodophyta, red algae; and Phaeophyta, brown algae) or by morphotype (e.g., filamentous, foliose, tubular) (Choudhary *et al*., 2021; Forero-López *et al*., 2024b). Macroalgae play a crucial role in coastal ecosystems, serving as primary producers and providing habitat for a wide variety of aquatic organisms. However, a recent study has shown that macroalgae are accumulating MDs, mainly MPs and APPs, becoming important potential sinks for these emergent contaminants in Argentine coastal ecosystems (Forero-Lopez *et al*. 2024b). For this reason, the main objective of this study was to investigate the abundance and physical composition of MDs and MeDs on intertidal macroalgae species and in surrounding water from the Estuary of Bahía Blanca, located in Buenos Aires Province. This research provides valuable insights into how these pollutants accumulate and impact macroalgae, crucial primary producers in the food chain.

2. MATERIALS AND METHODS

2.1. Sample collection and preparation

Samples were collected on 5 and 6 August 2024 (austral winter season) in the Bahía Blanca Estuary (BBE) (S 40◦ 28′; W 62◦ 22′). (**Fig. 1 and Table 1**). The sampling sites of BBE are located in the innermost and middle zone of this estuary: Coastal path of BBE (Cp) (38◦ 44′ S; 62◦ 19′ W), Club Náutico (CN) (38◦ 43′ S; 62◦ 16′ W), Villa del Mar (VM) (38◦ 47′ S; 62◦ 16′ W), and Puerto Rosales (RP) (38◦ 55′ S; 62◦ 04′ W) (**Table. 1**). Cp of BBE is located in the inner area of the estuary. In this sampling point is near a significant illegal dumpsite where is frequently burned plastic waste, tree trimmings, and other materials. CN is situated in the inner area of the estuary and is a nautical sports institution with approximately one hundred years of history. The commercial club features two commercial docks and accommodates a variety of vessels, including sailboats and small to medium-sized boats. Whereas VM and RP are located in the middle part of the BBE. VM is a small-scale artisanal fishing village affected by the industrial area of the port, and RP is the outermost port in the Bahía Blanca harbor system (PuertoBahiaBlanca, 2024).

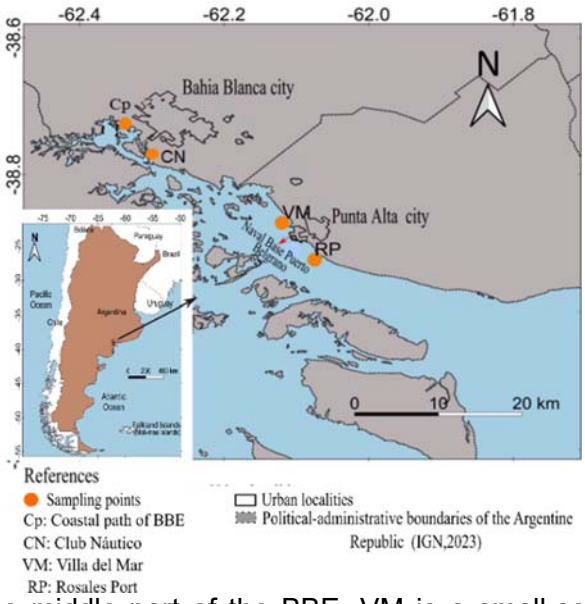


Figure 1*. Geographical position of the sampling sites along the Bahía Blanca Estuary (BBE) in Buenos Aires Province.*

The existence of macroalgae in the sampling sites from BBE is associated with tidal environments modified by the settlement of the exotic oyster *Crassostrea gigas* in these sampling points and by the presence of natural rock made of consolidated fine sedimentary particles (named outcrops) and artificial structures available for the settlement of these algae. In BBE, macroalgal assemblages inhabit the tidal pool or tidal channel, which remains filled with water during low tide (Croce *et al*., 2021; Forero-lópez *et al*., 2024b)

In order to investigate the abundance of MDs present in surface waters, approximately 10 L of

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water was collected in amber glass bottles at each sampling point at BBE. For the acquisition of macroalgae samples, the methodology described by Zhang *et al*. (2022) and Forero-Lopez *et al*. (2024b) was followed. Briefly, seven taxa of macroalgae were collected using a conditioned metal spoon being identified as: four red algae (Rhodophyta) i.e., *Polysiphonia morrowii*, *Ceramium diaphanum*, *Gelidium spp*. (G. crinale, G. carolinianum), and *Bangia sp*.; two green algae (Chlorophyta) i.e., *Ulva spp*. (*U. lactuca, U. prolifera, U. instestinalis, U. flexuosa*), and *Blidingia minima*; and one brown alga (Phaeophyta), i.e., *Planosiphon nakamurae* (**Table 1**). The collected macroalgae samples were rapidly placed in labeled small containers to impede MP pollution from the atmosphere. The containers used during sampling were washed three times with filtered deionized water (0.45 µm pore size), conditioned with previously filtered ethanol (70 %), and then with filtered deionized water following the methodology described by Forero-López *et al*. (2021b).

Tabla 1. *A summary of the information on the sampling stations and species of macroalgae was collected. Macroalgae samples were grouped based on their common morphological features (filamentous and non-filamentous).*

Station	Macroalgae type	Morphology(1)
Coastal path (Cp)	Green algae *Ulva spp.*	Blade-like
Club Náutico (CN)	Green algae *Ulva spp. (dock)*	Blade-like
	Green algae *Blidingia minima*	Tubular
	Brown algae *Planosiphon nakamurae*	Compressed with blade-like habit
	Green algae *Ulva spp. (Coastal)*	Tubular
Villa del Mar (VM)	Red algae *Polysiphonia morrowii*	Filamentous
	Red algae *Ceramium strictum*	Filamentous
	Red algae *Gelidium carolinianum*	Larger-sized corticated
Coronel Rosales (CR)	Green algae *Ulva spp.*	Blade-like and tubular
	Red algae *Bangia sp.*	Tubular

(1) Morpho-functional groups, according to Balata *et al*. (2011)

2.2. Laboratory procedures

For the water samples, 1 L of water was vacuum filtered using nitrocellulose filters (0.45 µm pore size). After filtration, the inner wall of the filtration vessel was rinsed with Milli-Q water and 70 % ethanol to collect any particles that may have adhered to the filter. Then, the filters with the samples were placed in Petri glass dishes that had been previously conditioned and dried at room temperature. MDs, MesPs, and MacroPs, were extracted from the different macroalgae species using the methodology described by Zhang *et al*. (2022) and Forero-López *et al*. (2024b).

In brief, a portion of algae with a fresh weight between 10 and 35 g (depending on biomass recollected) was placed in a previously cleaned and conditioned 500 mL beaker, and 50 mL of Fenton's reagent (Fe (II) solution (0.05 M) and 30 % v/v H_2O_2) were added. The samples were covered with aluminum foil and kept at 40 ◦C for 48 h with periodic shaking. This was done in triplicate for each type of algae sample. The result of the digestion of the algal samples is a yellow transparent solution, which was filtered under vacuum through a nitrocellulose filter (0.45 µm pore size). After filtration, the inner wall of the filter vessel was rinsed several times with 70 % ethanol to collect any elements outside the filter that could have adhered to the wall. All the filtered membranes with the sample were placed in clean, previously conditioned Petri dishes and dried at room temperature until visual inspection under the stereomicroscope.

2.3. MDs quantification

Morphological identification and counting of different anthropogenic particles on the obtained filters were conducted using a Leica S8APO stereomicroscope. All particles resembling MDs were photographed and sorted into their respective categories based on morphology, color, and size range. The morphology was classified into fibers, fragments, films, and pellets, as well as their color (blue, red, white, black, and yellow). Size ranges for MDs were defined as follows: <0.5 mm, 0.5–2.5 mm, 2.5–3.5 mm, 3.5–5 mm and >5 mm. The average abundance of MDs and MesDs in surface waters and macroalgae samples were expressed in items/ L and items/wet weight (w.w.), respectively. Statistical analyses of the abundance of MDs types in surface waters and macroalgae were performed using the free software R Development Core Team (2017). Also, an analysis of variances (ANOVA-one-way) was performed to evaluate the statistical differences between the concentrations of the sample stations.

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3. RESULTS AND DISCUSSION

A total of 97 MDs were found in surface waters, which were mostly MPs fiber (93.82%), and the 6±2.45 items/L was detected at Cp (**Fig. 2**). In terms of size, over 50% of MDs were primarily less than 0.5 mm in surface waters from CN and VM were primarily smaller than 0.5 mm, while those from Cp and CR sites were predominantly 0.5 to 2.5 mm.

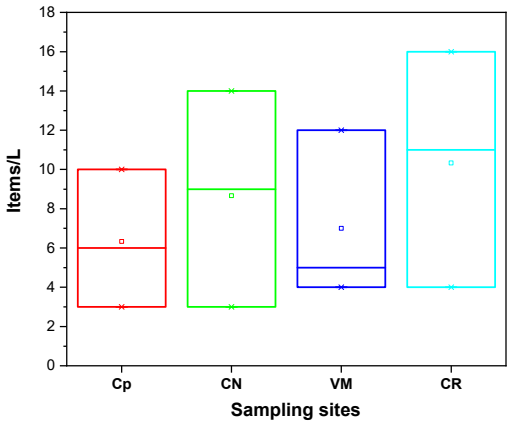


Figure 2. *Abundance (average ± SD) of MDs in water samples from Bahía Blanca Estuary (BBE).*

The concentration of MDs in surface waters showed no significant differences between the different sampling sites ($p > 0.05$). Finally, two MesoPs fibers were found in CR with size > 8.6 mm.

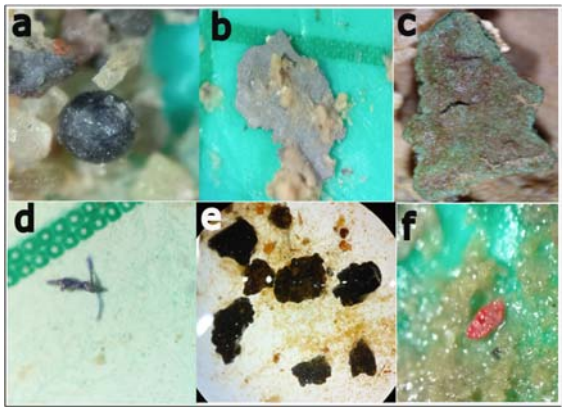


Figure 3. *Photograph MDs found in macroalgae: (a) microspheres metallic, (b) gray fragment, (c) green APPs fragment, (d) fiber MPs, (e) metallic fragment, and (f) red fragment*

In the case of macroalgae samples, a total of 184 MDs were found in seven species analyzed. Of these MDs, 52.71% were MPs (e.g., fibers, fragments, foams), followed by APPs at 26.63% and other MDs (black soot particles, fragments, and microspheres metallic) at 20.65% (**Fig. 3**). Black, white, and transparent MDs were the most abundant colors, accounting for 32.61%, 22.83%, and 17.39% of the total. MDs were most frequently remaining were fragments (6.18%). The range of MDs concentration was 3 items/L to 16 items/L, with the highest concentration found at the CR sampling station, with a mean value of 10,33±4.92 items/L, while a low mean value of abundance found in size ranges of 0.5–2.5 mm and <0.5 mm, comprising 61.96% and 24.46%, respectively.

A high average concentration of MPs was found in macroalgae *P. nakamurae* samples (1.47±0.13 items/g.w.w.) from CN, followed by *Gelidium spp*. (0.65±0.14 items/g.w.w.) from VM and *Bangia sp*. (0.42±0.51 items/g.w.w.) from CR (**Fig. 4**). Whereas high mean abundances of APPs were identified in *B. minima* (0.50 ±0.19 items/g.w.w.) from CN and *P. nakamurae* (0.28±0.16 items/g.w.w.) samples from CN (**Fig. 4**). Particularly, other MDs (e.g., black soot particles, metallic microspheres, and fragments) were also identified in green algae *Ulva spp.* from CN and Cp, with average concentrations 0.30±0.38 items/g.w.w. and 0.27±0.25 items/g.w.w., respectively (see ***Fig. 4***). According to the type of MDs, there are significant differences among the microalgae samples from each sampling site of BBE ($p < 0.05$), , with CN showing higher concentrations than Cp, CR, and VM. Finally, only one MacroPs fiber with a size of 3.8 cm was found in macroalgae samples from the VM. Additionally, 15 MesoPs fibers were found primarily in the VM (n=9), followed by the CN (n=3) and CR (n=3).

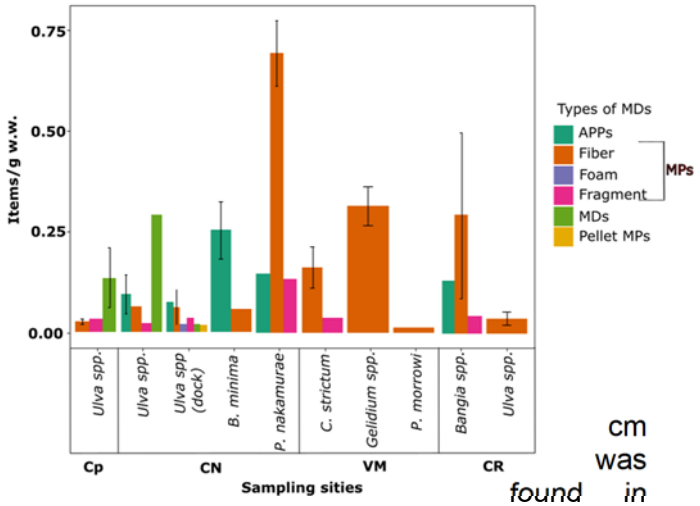


Figure 4. *Abundance (average ± SD) of MDs (APPs, MPs (fibers, fragments, foams) and other MDs) in different species of macroalgae from BBE.*

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4. CONCLUSIONS

This study evidenced the presence and abundance of MDs (APPs, and MPs, among others) and MesoPs in seven species of macroalgae from the Bahía Blanca estuary (BBE). MPs, APPs, and other types of (e.g., black soot particles, metallic microspheres, and fragments) were found in significantly higher concentrations within macroalgae than in surrounding waters.

Furthermore, sampling points such as CN, and CR with coastal structures, docks, harbors, berths for small vessels, and boatyards, exhibited high concentrations of MPs and APPs. Meanwhile, Cp, with an illegal dumpsite where plastic waste is frequently burned, exhibited the presence of black soot particles, evidencing that local sources change the composition of types of MDs in macroalgae samples. Finally, *Ulva spp.* tend to accumulate various types of MDs, while macroalgae species *P. nakamurae* and *Gelidium spp.* (non-filamentous morphotypes) accumulate the most MPs compared to the other species. This suggests that these primary producers act as crucial sinks for marine MDs, potentially facilitating their transfer and bioaccumulation throughout the food chain.

5. DECLARATIONS

5.1. Acknowledgements

This study was supported by BID PICT-2021–0220 granted to Dr. A.D. Forero-Lopez.

5.2. Open Access

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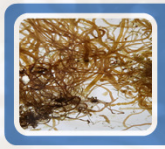
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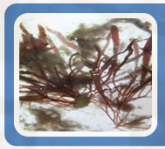
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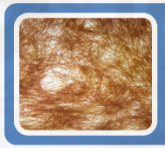
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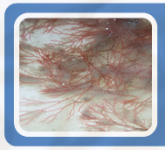
SUMMARY

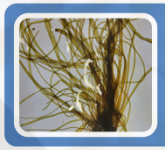

Introduction


Objetive


Methodology


Results and Discussion


Conclusions


Acknowledgement

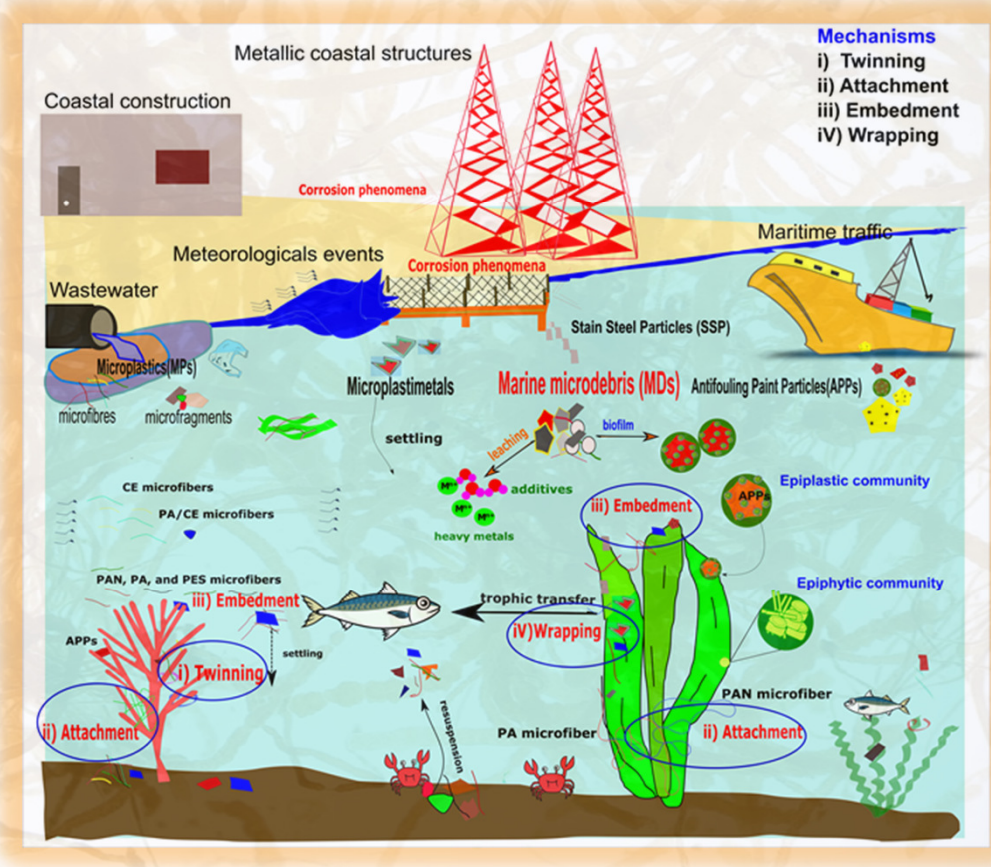


Fig. 1. marine microdebris (MDs) on the coastal environment.

INTRODUCTION

Marine Microdebris (MDs) are synthetic and semisynthetic particles persistent, manufactured, or processed solid material discarded or abandoned, which has been modified, or used by humans.

Macroalgae are photosynthetic organisms that inhabit in aquatic environments and are part of the primary trophic chain

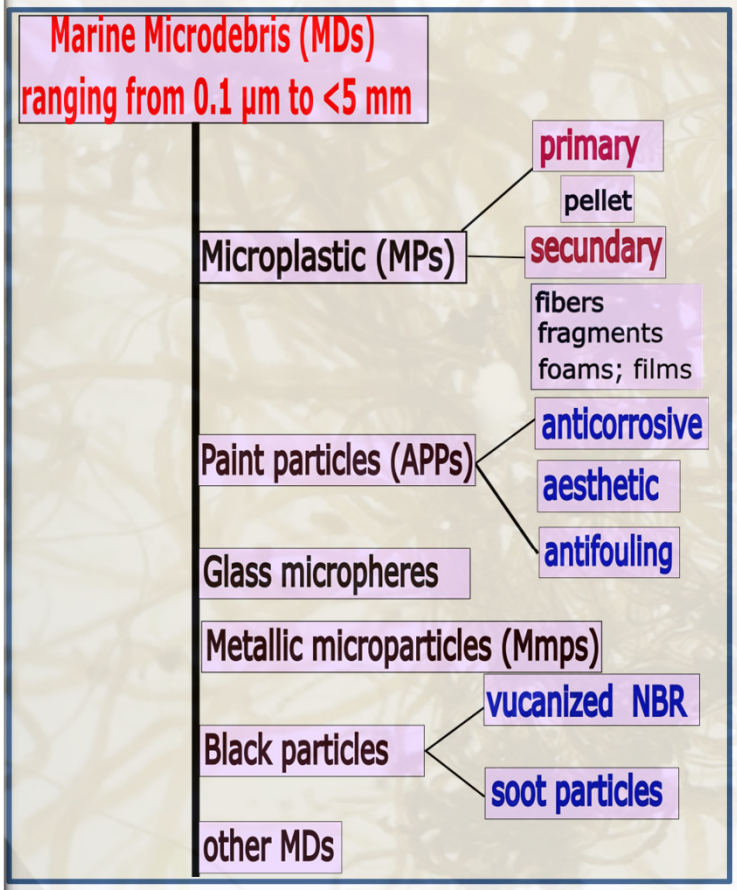


Fig. 2. *Types scheme of marine microdebris (MDs)*

MDs pollution

MesoPlastics

MesPs, 5 mm - 2.5 cm



Fig. 3. *Examples of macroalgae*

OBJETIVE



The objective of this study was to investigate the abundance and physical composition of **MDs** and **MeDs** on intertidal macroalgae species and in surrounding water from the Bahía Blanca Estuary (**BBE**), located in Buenos Aires Province.

METHODOLOGY

Sample collection

Samples were collected on 5 and 6 August 2024 (austral winter season) in the BBE (S 40◦ 28′; W 62◦ 22′).

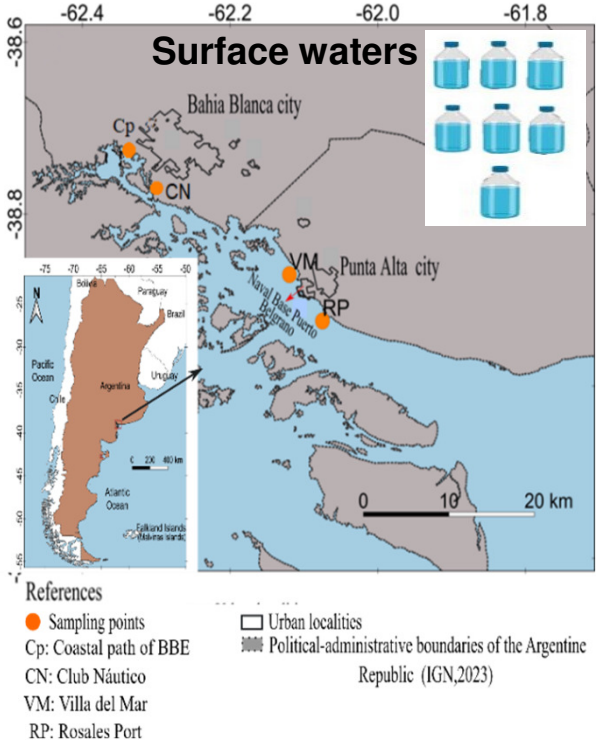


Fig. 4. (a) *Geographical position of the sampling sites along the Bahía Blanca Estuary (BBE) in Buenos Aires Province.*

Macroalgae samples

Station	Macroalgae type	Morphology
Coastal path (Cp)	**Green algae** *Ulva spp.*	Blade-like
Club Náutico (CN)	**Green algae** *Ulva spp. (dock)*	Blade-like
	Green algae *Blidingia minima*	Tubular
	Brown algae *Planosiphon nakamurae*	Compressed with blade-like habit
	Green algae *Ulva spp. (Coastal)*	Tubular
Villa del Mar (VM)	**Red algae** *Polysiphonia morrowii*	Filamentous
	Red algae *Ceramium strictum*	Filamentous
	Red algae *Gelidium carolinianum*	Larger-sized corticated
Coronel Rosales (CR)	**Green algae** *Ulva spp.*	Blade-like and tubular
	Red algae *Bangia sp.*	Tubular

Laboratory procedures

Surface waters

Filtration of water samples



Macroalgae samples



Weighing

15-35 g



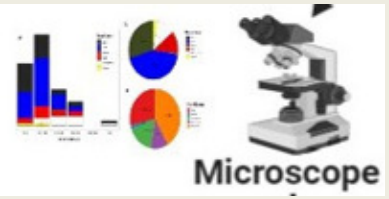
Digestion

Fenton reagent



Filtration

Quantification



RESULTS AND DISCUSSION

Abundance of MDs in surface waters

A total of 97 **MDs** were found in surface waters, which were mostly **MPs** fiber (93.82%), and the remaining were fragments (6.18%).

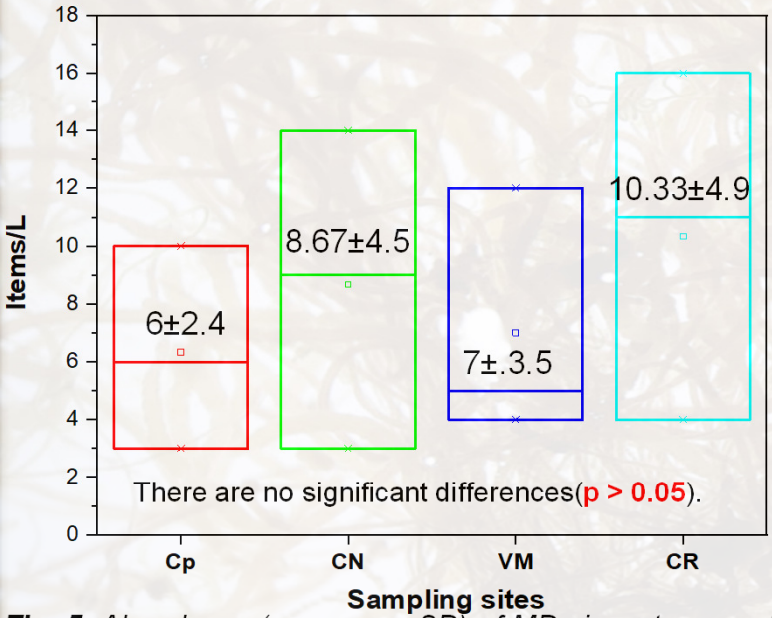


Fig. 5. *Abundance (average ± SD) of MDs in water samples from the BBE).*

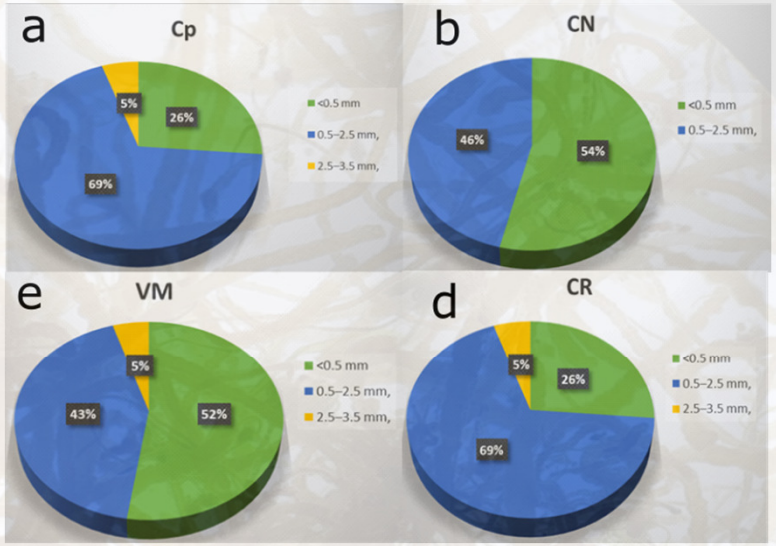


Fig. 6. *Percentage of MPs in water samples from the BBE).*

Abundance of MDs in macroalgae

A total of 184 **MDs** were found in seven species analyzed. Of these MDs, 52.71% were **MPs** (e.g., fibers, fragments, foams), followed by **APPs** at 26.63% and other MDs (black soot particles, fragments, and microspheres metallic) at 20.65%

RESULTS AND DISCUSSION

Abundance of MDs in macroalgae

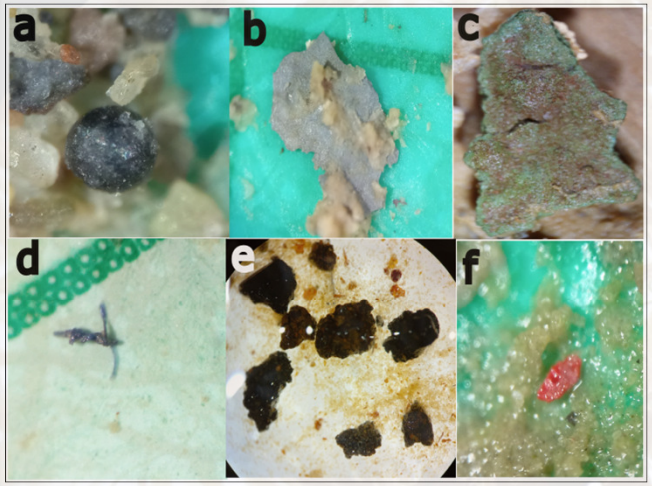


Fig. 7. *Photograph MDs found in macroalgae: (a) microspheres metallic, (b) gray fragment, (c) green APPs fragment, (d) fiber MPs, (e) metallic fragment, and (f) red fragment.*

Black (32.61%), white (22.83%), and **transparent (17.39%) MDs** were the most abundant colors

The size ranges **0.5–2.5 mm (61.96%)** and **<0.5 mm (24.46%)** were the most frequent range of **MDs** found in macroalgae samples.

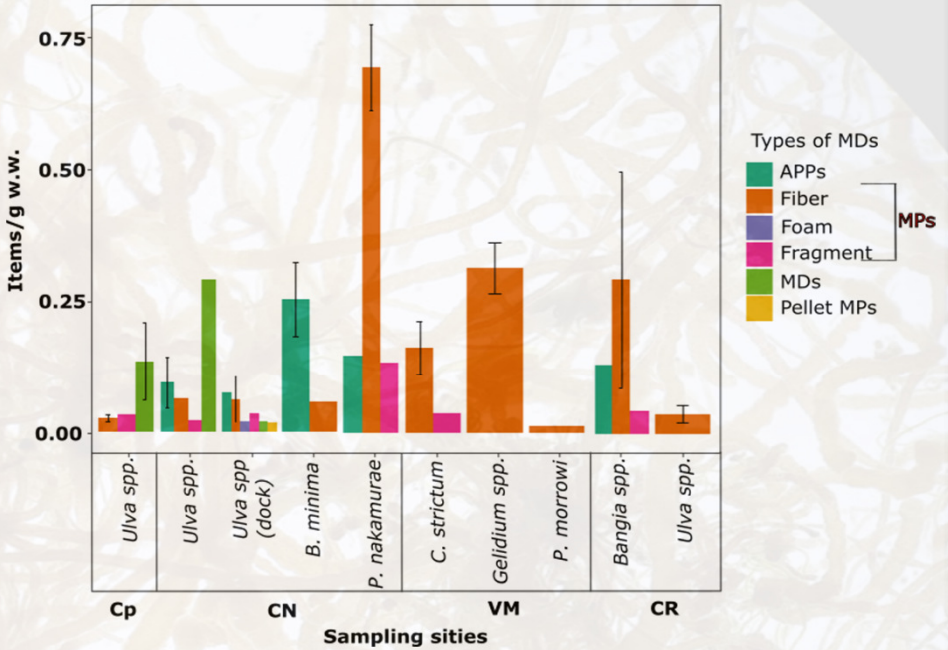


Fig. 8. *Abundance (average ± SD) of MDs (APPs, MPs (fibers, fragments, foams) and other MDs) in different species of macroalgae from the BBE.*

There are significant differences among the microalgae samples from each sampling site of **BBE** (**$p < 0.05$**)

CONCLUSIONS

❖This study evidenced the presence and abundance of **MDs** (**APPs**, and **MPs**, among others), and MesoPs in seven species of macroalgae from the Bahía Blanca estuary (**BBE**).

❖Highest concentrations of **MDs**, mainly **MPs** and **APPs,** were detected in macroalgae samples than in surrounding waters.

❖Local sources at sampling sites may change the composition of **MDs** types in macroalgae samples.

❖While ***Ulva spp.*** tend to accumulate various types of **MD**s, whereas macroalgae species ***P. nakamurae*** and ***Gelidium spp.*** tend to accumulate only **MPs**

ACKNOWLEDGEMENTS

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II SOUTHERN SCIENCE CONFERENCE
2024 - VIRTUAL CONFERENCE AND IN PERSON EDITION

STUDY OF THE ADSORPTION POTENTIAL OF NATURAL PEQUI SHELL AND ENDOCARP (*Caryocar Brasiliense*) FOR METHYLENE BLUE

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ABSTRACT

This study aimed to evaluate the adsorptive potential of the natural peel and endocarp of pequi (Caryocar brasiliense) for methylene blue adsorption in aqueous solutions, with the goal of promoting the adsorption method using bioadsorbents for treating contaminated aqueous effluents. Pequi is a fruit native to the Brazilian Cerrado and is widely found in the Central-West region. Its almond is sold in local markets, but much of the fruit is wasted due to the spines present around the endocarp, which make it difficult to consume. Thus, pequi was chosen due to its high availability, with the objective of reducing its waste by using it as a bioadsorbent. The experimental methodology included drying at 100 °C for 24 hours grinding the peel and endocarp with a knife mill. Particle size was determined using 42-mesh sieves, and sample analysis was conducted with a spectrophotometer at a wavelength of 660 nm. Experiments were performed in triplicate and in batch mode at different temperatures (25, 35, and 45 °C) and contact times (5, 10, 15, 20, 25, 30, and 40 minutes). Results showed that at 25 °C, the peel achieved a maximum removal of 84.70% (±1.41) and the endocarp 78.02% (±6.08) in 40 minutes. At 35 °C, the peel achieved a maximum removal of 89.95% (±0.80) and the endocarp 83.62% (±3.96). At 45 °C, the maximum removal was 87.97% (±0.87) and 85.16% (±5.10) for the peel and endocarp, respectively. It is worth noting that at 25 °C, equilibrium time was not observed for either adsorbent, indicating that adsorption sites were not saturated, requiring more time than the studied interval. Based on the results obtained, it can be concluded that adsorption using the natural peel and endocarp of pequi is an effective and promising method for treating aqueous effluents due to the low cost, high removal efficiency, and high availability of the bioadsorbent.

Keywords: *Bioadsorbent. Biomass. Kinetics. Dyes. Textile Effluent*.

1. INTRODUCTION

The first industrial revolution, which occurred in the mid-18th century, introduced significant advancements for humanity, such as the power loom. However, to keep up with society's demands, the industry was compelled to produce on an ever-larger scale (Sakurai and Zuchi, 2018). Consequently, the amount of aqueous effluents produced increased significantly. Among the industries that generate such waste, the textile industry stands out, as dyeing a single t-shirt consumes between 16 and 20 liters of water (Lee, 2009). Therefore, treating the aqueous effluents produced by it becomes necessary.

There are three main methods for treating aqueous effluents: chemical, biological, and physicochemical. Chemical methods involve processes where removal occurs through chemical reactions, such as oxidation, ozonation, or electrochemical destruction. However, they generally present high costs and environmental challenges related to the disposal of reagents and by-products (Wang et al., 2018). Biological methods are sustainable and economical, but they are highly sensitive to environmental changes, making large-scale implementation difficult (Silveira, 2013). Among physicochemical methods, adsorption stands out due to its low complexity and high removal capacity (Kwon and Lee, 2015).

In this context, adsorption is a physicochemical method involving the presence of

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an adsorbent, an adsorbate, and a solvent (Ruthven, 1984). Among various adsorbents, bioadsorbents are notable because, in addition to contributing to sustainability, they are readily available in nature.

Pequi can be divided into: epicarp (peel), external and internal mesocarp (pulp), endocarp, which has small, fine spines around it, making it difficult to consume, and an edible almond that is commercially used in local agriculture. The epicarp and external mesocarp are usually treated as by-products, often being discarded (Siqueira et al., 2013). The pulp has high antioxidant potential due to its composition, and the almond is widely used for oil extraction. According to Melo et al. (2021), 45 individuals/ha can produce about 180 kg of pulp, 119 kg of pulp oil, 33 kg of almonds, and 15 L of almond oil. Therefore, adsorption using the endocarp of pequi (Caryocar brasiliense), a fruit abundantly found in the Brazilian Cerrado and classified as a bioadsorbent, shows potential for treating aqueous effluents due to its high efficiency, operational simplicity, and low cost.

Thus, this study aims to investigate the potential of the natural shell and endocarp of pequi in the adsorption of methylene blue dye in aqueous solution at different temperatures and contact times.

2. MATERIALS AND METHODS

2.1. Adsorbent Preparation

Initially, the pequi parts were separated, selecting the peel and endocarp. They were washed with running water and left to air-dry for three days (at room temperature). Then, the samples were placed in an oven at 50 °C for 24 hours. Afterward, the bioadsorbent were ground separately in a knife mill (Tecnal, Te048) and left again in the oven under the same previous conditions. Finally, the samples were passed through a vibrating table (Bertel) with sieves of different meshes to separate the different particle sizes. The particle size chosen for this study was 42 mesh.

2.2. Batch Adsorption Potential Evaluation of the Adsorbent

All experiments presented in this study were performed in triplicate to assess the influence of contact time and temperature on the adsorption of natural peel and endocarp. Thus, experiments were conducted in 125 mL Erlenmeyer flasks containing 25 mL of methylene blue aqueous solution (100 mg/L adsorbate) and 0.05 g of adsorbent. The sample was subjected to different temperatures (25, 35, and 45 °C) and contact times (5, 10, 15, 20, 25, 30, and 40 minutes) under constant agitation in a shaker (Pro lab, Sk-O180-Pro digital) at 360 rpm connected to a thermostatic bath (Tecnal, TE2005) to maintain the temperature. After the desired time, the solution was filtered to stop contact between the adsorbent and adsorbate.

The filtered solution was analyzed in a UV-visible spectrophotometer (Bel UV-M51) at a wavelength of 660 nm. Based on the calibration curve constructed for the methylene blue solution, absorbance was converted to the final concentration (mg/L). To calculate the amount of material adsorbed at a given time (Qt) in mg adsorbed/g of adsorbent, equation 1 was used.

$$Qt = (Ci - Cf) * \frac{m}{V} \quad \text{(Eq. 1)}$$

where Ci and Cf (mg/L) are the initial and final concentrations, respectively, V is the volume (L) of the solution, and m is the mass (g) of the adsorbent.

3. RESULTS AND DISCUSSION:

3.1. Effect of Contact Time

The study of contact time is essential to determine the equilibrium time of an adsorption process, as it enables the assessment of the maximum adsorbed quantity under the tested conditions (Yu et al., 2013). The time range studied was between 0 and 40 min for experiments conducted using the endocarp and peel at 25°C. Within the selected range, it was not possible to establish the equilibrium time for either bioadsorbent, as the adsorbed quantity did not reach equilibrium; that is, the available adsorption sites were not fully occupied, requiring a longer adsorption time.

Figure 1 represents the kinetic curves of the amount adsorbed by the endocarp and peel at 25 °C. Since the experiments were performed in triplicate, the results presented represent the

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average of these trials.

It is noteworthy that between 5 and 40 min, the adsorbed quantity increased significantly over the interval. The process proved more effective over a longer duration; thus, 40 min would be the optimal time for treating the methylene blue solution using the peel and endocarp, providing speed and efficiency.

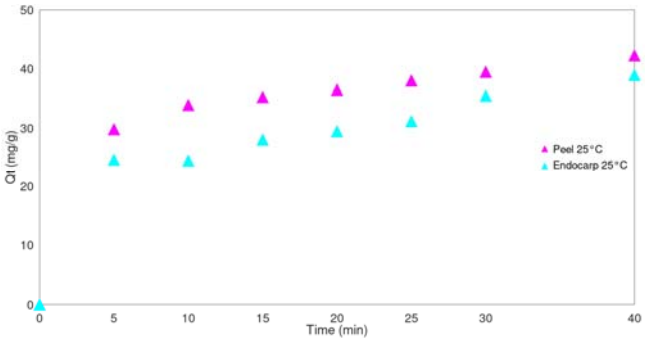


Figure 1. *Kinetic curves showing the adsorbed quantity as a function of contact time for adsorption using the natural endocarp and peel of pequi at 25 °C.*

Additionally, it can be observed that the peel exhibited a higher adsorbed quantity compared to the endocarp; this is due to the peel having a larger and more porous surface area, as well as more functional groups that facilitate adsorption (Amorim et al., 2016).

In Figure 2, the efficiency of the adsorption process using the natural endocarp at 25 °C can be seen through the change in color of the aliquots, indicating that the dye concentration decreased over time.

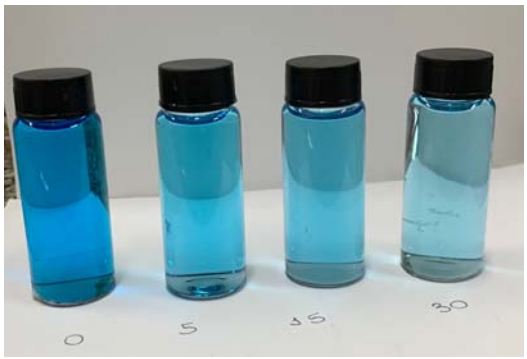


Figure 2. *Illustration of the solutions after 0, 5, 15, and 30 min at 25 °C.*

3.1. Effect of Temperature

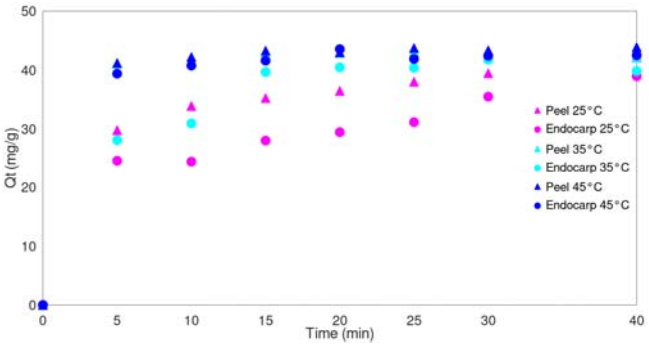


Figure 3. Effect of temperature on adsorbed quantity as a function of time using the natural endocarp and peel of pequi at 25, 35 and 45°C.

Figure 3 presents the average kinetic adsorption curve using the endocarp and the peel at times of 5, 10, 15, 20, 25, 30, and 40 minutes and at temperatures of 25, 35, and 45°C. From this figure, it is possible to observe that at 25°C, the endocarp presented a Qt of 38.93 (±2.99) mg/g, while the peel presented 42.27 (±0.65) mg/g. On the other hand, at a temperature of 35°C, the maximum amount removed by the peel was 44.03 (±0.66) mg/g, while the endocarp reached 41.76 (±1.97) mg/g. Finally, the temperature of 45°C proved to be the most effective for the adsorption process, as the peel achieved a maximum Qt of 43.90 (±0.87) mg/g and the endocarp, 42.50 (±2.48) mg/g

After analyzing the results across all temperatures, it was found that the adsorption process proved more efficient at higher temperatures, achieving equilibrium faster. Additionally, the maximum adsorbed quantity varied little between 35 °C and 45 °C, demonstrating that temperature changes affect the speed of the adsorption process but not the maximum adsorbed quantity.

The equilibrium time is reached when the removal after that point does not vary significantly, meaning all sites have been occupied. Thus, within the studied range, no equilibrium time was observed at a temperature of 25°C, requiring a longer time. At 35°C, the equilibrium time was reached in 15 minutes for the peel and 20 minutes for the endocarp. At 45°C, the sites became saturated more quickly, being 10 minutes for the peel and 15 minutes for the endocarp.

Thus, the high efficacy of the process using natural bioadsorbents is evident, reducing costs for implementing the process at an industrial level, as no thermal treatment is required to achieve satisfactory results.

For future research, it is recommended to

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test the adsorption process with thermal treatment and at different pH ranges. Additionally, it is worthwhile to study adsorption in continuous operation mode using an adsorption column.

4. CONCLUSIONS:

The adsorption method using the natural peel and endocarp of pequi for the removal of methylene blue dye in an aqueous solution proved technically viable. Among the three temperatures studied, 45 °C was the most effective, adsorbing the largest amount (87,97 % for peel and 85,16% for endocarp). Therefore, it can be concluded that the process at 25 °C is not spontaneous. In this context, the use of biomass as an adsorbent is considered viable, as it is cost-effective and abundant compared to other synthetic materials.

5. DECLARATIONS

5.1. Acknowledgements

Acknowledgments to FAPERJ for the scientific initiation scholarship and financial support.

CAPES for financial assistance, funding code 001.

CNPq for the post-doctoral scholarship.

5.2. Open Access

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Southern Science Conference, 2024.

STUDY OF THE ADSORPTION POTENTIAL OF NATURAL PEQUI PEEL AND ENDOCARP (*Caryocar Brasiliense*) FOR METHYLENE BLUE

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October/2024

INTRODUCTION

In this study, the adsorption process was investigated using the raw peel and endocarp of *pequi* (*Caryocar brasiliense*) as adsorbent, with the objectives of:

•Promoting an understanding of the adsorption process as a method for treating aqueous effluents produced by the textile industry;

•Encouraging the use of natural adsorbents that are low-cost, highly available, operationally simple, and sustainable;

•Studying the influence of contact time on the adsorption process;

•Examining the adsorption behavior using *pequi* endocarp and peel at different temperatures;

•Enabling the treatment of aqueous effluents through adsorption."

BACKGROUND

- Melo et al. (2023) achieved a removal of 22.32 mg/g using raw *pequi*, while the experiment with thermal treatment achieved 500 mg/g.
- Melo et al. (2022) achieved a maximum removal of 7.78 mg/g using the raw endocarp and 476.19 mg/g with the calcined endocarp."

AIM/OBJETIVE/PURPOSE

Promote the adsorption process to treat aqueous effluents in a sustainable way

METHODOLOGY

- **Raw material pre-treatment**
  - Grinding and drying of the pequi peel and endocarp;
  - Selection of the particle size range at 42 mesh;

- **Sample analysis before and after adsorption**
  - Construction of the methylene blue calibration curve

- **Experimental Procedure**
  - 0,05 g of adsorbent mass in 25 mL of aqueous methylene blue solution at 100 mg/L;
  - Strirring at 360 rpm in a shaker at different times and temperatures
  - Filtration
  - Solution analysis after adsorption.

METHODOLOGY

Figure 1. Pequi fruit without peel.



Source: Adapted from Google Images (2007)

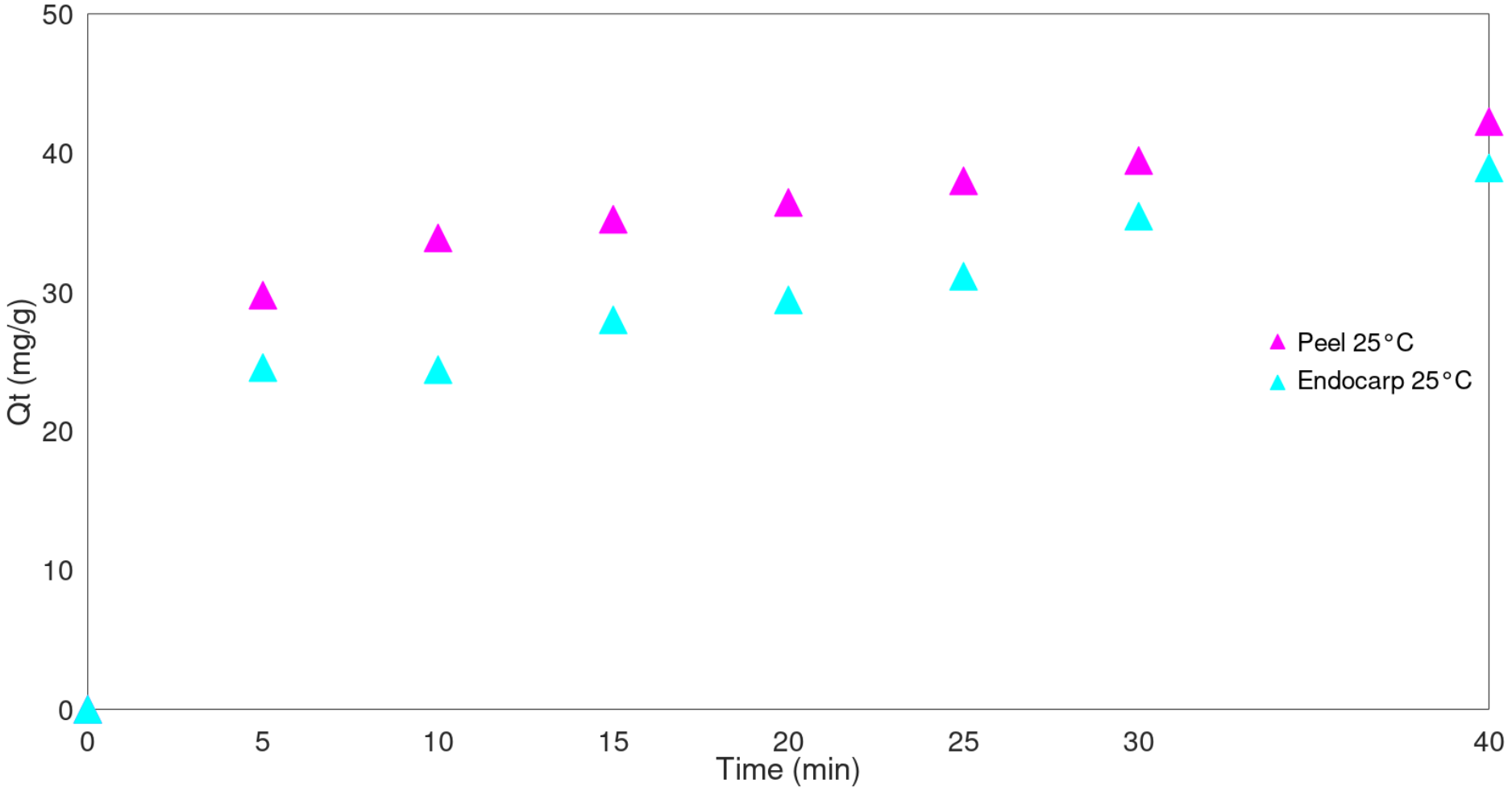
Figure 2. Ground and dried pequi endocarp



Source: the author (2024).

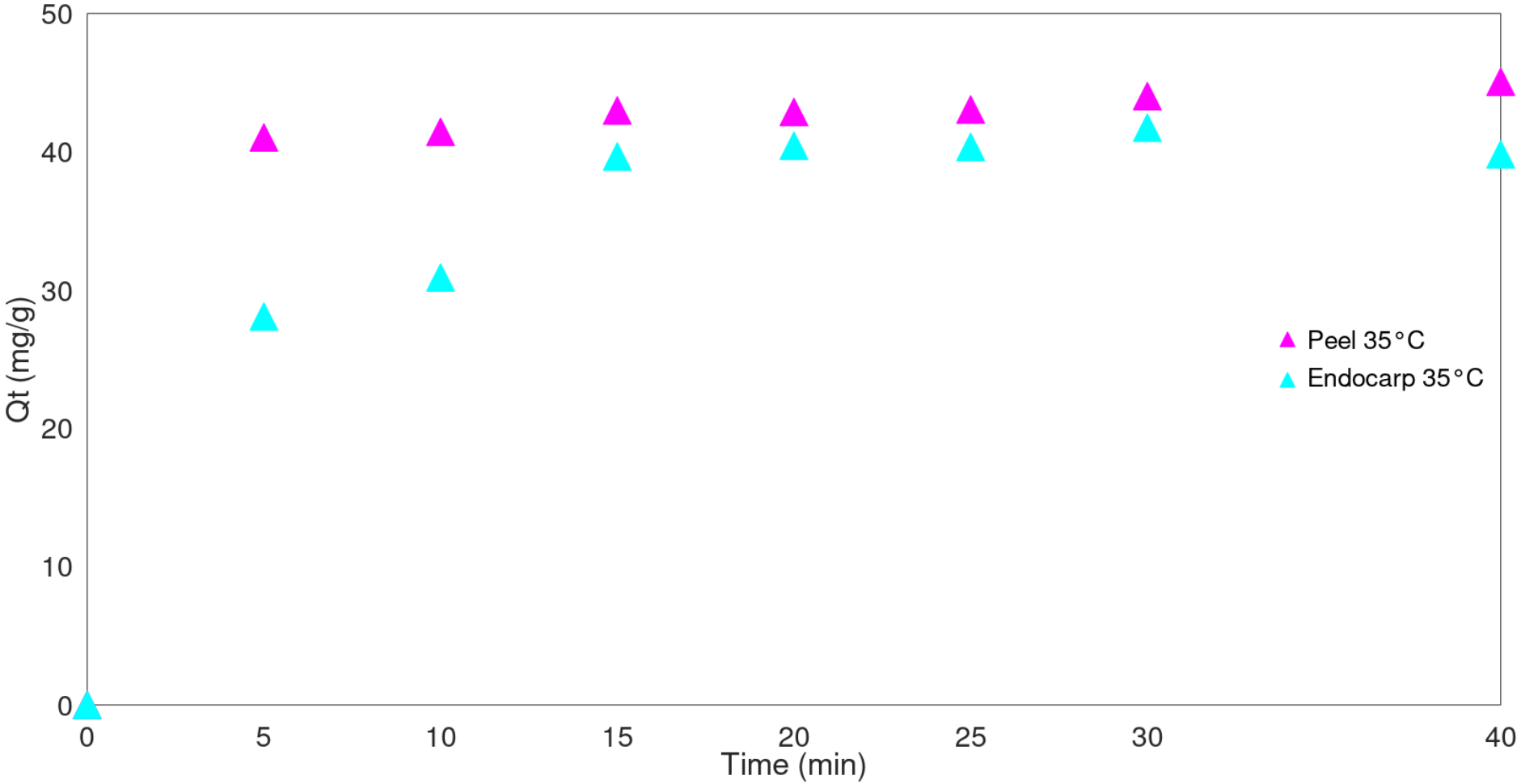
RESULTS AND DISCUSSION

Figure 3. Effect of temperature on adsorbed quantity as a function of time using the natural endocarp and peel of pequi at 25 °C.



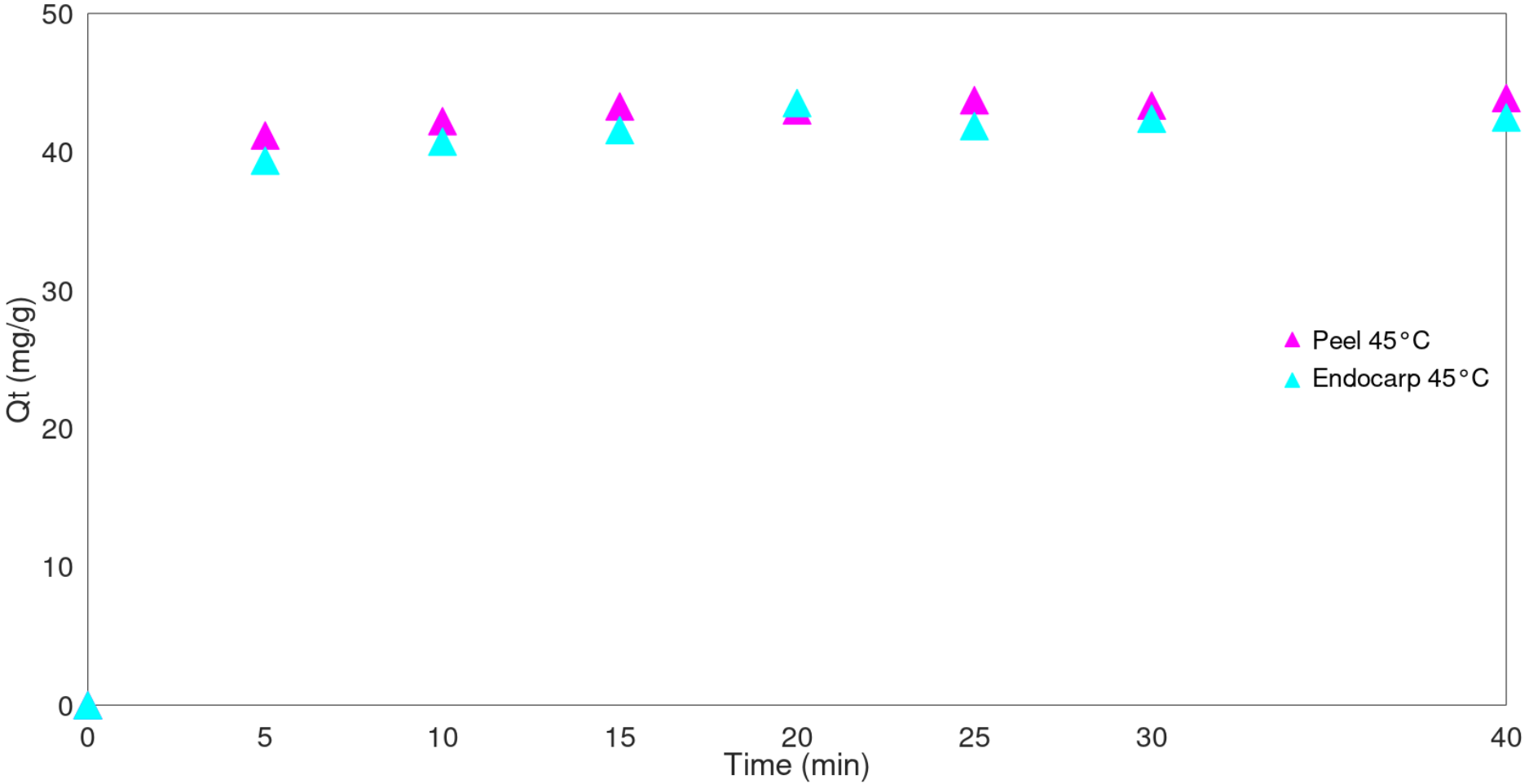
RESULTS AND DISCUSSION

Figure 4. Effect of temperature on adsorbed quantity as a function of time using the natural endocarp and peel of pequi at 35 °C.



RESULTS AND DISCUSSION

Figure 5. Effect of temperature on adsorbed quantity as a function of time using the natural endocarp and peel of pequi at 45 °C.



CONCLUSIONS

- The adsorption process was better at 45°C.

- The raw pequi bioadsorbent proved effective, achieving a removal potential of approximately 85% for the endocarp and 90% for the peel.

- The equilibrium time at 35 and 45°C was approximately 10 minutes. No equilibrium time was observed at 25°C.

- The method proved to be effective and promising.

ACKNOWLEDGEMENTS

•Acknowledgments to FAPERJ for the scientific initiation scholarship and financial support .

•CAPES for financial assistance, funding code 001.

•CNPq for the post-doctoral scholarship

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NEUROMODULATORY EFFECTS OF ESTRADIOL AND PROGESTERONE ON KETAMINE'S ACTION IN FEMALE RAT BRAIN

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ABSTRACT

Ketamine-induced psychotic episodes with hallucinations and sensory dissociation when abused. In rats, prolonged intraperitoneal ketamine (K) administration increases locomotor activity. Neuroactive steroids modulate responses to such drugs. This study aimed to investigate ketamine-induced neuroadaptive effects and neuromodulatory phenomena from Estradiol (E2) and Progesterone (P4) in female rats. Female rat ovariectomies (OVX) were performed, followed by open field behavioral tests to assess locomotor activity (LA), which were analyzed using the EthoWatcher software. Significant LA increases were observed in control EP and K groups vs. C. E2 and P4 further raised LA in sensitized OVX animals. The results demonstrate that E2 and P4 supplementation enhances potentiation, indicating genomic and non-genomic interactions, leading to positive neuroadaptive plasticity with K.

Keywords: *ketamine (K), neuroprotection, estradiol (E2), progesterone (P4).*

1. INTRODUCTION

Ketamine (K) is an anesthetic drug that, when abused by humans, induces psychotic episodes marked by hallucinations, sensory dissociation, and delusional thinking. In rats, prolonged intraperitoneal (i.p.) administration of ketamine causes psychotomimetic behaviors and adaptive changes in the Central Nervous System, often reflected by increased locomotor activity. This sensitization process modifies neuronal networks involving dopamine, glutamate, and GABA in the mesocorticolimbic pathway. Our laboratory has demonstrated that neuroactive steroids play a neuromodulatory role in the differential response to drugs.

The aim of this work is to study the neuroadaptive effects induced by ketamine and the neuromodulatory actions of subcutaneous (s.c.) administration of Estradiol (E2) and Progesterone (P4) in female rats.

2. MATERIALS AND METHODS

2.1. Materials

Ovariectomized (O) female Sprague-Dawley rats were used. Drugs like ketamine (K), estradiol (E), and progesterone (P) were administered. The groups were: Ovariectomized: Control OVX (CO), Control Estradiol Progesterone OVX (CEPO), Ketamine OVX (KO), Ketamine Estradiol Progesterone OVX (KEPO). No ovariectomized: Control (C), Control Estradiol Progesterone (CEP), Ketamine (K), Ketamine Estradiol Progesterone (KEP). Behavioral tests were conducted in open field, and the video data were processed using EthoWatcher software.

2.2. Methods

Female rats, aged 60 days, were subjected to ovariectomy. A 5-day period of K (25mg/kg) addiction was induced. An abstinence period followed. On day 88, E2 (4mg/kg) and P4 (0.1mg/kg) were administered, and open-field behavioral tests were conducted on day 90. The resulting behavioral data were analyzed using EthoWatcher software.

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3. RESULTS AND DISCUSSION:

3.1. Results

We observed a significant increase in LA in the CEP group compared to the C group ($p<0.0001$). Similarly, the K group exhibited significantly higher LA compared to the C group ($p<0.0001$). Administration of E2 and P4 to ketamine-sensitized animals resulted in increased LA compared to the C group ($p<0.0001$). Sensitized OVX animals treated with E2 and P4 also showed significantly increased LA compared to the C group ($p<0.0001$). However, steroid supplementation significantly increased LA in the KEPO group compared to the KO group ($p<0.0001$). Furthermore, the KEPO group exhibited significantly higher LA compared to the KEP group.

3.2. Discussion

Our results indicate that E2 and P4 significantly potentiate the effects of K on LA in female rats. This synergy suggests that neurosteroids modulate the neuronal response to ketamine, possibly through the interaction with key neurotransmitter receptors. These findings highlight the importance of considering the role of sex hormones in the effects of drugs and open new avenues for investigating the treatment of ketamine-related disorders.

4. CONCLUSIONS:

Supplementation with E2 and P4 amplifies this potentiation, suggesting a significant interaction through both genomic and non-genomic mechanisms, indicating positive neuroadaptive plasticity in response to ketamine-induced changes.

5. DECLARATIONS

5.1. Acknowledgements

I would like to express my sincere gratitude to INBIOMED and the University of Mendoza for the invaluable support provided during our research. The opportunity to work in such an excellent academic environment has been an enriching experience.

5.2. Open Access

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Southern Science Conference, 2024.

NEUROMODULATORY EFFECTS OF ESTRADIOL AND PROGESTERONE ON KETAMINE'S ACTION IN FEMALE RAT BRAIN

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November/2024



INTRODUCTION

- **Ketamine**: An anesthetic that induces **psychotic episodes** in humans when abused (hallucinations, dissociation, delusions).
- In rats, **prolonged i.p. ketamine** leads to **psychotomimetic behaviors** and **CNS changes** (increased locomotion).
- **Neuronal networks** in the **mesocorticolimbic pathway** involving dopamine, glutamate, and GABA are affected by this sensitization.
- **Neuroactive steroids** (e.g., estradiol and progesterone) play a **neuromodulatory role** in response to drugs.
- Study focus: **Neuroadaptation** from ketamine, alongside **E2 and P4 neuromodulation** in female rats.

AIM/OBJETIVE/PURPOSE

Ketamine-induced neuroadaptation and the

neuromodulatory effects of E2 and P4 in female rats



METHODOLOGY

2.1. Materials

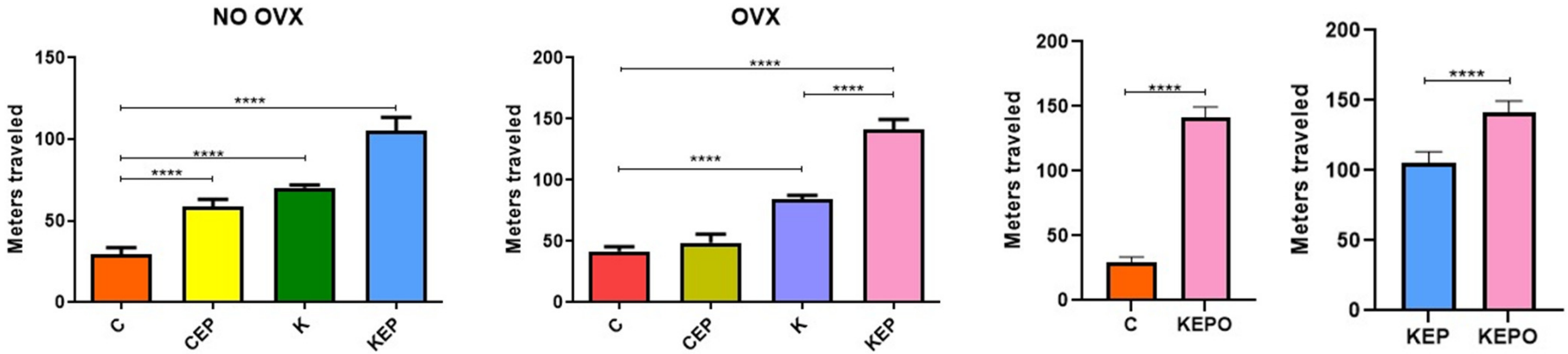
- Ovariectomized(OVX) female Sprague-Dawley rats were used.
- Drugs like ketamine(K), estradiol(E), and progesterone(P) were administered.
- The groups were:
  - OVX: Control(CO), Control EP(CEPO), Ketamine(KO), Ketamine EP(KEPO).
  - No OVX: Control (C), Control EP (CEP), Ketamine(K), Ketamine EP(KEP).
- Behavioral tests were conducted in open field, and the video data were processed using EthoWatcher software.

2.2. Methods

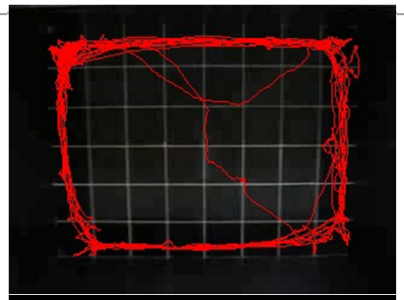
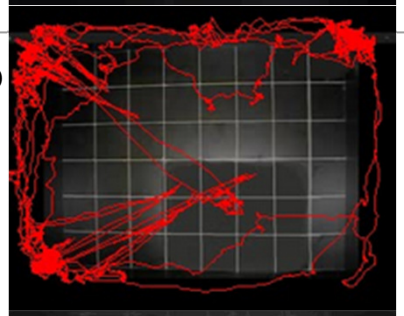
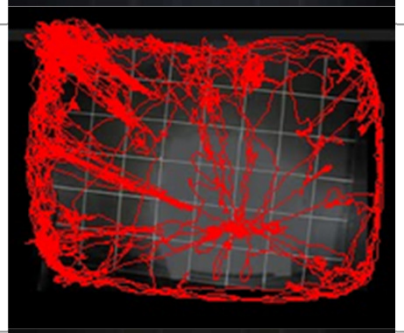
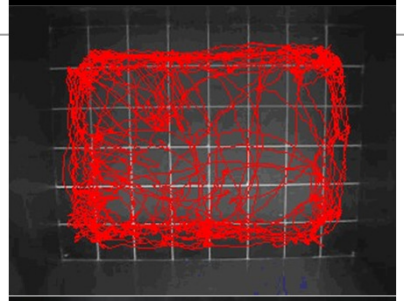
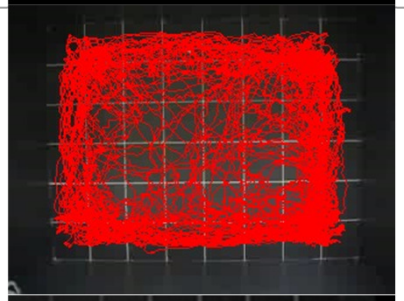
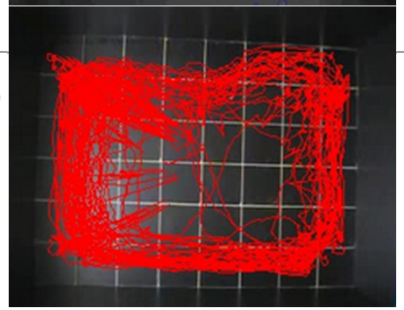
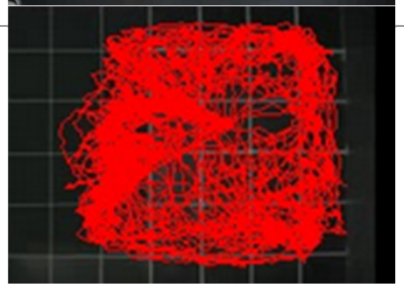
Female rat ovariectomices were performed, followed by open field behavioral tests, which were analyzed using the EthoWatcher software.

RESULTS AND DISCUSSION

- **CEP group**: Significant increase in locomotor activity (LA) compared to control (C) group ($P<0.0001$).
- **K group**: Significant LA increase compared to C group ($P<0.0001$).
- **E2 + P4 in ketamine-sensitized animals**: Increase in LA compared to C ($P<0.0001$).
- **Sensitized OVX animals with E2 + P4**: Significant LA rise compared to C ($P<0.0001$).
- **KEPO group vs. KO**: Steroid supplementation led to a significant LA increase ($P<0.0001$).
- **KEPO vs. KEP**: Significant LA difference observed.



RESULTS AND DISCUSSION

	NO OVX		OVX
C group		C group	
CEP group		CEP group	
K group		K group	
KEP group		KEP group	

CONCLUSIONS

- **E2 + P4 supplementation**: Enhances the potentiation effect.
- **Mechanisms**: Involves both **genomic and non-genomic** pathways.
- **Implication**: Suggests **positive neuroadaptive plasticity** in response to ketamine-induced neural changes.

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POTENTIAL USE OF THE STERILE FROM IPUEIRA MINE, BAHIA, BRAZIL, AS A CORRECTIVE ACID SOIL

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*** In Memoriam*

ABSTRACT

The use of corrective soil agriculture has a significant impact on agricultural productivity, whether by correcting acidity or by providing calcium and magnesium. Rocks for crops are a soil remineralization technique that involves adding rock powder to the soil to promote acidity correction and increase fertilization. The beneficial effects of using this technique have expanded the potential use of rocks as corrective soil and added value to alternative input sources. In this context, the objective of this study was to evaluate the waste rock from the Ipueira Mine, Bahia, Brazil, for use in agriculture as a soil amendment for acidic soils, according to the characteristics specified by the regulations of the Ministry of Agriculture and Livestock. The characteristics of the rock were evaluated in terms of reactivity (RE), neutralization power (PN), total neutralization relative power (PRNT), and calcium and magnesium contents as their respective oxides. The analysis of the results showed that the waste rock from the Ipueira Mine meets the limits specified by the current regulations for acidity correctives, with 57% PRNT, and that particles with sizes smaller than 0.30 mm present a reduction in CaO content and an increase in MgO content, compared to the other granulometric fractions. Thus, given the results obtained, it is possible to state that the waste rock from the Ipueira mine has the potential for application in agriculture as a corrective for acidic soils, which makes the study of this rock a contribution to the growth of sustainable agriculture in the country.

Keywords: *Serpentine marble. Rocks for crops. Neutralization power. Sustainable agriculture*.

1. INTRODUCTION

Soil acidity is related to a combination of factors that occur due to its own nature and/or its continuous use. To achieve efficiency in the productive capacity of plants, it is necessary to neutralize soil acidity. The use of rock powder in agriculture is called rocks for crops or remineralization and consists of adding rock powder to the soil to promote acidity correction and increase soil fertilization. The use of silicate rocks to correct soil acidity also reveals positive effects as an alternative source, with the release of silicon to plants that accumulate this element (Filho *et al.*, 2004; Korndörfer *et al.*, 2003; Martins *et al.*, 2005; Viana *et al.*, 2024; Silverol and Filho, 2007). The use of these new mineral inputs in agriculture, in addition to corrected soil acidity, contributes to the replacement of nutrients, which reduces the consumption of industrial fertilizers. Thus, the beneficial effects on soil fertility and plant nutrition can increase the potential for using rocks as a corrective soil and, in this way, add value to these new sources of alternative inputs due to their multi-nutrient and soil conditioning effect (Silverol and Filho, 2007).

In Brazil, the Normative Instruction of July 4th, 2006, establishes standards to be followed regarding the definition, specification, analytical methods, and marketing of acidity, alkalinity, and sodicity correctors, as well as soil conditioners intended for agriculture (Brazil, 2006). This Normative Instruction defines acidity correctors as

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the product that promotes the correction of soil acidity, in addition to providing calcium and/or magnesium. The standard establishes, according to the characteristics of each material, the specifications for acidity correctors regarding neutralization power (PN), the sum of the percentages of calcium and magnesium oxides (CaO+MgO), and the Total Neutralization Relative Power (PRNT).

The rock under study is sterile from the Ipueira Mine, belonging to the FERBASA group, located in Andorinha City, Bahia, Brazil. This rock is mined and accumulated in yards, with no defined application, since it is not used as raw ore and/or has no economic interest. However, this rock has aroused interest for its use in agriculture as a corrective for acidic soils since its composition is mainly formed by dolomite [$CaMg(CO_3)_2$], calcite ($CaCO_3$), diopside ($CaMgSi_2O_6$), muscovite [$KAl_2Si_3AlO_{10}(OH,F)_2$] and antigorite [$(Mg, Fe)_3Si_2O_5(OH)_4$], indicating that mineralogical changes occurred in the composition of the rock, preserving antigorite as the original mineralogical compound (Blaskoski *et al.*, 2019; Carmignano, 2020; Teixeira *et al.*, 2010; Viana *et al.*, 2024). In the study of the classification of the rock according to environmental risk, because the waste comes from a chromite mine, it was found that in granulometry below 2 mm, it is an inert residue and does not present amounts of chromium above the limits established by legislation (Andrade and Abreu, 2006; Apolaro *et al.*, 2011; Brazil, 2009; Carmignano, 2020; Marchi *et al.*, 2009; Teixeira *et al.*, 2012). In this context, the study aimed to evaluate the waste rock from the Ipueira Mine, Bahia, Brazil, for use in agriculture as a corrective for acidic soils, according to the characteristics specified by Brazilian legislation.

2. MATERIALS AND METHODS

The rock was subjected to the crushing, grinding, and homogenization stages to obtain the final sample with a granulometry suitable for testing, according to the standard procedure developed at the Mineral Technology Center (CETEM) (Oliveira and Aquino, 2007). Afterward, the chemical and physical characteristics of the rock were evaluated according to the normative instruction of the Ministry of Agriculture and Livestock for acidity corrector (Brazil, 2006). To this end, it was necessary to comminute the rock to a granulometry of less than 2 mm to adapt it to the granulometric limits established by the normative instruction.

The characterization of the rock as a soil corrective was carried out according to the procedures described in the Manual of Official Analytical Methods of the Ministry of Agriculture and Livestock (Brazil, 2023). The moisture content of the material was determined at 100 ºC until constant mass. RE was determined by performing the rock granulometric distribution using sieves 2.00, 0.84, and 0.30 mm. PN was defined by alkalimetry and is expressed in pure calcium carbonate equivalent (% E_{CaCO3}). PRNT was calculated by correlating RE and PN of the soil amendment. The calcium and magnesium contents in the rock were determined by inductively coupled plasma optical emission spectrophotometry (ICP-OES), and the values converted to the respective oxides (CaO and MgO), to sum the percentages of these oxides, as specified in Normative Instruction No. 35 of July 4th, 2006, of the Ministry of Agriculture and Livestock (Brazil, 2006). Furthermore, to verify differences in mineralogical characteristics, the rock fractions were also evaluated according to Ca and Mg contents, as well as PN.

3. RESULTS AND DISCUSSION:

The data on the characterization of the rock under study as a soil corrective are recorded in Table 1, and were compared with the minimum specification established by the current Normative Instruction.

Table 1. *Characterization of serpentinite marble as a corrective soil.*

Parameters	Serpentine marble (%)	Technical specification (%)
RE	71.9	-
PN (%E_{CaCO3})	79.3	67.0
CaO + MgO	37.8	38.0
PRNT	57.0	45.0
Humidity (100 °C)	0.38	-
Passant (%)		
2.00 mm	100.0	95.0
0.84 mm	77.0	66.5
0.30 mm	52.7	47.5

The results obtained in the granulometric distribution of the serpentine marble meet the tolerance limits of the guarantees for acidity correctives, according to the current Normative Instruction (Brazil, 2006), showing that it is possible to adapt the rocks particle size. The granulometric distribution showed proportional behavior for the rock with particle size below 4.7

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mm (Teixeira *et al.*, 2010). The granulometric distribution results were also used to calculate the reactivity of the material, which corresponds to the percentage of the corrective that reacts in the soil in a period of 3 months (Brazil, 2023). Thus, the finer the material, the greater the contact area with the soil and the faster its neutralizing action, favoring the solubility of the acidity corrector, this measurement being essentially dependent on the size of the particles.

The PN indicates the total capacity of the neutralizing bases contained in the acidity corrector, and for the rock under study, a value of 79.3% E_{CaCO3} is higher than the minimum specification for soil correctives. The same fact occurred for the analysis of the rock fractions, presenting relatively close PN values, Table 2. Analyzing $\%E_{CaCO3}$ converted to carbonate, 47.6%, a value higher than that determined by ATG, 40%, is verified for the same material (Teixeira *et al*., 2010), suggesting the neutralizing effect of other basic forms present in the rock composition, such as diopside ($CaMgSi_2O_6$), muscovite [$KAl_2Si_3AlO_{10}(OH,F)_2$] and antigorite [$(Mg,Fe)_3Si_2O_5(OH)_4$].

Table 2. *Fractions characterization parameters.*

Granulometric fraction (mm)	Weight (% w/w)	CaO + MgO (%)	PN (%)
- 2.00 + 0.84	23.0	41.7	84.4
- 0.84 + 0.30	24.3	39.1	78.8
- 0.30	52.7	38.6	84.3

It is worth noting that during the determination of PN, both in the analysis of the overall sample and of the fractions, the formation of colloids was observed, which hindered the identification of the endpoint of the titration since the titrate was cloudy. Thus, the volumes of the titrant (NaOH) used in the sample titrations were uncertain, which generated uncertain or less accurate results. These facts reveal that the characterization of these rocks by classical methods may not be adequate (Alcarde and Rodella, 1996; Alcarde, 2005), since hydrochloric acid is also consumed by the dissolution of part of the silicates, which may, in principle, result in overestimated PN values (Martins *et al.*, 2000).

In relation to PRNT, the rock under study presented 57% and, considering the classification of agricultural limestones sold in Brazil, it can be classified as group A, with PRNT between 45 and 60%, as well as magnesian limestone, since the MgO content is between 5 and 12% of this oxide (Kappes, 2008). It is worth noting that, although the water solubility of $CaCO_3$ (25 °C, 0.014 $g.L^{-1}$) is lower than that of $MgCO_3$ (25 °C, 0.106 $g.L^{-1}$), dolomitic limestones, despite having greater neutralization power, react more slowly with acidic soils than calcitic limestones, which demonstrates a different behavior between pure salts and the minerals that contain these carbonates (Alcarde and Rodella, 1996; Apollaro *et al.*, 2012; Holzschuh, 2007; Viana *et al.*, 2024), which may be interesting for the application of this material for long-term crops.

The results obtained for the CaO and MgO contents were 28.1% and 9.7%, respectively, for the sample evaluated as a soil amendment. These results were obtained according to the procedure described in the official analytical method (Brazil, 2023), which is different from the analytical method used to determine the total CaO and MgO contents contained in the rock. The analytical methods differ in the reagents used and the sample digestion time. The official analytical method (Brazil, 2023) describes a specific procedure for calcium or magnesium carbonates. Therefore, the difference between the results obtained by the official analytical method and the method for the total determination of CaO and MgO contents can be explained by the existence of these cations (Ca^{2+} and Mg^{2+}) in the minerals diopside, antigorite, and muscovite, which are part of the composition of the rock under study, but are associated with other types of neutralizing bases (Alcarde and Rodella, 1996; Blaskoski *et al.*, 2019; Carmignano, 2020; Teixeira *et al.*, 2010).

The analysis of the results of the rock fractions indicates that the finest part of the material, with particle size below 0.30 mm, has a lower CaO content and a higher MgO content. In general, it is observed that the CaO content decreases, and the MgO content increases for the finest fractions. Figure 1 illustrates the distributions of CaO and MgO in the fractions obtained from the correlation between the content of these oxides in the fractions in relation to the overall sample. It was found that the finest fraction, particles below 0.30 mm, has the largest part of CaO and MgO, approximately 47% and 67%, respectively.

The analysis of the characterization of the rock distribution fractions and the results for the evaluation of the rock as an acidity corrective show that the characteristics obtained for the rock correspond to the reference indexes defined by the regulations (Brazil, 2006), for other acidity correctives, as well as for agricultural limestone.

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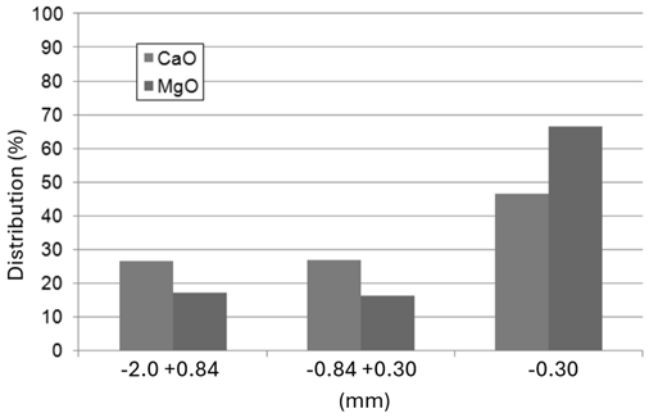


Figure 1. *Distributions of CaO and MgO contained in the serpentine marble fractions.*

4. CONCLUSIONS:

The characteristics of the rock, when evaluated as acidity correctives, meet the limits specified by the current Normative Instruction of the Ministry of Agriculture and Livestock, with 57% PRNT. Furthermore, the finest fraction of the material, with a particle size smaller than 0.30 mm, presents a reduction in CaO and an increase in MgO. In view of the results obtained, it is possible to state that the waste rock from the Ipueira Mine has the potential for application in agriculture as a corrective for acidic soils, which makes the study of this rock a contribution to the growth of sustainable agriculture in the country. This indicator even allows for the full use of the chromite mine in Andorinha City, Bahia, Brazil, at a reduced cost since the processing of the rock for use in agriculture consists only of grinding and screening the rock. However, additional tests are necessary to evaluate its solubility, as well as its residual effect on crops.

5. DECLARATIONS

5.1. Acknowledgements

Thanks to CETEM/MCTI for analysis and mineral processing and FERBASA S.A. for providing the rock sample.

5.2. Open Access

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POTENTIAL USE OF THE STERILE FROM IPUEIRA MINE, BAHIA, BRAZIL, AS A CORRECTIVE ACID SOIL

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INTRODUCTION

The use of the corrective soil in agriculture has a significant impact on agricultural productivity, whether by correcting acidity or by providing calcium and magnesium.

Rocks for crops is a soil remineralization technique by adding rock powder to the soil to promote acidity correction and increase fertilization.

The beneficial effects of using this technique have expanded the potential use of rocks as a corrective soil and added value to alternative input sources, one example is silicate rocks.

BACKGROUND

Positive effects the use of rocks for crops in the agriculture:

- increase in rice production due to the application of silicate slag;
- increased the availability of exchangeable silicon, phosphorus and calcium to the crop;
- replacement of nutrients and reduce the consumption of industrial fertilizers;
- add value to new sources of alternative inputs, due to their multinutrient and soil conditioning effect.

Serpentinite Marble

Is the sterile rock from Mine
Is mined and accumulated in yards, with no defined application



Composition mainly:

- dolomite [$CaMg(CO_3)_2$]
- calcite ($CaCO_3$)
- diopside ($CaMgSi_2O_6$)
- muscovite [$KAl_2Si_3AlO_{10}(OH,F)_2$]
- antigorite [$(Mg,Fe)_3Si_2O_5(OH)_4$]

Classification according to environmental risk: it is an inert residue and does not present amounts of chromium above the limits established by Brazilian legislation

OBJETIVE

Evaluate the waste rock from the Ipueira Mine, Bahia, Brazil, for use in agriculture as a corrective for acidic soils, according to the characteristics specified by the regulations of Brazilian legislation.

METHODOLOGY

Rock beneficiation: crushing and grinding to obtain material with granulometry suitable, below 2.00 mm.

Characterization parameters as a corrective soil according Brazilian legislation:

- **Humidity** at 100ºC, until constant mass.
- **Reactivity** (RE) – its determined by performing the rock granulometric distribution using sieves 2.00, 0.84 and 0.30 mm.
- **Neutralization power** (PN) - alkalimetry titration

  expressed in carbonate equivalent (% E_{CaCO3})
- **Relative Power Total Neutralization** (PRNT) - by correlating RE and PN
- **Calcium and magnesium contents** – obtained by inductively coupled plasma optical emission spectrophotometry (ICP-OES)

- Fraction analysis - Ca and Mg contents, as well as PN.

RESULTS AND DISCUSSION

the serpentine marble meet the tolerance limits of the guarantees for acidity correctives both for particle size distribution and for other parameters (RE, PN, PRNT and Cao+MgO)

Table 1. *Granulometric distribution.*

Sieve opening (mm)	Passant (%)	Technical specification (%) minimum
2.00	100.0	95.0
0.84	77.0	66.5
0.30	52.7	47.5

Table 2. *Characterization parameter as a corrective soil.*

Parameters	Serpentine marble (%)	Technical specification (%)
RE	71.9	-
PN (%E_{CaCO3})	79.3	67.0
CaO + MgO	37.8	38.0
PRNT	57.0	45.0
Humidity (100 °C)	0.38	-

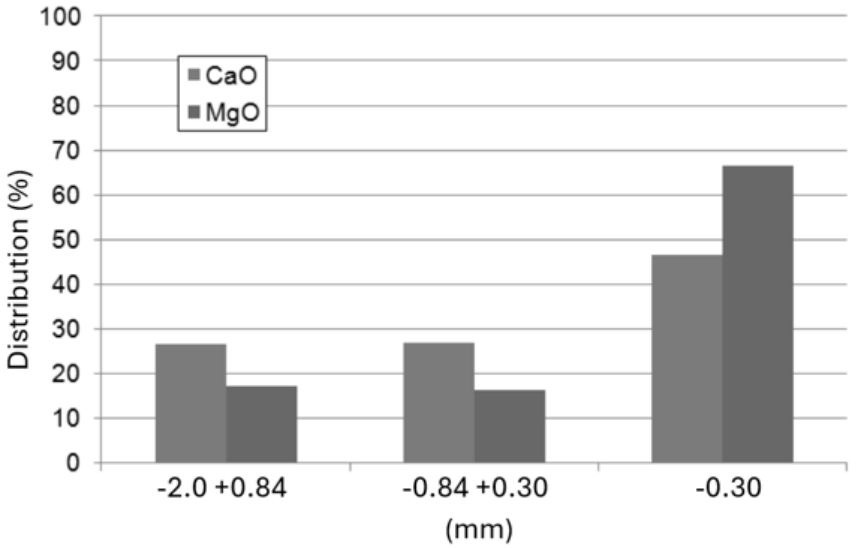
RESULTS AND DISCUSSION

The PN indicates the total capacity of the neutralizing bases contained in the acidity corrective and for the rock under study a value of 79.3% E_{CaCO3}, higher than the minimum specification for soil correctives.

Results of the rock fractions indicates that particle size below 0.30 mm, has a lower CaO content and a higher MgO content. In general, it is observed that the CaO content decreases and the MgO content increases for the finest fractions, approximately 47 and 67% respectively.

Table 3. *Fractions characterization parameters.*

Granulometric fraction (mm)	Weight (% w/w)	CaO + MgO (%)	PN (%)
- 2.00 + 0.84	23.0	41.7	84.4
- 0.84 + 0.30	24.3	39.1	78.8
- 0.30	52.7	38.6	84.3
Global sample	-	37.8	79.3



CONCLUSIONS

- The characteristics of the rock, when evaluated as acidity correctives, meet the limits specified by the current Normative Instruction of the Ministry of Agriculture and Livestock, with 57% PRNT.

- The finest fraction of the material, with a particle size smaller than 0.30 mm, presents a reduction in CaO and an increase in MgO.

In view of the results obtained, it is possible to state that the waste rock from the Ipueira Mine has potential for application in agriculture as a corrective for acidic soils, which makes the study of this rock a contribution to the growth of sustainable agriculture in the country.

This indicator even allows for the full use of the chromite mine in the Andorinha City, Bahia, Brazil, at a reduced cost, since the processing of the rock for use in agriculture consists only of grinding and screening the rock.

However, additional tests are necessary to evaluate its solubility, as well as its residual effect on crops

ACKNOWLEDGEMENTS

Thanks to Mineral Analysis Coordination and Mineral Processing Coordination at CETEM/MCTI

Thanks to FERBASA S.A. for providing the rock sample.

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II SOUTHERN SCIENCE CONFERENCE
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COMPUTATIONAL THINKING AND SCIENCE VALUE: PREDICTORS OF SENIOR SCHOOL PHYSICS STUDENTS SCIENCE IDENTITY IN ILORIN, NIGERIA

.

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ABSTRACT

Knowledge acquisition and positive learning outcomes serve as the major output of teaching-learning activities. To be able to think differently, independently, and creatively in nature for the decision-making process constitutes what is called computational thinking. The present study searched the senior school students' science value as a mediating variable between computational thinking and science identity. Computational thinking as a multi-dimensional construct consists of creativity, algorithmic thinking, cooperativity, critical thinking, and problem-solving skills, as theorized in previous literature. The structural equation model approach was employed to analyze the collected data from 243 physics students. The findings of the study revealed that computational thinking dimensions had a weak and non-significant relationship with students' science identity ($p>.05$, $t<1.96$). The study further revealed that the science value held by students does not significantly mediate the relationship between computational thinking dimensions and science identity. The study concluded that computational thinking does not portray students as being scientists. It is recommended to work on other determinant variables so as to determine the factors responsible for students science identity.

Keywords:*Science Identity, Science Value, Computational Thinking, Physics Student*

1. INTRODUCTION

The student computational thinking skill is an essential component of knowledge acquisition, problem-solving approach, decision-making, and logical reasoning. Angeli and Giannakos (2020) asserted that students' knowledge development, computational solutions to problems, algorithmic thinking, coding, abstract thinking development, problem-solving approach, pattern recognition, and logical reasoning are the main focuses of student computational thinking. Wing (2008) asserted that computational thinking is a factor that influences every field of endeavor and poses a new challenge in education.

Cheng *et al.* (2022) posited that computational thinking integration in science, technology, engineering, and mathematics has a large effect size on students' STEM learning outcomes. Computational thinking integration into high school biology units leads to both science and computational learning, improves thinking performance, enhances students' understanding of complex systems, and supports data gathering and analysis activities (Irgens et al., 2020 & Waterman et al., 2019). Li et al. (2020) posited that computational thinking is an important model of thinking in computer science, mathematics, and other STEM disciplines. Winthrop et al. (2016) believe that mathematics and science computational thinking involves data, simulation and modeling, problem-solving, and system thinking practices.

Ogegbo and Ramnarain (2021) view computational thinking as an essential part for teaching and learning science subjects at both elementary and high school levels. Korkmaz et al. (2017) theorized that computational thinking is a multi-faceted and multi-dimensional variable that includes creativity, algorithmic thinking,

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cooperativity, critical thinking, and problem-solving skills.

Hypotheses:

HO_1: Creativity, Algorithmic thinking, Cooperativity, Critical Thinking Skills, and Problem-solving Skills significantly predict students' science identity

HO_{2B}: Science Value significantly mediates the relationship between creativity, algorithmic thinking, cooperation, critical thinking skills, and problem-solving skills, significantly predicting students' science identity.

2. MATERIALS AND METHODS

This research was a correlational study of descriptive type that used a multivariate statistical technique to analyze the collected data. Senior school students who are currently in their ultimate year are the sample and were selected through a simple random technique. The analysis utilized 243 of the responses retrieved from the respondents. A general criterion for sample size selection is encouraged by multivariate methods like structural equation modeling.

3. RESULTS AND DISCUSSION

Table 1 describes the demographic profiles of the respondents. One hundred fourteen respondents, representing 46.9%, were female, while 129 respondents representing 53.1% were male.

Measures of Construct

This study determines the relationship between computational thinking' dimensions, science value, and science identity. The details of the constructs are described in Table 1 below. The items of the constructs were rated on 5 Likert scales. Table 2 shows constructs' description, item's code, and sources of the items.

Tabel 3 and 4 explains the divergent and convergent validities of the adopted items. Table 5 below explains the relationship that exists between computational thinking and students' science identity. The path coefficients in the table revealed that computational thinking dimensions had a weak and non-significant relationship with students' science identity ($p>.05$, $t<1.96$).

Table 6 below explains the mediating role of students' science value on the relationship that existed between computational thinking and students' science identity. The path coefficients in the table revealed that computational thinking dimensions had a weak and non-significant relationship with students' science identity when mediated by the science value held by students ($p>.05$, $t<1.96$).

Table 7 revealed that 14.7% of students' science identity was explained by computational thinking and science value.

4. CONCLUSIONS:

The study concluded that computational thinking does not portray students as being scientists.

5. DECLARATIONS

5.1. Acknowledgements

The sample students and schools where the data was collected were acknowledged.

5.2. Open Access

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Table 1: *Demographic Profile of the Respondents*

Gender		N	%
	Female	114	46.9
	Male	129	53.1
	Total	**243**	**100**

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Table 2: *Construct description, item's code, and source of the items' table*

Construct	Number of Items	Items code	Source of Instrument
Creativity	Seven	CRE1-CRE7	Korkmaz et al., (2017)
Algorithms Thinking	Six	ALG1-ALG6	Korkmaz et al., (2017)
Cooperativity	Four	Coop1-Coop4	Korkmaz et al., (2017)
Critical Thinking Skill	Five	CRI1-CRI5	Korkmaz et al., (2017)
Problem-Solving Skill	Six	PRB1-PRB6	Korkmaz et al., (2017)
Science Value	Two	SV1-SV2	Aghekyan (2019)
Science Identity	Seven	SI1-SI7	Aghekyan (2019)

Table 3:*FornellLarcker discriminant correlations of the constructs*

Construct	Algorithm Skill	Cooperativity	Creativity	CriticalThinking	Problem-Solving Skill	Science Identity	Science Value
Algorithm Skill							
Cooperativity	0.720						
Creativity	0.682	0.987					
Critical Thinking	1.027	0.749	0.863				
Problem-Solving Skill	0.587	0.494	0.525	0.482			
Science Identity	0.283	0.251	0.338	0.236	0.244		
Science Value	1.086	1.069	0.934	1.172	0.738	0.953	

Table 4: *Convergent Validity of the first-order constructs' measure*

Construct	Cronbach Alpha (CA)	Composite Reliability (CR	Average Variance Extracted (AVE)
Algorithm Skill	0.812	0.829	0.862
Cooperativity	0.757	0.818	0.838
Creativity	0.826	0.837	0.868
Critical Thinking	0.747	0.853	0.825
Problem Solving Skill	0.801	0.897	0.843
Science Identity	0.753	0.800	0.809
Science Value	0.154	-0.225	0.195

Table 5: Direct relationship results of computational thinking's dimensions and science identity

Path Relationship	Path Coeff. (β)	Coeff. Mean	Remark	t-value	p-value	Remark
Algorithm Skill -> Science Identity	0.075	0.059	Weak/Positive	1.635	0.102	HO_{1A} Not Significant
Cooperativity -> Science Identity	0.059	0.026	Weak/Positive	1.015	0.310	HO_{1B} Not Significant
Creativity -> Science Identity	0.012	0.029	Weak/Positive	0.420	0.675	HO_{1C} Not Significant
Critical Thinking -> Science Identity	0.081	0.063	Weak/Positive	1.395	0.163	HO_{1D} Not Significant
Problem Solving skill -> Science Identity	0.038	0.009	Weak/Positive	0.994	0.320	HO_{1E} Not Significant

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Table 6: Indirect relationship results of computational thinking's dimensions, science value, and science identity

Path Relationship	Path Coeff. (β)	Coeff. Mean	Remark	t-value	p-value	Remark
Problem Solving skill -> Science Value -> Science Identity	0.038	0.009	Weak/Positive	0.994	0.320	HO_{2A} Not Significant
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Table 7: Variance of students' science identity been predicted by computational thinking and science value

	R-Square	Adjusted R-Square
Science Identity	0.147	0.145

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Southern Science Conference, 2024.

Computational Thinking and Science Value: Predictors of Senior School Physics Students Science Identity in Ilorin, Nigeria

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November/2024

INTRODUCTION

- **Concept of Computational Thinking;**
- **Science Identity;**
- **Science Value;**
- **Structural Equation Model; and**
- **Justification for the study.**

  - Cheng et al. (2022);
  - Ogegbo and Ramnarain (2021);
  - Angeli and Giannakos (2020).

AIM/OBJETIVE/PURPOSE

The main aim of this study was to determine if computational thinking predicted the physics students' science identity.

Specifically;

1. The study determines the prediction of physics study identity through computational thinking dimensions;

2. The study determines the prediction of physics study identity through computational thinking dimensions when mediated by science value.

METHODOLOGY

This research was a co-relational study of descriptive type that used a multivariate statistical technique to analyzed the collect data. Senior school students who are currently in their ultimate year are the sample and were selected through simple random technique. The analysis utilized 243 of the responses retrieved from the respondents. A general criterion for sample size selection is encouraged by multivariate methods like structural equation modeling.
The table 1 described the demographic profiles of the respondents. 114 respondents representing 46.9% were female while 129 respondents representing 53.1% were male.

Construct description, item's code, and source of the items' table

Construct	Number of Items	Items code	Source of Instrument
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Cooperativity	Four	Coop1-Coop4	Korkmaz et al., (2017)
Critical Thinking Skill	Five	CRI1-CRI5	Korkmaz et al., (2017)
Problem-Solving Skill	Six	PRB1-PRB6	Korkmaz et al., (2017)
Science Value	Two	SV1-SV2	Aghekyan (2019)
Science Identity	Seven	SI1-SI7	Aghekyan (2019)

RESULTS AND DISCUSSION

Path Relationship	Path Coeff. (β)	Coeff. Mean	Remark	t-value	p-value	Remark
Algorithm Skill -> Science Identity	0.075	0.059	Weak/Positive	1.635	0.102	HO_{1A} Not Significant
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CONCLUSIONS

- Computational thinking dimensions' and science identity
- The mediating role of science value on the prediction of physics students' science identity by computational thinking

ACKNOWLEDGEMENTS

The sampled students and schools where the data was collected were acknowledged.

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II SOUTHERN SCIENCE CONFERENCE
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FLASH VACUUM PYROLYSIS (FVP) OF DIMETHYL 5-METHYL-3-PHENYL-1H,3H-PYRROLO[1,2-C]THIAZOLE-6,7-DICARBOXYLATE 2,2-DIOXIDE: KINETIC AND THERMAL PARAMETERS

VELAZCO MONTAGNA, Federico Juan[1,2]; CAMARGO SOLORZANO, Gloria Patricia[1,2]; SOARES, María Isabel[3]; PINHO E MELO, Teresa María V. D.[3] and PELÁEZ, Walter José[1,2*].

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ABSTRACT

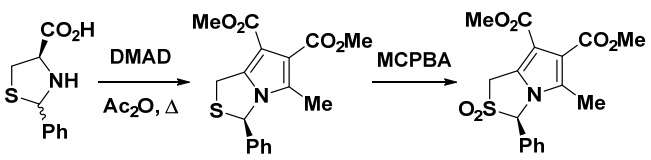
The generation through FVP and reactivity of an azafulvenium derived from thermal SO_2 extrusion of dimethyl 5-methyl-3-phenyl-1H,3H-pyrrolo[1,2-c]thiazole-6,7-dicarboxylate 2,2-dioxide (compound **1**) is described. Synthesis of **1** is briefly shown (Scheme 1, Sutcliffe *et al*., 2001). The intermediate azafulvenium was previously shown to be trapped by dipolarophiles, acting either as a 4π or 8π dipole (Pinho e Melo *et al*., 2004). A pyrolysis mechanism is proposed (Scheme 2). Three products were found, two of which were not previously reported (Scheme 3, **2***cis* and **3**). The characterization by NMR, UV-Vis, and GC-MS of the substrate and products was performed. Molar absorptivities from **1** are informed (Figure 1, Table 1), along with ^{1}H-NMR signals (Figure 2). Conditions of pyrolysis reactions are informed in Tables 2 and 3. These data allowed us to obtain the Arrhenius parameters corresponding to the reaction extrusion of SO_2 (Figure 3, Table 4). Besides, thermodynamic parameters from the equilibrium between both styrylpyrroles (**2***trans* and **2***cis*) obtained as main products are also reported for the very first time (Figure 4, Table 4).

Keywords: *Azafulvenium, Styryl pyrroles, Thermolysis, Arrhenius Parameters, SO_2 extrusion.*

1. INTRODUCTION

This research work addresses the spectroscopic, thermal, and kinetic characterization of dimethyl 5-methyl-3-phenyl-1H,3H-pyrrolo[1,2-c]thiazole-6,7-dicarboxylate 2,2-dioxide (Sutcliffe *et al.*, 2001); as well as the theoretical computations of kinetic parameters.

This compound was previously synthesized from the thiazolidine derived from L-cysteine, as shown in Scheme 1 (Pinho e Melo *et al.*, 2004).



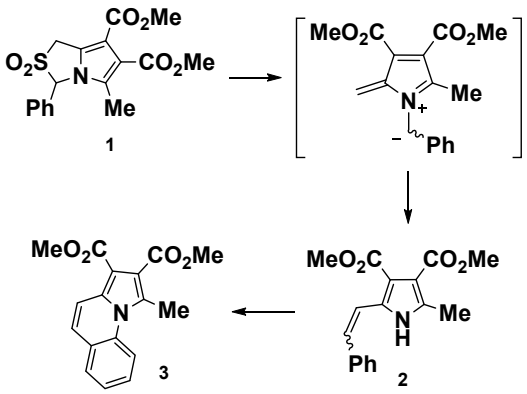
Scheme 1. *Synthesis of the studied compound.*

Heterocyclic ring systems like this are known to extrude SO_2 under different conditions by conventional heating in solution (reflux), under microwave irradiation, and in the gas phase. All of these techniques generate azafulvenes intermediates, which, in turn, produce new heterocyclic compounds with many synthetic and pharmaceutical properties (Soares *et al.*, 2015).

The azafulvene we studied consists of an extended dipolar system that experiences [1,8]H sigmatropic rearrangements, leading to the formation of vynylpyrroles (Scheme 2). It may as well be attacked by dipolarophiles in cycloaddition reactions [8π + 2π] to give 1,7-addition products.

In this work, we present, foremost, the characterization of the studied compound using the usual techniques (UV-Vis, NMR, GC-MS).

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***Scheme 2**. Proposed mechanism of pyrolysis-induced sulfur dioxide extrusion.*

In a second instance, we present the gas phase pyrolysis reactions carried out as part of the thermal and kinetic characterization.

2. MATERIALS AND METHODS

2.1 Physical and chemical characterization

2.1.1. UV-Vis

Stock solutions of the compounds to be analyzed were prepared by dissolving 5 mg in 25 mL of acetonitrile. In a quartz cell, 2 mL of acetonitrile was added, followed by 10 µL of stock solution with a final volume of 90 µL.

2.1.2. ^{1}H-NMR

NMR spectra were performed on a Bruker DRX 400 MHz spectrometer in 10 mM CDCl. Chemical shifts are expressed in relative ppm (δ) with TMS as an internal reference, and coupling constants J values are reported in Hz.

2.1.3. GC-MS

GC-MS chromatograms and patterns were performed using a Shimadzu GC-MS-QP 5050 with a SE-30 column, He as the elution gas at a flow rate of 1 mL/min, coupled to an EI mass spectrometer (70 eV). Injections were performed from stock solutions prepared in ethyl acetate at a sample concentration of 0.2 g/L.

2.1.4. Pyrolytic reactions

FVP reactions were carried out in a Vycor glass reactor using a tube furnace with a temperature-controller device. Oxygen-free dry nitrogen was used as a carrier gas. Approximately 50 mg samples were pyrolyzed. Contact times were around 10-1 s and a pressure of 0.4 torr. Products were trapped at liquid air temperature, extracted with solvent, and subjected to different analyses or separation techniques. In all FVP experiments, the recovery of material was >80%.

3. RESULTS AND DISCUSSION:

The UV-Vis spectra of compound **1** were used to obtain the molar absorptivity in ACN, as shown in Figure 1 and Table 1. There are two well-defined bands at 262 nm and 199 nm. There is also a poorly defined band at 223 nm.

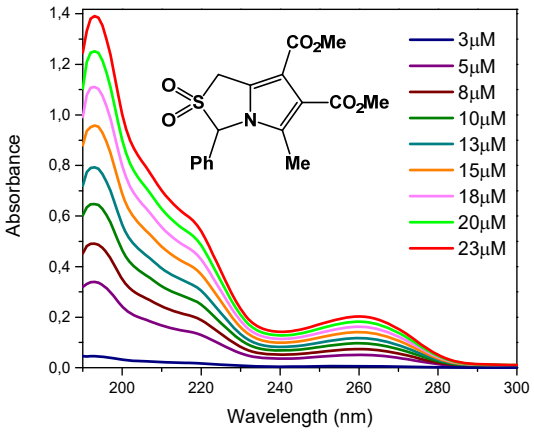


***Figure 1.** UV-Vis spectrum of compound **1** with increasing concentrations.*

These data were used to determine the molar absorptivity coefficients of the compound, shown in Table 1.

***Table 1.** Molar absorptivities of compound **1** from UV-Vis spectra in ACN at 25°C.*

ε 10^6x(M^{-1} cm^{-1})	λ (nm)	Band Observations
63,5 ± 0,4	193	Most intense.
20,6 ± 0,1	223	Poorly defined.
9,11 ± 0,07	260	Defined and assigned to the H →L transition

Another characterization performed to sulfone **1** was through the ^{1}H-NMR spectroscopy. In Figure 2, chemical shifts are shown along with the corresponding assignations.

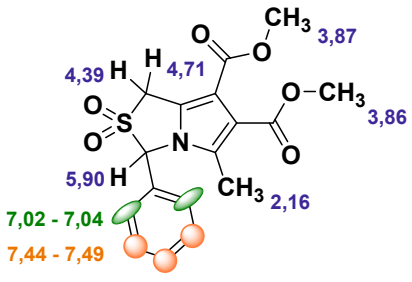
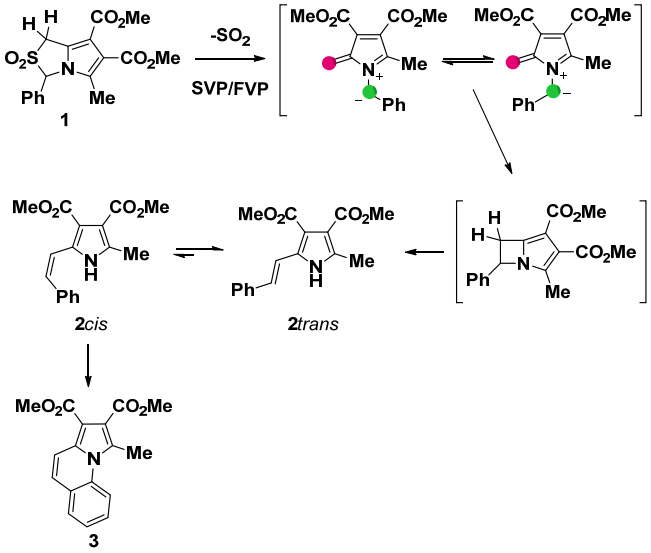


***Figure 2.** ^{1}H-NMR chemical shifts observed.*

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Regarding the pyrolytic reactions, they were performed with a temperature ranging from 250°C to 475°C. Pyrolysis from **1** (Scheme 3) yielded the styrylvynylpyrroles **2***trans* and **2***cis*, characterized by ^{1}H-NMR and GC-MS, and a small quantity of the polycycle **3**, characterized by GC-MS.



Scheme 3. *Proposed mechanism for the observed products in the* FVP *of* ***1***.

FVP conditions are shown in Table 2 with the corresponding yields. Further reactions were performed to unravel the mechanism occurring in this reaction. It is important to note that from the analysis of this Table, at lower temperatures (250 – 325°C), reagent **1** is converted to a unique product, the styrylpyrrole **2***trans*, producing an almost total conversion at 325°C. On the other hand, at higher temperatures, a mixture of the styrylpyrroles **2***trans* and **2***cis* is obtained together with the appearance of the tricyclic compound **3**, most likely generated from the cyclization reaction of the isomer **2***cis*.

Table 2. *Reaction conditions for the pyrolysis of* ***1*** *and the proportion of products obtained.*

Temperature (°C)	1	2*trans*	2*cis*	3
250	93%	7%	-	-
275	67%	33%	-	-
300	57%	43%	-	-
325	6%	94%	traces	-
375	traces	87%	12%	1%
400	-	82%	16%	2%
425	-	80%	17%	3%
450	-	75%	22%	4%
475	-	70%	20%	10%

These results allowed the kinetic (Figure 3) and thermal (Figure 4) characterization of both reactions occurring, i.e. the thermal extrusion of SO_2 and the isomerization between both styrylpyrroles.

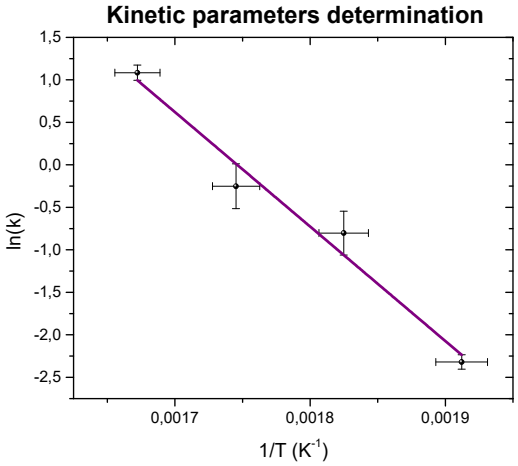
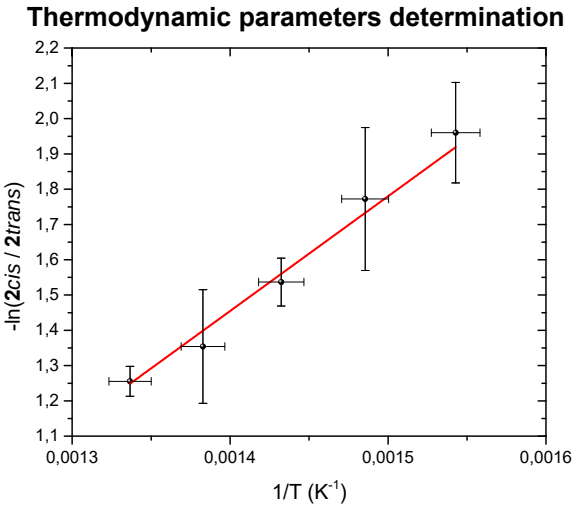


Figure 3. *Arrhenius linear plot used to determine the kinetic parameters.*

Figure 4. *Van't Hoff linear plot used to determine*



the thermal parameters.

Experimental parameters from the reactions are informed in Table 3. Results of the characterization are summarized in Table 3.

Table 3. *Experimental parameters for the pyrolysis reactions of compound* ***1***.

T (K)	C_{2trans}/C_1	t (s)	k (s^{-1})
523	14,42	0,75	0,098
548	0,77	0,91	0,448
573	0,50	0,73	0,778
598	0,077	0,93	2,956

From the results of Figure 3 we were able

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to determine all parameters presented in Table 4. It is important to note that the kinetic characterization refers to SO_2 extrusion from **1**, while the thermal characterization refers to the equilibrium between **2***trans* and **2***cis*.

According to the ΔS‡ value (-70 eu), the transition state is achieved with a high order compared to the reagent, requiring 112 kJ/mol (E_a) in order to occur.

Table 4. *Results from the kinetic and thermal characterization.*

Kinetic characterization		**Thermal characterization**	
E_a (kJ/mol)	112	-	-
ln(A)	23	-	-
ΔH‡ (kJ/mol)	114	$\Delta_r H°$ (kJ/mol)	27,0
ΔG‡ (kJ/mol)	135	$\Delta_r G°$ (kJ/mol)	28,3
ΔS‡ (J/K mol)	-70	$\Delta_r S°$ (J/K mol)	-25,7

It is important to bear in mind that, as all reactions were performed in gas-phase and high temperature, the ΔG‡ describes the process better than the E_a. It can be seen from Equations 1 and 2, that high temperatures raise the E_a and the entropic term, which cannot be negliged. Thus, the ΔG‡ obtained value (135 kJ/mol) characterizes the reaction.

$$\Delta G^{\ddagger} = \Delta H^{\ddagger} - T\Delta S^{\ddagger} \quad \text{(Eq. 1)}$$

$$E_a = \Delta H^{\ddagger} + RT \quad \text{(Eq. 2)}$$

On the other hand, the results from Table 2 at higher temperatures made possible to calculate the thermodynamic parameters from Equations 3 and 4 for the isomerization of both styrylpyrrols **2***trans* and **2***cis*.

$$-lnK = \frac{\Delta_r H^{\circ}}{RT} - \frac{\Delta_r S^{\circ}}{R} \quad \text{(Eq. 3)}$$

$$\Delta_r G^{\circ} = \Delta_r H^{\circ} - T\Delta_r S^{\circ} \quad \text{(Eq. 4)}$$

4. CONCLUSIONS:

The pyrolysis reaction from Scheme 3 was thoroughly characterized. Arrhenius parameters corresponding to the reaction extrusion of SO2 from **1** to generate the corresponding azafulvenium and later **2***trans* were obtained, In addition, thermodynamic parameters from equilibrium between **2***trans* and **2***cis* were also obtained for the very first time. Compound **3** was detected with GC-MS. This is a new product that could undergo further transformations, leading to new interesting heterocyclic compounds.

5. DECLARATIONS

5.1. Acknowledgements

FVM thanks to the Consejo Interuniversitario Nacional (CIN) for the fellowship. This work was supported by Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET-11220200101308CO), Fondo para la Investigación Científica y Tecnológica (FONCYT-PICT-2020-SERIE-A-01862) and Secretaría de Ciencia y Tecnología (SeCyT-UNC-Nº258/23).

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Southern Science Conference, 2024.

FLASH VACUUM PYROLYSIS (FVP) OF DIMETHYL 5-METHYL-3-PHENYL-1H,3H-PYRROLO[1,2-C]THIAZOLE-6,7-DICARBOXYLATE 2,2-DIOXIDE: KINETIC AND THERMAL PARAMETERS

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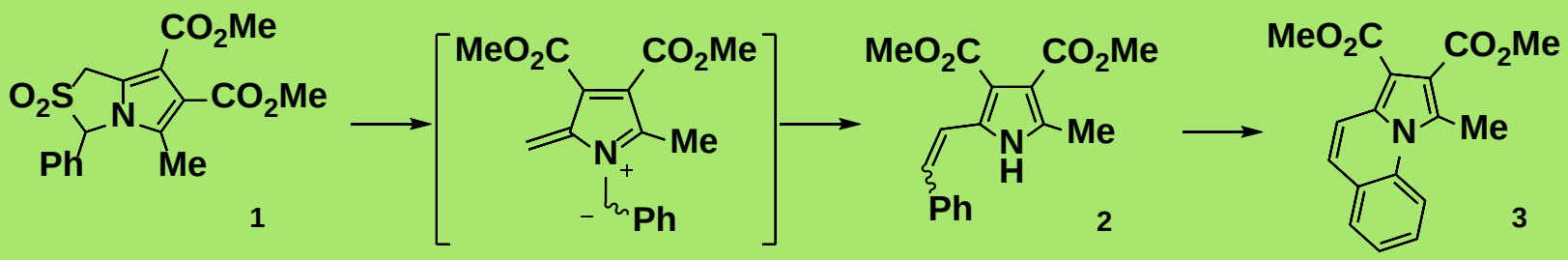
[1] Universidad Nacional de Córdoba. Facultad de Ciencias Químicas. Departamento de Fisicoquímica, X5000HUA, Córdoba, Argentina.

[2] Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Instituto de Investigaciones en Fisicoquímica de Córdoba (INFIQC), X5000HUA, Córdoba, Argentina.

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November/2024

INTRODUCTION



- Spectroscopic, thermal, and kinetic characterization of **1**;
- Production of azafulvene intermediates via SO_2 extrusion;
- Formation of vynylpyrroles and cycloaddition reactions [8π + 2π];
- Possible formation of 1,7-addition products with many synthetic and pharmaceutical properties.

OBJECTIVES

This work aims at:

•Characterization of **1** using the usual techniques (UV-Vis, NMR, GC-MS), along with gas phase pyrolysis reactions;

•Discuss the possibility of 1,7-cycloadditions from the intermediate azafulvene;

•Further exploration of pyrolysis products from **1**.

METHODOLOGY

Characterization

UV-Vis

5 mg of compound in 25 mL of acetonitrile

2 mL ACN in cell, followed by additions of 10 µL of stock solution (max. 9 additions).

^{1}H-NMR

DRX 400 MHz spectrometer (10 mM $CDCl_3$). Chemical shifts are expressed in relative ppm (δ) with TMS as an internal reference, and coupling constants J values are reported in Hz.

GC-MS

Shimadzu GC-MS-QP 5050, SE-30 column.

He as elution gas (1 mL/min).

EI mass spectrometer (70 eV).

Stock solutions (AcOEt, 0.2 g/L).

Pyrolytic reactions

Vycor glass reactor, tube furnace with a temperature-controller device.

Oxygen-free dry nitrogen as carrier gas.

50 mg samples pyrolyzed.

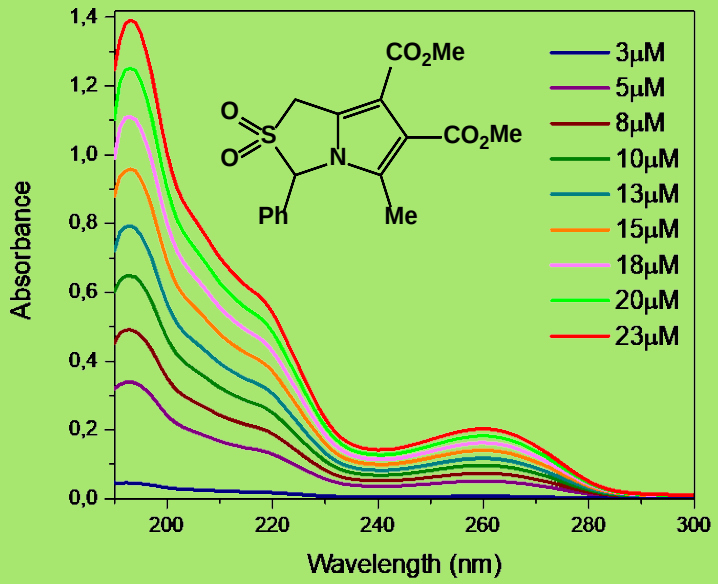
Contact times around 10^{-1} s and pressure of 0.4 torr.

Products trapped at liquid air temperature, extracted with solvent, and subjected to analyses or separation techniques.

Recovery of material >80%.

RESULTS AND DISCUSSION

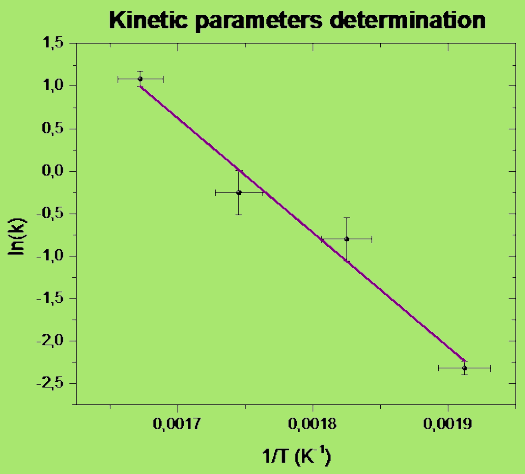
UV-Vis



ε 10^6x(M^{-1} cm^{-1})	λ (nm)	Band Observations
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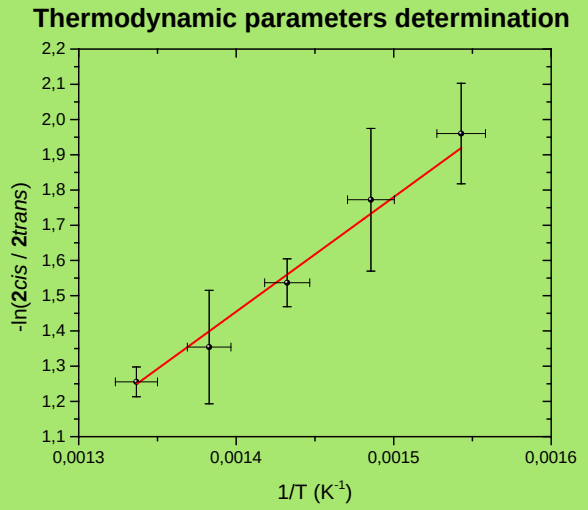
RESULTS AND DISCUSSION

Kinetic characterization

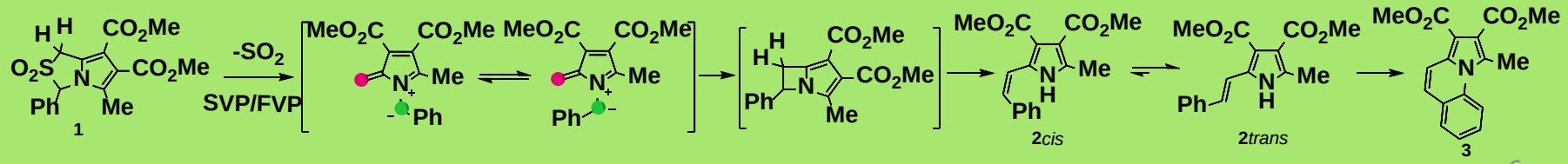


Kinetic characterization		Thermal characterization	
E_a	112	-	-
ln(A)	23	-	-
$\Delta H^{\ddagger}$	114	$\Delta_r H°$	27,0
$\Delta G^{\ddagger}$	135	$\Delta_r G°$	28,3
$\Delta S^{\ddagger}$	-70	$\Delta_r S°$	-25,7

Thermodynamic characterization



Proposed mechanism



CONCLUSIONS

- Pyrolysis reaction from 1 was thoroughly characterized;
- Compounds 2*cis* and 3 were reported for the first time;
- Transition state is achieved with a high order in relation to the reagent;

ACKNOWLEDGEMENTS

- FVM thanks to the Consejo Interuniversitario Nacional (CIN) for the fellowship;
- The team thanks the support from the Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET-1122020010130 8CO);
- We acknowledge the finantial support from the Fondo para la Investigación Científica y Tecnológica (FONCYT-PICT-2020-SERIE-A-01862);
- We also thank the Secretaría de Ciencia y Tecnología (SeCyT-UNC-N°258/23).

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II SOUTHERN SCIENCE CONFERENCE
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EVALUATION OF OXAZINES AS A POTENTIAL TREATMENT FOR GONORRHEA

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ABSTRACT

Sexually transmitted infections pose serious public health challenges, with gonorrhea, caused by *Neisseria gonorrhoeae*, being a common concern, especially due to increasing antibiotic resistance. This study focused on identifying molecules that inhibit *N. gonorrhoeae* growth or act as antibiotic adjuvants, with parallel testing in other Gram-negative bacteria. Synthetic organic molecules were evaluated through in-silico structural analysis and validated through in vitro assays. Microdiffusion assays showed that molecules WpD, WpF, Wp55, and Wp56 demonstrated antimicrobial activity against Salmonella. When testing adjuvant effects with antibiotics, molecules WpB, WpD, WpE, WpF, Wp3, Wp8, Wp55, Wp56, WpG40, and T10 showed adjuvant activity in Salmonella, while only H07 and H08 showed adjuvant activity in *N. gonorrhoeae* strains L and F. These findings suggest these adjuvant molecules could reduce required antibiotic doses in gonorrhea treatment, potentially decreasing bacterial resistance development.

Keywords: *Gonorrhea, STI; Antibiotics, oxazines.*

1. INTRODUCTION

Gonorrhea is a sexually transmitted disease caused by the bacteria Neisseria gonorrhoeae. After exposure, the bacteria infect the most exposed mucous membranes, such as the urogenital tract, rectum, pharynx, and conjunctiva (1). Urethral infection in men is symptomatic in about half of the cases (2), producing purulent and painful urine. Although in women, the percentage of asymptomatic presentations is higher (3), female urethral, rectal, pharyngeal, and conjunctival infections are asymptomatic, so early diagnosis is essential.

If gonorrhea is not treated in time, it can result in complications of varying severity, ranging from pelvic inflammatory disease (PID) chronic pelvic pain, tubal obstruction, and sterility. It also increases the transmission of HIV by up to 5 times. Among other critical implications for reproductive health, they can also cause ectopic pregnancies, abortions in the first trimester of pregnancy, and sterility. The greatest risk for the newborn is eye infections that can lead to blindness (1,4,5).

Since the beginning of the use of antibiotics for the treatment of gonorrhea in 1930, until today, the bacteria has been able to evolve, using various mechanisms, to generate resistance (6). A characteristic of *N. gonorrhoeae* is its ability to modulate its antigenic surface at high speed. This is the basis of its success as a specific pathogen in humans since its constant modulation of the antigenic surface (7) (and its point mutations) (8) or through plasmid DNA (9) improve the bacteria's ability to avoid immune defense mechanisms in humans. It is this same modulation capacity that leads to a major problem in the development of effective vaccines against different strains of N. gonorrhoeae. In recent years, the emergence of new strains of N. gonorrhoeae resistant to a broad spectrum of antibiotics, including the most commonly used ones such as cephalosporins and fluoroquinolones, has been reported, giving rise to the name "superbacteria" or "superbugs" (6). The

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continued emergence of multidrug-resistant (MDR) and extensively drug-resistant (XDR) strains suggests that treatments will not always be effective (10). Resistant strains have been found in Argentina in different research carried out by Dr. Galarza's laboratory (11–15). In 2017, the World Health Organization (WHO) included N. gonorrhoeae as one of the 12 priority bacteria for finding effective treatments (16).

Cyclic molecules as oxazines and their derivatives have been shown to have antibacterial and antiparasitic activity, being effective in inhibiting the growth Gramm positive and negative bacteria (17) in addition to their antioxidant activity (18) being a family of compounds of recent interest in pharmacology (19). The same compounds are fully synthesized by our collaborating group, led by Dr. Walter Peláez, in Córdoba (20,21).

In the present work, we have evaluated the antibacterial activity of the isolated compounds and supplemented the usual antibiotics. They were tested in inhibition discs on the culture medium of bacteria isolated from N. gonorrhoeae on reference strains from the World Health Organization (22), using *E. col*i and *Salmonella enterica* strains as controls.

Our hypothesis is that the molecules to be tested will have different degrees of inhibitory power on the growth of *N. gonorrhoeae* in isolated cultures, with antibacterial activity per se or as an adjuvant to other antibiotics. Our main objective is to test the antibacterial activity of the different oxazines on *N. gonorrhoeae* isolated in culture.

2. MATERIALS AND METHODS

2.1. Materials:

Bacterial strains: we used WHO reference strains of *N. gonorrhoeae* (F, G, K, L, M, P), *E. coli* DH5α , and *Salmonella enterica* Hadar and Heidelberg were used

Bacterial cultures. Bacterial cultures of *N. gonorrhoeae* from commercial and/or modified strains will be performed in a modified Tayer-Martin medium in a thermostatically controlled incubator at 37ºC with 5% CO2. The E. coli and *Salmonella enterica* strains were grown in LB-agar medium, in a thermostatically controlled incubator at 37ºC.

2.2. METHODS

The antibacterial activity and the potential as an adjuvant were assessed using inhibition disks and measuring the inhibition zones. The inhibition disks are charged with known concentrations of antibiotics and/or the molecules to be tested. The dried disk is situated over the freshly cultured bacteria on semi-solid media. After that, it is incubated 24hs, and the halo of inhibition is measured. The experiments are repeated three times.

2.2.1. Antimicrobial Assays:

Antimicrobial activity was assessed via microdiffusion assays, in which filter disks soaked with solutions of the compounds were incubated on media inoculated with bacterial strains. Zones of inhibition around the disks indicated antibacterial activity.

2.2.2. Adjuvant Activity:

In the second phase, the potential adjuvant effect of the molecules was tested in combination with antibiotics. This involved adding the minimum bactericidal concentration (MBC) of antibiotics to the assay alongside the candidate molecules.

3. RESULTS AND DISCUSSION:

No Antibacterial Activity Observed for Tested Oxazines

A total of 25 oxazine molecules were evaluated for antibacterial activity using microdiffusion assays against *Neisseria gonorrhoeae* (strains L and M), *Escherichia coli* DH5α, and *Salmonella enterica* serovars Hadar and Heidelberg. Serial dilutions (base 10) were performed with a maximum concentration of 1 mg/mL. No antibacterial activity was detected for any of the compounds under the tested conditions.

Oxazines Exhibit Potential Adjuvant Activity

The Minimum Bactericidal Concentrations (MBC) of penicillin, Streptomycin (for *N. gonorrhoeae*), and Kanamycin (for *E. coli* and *S. enterica*) were first established. Notably, *N. gonorrhoeae* strains L and M were resistant to penicillin. In subsequent assays, 5 µL of each antibiotic was supplemented with 5 or 10 µL of oxazine molecules. Three independent experiments confirmed all positive results.

Several oxazines enhanced the activity of

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Kanamycin, specifically against *S. enterica* Heidelberg, including molecules WpB, WpD, WpE, WpF, Wp3, Wp8, Wp55, Wp56, WpG40, and T10 (Table 1). Additionally, molecules H07 and H08 exhibited adjuvant activity with penicillin against the Penicillin-resistant *N. gonorrhoeae* strain L (Figure 2) and enhanced the efficacy of Streptomycin against *N. gonorrhoeae* strain F.

3.2. DISCUSSIONS:

The terms multidrug-resistant (MDR) and extensively drug-resistant (XDR) refer to bacteria that exhibit resistance to multiple antimicrobial classes or nearly all available treatments, respectively. The continued emergence of MDR and XDR strains of N. gonorrhoeae presents a critical public health concern, reinforcing the urgent need for novel therapeutic interventions. In response, the WHO has listed *N. gonorrhoeae* as a priority pathogen in the search for new treatments.

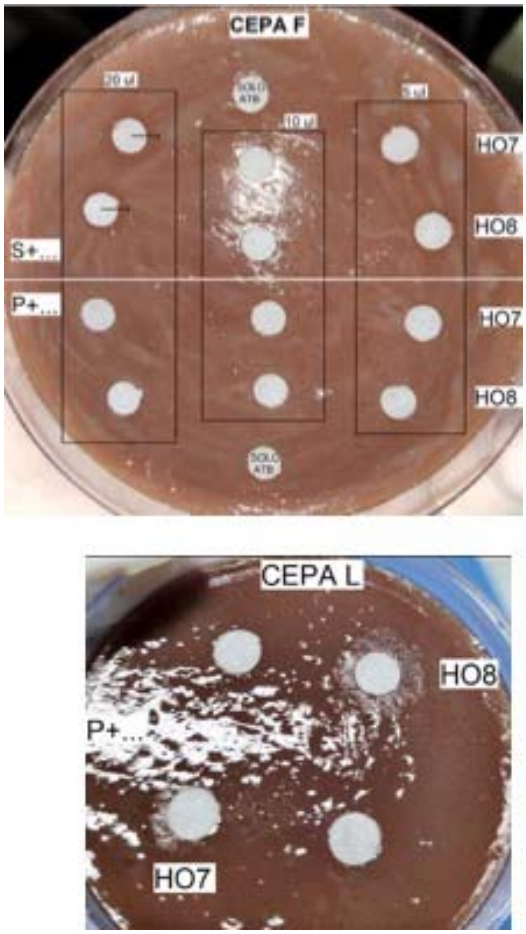


Figure 1. *Determination of potential adjuvant activity of selected molecules. In concentrations under the MBC of the antibiotic, the organic molecules were added. Determination for Neisseria gonorrhoeae strains L and F*

In this study, we identified oxazine-derived molecules with potential as adjuvants in antibiotic therapy. Although these compounds do not exhibit significant antibacterial activity on their own, they may enhance the efficacy of conventional antibiotics, offering a strategy to reduce antibiotic doses and combat resistance. Future research will aim to determine whether these molecules can act on intracellular bacteria without harming host cells and elucidate their mechanisms of action.

Table 1. *Molecules with adjuvant activity*

Adjuvant activity	***S. entérica* Heidelberg**	***N. gonorrhoeae* strain L/F**
WpB, WpD, WpE, WpF, Wp3, Wp8, Wp55, Wp56, WpG40, T10	**+**	**-**
HO7, HO8	**-**	**+**

The table summarizes the molecules exhibiting adjuvant activity over the different bacteria.

4. CONCLUSIONS:

Our results indicate that H07 and H08 are promising adjuvant candidates for spectinomycin and penicillin in the treatment of gonorrhea, potentially reducing the dosage needed for effective therapy. This reduction could play a critical role in minimizing the development of antibiotic resistance. Moreover, similar molecules showed adjuvant activity against *Salmonella enterica*, enhancing the activity of kanamycin.

Overall, our findings highlight oxazine derivatives as a promising family of molecules with high potential for treating bacterial infections, particularly in cases of antibiotic resistance

5. DECLARATIONS

5.1. Study Limitations

No limitations were known at the time of the study.

5.2. Acknowledgements

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We thank Stella Galfre for the support from the Central Laboratory of Universidad Maza.

5.3. Funding source

The work was supported by an internal grant from Universidad JA Maza and an internal grant from Universidad de Mendoza.

5.4. Competing Interests

The authors declare that they have no competing interests.

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Southern Science Conference, 2024.

EVALUATION OF OXAZINES AS A POTENTIAL TREATMENT FOR GONORRHEA

Perlbach, Agostina[1]; Quiroga, Agustina[1]; Gonzalez, Andrés1; Cabrini, Micaela[1]; Cambulli Bianchi, Paula[2], Díaz, Sofía[2], Hualpa, Mauricio[1]; Pinilla Peña, Diana Carolina[3]; Ceballos, Noela M.[3]; Pelaez, Walter[3], Quintero, Cristián Andrés,[1,2]

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November/2024

INTRODUCTION

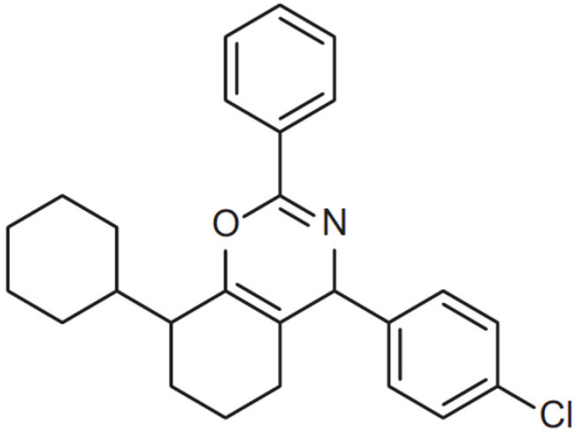
- Gonorrhea is a sexually transmitted disease caused by the bacteria *Neisseria gonorrhoeae.*
- More than 1 million curable STIs are acquired every day. In 2020, WHO estimated 82 million new infections with gonorrhoea
- *N. gonorrhoeae* have generated resistance to the current treatments.
- In 2017 and 2024, he World Health Organization (WHO) included N. gonorrhoeae as one of the 12 priority bacteria for finding effective treatments.

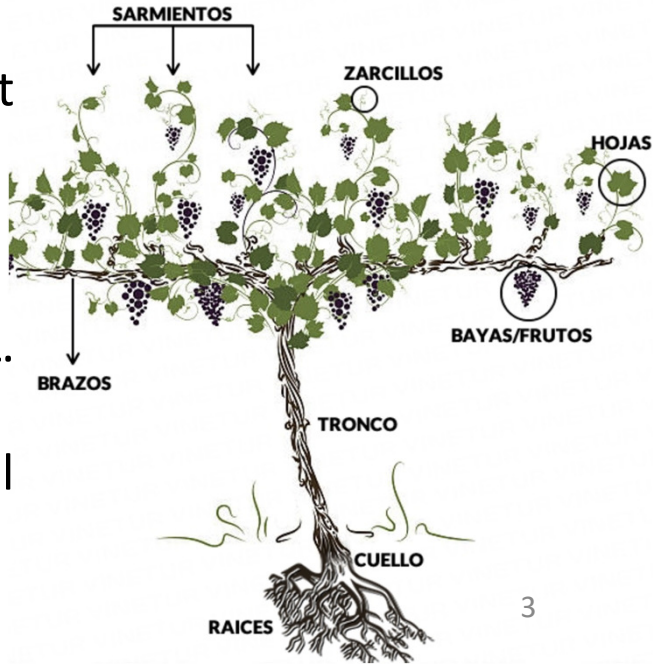


World Health Organization

BACKGROUND

- Cyclic molecules as oxazines and their derivatives have been shown to have antibacterial and antiparasitic activity
- An important approach to finding new and effective treatments for infectious diseases is using plant extracts and natural compounds.
- Byproducts of the wine industry from *Vitis vinífera* L. (Vitaceae) have been succesfuly tested against several bacteria





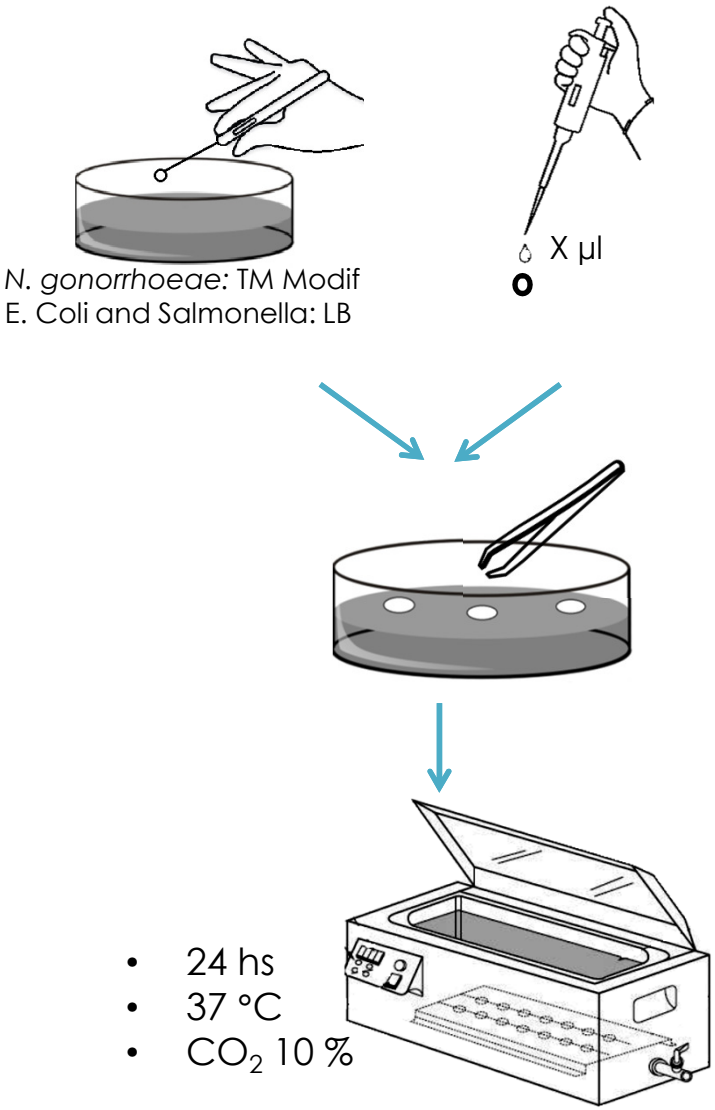
OBJETIVE

Our aim is determine the antibacterial activity of the oxazines and their related molecules, either isolated compounds and supplemented the usual antibiotics

METHODOLOGY

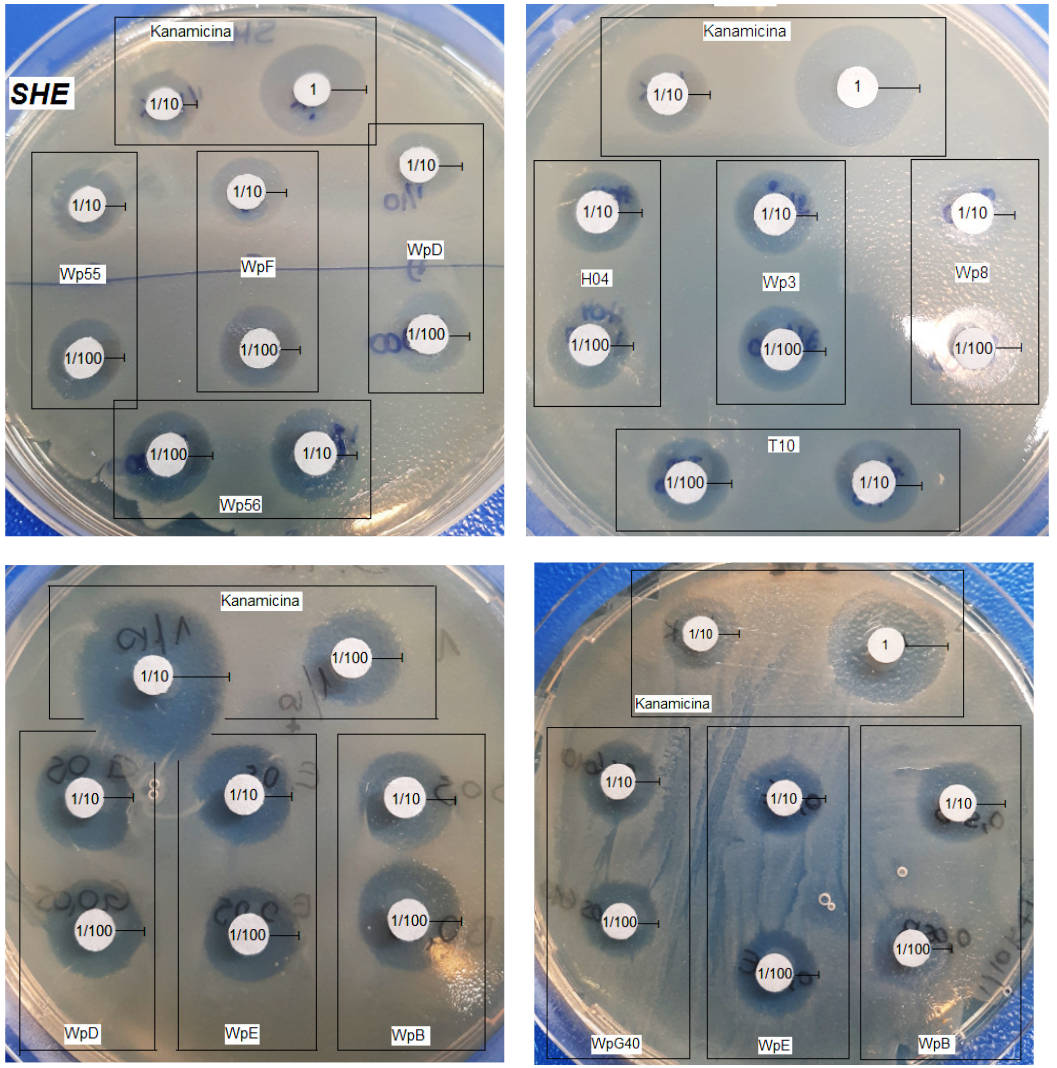
MICRODIFFUSION TESTS

1. Prepare a pre-culture of each microorganism.
2. Soak sterilized filter paper discs with the exact amount (µl) of the corresponding solution to build the inhibition discs. Allow to dry.
3. Place the discs on recently seeded plates in bulk.
4. Incubate at 37 °C.
5. After 24 hours, observe the growth pattern in the presence of synthetic molecules.
6. Measure the diameter of the inhibition zone, if present.



RESULTS AND DISCUSSION

- No compound showed microbial activity by itself.
- Molecules such as WpB, WpD, WpE, WpF, Wp3, Wp8, Wp55, Wp56, WpG40 and T10 **showed activity as adjuvants for Kanamycin** in *Salmonella* (SHE).

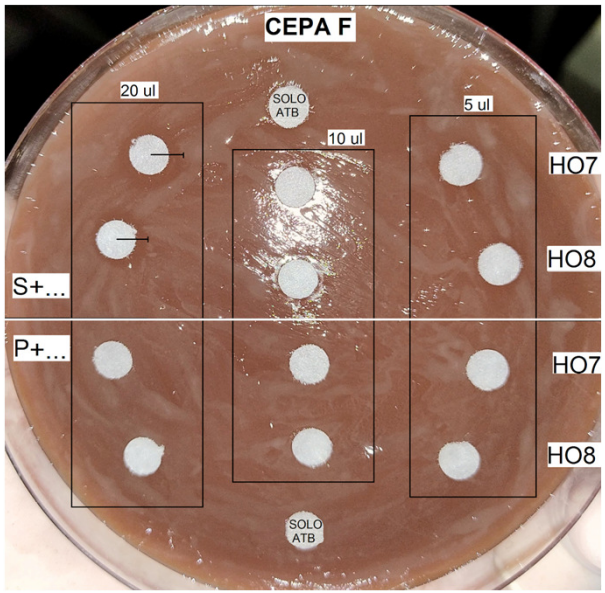


RESULTS AND DISCUSSION

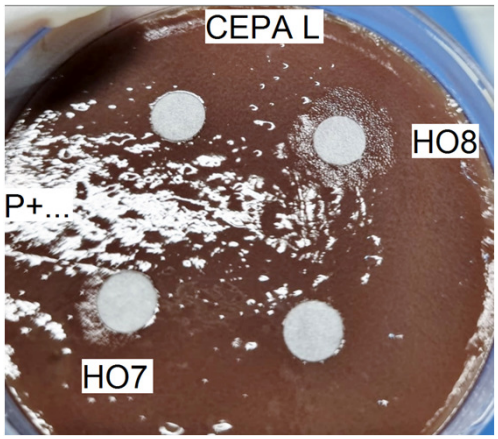
For ***N. gonorrhoeae***, the molecules **HO7** and **HO8** would have activity as adjuvant in the **F** strain with Streptomycin, and in the **L** strain with Penicillin.

The diameters of the inhibition zones would indicate that it is **dose-independent.**

On the contrary, the growth of *Salmonella* and *E. coli* was not altered by the presence of these molecules.



Molecules with Adjuvant activity	*Salmonella Heidelberg*	*Neisseria gonorrhoeae*
WpB, WpD, WpE, WpF, Wp3, Wp8, Wp55, Wp56, WpG40 y T10		X
HO7, HO8	X	



CONCLUSIONS

•Our results indicate that H07 and H08 ***are promising adjuvant candidates*** for spectinomycin and penicillin in the treatment of gonorrhea, potentially reducing the dosage needed for effective therapy.

•This ***reduction could play a critical*** role in minimizing the development of antibiotic resistance.

•Moreover, similar molecules showed adjuvant activity against *Salmonella enterica*, enhancing the activity of kanamycin.

•Overall, our findings highlight ***oxazine derivatives as a promising family of molecules*** with high potential for treating bacterial infections, particularly in cases of antibiotic resistance.

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THEORETICAL STUDY OF SO_2 EXTRUSION REACTION FOR THE PRODUCTION OF DIAZAFULVENES AND ITS CYCLOADDITION REACTION WITH SEVERAL POLAROPHILES

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ABSTRACT

For the first time, a theoretical study about the thermodynamic parameters of the SO_2 extrusion reaction for two pyrazolo[1,5-c]thiazole derivatives and a thiazolo[3,4-b]indazole derivative is carried out. It is evaluated as the substituents of substrates affect the stability of the diazafulvene intermediates formed; in addition, the energy gaps are calculated between the $HOMO_{dipole}$-$LUMO_{dipolarophile}$ orbitals to explore their possible incidence in obtaining heterocyclic products by cycloaddition reactions of diazafulvenes and different polarophiles are explored.

Keywords: *so_2 extrusion, diazafulvenes, FVP, indazole, pyrazole, theoretical study, cycloaddition reaction.*

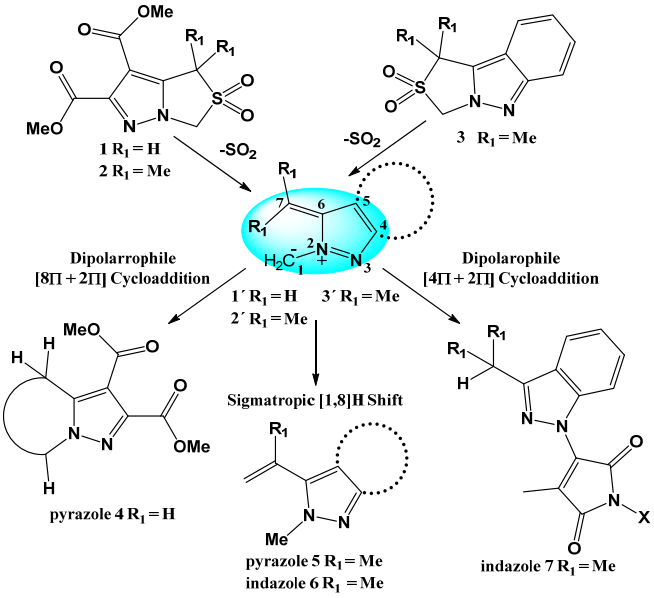
1. INTRODUCTION

In recent years, the versatility of aza- and diazafulvenium methides systems has been demonstrated as building blocks for the synthesis of stable heterocyclic compounds and macrocycles with potential use in various biomedical applications (Pereira *et al.*, 2010; Pereira *et al.*, 2011).[1]

Diazafulvenium methides are generated from 2,2-dioxo-pirazolo[1,5-*c*][1,3]tiazoles **1 and 2** by thermal extrusion of sulfur dioxide. The diazafulvenium methides unsubstituted at C-7 participate in [8π + 2π] cycloadditions, giving pyrazolo[1,5-*a*]pyridine derivatives **4** resulting from the addition across the 1,7- position. In the absence of dipolarophiles 7,7-dimethyl-diazafulvenium methides undergo intramolecular sigmatropic [1,8]*H* shifts, giving *C*-vinyl-1*H*-pyrazoles **5** (Pinho e Melo *et al.*, 2007).[2]

For their part, the 7,7-dimethylbenzo-2,3-diazafulvenium methides **3´** show 1,3-cycloaddition with maleimides and experiment

sigmatropic [1,8]*H* shifts under flash vacuum pyrolysis or under microwave irradiation allowing the efficient synthesis of indazoles **6 and 7** (Soares *et al.*, 2013).[3]



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Figure 1. *Pericyclic and cycloaddition reactions of diazafulvenium methides 1´- 3´.*

Although the chemistry of diazafulvenium methides **1´- 3´** has been known for some years, there are no reports about the thermodynamic parameters that characterized the SO_2 extrusion reaction from the pyrazolo-thiazoles and thiazolo-indazoles derivatives. No information has been described on how the different substituents affect the stability of the diazafulvene formed and, consequently, the distribution of the products obtained.

For this reason, here we carry out a theoretical study of the thermodynamic parameters of the SO2 extrusion process for two derivatives of pyrazolo [1,5-*c*]thiazoles **1** and **2** and one derivative of thiazolo [3,4-*b*] indazole **3**. It is described as the substituents of the reactants affecting: 1) the stability of the diazafulvene intermediary formed and 2) the cycloaddition reactions with different dipolarophiles. For this, the energy difference between the HOMO of the dipoles and the LUMO of different dipolarophiles was evaluated.

2. MATERIALS AND METHODS

2.1 DFT Calculations.

The optimization of the geometries of substrates **1 – 3** and the diazafulvenium methides **1´- 3´,** the transition states (TS), and the HOMO-LUMO energies were performed with Gaussian16 (Frisch *et al.*, 2016)[4] at the DFT level of theory, using the standard 6311+g (d,p) base set (Pople *et al.*, 1990),[5] and the three-parameter density functional B3LYP (Becke, 1988; Lee *et al.*,1988).[6]

Frequency calculations were also performed for the structures of each molecule, and it was determined whether the transition states had a single negative frequency value. All calculations were performed in the gas phase.

3. RESULTS AND DISCUSSION:

The value of de $\Delta G^{\#}$ for the extrusion reaction of molecules **1** – **3** was examined by quantum chemical calculations and is presented in Table 1. Similar energy values were found for the extrusion reaction of pyrazolo[1,5-*c*]thiazole derivatives **1** and **2**, but thiazolo[3,4-*b*]indazole derivative **3** showed a decrease of 20 kJ/mol in the $\Delta G^{\#}$ value. This could be due to the presence of an aromatic ring in the molecule, which favors the stability of the dipole intermediate **3´** formed.

Table 1. *Theoretical* $\Delta G^{\#}$ *for the* SO_2 *extrusion reaction of pyrazolo[1,5-c]thiazoles* ***1-2*** *and thiazolo[3,4-b]indazole* ***3***

Molecule	$\Delta G^{\#}$ (kJ / mol)
1	92,14
2	91,67
3	72,16

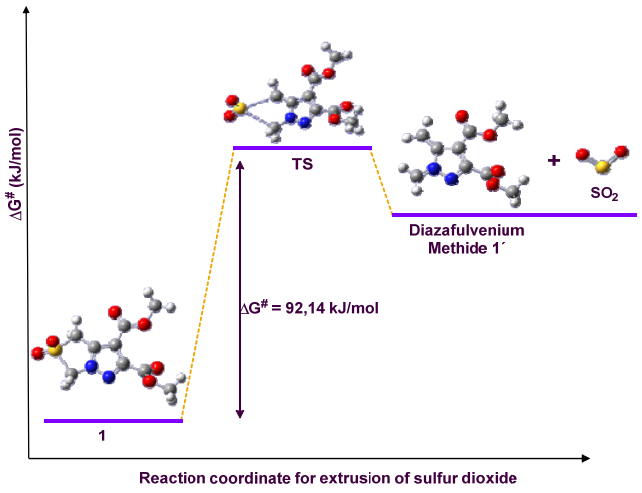


Figure 2. *Theoretical* $\Delta G^{\#}$ *required for the formation of diazafulvenium methide* ***1´***

To be able to rationalize the different chemical behavior of diazafulvenium methides **1´- 2´** and benzodiazafulvenium methides **3´** toward dipolarophiles (**DIPO1 - DIPO 4**), frontier molecular orbital (FMO) analysis was carried out as shown in Table 2 and Figure 3.

Table 2. *Frontier orbital energies for diazafulvenium* ***1´- 3´*** *and dipolarophiles* ***1 - 4***

Molecule	HOMO (eV)	LUMO (eV)
1´	-5,68	-3,09
2´	-5,42	-2,63
3´	-4,9	-2,17
DIPO1	-6,94	-3,08
DIPO2	-7,84	-3,02
DIPO3	-8,25	-1,91
DIPO4	-6,06	-1,68

Theoretically, it was found that energy gaps between the $HOMO_{dipole}$ - $LUMO_{dipolarophile}$ orbitals are similar in all cases for **1´**and **2´**. However, according to the experimental results reported (Pinho e Melo *et al.*, 2007) [2], only diazafulvene **1´** forms cycloaddition products with the

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dipolarophiles **DIPO1** and **DIPO3**.

Although **1´** presents HOMO energy values similar to **2´**, the absence of cycloaddition products for diazafulvenium methide **2´** in front of these same dipolarophiles, may be due to steric hindrance caused by the two methyl groups present at carbon 7 of the dipole.

The **3´** dipole presents the lowest energy gaps between $HOMO_{dipole}$ - $LUMO_{dipolarophile}$ with the dipolarophiles **DIPO1** and **DIPO2**, which is consistent with the experimental data that report cycloaddition products between **3´** and these dipolarophiles(Soares *et al.*, 2013). There are no experimental reports of the reaction of **3´** with the acetylenes **DIPO3** or **DIPO4**, but it has been reported that this benzodiazafulvenium methides does not form cycloaddition products with bis(trimethylsilyl)acetylene under thermolysis conditions.

4. CONCLUSIONS:

The thermodynamic parameters of SO_2 extrusion are presented for the first time in a theoretical form, obtaining higher $\Delta G^{\#}$ values for the pyrazolo[1,5-*c*]thiazole derivatives **1** and **2**. This could be due to the presence of an aromatic ring in **3** that would favor the stabilization of the TS that generates diazafulvene **3'**.

Dipoles **1´**and **2´** have very similar $HOMO_{dipole}$-$LUMO_{dipolarophile}$ energy gaps. However, diazafulvene **1´** forms cycloaddition products with conventional polarophiles, while dipole **2´** does not present cycloaddition reaction products. This may be due to the presence of two methyl groups on carbon 7 of dipole **2´**, which, due to steric hindrance would not allow the formation of the [8Π + 2 Π] cycloadduct.

5. DECLARATIONS

5.1. Acknowledgements

This work was partly supported by the Universidad Nacional de Cordoba (UNC), the Consejo Nacional de Investigaciones Cientificas y Tecnicas (CONICET) and Secretaria de Ciencia y Tecnologia, Universidad Nacional de Cordoba (SECyT).

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2. Pinho e Melo, T. M. V. D.; Nunes, C. M.; Soares, M. I. L.; Paixao, J. A.; Beja, A. M.; Silva Ramos, M. *J. Org. Chem*. **2007**, 72, 4406.
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7. *B.* **1988,** 37, 785.

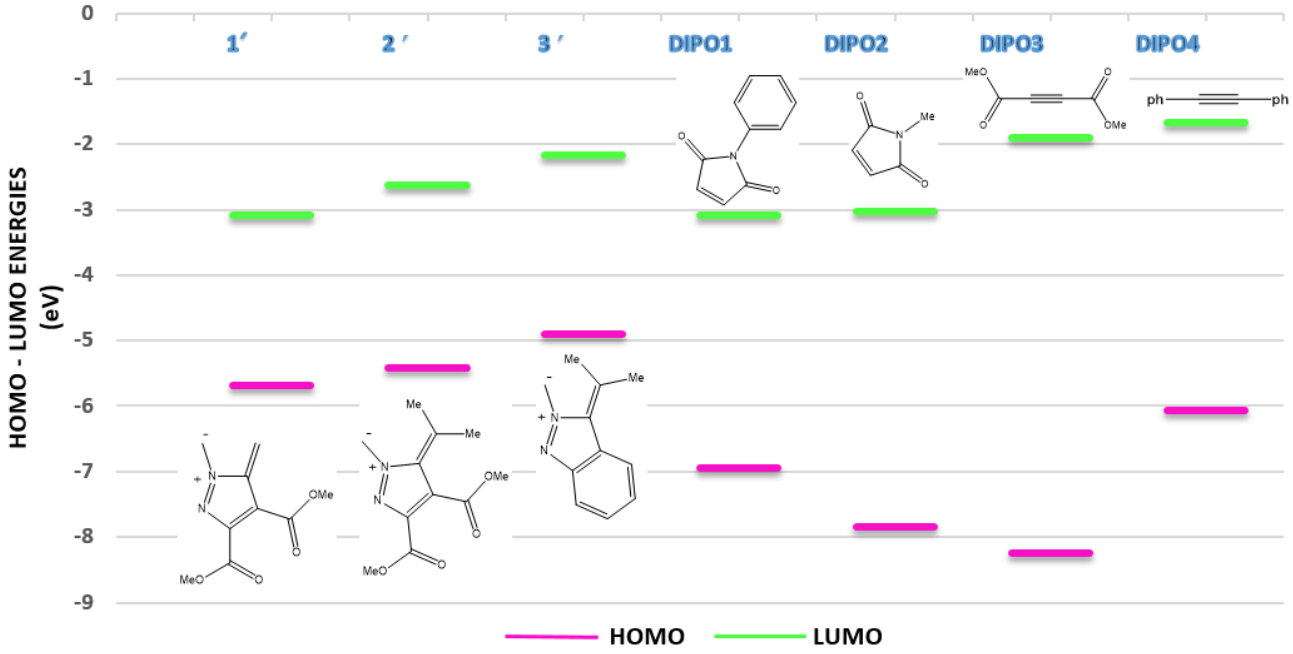


Figure 3. *Theoretical Homo-Lumo Energies of Diazafulvenium* ***1´- 3´*** *and Dipolarophiles (****DIPO 1 - 4****)*

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Southern Science Conference, 2024.

THEORETICAL STUDY OF SO_2 EXTRUSION REACTION FOR THE PRODUCTION OF DIAZAFULVENES AND ITS CYCLOADDITION REACTION WITH SEVERAL POLAROPHILES

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Universidad de Coímbra, Departamento de Química – Coímbra, Portugal.

Walter José Peláez,
Universidad Nacional de Córdoba, Facultad de Ciencias Químicas – Córdoba, Argentina

October/2024

INTRODUCTION

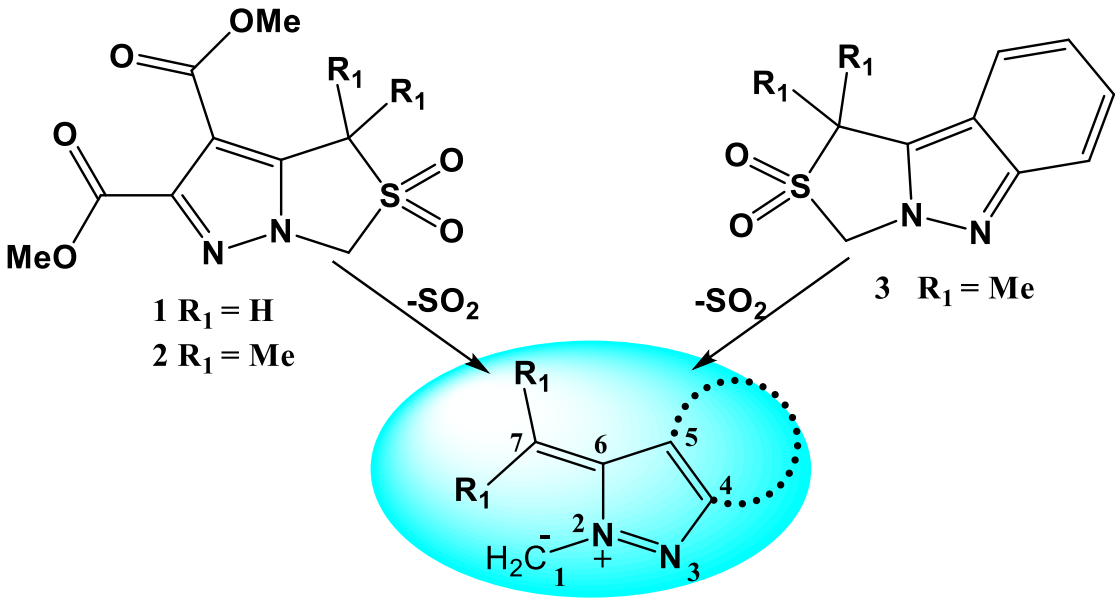


Figure 1.

Formation of diazafulvenium methides by SO_2 extrusion reaction

- **In recent years, the versatility of aza- and diazafulvenium methides systems has been demonstrated as building blocks for the synthesis of stable heterocyclic compounds and macrocycles with potential use in various biomedical applications.[1]**
- **Diazafulvenium methides are generated from 2,2 dioxo-pirazolo[1,5-*c*][1,3]tiazoles 1 and 2,[2] or from thiazolo - indazoles 3[3] by thermal extrusion of sulfur dioxide (SO_2).**

1. (**a**) Pereira, N. A. M.; Serra, A. C.; Pinho e Melo, T. M. V. D. *Eur. J. Org. Chem.* **2010**, 6539. (**b**) Pereira, N. A. M.; Fonseca, S. M.; Serra, A. C.; Pinho e Melo, T. M. V. D.; Burrows, H. D. *Eur. J. Org. Chem*. **2011**, 3970.
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INTRODUCTION

- The diazafulvenium methides unsubstituted at C-7 participate in [8π + 2π] cycloadditions, giving pyrazolo[1,5-a]pyridine derivatives **4**.
- In the absence of dipolarophiles 7,7-dimethyl-diazafulvenium methides **2´** and 7,7 dimethylbenzo-2,3-diazafulvenium methides **3´** are undergo intramolecular sigmatropic [1,8]H shifts, giving vinyl-pyrazoles **5**[2] and vinyl-indazoles **6.**[3]
- The 7,7 dimethylbenzo-2,3-diazafulvenium methides **3´** show 1,3-cycloaddition with maleimides to form indazole derivates **7.**[3]

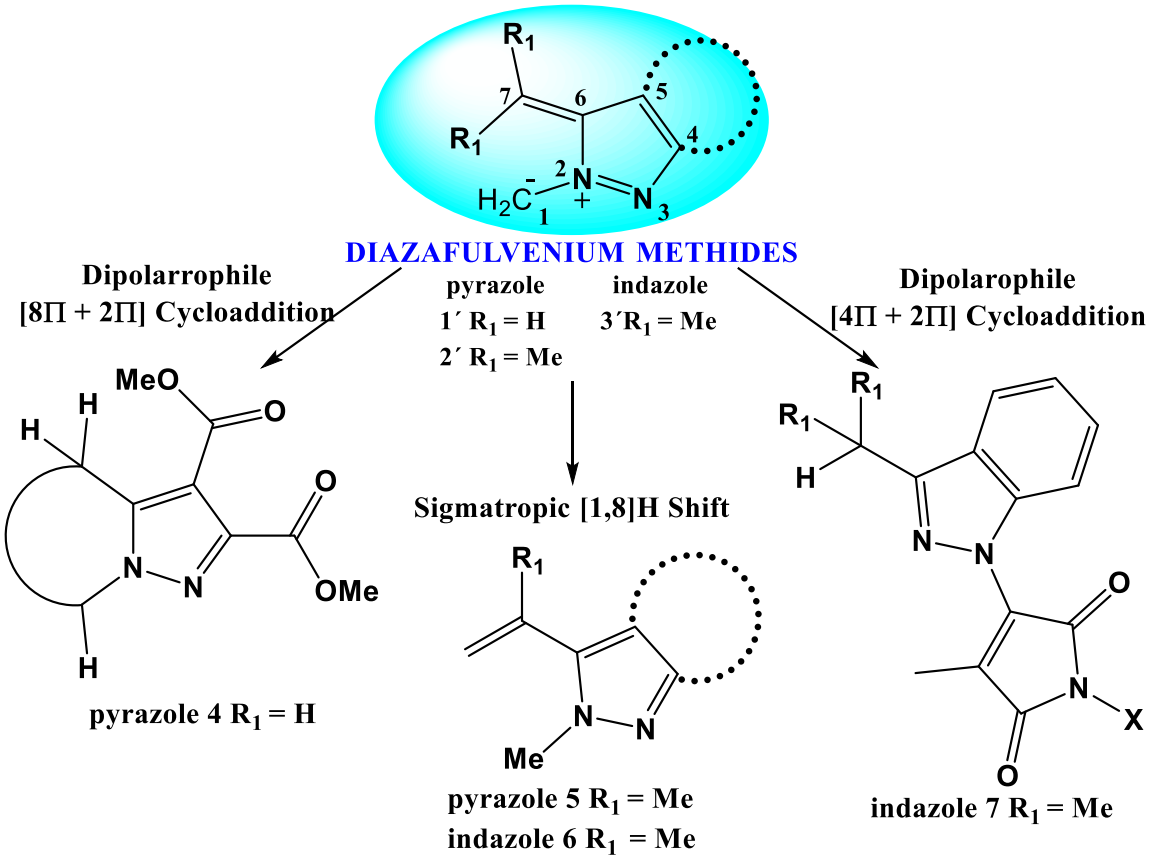


Figure 2.

Pericyclic and cycloaddition reactions of diazafulvenium methides 1´- 3´

3. Soares, M. I. L.; Nunes, C. M.; Gomes, C. S. B.; Pinho e Melo, T. M. V. D. *J. Org. Chem.* **2013**, 78, 628.

OBJETIVE

Although the chemistry of diazafulvenium methides **1´- 3´** has been known for some years, there are no reports about the thermodynamic parameters that characterized the SO_2 extrusion reaction from the pyrazolo-thiazoles and thiazolo- indazoles derivatives. No information has been described on how the different substituents affect the stability of the diazafulvene formed and, consequently, the distribution of the products obtained. For this reason, here we propouse:

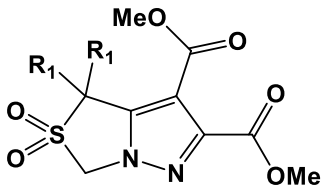
❖ Carry out a theoretical study of the thermodynamic parameters of the SO_2 extrusion process for :two derivatives of pyrazolo [1,5-*c*]thiazoles **1** and **2** and one derivative of thiazolo [3,4-*b*] indazole **3**.

❖ Observe the influence of the reactant´s substituents on the stability of the diazafulvene intermediate formed.

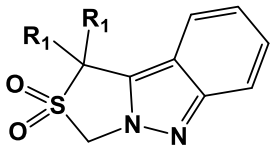
❖ Describe as the substituents of the diazafulvene intermediates affect the cycloaddition reactions with different dipolarophiles, by means of the evaluation of HOMO_dipole and LUMO_dipolarophile energies.

RESULTS AND DISCUSSION

Table 1.
Theoretical $\Delta G^{\#}$ for the SO_2 extrusion reaction of molecules 1 - 3



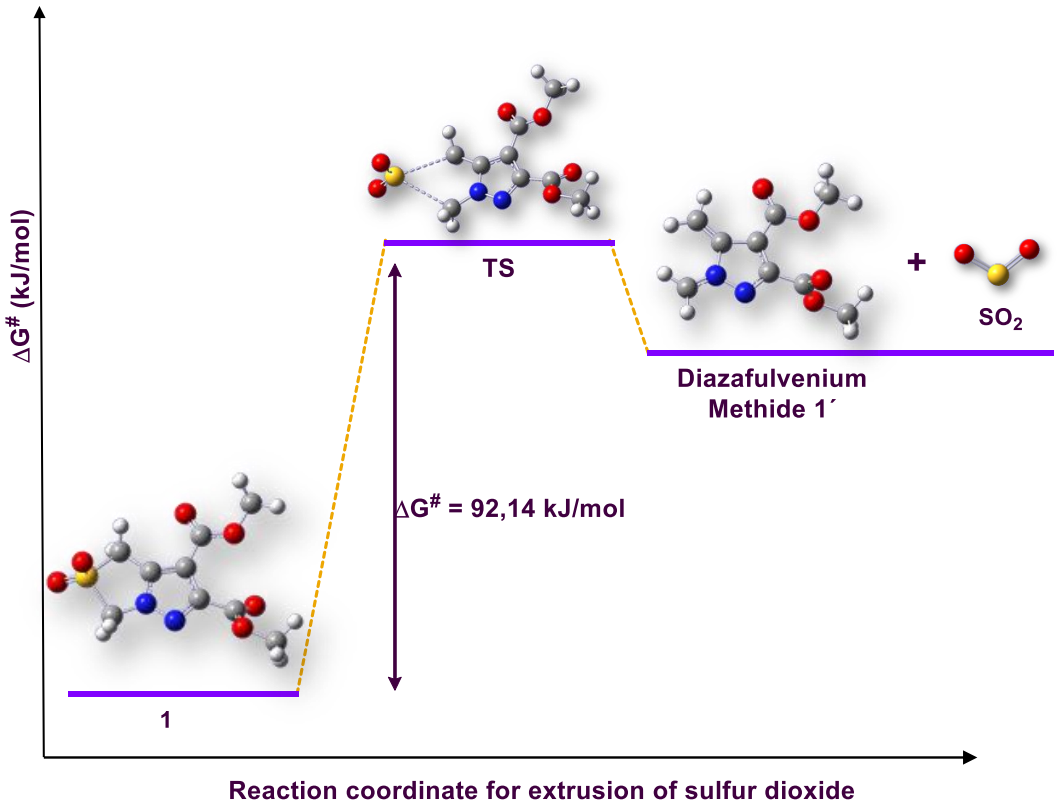
pyrazole
1 R_1 = H
2 R_1 = Me



indazole
3 R_1 = Me

Molecule	$\Delta G^{\#}$ (kJ / mol)
1	92,14
2	91,67
3	72,16

Figure 3.
Theoretical $\Delta G^{\#}$ required for the formation of diazafulvenium methide 1´

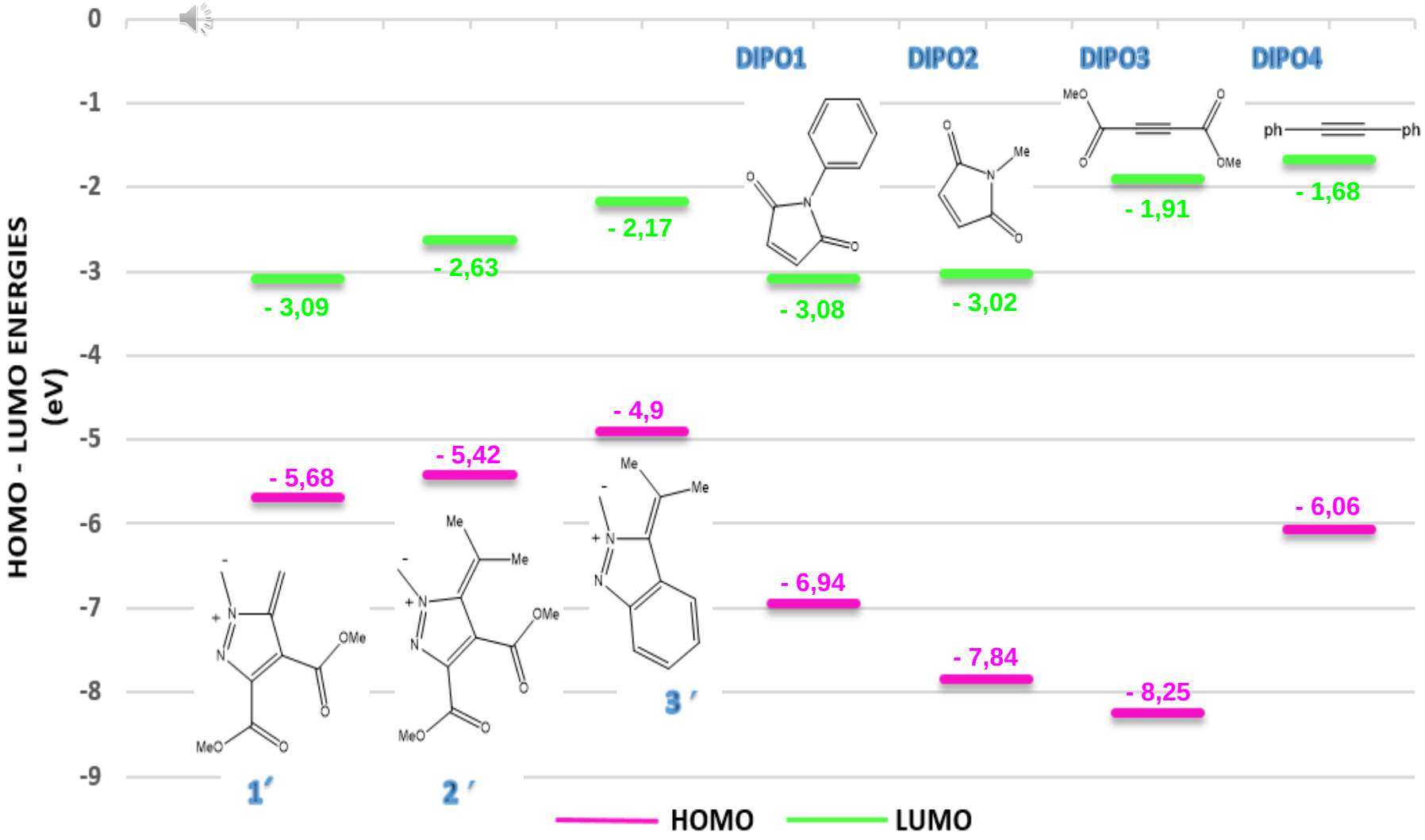


Program: Gaussian16[4] - Method: DFT/6-311+g (d,p)[5]/B3LYP[6]

[4] **Gaussian 16,** Revision C.01, Frisch, M. J. *et al.* ; Gaussian, Inc., Wallingford CT, **2016**.
[5] Frisch, M.; Head-Gordon, M.; Pople, J. A. *Chem. Phys. Lett.* **1990**, 166, 281.
[6] (**a**) Becke, A. *Phys. Rev. A* **1988**, 38, 3098. (**b**) Lee, C.; Yang, W.; Parr, R.; *Phys. Rev. B.* **1988,** 37, 785

RESULTS AND DISCUSSION

Figure 4. **Theoretical HOMO-LUMO Energies of Diazafulvenium 1´- 3´ and Dipolarophiles (DIPO 1 - 4)**



Program: Gaussian16[4] - Method: DFT/6-311+g (d,p)[5]/B3LYP[6]

CONCLUSIONS

- ✓ The thermodynamic parameters of SO_2 extrusion are presented for the first time in a theoretical form, obtaining higher $\Delta G^{\#}$ values for the pyrazolo[1,5-*c*]thiazole derivatives **1** and **2**. This could be due to the presence of an aromatic ring in **3** that would favor the stabilization of the TS that generates diazafulvene **3'**.

- ✓ Dipoles **1´**and **2´** have very similar $HOMO_{dipole}$-$LUMO_{dipolarophile}$ energy gaps. However, diazafulvene **1´** forms cycloaddition products with conventional polarophiles, while dipole **2´** does not present cycloaddition reaction products. This may be due to the presence of two methyl groups on carbon 7 of dipole **2´**, which, due to steric hindrance would not allow the formation of the [8P + 2 P] cycloadduct.

- ✓ The extension of the results presented in this theoretical study leads to predictive approaches that optimize the design and reduce costs in synthetic exploration by pyrolysis of new heterocyclic compounds with biomedical and technological applications.

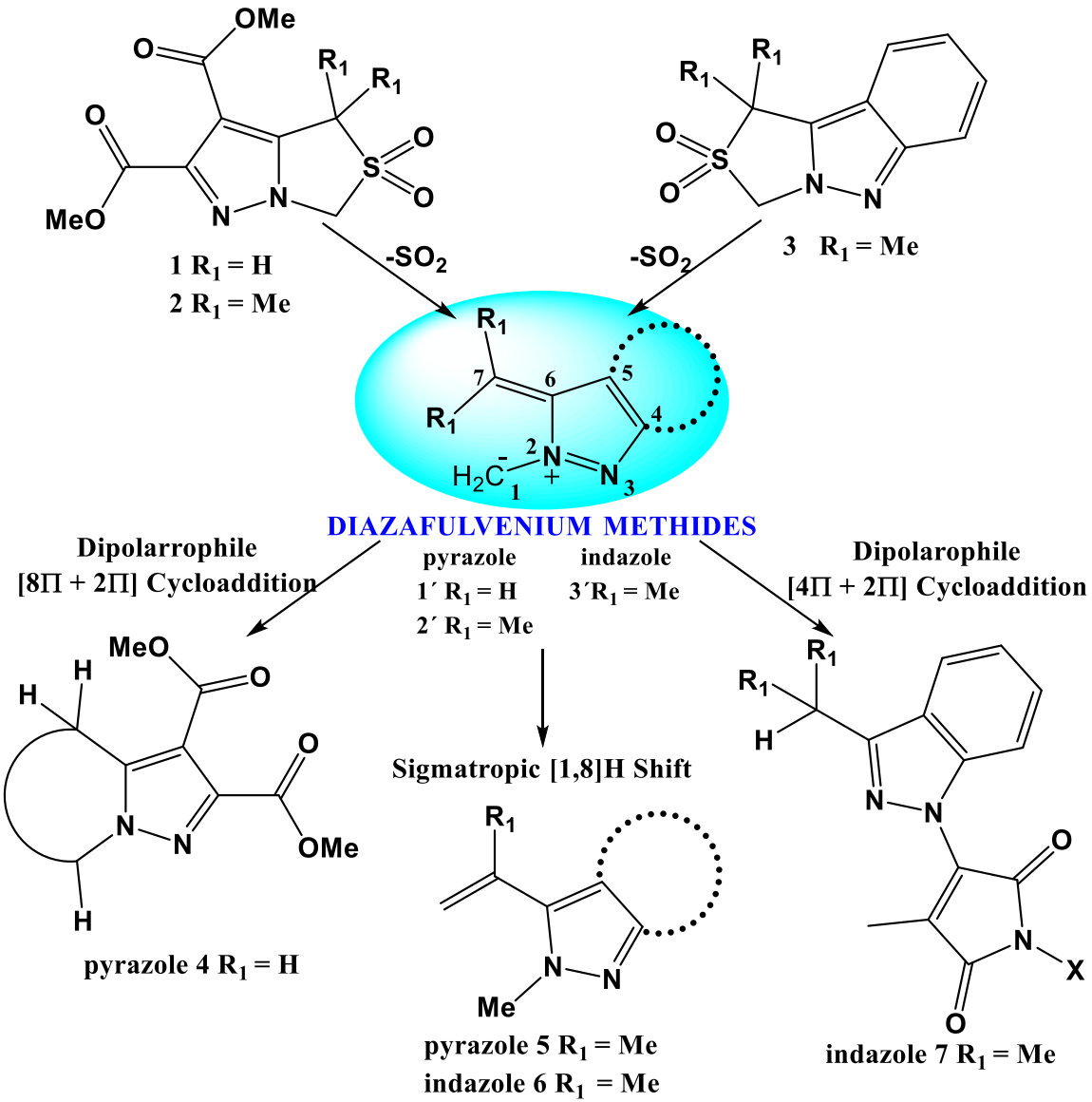


ACKNOWLEDGEMENTS








1 R1 = H
2 R1 = Me
-SO2
-SO2
3 R1 = Me
DIAZAFULVENIUM METHIDES
Dipolarrophile
[8Π + 2Π] Cycloaddition
pyrazole
1´ R1 = H
2´ R1 = Me
indazole
3´R1 = Me
Dipolarophile
[4Π + 2Π] Cycloaddition
pyrazole 4 R1 = H
Sigmatropic [1,8]H Shift
pyrazole 5 R1 = Me
indazole 6 R1 = Me
indazole 7 R1 = Me

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CHARACTERIZATION OF AEROSOL PARTICLES IN ILORIN, NIGERIA: GROUND-BASED MEASUREMENT APPROACH

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ABSTRACT

The present study investigated the changes in aerosol optical characteristics and their impact on climate change risks in Ilorin, Nigeria, focusing on the physical characteristics, spatial distribution, and relationships between aerosol properties. The research utilized ground-based measurements from AERONET data archives to analyze aerosol optical depth and angstrom exponent data, along with single scattering albedo and aerosol size distribution parameters for 2019 and 2021. Analysis was conducted using mean, percentages, and correlation analysis to determine seasonal and annual aerosol properties. The findings revealed four distinct types of aerosol particles: urban industrial (29.22%), desert dust (37.08%), biomass burning (10.67%), and urban mix (23.03%). The study demonstrated statistically insignificant annual and seasonal variations (p value>0.05), with low Angstrom exponent values (<1) indicating a predominance of coarse particles over Ilorin. The average annual single scattering albedo at wavelengths 440/675/870/1020 was 0.05/0.09/0.23/0.25. A positive correlation between aerosol properties and particle concentration was observed, highlighting the significant impact of spatiotemporal aerosol changes on climate change risks. These findings suggest that increasing changes in Ilorin's aerosol properties may exacerbate future climate risks, emphasizing the growing contribution of anthropogenic emissions to urban climate challenges. This research contributes to our understanding of aerosol optical characteristics in urban environments and their implications for climate change mitigation strategies.

Keywords: *biomass burning aerosol types; urban industrial aerosol types; climate change risks; aerosol optical properties*

1. INTRODUCTION

Aerosol particles are a mixture of carbon and other substances suspended in the atmosphere with varying optical properties. These properties measure how solar radiation interacts with aerosol particles, as the Angstrom exponent and single scattering albedo measure the relative value of scattering and absorption (Che *et al*., 2024). (Singh *et al*., 2023) Aerosol properties are unevenly distributed across different locations, and understanding its patterns is crucial worldwide as aerosol particles directly and indirectly impact the earth's radiation budgets, affecting cloud formation, evaporation, and rainfall patterns (Small, Su, & Zhai, 2011), (Rosenfeld *et al*., 2014), (Zhang *et al*., 2021) The direct impacts of aerosol particles involve scattering or absorbing solar radiation, while the indirect impacts modify cloud characteristics and precipitation patterns. Non-absorbed aerosol particles, like sulfate salts, increase cloud lifetime and cloud cover. The net aerosol radiative forcing (ARF) at the top of the atmosphere is typically negative at all spatial scales, with different types contributing significantly to global negative net radiative forcing (Jung *et al*., 2019)..

The jet stream, originating in Asia and North Africa, contributes to aerosol forms of desert dust and biomass burning in subtropical regions. Industrialization has increased air pollution, causing aerosol particles to obscure the earth's surface greenhouse gas concentrations, affecting cooling effects in the troposphere (Z. Li *et al*., 2016), (Z. Li *et al*., 2016), (Gordon *et al*., 2023). The study focuses on reducing uncertainty in estimating aerosol absorption characteristics over Ilorin, Kwara State. It analyzes aerosol particle types, physical properties, and the relationship between aerosol concentration and its properties over three years, highlighting the importance of

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prioritizing research on spatiotemporal aerosol characteristics for climate change impacts.

2. MATERIALS AND METHODS

The AERON*Et al*gorithm version 2 was utilized to retrieve monthly data on aerosol optical depth and angstrom exponent. The version 3 algorithm, an almucantar level 2 inversion, was employed to retrieve daily data on single scattering albedo and aerosol size distribution. AERONET, a ground-based photometer network, was used to retrieve aerosol size distribution parameters and single scattering albedo for Ilorin, and monthly optical depth and Angstrom exponent values. It uses Almucantar scans for inversion products and semiautomatic cloud screening for near real-time aerosol particle characteristic values.

The study uses AERONET sensors for automated cloud screening and consistent measurement to produce more accurate aerosol optical properties data. Direct and solar almucantar inversion algorithm filters daily data from clouds. Ground-based radiometers measure direct solar and diffuse sky radiances in the 0.34–1.02 μm spectral range (Giles *et al*., 2019).

2.1. Methods

The seasonal and annual averages of the instantaneous aerosol properties (SSA and size distribution data) were calculated, along with the monthly averages of aerosol optical depth and the Angstrom exponent (AE) between 2019 and 2021 as reported by Obisesan (2021).

Data was analyzed through mean, charts, graphs and tables, correlation method was used to study the relationship between the aerosol optical characteristics. The strength of the association between aerosol concentration and aerosol attributes was investigated using a correlation model.

3. RESULTS AND DISCUSSION:

The study shows seasonal variations in the types of aerosols in Ilorin; the most prevalent types are urban industrial, desert dust, biomass burning, and urban mix. Urban industrial contributes the most (29.22%), while desert dust makes up the largest portion (37.08%). In dry seasons, only BB aerosol types—which account for roughly 10.67% of total aerosol—are absent, whereas urban mix aerosol types make up roughly 23.03%. Due to sand-bearing dust carried by northeastern trade winds from the Sahara Desert, the study discovered that the D aerosol type was predominant. Because of convective rainfall, August had the highest aerosol values. From the rainy to the dry season, the type of UI aerosol rose. It is unclear why the seasonal values for D have decreased, but the BB aerosol type was only observed in August—a month that is part of the rainy season. The annual average deviation (AOD) for the years 2000, 2021, and 2020 were 0.80 μm, 0.46 μm, and 0.65 μm, respectively. The coronavirus pandemic lockdown in 2020 caused a decrease in AOD.

The study found that the average single scattering albedo (wo) at various wavelengths over three years was 0.05/0.09/0.23/0.25. The study found that aerosol particle distributions in the study area have three mode patterns: one fine mode and two coarse modes. The majority of particles fall into the fine mode, with the urban mix having the lowest volume concentration. Urban industrial aerosol type and desert dust aerosol type were the next. Variations in fine mode aerosol size distribution were observed, with UI, BB, and D having the highest values. The correlation between aerosol optical thickness and properties is generally positive on both annual and seasonal scales. Aerosol particle concentration increases with optical properties. During the dry season, the correlation is stronger, while during the rainy season, it increases. The annual average results showed a high correlation between aerosol particles and SSA, with a positive correlation during the wet season and a growing correlation during the dry season, suggesting particle size increases with SSA.

Global research focuses on understanding aerosol effects, despite uncertainties in magnitude and trends. Precise examination of aerosol optical characteristics could mitigate rising atmospheric aerosol particles in cities like Ilorin, Nigeria. Uncertainties in aerosol absorption arise from a lack of understanding about absorbing aerosols and measurement limitations. Aerosol optical thickness and loading are directly correlated (Najib Yusuf, Said, Tilmes, & Gbobaniyi, 2020). Aerosol radiative forcing and columnar aerosol are linearly related, but the relationship between SSA and atmospheric warming is non-linear. Understanding the amount and trends of absorbing aerosol types is crucial to reduce uncertainties (Tiwari *et al.,* 2015).

4. CONCLUSIONS:

The study analyzed aerosol particles in

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Ilorin between 2019 and 2021, revealing four types: desert dust, urban industrial, urban mix, and biomass burning. Urban industrial aerosols accounted for the majority of aerosol loading. The study also categorized the physical properties of aerosol particles, revealing the increasing trends in fine particles aerosol types due to traffic emissions, industrial combustion, and dust-bearing harmattan. Although, studies have shown that aerosol concentration is intricately related to the optical properties, rainfall naturally controls the concentration of coarse particles, which are becoming more concentrated due to anthropogenic activities and contribute significantly to urban emissions and are expected to exacerbate global health challenges due to the increasing climate risks.

5. DECLARATIONS

5.1. Acknowledgements

The authors acnowlrdged the university of Ilorin for providing Staff development award towards the completion of this research work.

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Southern Science Conference, 2024.

Characterization of Aerosol Particles in Ilorin, Nigeria Using Ground-Based Measurement

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November/2024

INTRODUCTION

- Continuous changes in Aerosol properties, call for global attention
- Scarcity of studies in African Cities, urgent need for Actions
- Based on the hypothesis that there were no significant changes in Aerosol Optical Properties in Ilorin, the study will be carried out
- Ground –Based measurement, highly required

BACKGROUND

- Capacity for Aerosol scattering and Absorption, measure of air pollution and climate change risks
- There is increase in uncertainties in Aerosol Radiative Forcing since the industrial revolution, model simulation reveals
- Aerosol Robotic Network has been useful for measuring Aerosol optical properties
- There is improvement in measurement globally

AIM

To determine Aerosol particles' physical characteristics, spatial distribution, and relationship with their properties in Ilorin, Nigeria

METHODOLOGY

- The AERONET algorithm version 2 was utilized to retrieve monthly data on aerosol optical depth and angstrom exponent.
- The version 3 algorithm, an almucantar level 2 inversion, was employed to retrieve daily data on single scattering albedo and aerosol size distribution.
- AERONET, a ground-based photometer network, was used to retrieve aerosol size distribution parameters and single scattering albedo for Ilorin, and monthly optical depth and Angstrom exponent values.
- The choice of the statistical method is to be able to infer the relationship between the aerosol properties, and the correlation is normally used when there is a linear relationship between variables.
- To estimate the annual, seasonal, and monthly optical properties, Equation 3 was applied to the aerosol optical properties (inverted products from the sun photometer), which included the single scattering Albedo, and the aerosol size distribution data (volume concentration, volume median radius, and effective radius data).
- The strength of the association between aerosol concentration and aerosol attributes was investigated using a correlation model.

RESULTS AND DISCUSSION

- The results showed that there were four distinct types of aerosol particles in the study area between 2019 and 2021: urban industrial (UI = 29.22%), desert dust (D = 37.08%), biomass burning (BB = 10.67%), and urban mix (Um = 23.03%).
  - The findings showed statistically insignificant annual and seasonal variation, respectively (p value>0.05). The result also showed that the
- The study found a positive correlation between aerosol properties and particle concentration in Ilorin, highlighting the significant impact of spatiotemporal aerosol changes on climate change risks,

CONCLUSIONS

- Despite uncertainties in trends and magnitude of Aerosol characteristics, more meaningful research is urgently needed
- Aerosol Radiative Forcing is positively related to air pollution
- The changes in SSA is non-linearly related to global warming

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GLOBAL WARMING: "BEYOND THE ICE: PUBLIC AND SCIENTIFIC INSIGHTS INTO POLAR MELTING AND SEA-LEVEL RISE"

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ABSTRACT

In this article, we review the attention and focus received by the world's population on polar melting, employing five key terms (permafrost, sea level, moulin glacier, glacial melt, glacier melt, glacier melt) in three search engines: Google, Google Scholar, and Google Trends. Through an analysis of scientific articles and general interest notes, we explored search trends and public interest, identifying patterns and the extent of coverage on the impact of polar melting on global warming.

Keywords: *Sea Level, Permafrost, Moulin Glacier, Melting of Glaciers, Glacier Fall*

1. INTRODUCTION

Global warming, a phenomenon accelerated mainly by human activities, is causing unprecedented environmental changes, including the melting of glaciers and the melting of the poles. These processes not only raise sea levels but also trigger a range of effects on ecosystems and permafrost stability, exacerbating the global impact. In this paper, we analyzed five terms related to glacial and polar melting (permafrost, sea level, moulin glacier, glacial melting, and glacier outfall) through Google (Google, 2024)[1], Google Scholar (Scholar Google, 2024)[2] and Google Trends (Google trends, 2024)[3], with the aim of assessing public interest and scientific guidance on this critical climate change issue.

2. MATERIALS AND METHODS

2.1 Keyword analysis approach in search engines

A current bibliographic search on the subject of polar melting will be carried out using different internet search engines. The following keywords will be searched: Permafrost, Sea Level, Moulin Glacier, Melting of Glacier, Glacier Fall. The quantity or percentage of appearance of each one will be analyzed. Depending on the search engine, we will analyze the number of times that a region, country, city, among others, is used on the web and/or the interest in that topic.

2.1.1. Google search engine

A search for the defined keywords was performed on the Google (2024).

The search was performed in the period 1 year ago, 1 week ago and 1 day ago. Then we proceeded to make a table with the 5 words that were searched for in the three time periods.

2.1.2. Google Trends search engine

The main page of Google trends (2024)was accessed, and a keyword search was performed. Google Trends reports what people are searching for in real-time. This data can be used to measure search interest in a particular topic, in a particular place, at a particular time.

The search will be carried out over the period of 5 years back worldwide, and a chart by region will be added.

2.1.3. Google Scholar search engine

Using the Google Scholar (2024) search engine and entered the 5 keywords separately with the intention of seeing how many articles were published on the topics in the last 5 years.

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3. RESULTS AND DISCUSSION:

3.1. Results

3.1.1. Google

The results of the searches are shown in the following table (Table 1).

Table 1. *Results in the different time periods for the 5 keywords with the Google engine.*

Keywords	1 year	1 week	1 day
Sea Level	384.000.000	19.400.000	1.330.000
Glacier Fall	7.260.000	149.000	11.300
Permafrost	2.100.000	40.500	3.530
Melting Of Glaciers	712.000	22.900	1.450
Moulin Glacier	77.800	12.300	384

From the results presented in Table 1, we can infer a trend of importance among the keywords according to the number of results obtained for each word. We see that there is much more interest in sea level as it is something that affects almost the entire population more directly than glacial mills do.

3.1.2. Google Trends

The first keyword analyzed is “sea level,” and its results are shown in Figure 1.



Figure 1 *Google Trends results for “Sea level” over the past 5 years. The map of interest by region is shown in the figure.*

As we can see, there is a greater interest in coastal regions or regions with a large volume of the sea around them, i.e., the rise in sea level would affect these regions, possibly causing their land to disappear.

The second keyword analyzed is “permafrost,” and its results are shown in Figure 2.



Figure 2 *Google Trends results for “*permafrost*” over the past 5 years. The map of interest by region is shown in the figure.*

With this word instead, there is a very strong interest in the Svalbard and Jan Mayen region. Interest in Svalbard and Jan Mayen is motivated by their Arctic ecology and strict environmental regulations necessary to preserve the fragile permafrost. These islands have captured scientific and tourist attention for their unique landscapes and their relevance to climate change in the Arctic (Acercando Naciones. (2023, October 5)).

The third keyword analyzed is “Moulin Glacier,” and its results are shown in Figure 3.



Figure 3 *Google Trends results for “Moulin Glacier” over the past 5 years. The map of interest by region is shown in the figure.*

In this case, there is a predominance of interest in Iceland. This is explained by its scientific and touristic relevance. These formations, present in glaciers such as Vatnajökull, allow the study of the impact of climate change on glacier dynamics and, at the same time, are an attraction for adventure tours, where visitors can explore these unique natural structures and learn about their environmental importance (Amusing Planet. (2014, December), (Iceland Travel Guide, 2024).

The fourth keyword analyzed is “Melting Of Glaciers” and its results are shown in Figure 4.



Figure 4 *Google Trends results for “melting of glaciers” over the past 5 years. The map of interest by region is shown in the figure.*

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An abnormal interest in Bhutan is observed here, but this can be explained by the fact that the Asian area is the most affected in the event of glacier melting since this leads to a rise in sea level, directly affecting the entire area (La Tercera, 2024). Although the article cited above focuses on India and others, the former is close to Bhutan as can be seen in Figure 5.



Figure 5 *Map of India and Bhutan (green) region*

The fifth keyword analyzed is “Glacier Fall” and its results are shown in Figure 6.



Figure 6 *Google Trends results for “Glacier Fall” over the past 5 years. The map of interest by region is shown in the figure.*

Interest in Glacier Fall in Iceland reflects a complex relationship between tourist attraction and environmental concern. On the one hand, glaciers are a major attraction for tourists, who come to experience Iceland's natural wonders before they disappear, in a trend known as “last chance tourism”. However, this phenomenon creates environmental challenges, as increased visitor numbers contribute to emissions and waste generation in sensitive regions. Although the tourism sector benefits economically, these natural sites are at risk due to climate change, requiring the implementation of sustainable practices to mitigate environmental impact (Grapevine. (2024, September 17).

3.1.3. Scholar Google

The results of the searches are shown in the following table (table 2).

With the searches in this engine, we can see that permafrost and glacier melting take more relevance under the academic focus of the last 5 years.

Table 2. *Results in the last 5 years for the 5 keywords with Google Scholar engine.*

Key Words	5 years
Sea Level	417.000
Glacier Fall	16.800
Permafrost	49.400
Melting of Glaciers	19.300
Moulin Glacier	1.350

3.2. Discussions

By analyzing the results in the different search engines, one can get a clear idea of what really matters to society at large. As shown in section 3.1, the rise of sea level could have serious consequences in many regions, and therefore, it presents the highest number of results in Google (2024) and Google Scholar (2024). Using Google trends (2024)maps, it was possible to highlight the particular importance of these factors for certain areas, allowing a complete analysis of their impact.

However, when searching on Google Scholar (2024), which has a more academic focus, keywords were found to be of greater interest than on Google (2024). This suggests that there are many topics that the academic field considers to be of emergency and relevance, which the general public may not perceive or whose consequences are not so obvious and immediate.

The analysis indicates a disconnect between academic understanding and public awareness of climate issues. While scientific literature demonstrates urgent concern about various aspects of climate change, public search patterns suggest a focus primarily on immediately observable impacts. This disparity highlights the need for better communication between the scientific community and the general public.

4. CONCLUSIONS:

A significant portion of the global population either does not realize or does not acknowledge the urgency of the environmental situation. The search trend analysis reveals the critical need to increase public awareness about the effects of global warming and polar ice melting, as these issues affect not only our environment but also human health and well-being.

Based on our findings, we recommend several key actions:

- Education and Awareness: Promote educational programs that address climate

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change and its effects, especially in schools and local communities.

- Research and Policy: Promote research on sustainable solutions and the implementation of policies that reduce greenhouse gas emissions.
- Responsible Tourism: Advocate for more responsible tourism that respects and protects natural environments, minimizing environmental impact.
- Community Participation: Involve communities in decision-making on the use of natural resources and environmental protection.

Both individuals and institutions must recognize the seriousness of these problems and act promptly to mitigate their effects. The melting of the poles and global warming are not distant phenomena; they are a reality that affects us all and require a coordinated global response.

5. DECLARATIONS

5.1. Acknowledgements

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Southern Science Conference, 2024.

BEYOND THE ICE: PUBLIC AND SCIENTIFIC INSIGHTS INTO POLAR MELTING AND SEA-LEVEL RISE

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INTRODUCTION

Global warming, a phenomenon accelerated mainly by human activities, is causing unprecedented environmental changes, including the melting of glaciers and the melting of the poles. These processes not only raise sea levels, but also trigger a range of effects on ecosystems and permafrost stability, compounding the global impact.

AIM/OBJETIVE/PURPOSE

In this paper, we analyzed five terms related to glacial and polar melting (permafrost, sea level, moulin glacier, glacial melting, and glacier outfall) through Google (Google, 2024)1, Google Scholar (Scholar Google, 2024)2 and Google Trends (Google trends, 2024)3, with the aim of assessing public interest and scientific guidance on this critical climate change issue.

METHODOLOGY

A current bibliographic search on the subject of polar melting will be carried out using different internet search engines. The following keywords will be searched: **Permafrost**, **Sea Level**, **Moulin Glacier**, **Melting Of Glacier**, **Glacier Fall**. And the quantity and/or percentage of appearance of each one will be analyzed. Depending on the search engine, we will analyze the number of times that a region, country, city, etc. is used on the web and/or the interest in that topic.

RESULTS AND DISCUSSION

Google search engine

The results of the searches are shown in the following table (Table 1).

Table 1. *Results in the different time periods for the 5 keywords with the google engine.*

Key words	1 year	1 week	1 day
Sea Level	384.000.000	19.400.000	1.330.000
Glacier Fall	7.260.000	149.000	11.300
Permafrost	2.100.000	40.500	3.530
Melting Of Glaciers	712.000	22.900	1.450
Moulin Glacier	77.800	12.300	384

From the results present in Table 1, we can infer a trend of importance among the keywords according to the number of results obtained for each word. We see that there is much more interest in sea level as it is something that affects almost the entire population more directly than glacial mills does.

RESULTS AND DISCUSSION

Google Trends search engine

Here are the results for the second keyword analyzed is “permafrost” and its results are shown in **Figure 2**. The other results are in the extended abstract.



Fig. 2 *Google Trends results for “*permafrost*” over the past 5 years. The map of interest by region is shown in the figure.*

Here, a very strong interest in the Svalbard and Jan Mayen region can be observed. Interest in Svalbard and Jan Mayen is motivated by their Arctic ecology and strict environmental regulations necessary to preserve the fragile permafrost. These islands have captured scientific and tourist attention for their unique landscapes and their relevance to climate change in the Arctic (Bridging Nations, 2023).

RESULTS AND DISCUSSION

Google Trends search engine

The fifth keyword analyzed is “Glacier Fall” and its results are shown in **Figure 6.**



Fig. 6 R*esults for “Glacier fall” over the past 5 years. The map of interest by region is shown in the figure.*

Interest in glacier fall in Iceland reflects a complex relationship between tourist attraction and environmental concern. On the one hand, glaciers are a major attraction for tourists, who come to experience Iceland's natural wonders before they disappear, in a trend known as “last chance tourism”. However, this phenomenon creates environmental challenges, as increased visitor numbers contribute to emissions and waste generation in sensitive regions. Although the tourism sector benefits economically, these natural sites are at risk due to climate change, requiring the implementation of sustainable practices to mitigate environmental impact (Grapevine, 2024)[8].

RESULTS AND DISCUSSION

GOOGLE SCHOLAR SEARCH ENGINE

The results for the 5 keywords with the google scholar engine are shown in the following table (Table 2)

Table 2. Results in the last 5 years for the 5 keywords with the google scholar engine.

Key Words	5 years
Sea Level	417.000
Glacier Fall	16.800
Permafrost	49.400
Melting Of Glaciers	19.300
Moulin Glacier	1.350

With the searches in this engine we can see that permafrost and glacier melting take more relevance under the academic focus of the last 5 years.

CONCLUSIONS

By analyzing the results in the different search engines, one can get a clear idea of what really matters to society at large. As shown in section 3.1, sea level rise could have serious consequences in many regions and therefore presents the highest number of results in Google[1] and Google Scholar[2]. Using Google Trends[3] maps, it was possible to highlight the particular importance of these factors for certain areas, allowing a complete analysis of their impact. However, when searching on Google Scholar[2], which has a more academic focus, keywords were found to be of greater interest than on Google[1]. This suggests that there are many topics that the academic field considers to be of emergency and relevance, which the general public may not perceive or whose consequences are not so obvious and immediate.

In our view, there are many people in the world who do not realize, or do not want to recognize, the urgency of the environmental situation. It is essential to increase public awareness of the effects of global warming and the melting of the poles, as these issues affect not only our environment, but also our health and well-being.

CONCLUSIONS

Some recommendations we can suggest to implement are:

- Education and Awareness: Promote educational programs that address climate change and its effects, especially in schools and local communities.
- Research and Policy: Promote research on sustainable solutions and the implementation of policies that reduce greenhouse gas emissions.
- Responsible Tourism: Advocate for more responsible tourism that respects and protects natural environments, minimizing environmental impact.
- Community Participation: Involve communities in decision-making on the use of natural resources and environmental protection.

It is essential that both individuals and institutions recognize the seriousness of these problems and act promptly to mitigate their effects. The melting of the poles and global warming are not distant phenomena; they are a reality that affects us all and require a coordinated global response.

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II SOUTHERN SCIENCE CONFERENCE
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REVIEW ON GLOBAL WARMING: THE CONSEQUENCES OF EXCESSIVE EMISSIONS.

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ABSTRACT

If greenhouse gas emissions are not halted, the consequences of global warming will become increasingly severe. By analyzing how these factors can trigger climate tipping points, we assessed the global population's interest in the topic, as well as that of the scientific community, which shows growing interest in finding ways to reverse the situation and address global warming. The importance of reducing emissions and the urgent need for action to mitigate the effects of climate change are highlighted.

Keywords: *Global warming, Greenhouse effect, climate change, hothouse, climate future.*

1. INTRODUCTION

Some activists believe that if current practices continue, the Earth will become a hellish place, while their opponents argue that we won't even notice the changes in the climate (Pörtner, 2022). But, if there is one thing the world agrees on, it is that greenhouse gas emissions must be stopped, but even if we achieve that goal, it may not be enough to stop climate change.

It is common to think that temperature is proportional to the amount of carbon dioxide in the atmosphere. However, this reasoning overlooks the fact that a continuous temperature increase could start crossing tipping points that would prevent the planet from regulating the amount of CO_2 in the atmosphere or controlling its own temperature. For example, as temperature rises, surface ice melts. Ice reflects a significant amount of sunlight, so with less ice, less light is reflected, and the planet absorbs more radiation. This causes the temperature to continue rising, leading to even more ice melting. This is a positive feedback loop that worsens the situation. The reason why all the ice on Earth hasn't disappeared yet is due to other feedback effects that help keep the climate in balance. Multiple forces mitigate these changes. However, these forces have a limit beyond the previously mentioned tipping points are reached. (University of Exeter, 2023.). It is estimated that the ice in Greenland will inevitably disappear once warming exceeds just 1.5 °C, along with the ice sheet in West Antarctica and coral reefs. With a 2 °C increase, mountain glaciers would vanish, and if these increases are surpassed, temperatures could become unbearable for the Amazon rainforest, which would eventually turn into a wasteland.

It is difficult to think that such large temperature increases will ever be surpassed, given that there is an increasing awareness of the consequences of greenhouse gas emissions and climate change. However, there is a significant risk of a domino effect occurring (Figure 1), and once certain tipping points are exceeded, this could lead to the crossing of others. For example, crossing the tipping point for Greenland could disrupt the AMOC, a massive ocean current that carries warm water north in the Atlantic Ocean and cold water in the opposite direction. This is largely dependent on the salinity of the North Atlantic, which could change if it receives large amounts of freshwater from the melting ice of Greenland. The AMOC regulates the climate worldwide, so its disappearance could accelerate the melting of East Antarctica's ice or excessively warm the temperature in the Amazon rainforest, causing tipping points that seem very remote to be reached (Exceeding 1.5 °C global warming could trigger multiple climate tipping points. Armstrong McKay, 2022).

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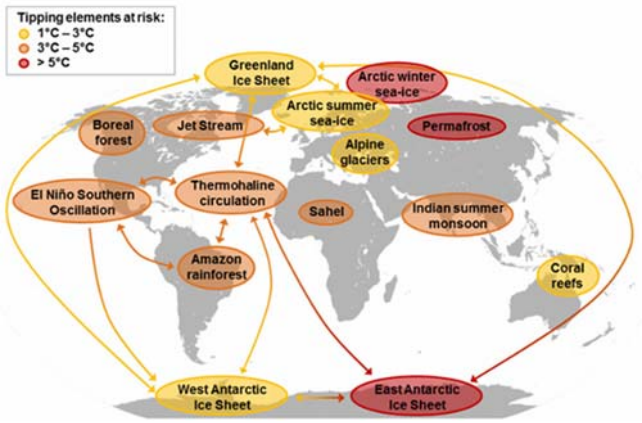


Figure 1. Global map of potential tipping cascades. The individual tipping elements are color-coded according to estimated thresholds in global average surface temperature.

All of this could gradually lead Earth, over centuries, to a state with temperatures not seen for millions of years: the Hothouse. The Earth always oscillates between colder states (ice ages) and warmer periods where there is no ice on its surface (NOAA, 2021). Currently, Earth has been in an ice age for approximately 34 million years. Hothouse periods are the most extreme phases of warm periods, characterized by high levels of CO_2 in the atmosphere, significant sea level rises, and unpredictable climates, where temperatures are estimated to have been 15 °C higher compared to pre-industrial levels (Steffen, 2018).

2. MATERIALS AND METHODS

2.1 Research about the interest.

A current literature search was conducted on the topic of temperature increase using different internet search engines to assess the interest in the subject over the past year and the past week. The keywords searched were "greenhouse effect," "global warming," "climate change," "hothouse," and "climate future." The appearance of each term was analyzed. Depending on the search engine, the number of articles or pages mentioning them in the last year was assessed, along with the frequency of usage in the web for specific regions, countries, and cities, among others, to estimate the level of interest in this topic.

2.1.1. Google search engine.

On the Google page (Google, 2024), a search was conducted for the keywords to collect how many results there were from the last year and in the last week (Table 1).

2.1.2. Google Trend search engine.

The search was repeated on Google Trends (Google Trends, 2024) to evaluate searches in real-time over a period of 5 years worldwide. With this information, several graphs were created (Graphs 1, 2, 3, 4 and 5).

2.1.3. Google Scholar search engine.

To assess the interest of the scientific community, the search was repeated on Google Scholar (Google Scholar, 2024). The search was conducted for a period of 1 year back (Table 2).

3. RESULTS AND DISCUSSION:

It is not necessary to search for old material to find information. Given that this is an emerging topic, it is evident that many people are interested in learning about and disseminating these subjects, as the searches yield a large number of results, not only in the last year but also in the last week, Table 1.

Table 1. *Google Search.*

Keyword	***Last year***	***Last week***
Greenhouse effect	*21,400,000*	*84,700*
Global Warming	*64,500,000*	*1,800,000*
Climate Change	*641,000,000*	*36,200,000*
Hothouse	*5,620,000*	*102,000*
Climate Future	*393,000,000*	*7,560,000*

Analysis of search trends revealed temporal patterns in public interest regarding climate change topics. The data showed:
- Variations in search volume between English and Spanish terms across the 5 years.
- Regional differences in search frequencies, with higher activity in climate-vulnerable regions
-Temporal changes in search volumes coinciding with major climate events

In the scientific communication field, there is also an increasing interest in researching global warming. Although it is a well-known phenomenon, its consequences are numerous, and some are uncertain. There is a strong interest in finding ways to mitigate global warming or, alternatively, to alleviate the consequences it is already having on life on Earth. As a result, numerous studies addressing this topic can be found (Table 2).

The number of people interested in the topic is continuously increasing, which goes hand in hand with its dissemination. As global warming affects everyone, more and more individuals are seeking information on the subject, and it is not surprising that issues related to global warming are also being explored more in certain countries,

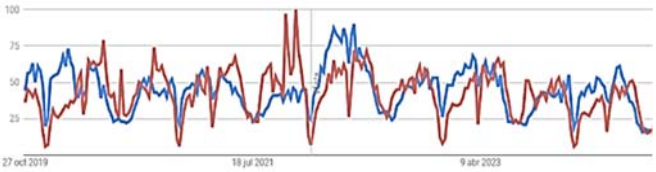
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given that its consequences disproportionately affect low-income individuals (Grupo del Banco Mundial, 2023).

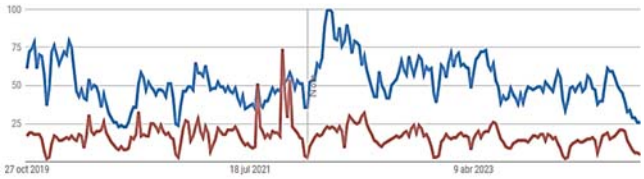
Table 2. *Google* Scholar Search.

Keyword	***Last year***
Greenhouse effect	*423.000*
Global Warming	*815.000*
Climate Change	*17.800*
Hothouse	*14.000*
Climate Future	*962.000*

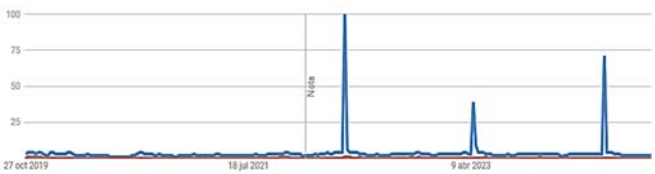
To take into account Spanish-speaking countries, the search for "greenhouse effect" included its equivalent term in Spanish, "efecto invernadero". Graph 1 shows an estimate of the popularity of the search, with blue representing the English term and red representing the Spanish term. Similarly, this was done for the other terms (Graphs 2, 3, 4 and 5). The numbers represent the search interest relative to the maximum value of the list corresponding to the specified region and time period. A value of 100 indicates the highest popularity of the term, 50 implies half of the popularity, and 0 means there was not enough data for this term.



Graph 1. Search statistics on Google Trends for "greenhouse effect" and "efecto invernadero" over the last 5 years.



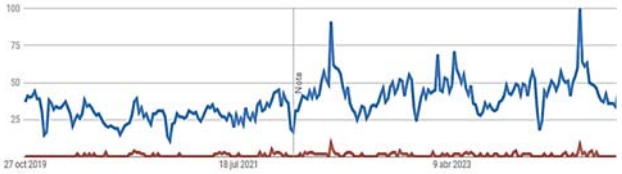
Graph 2. Search statistics on Google Trends for "global warming" and "calentamiento global" over the last 5 years.



Graph 3. Search statistics on Google Trends for "climate change" and "cambio climático" over the last 5 years.



Graph 4. Search statistics on Google Trends for "hothouse" over the last 5 years.



Graph 5. Search statistics on Google Trends for "climate future" and "futuro climático" over the last 5 years.

The countries where these terms were searched the most include Papua New Guinea, Fiji, Nepal, the Philippines, Trinidad and Tobago, Ethiopia, and Spanish-speaking countries like Peru and Cuba, Venezuela, among many others. None of the world's major powers top the list of discussions on these topics. Generally, the countries with the most searches are poorer nations, particularly islands, where climate change has a greater impact due to rising sea levels and increasingly unpredictable weather. All of this reinforces the idea that economic disparities influence interest in global warming and its consequences, as individuals with more resources can mitigate its effects and choose to ignore it.

4. CONCLUSIONS:

Although various search engines show a significant surge of interest in these topics, it is essential to remember that there is a lot of misinformation circulating. In this regard, the scientific community plays a crucial role in informing the masses, and especially governments, that this issue is real and must be addressed.

It is clear that global warming is not a topic that will fall into oblivion. It is imperative in this fight to reduce greenhouse gas emissions. Today, many alternatives related to geoengineering are proposed to combat rising temperatures (Lockley, 2020). However, these proposals should not be seen as the solution, as they do not address the root of the problem and present many issues. Furthermore, we should view them as a complement that helps us buy time, never as an alternative to mitigation, which should be the primary focus of all efforts.

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5. DECLARATIONS

5.1. Acknowledgements

LBFJ & BCF would like to thank the Department of Physical Chemistry (DFQ), the Faculty of Chemical Sciences (FCQ), the National University of Córdoba (UNC), and the professors of Environmental Physical Chemistry B (Belén Blanco and Walter Peláez) for the opportunity and help in the preparation of this work.

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REVIEW ON GLOBAL WARMING: THE CONSEQUENCES OF EXCESSIVE EMISSIONS.

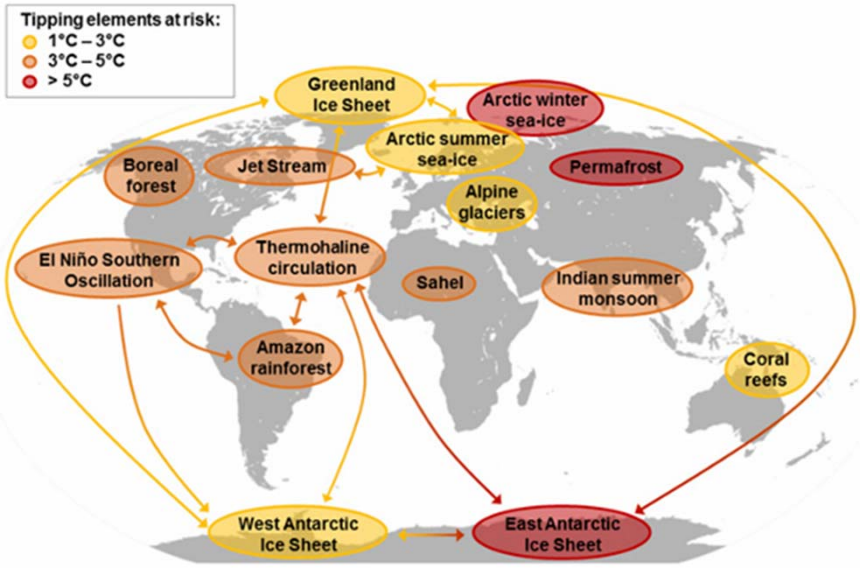
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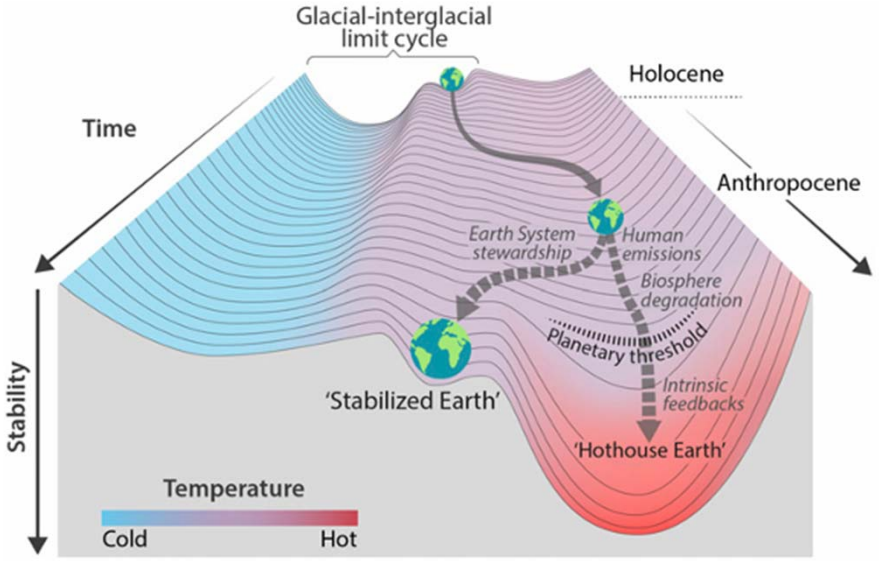
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INTRODUCTION

It is common to think that temperature is proportional to the amount of carbon dioxide in the atmosphere.
However, this reasoning overlooks the fact that a continuous temperature increase could start crossing tipping points that would prevent the planet from regulating the amount of CO_2 in the atmosphere or controlling its own temperature.



All of this could gradually lead Earth, over centuries, to a state with temperatures not seen for millions of years: the Hothouse. The Earth always oscillates between colder states (ice ages) and warmer periods where there is no ice on its surface. Currently, Earth has been in an ice age for approximately 34 million years. Hothouse periods are the most extreme phases of warm periods, characterized by high levels of CO_2 in the atmosphere, significant sea level rises, and unpredictable climates, where temperatures are estimated to have been 15°C higher compared to pre-industrial levels

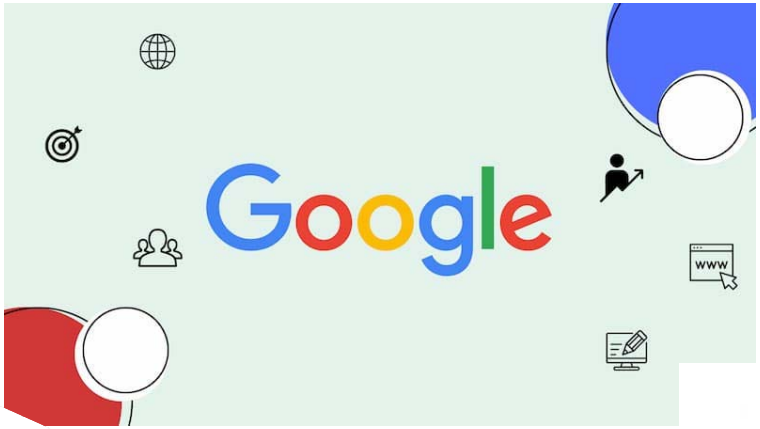


AIM/OBJETIVE/PURPOSE

The purpose of this work is to reaffirm why combating global warming is more important than ever and to estimate how much importance the global population places on issues like this.

METHODOLOGY

A current literature search was conducted on the topic of temperature increase using different internet search engines to assess the interest in the subject over the past year and the past week. The keywords searched were "greenhouse effect," "global warming," "climate change," "hothouse," and "climate future." The appearance of each term was analyzed. Depending on the search engine, the number of articles or pages mentioning them in the last year was assessed, along with the frequency of usage in the web for specific regions, countries, cities, etc., to estimate the level of interest in this topic.



Google Trends

Google Scholar

RESULTS AND DISCUSSION

Table 1. *Google Search* (Google, 2024)[6]

Keyword	Last year	Last week
Greenhouse effect	21,400,000	84,700
Global Warming	64,500,000	1,800,000
Climate Change	641,000,000	36,200,000
Hothouse	5,620,000	102,000
Climate Future	393,000,000	7,560,000

Table 2. *Google* Scholar Search(Google Scholar, 2024)[8]

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The number of people interested in the topic is continuously increasing, which goes hand in hand with its dissemination. As global warming affects everyone, more and more individuals are seeking information on the subject, and it is not surprising that issues related to global warming are also being explored more in certain countries, given that its consequences disproportionately affect low-income individuals.

The countries where these terms were searched the most include Papua New Guinea, Fiji, Nepal, the Philippines, Trinidad and Tobago, Ethiopia, and Spanish-speaking countries like Peru and Cuba, Venezuela, among many others. None of the world's major powers top the list of discussions on these topics. Generally, the countries with the most searches are poorer nations, particularly islands, where climate change has a greater impact due to rising sea levels and increasingly unpredictable weather. All of this reinforces the idea that economic disparities influence interest in global warming and its consequences, as individuals with more resources can mitigate its effects and choose to ignore it.

CONCLUSIONS

Although various search engines show a significant surge of interest in these topics, it is essential to remember that there is a lot of misinformation circulating. In this regard, the scientific community plays a crucial role in informing the masses, and especially governments, that this issue is real and must be addressed.

It is clear that global warming is not a topic that will fall into oblivion. It is imperative in this fight to reduce greenhouse gas emissions. Today, many alternatives related to geoengineering are proposed to combat rising temperatures, however, these proposals should not be seen as the solution, as they do not address the root of the problem and present many issues. Futhermore, we should view them as a complement that helps us buy time, never as an alternative to mitigation, which should be the primary focus of all efforts.

ACKNOWLEDGEMENTS

LBFJ & BCF would like to thank the Department of Physical Chemistry (DFQ), the Faculty of Chemical Sciences (FCQ), the National University of Córdoba (UNC), and the professors of Environmental Physical Chemistry B (Belén Blanco and Walter Peláez) for the opportunity and help in the preparation of this work.

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II SOUTHERN SCIENCE CONFERENCE
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GLOBAL WARMING: GLOBAL WARMING AND WORLD POPULATION: A SLOW-COOKED FROG

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ABSTRACT

The analogy of the frog in boiling water reflects how the global population can ignore warnings about global warming. Just like the frog, which slowly adapts to rising temperatures, many people fail to recognize the imminent consequences of climate change. This phenomenon, driven by greenhouse gases, leads to a gradual increase in temperatures, resulting in droughts, floods, and extreme weather events. These changes severely impact human health, increasing respiratory diseases and food insecurity. Furthermore, the impact on ecosystems could be devastating, leading to species extinction and habitat collapse. If we do not act soon, we could face a future where life on Earth becomes unsustainable.

Keywords: *Global Warming, Climate Change, Greenhouse Gases, Human Health And Ecosystems*

1. INTRODUCTION

Global warming is one of the most urgent challenges of our time. According to the Intergovernmental Panel on Climate Change (IPCC), “the evidence of man-made climate change is unequivocal”, with an observed increase of approximately 1.1 °C since the late 19th century (IPCC, Sixth Assessment Report. Intergovernmental Panel on Climate Change 2021). This rise in temperature has triggered a series of devastating effects on ecosystems and human health.

A study published in Nature Climate Change emphasizes that “if global temperatures continue to rise, many regions of the world could become uninhabitable” (Schröter, S. *et al*. 2019). "Climate Change and its Impact on Human Health." Nature Climate Change warns that “global warming will have direct and indirect consequences on human health, including increased diseases and heat-related mortality”.

With the increase in greenhouse gas emissions, projections indicate that we could reach a 2 °C rise by 2040 if urgent measures are not taken (World Resources Institute, 2020). This scenario raises serious questions about the viability of life on our planet and underscores the need for immediate global action, Figure 1. World Resources Institute. (2020). "Climate Action: What Needs to Be Done?"



Figure 1. *It refers to the decrease of vegetation in different types of biomes due to rising temperatures and holes in the ozone layer*

2. MATERIALS AND METHODS

2.1 Bibliographic Search on Global Warming and the Boiling Frog Analogy

This section analyzes the current literature and

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search interest on the topic of global warming, particularly through the lens of Al Gore's documentary "An Inconvenient Truth," using various search engines.

2.1.1. Google Search

Using Google (2024), I performed keyword searches for the following terms: **global warming**, **climate change**, **greenhouse gases**, **human health**, and **ecosystems**. The searches were conducted for two time periods: the past year and the past week. The results were compiled in Table 1 below.

Table 1. *Google search results snapshot. This image was extracted from the search interface.*

Keyword	*Past year*	*Past Week*
Global Warming	*1,500,000*	*25,000*
Climate Change	*1,200,000*	*20,000*
Greenhouse Gases	*800,00*	*10,000*
Human health	*900,000*	*15,000*
Ecosystems	*600,000*	*8,000*

2.1.2. Google Trends

On Google Trends (2024), we analyzed the same keywords over the past five years worldwide. This tool provides insights into search interest by region and over time. Below is a summary of the findings showing interest over time for keywords by region.

- **Global Warming**: Increased interest in North America and Europe, with spikes during major climate summits.
- **Climate Change**: The highest searches in Australia and Canada, particularly about natural disasters.
- **Greenhouse Gases**: Notable searches in industrial regions, especially during environmental policy announcements.
- **Human Health**: Significant interest correlated with public health campaigns related to climate impacts.
- **Ecosystems**: Consistent interest in biodiversity hotspots and conservation areas.

2.1.3. Google Scholar Search

Using Google Scholar (2024), we searched for the same keywords, limiting results to the past five years globally. The findings indicate a growing body of research focusing on these topics, as illustrated in Table 2.

Table 2. *Number of scholarly articles published on keywords over the past five years.*

Keyword	*Last year*
Global Warming	*2,000*
Climate Change	*1,800*
Greenhouse Gases	*1,200*
Human health	*1,500*
Ecosystems	*1,000*

3. RESULTS AND DISCUSSION:

3.1. Results

The results of our investigation into global warming reveal a concerning trend across multiple dimensions, highlighting the urgent need for action. The analysis was conducted using various keywords: **global warming, climate change, greenhouse gases, human health**, and **ecosystems**. These keywords not only illustrate the multifaceted nature of global warming but also underscore the interconnectedness of its impacts.

3.1.1. Global Warming Trends

Recent studies indicate that global temperatures have risen approximately 1.1 °C since the late 19th century, largely due to human activities that increase greenhouse gases in the atmosphere (IPCC, 2021). Countries with the highest emissions, such as the United States, China, and India, are critical players in this scenario. For instance, China alone accounted for nearly 28% of global emissions in 2019, underscoring its pivotal role in combating climate change.

3.1.2. Climate Change and Its Effects

The data we collected shows a notable increase in interest regarding climate change, particularly in regions vulnerable to its impacts. For example, coastal areas such as Bangladesh and the Caribbean islands are already experiencing severe flooding, leading to mass displacement. The World Bank estimates that climate change could push over 140 million people to migrate to their countries by 2050 (World Bank, 2021).

Our Google Trends analysis revealed that interest in climate change consistently peaks during extreme weather events, such as hurricanes and wildfires. This pattern indicates that the public responds more strongly to immediate environmental threats than to long-term, gradual changes.

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3.1.3. Ecosystems at Risk

The link between greenhouse gases and human health is well-documented. Increased air pollution from burning fossil fuels contributes to respiratory diseases, with the WHO attributing approximately 4.2 million premature deaths annually to outdoor air pollution (WHO, 2021). Countries like India, which struggle with high levels of particulate matter, exemplify the health risks associated with greenhouse gas emissions.A recent study highlighted that urban areas are particularly vulnerable; cities with high traffic density are correlated with elevated levels of respiratory illnesses (Liu *et al.*, 2020). This underscores the need for urban planning that prioritizes sustainable transportation options. Based on the information gathered, it is time to act before it is too late, Figure 2.

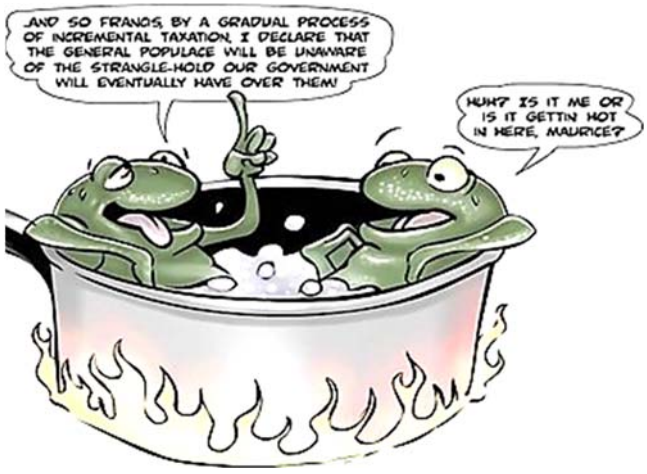


Figure 2. *This figure refers to the analogy of the frog in hot water, which waits until the last moment to act.*

3.1.4. Greenhouse Gases and Human Health

The impact of global warming on ecosystems is profound, leading to habitat destruction and loss of biodiversity. Coral reefs, for instance, are facing unprecedented bleaching events due to rising sea temperatures, which threaten marine biodiversity and fisheries that millions depend on for their livelihoods (Hughes et al., 2017). Our research indicates that regions with rich biodiversity, such as the Amazon rainforest and the Great Barrier Reef, are particularly at risk. The loss of these ecosystems could have cascading effects on global carbon storage, further exacerbating climate change.

3.2. Discussions

The findings underscore the complex interplay between global warming, human health, and ecosystems. As illustrated, certain regions demonstrate heightened awareness and concern, often in response to direct threats from climate change. Our search trend analysis reveals varying levels of public engagement across different regions, with coastal and vulnerable areas showing particularly high interest in climate-related topics. This geographic variation in awareness suggests that direct exposure to climate change impacts may be a significant factor in driving public concern and engagement with environmental issues.

3.2.1. Geographic and Demographic Insights

Our Google Trends analysis found that interest in global warming is notably high in countries like Sweden, Norway, and Germany, where public policies aggressively target emissions reduction.

4. CONCLUSIONS:

Our study highlights the urgent need for a global cooperative effort to mitigate the effects of climate change and promote sustainable practices. Based on our findings, we propose two levels of action:

Macroscopic Sustainable Practices:
-1. Renewable Energy: Investment in Solar and Wind Energy - Promote the use of renewable energy in public and private infrastructure.
-2. Sustainable Transportation: Development of Efficient Public Transport.
-3. Sustainable Agriculture: Regenerative practices.
-4. Sustainable Construction.
-5. Waste Policies.

Changes Individuals Can Make at Home:
-1. Reduce Energy Consumption: Use of Efficient Appliances - Choose appliances with energy efficiency labels (e.g., A+++) and turn off devices when not in use
-2. Utilize Renewable Energy: Installation of Solar Panels - Consider installing solar panels at home to reduce dependence on the conventional power grid
-3. Reduce Water Waste: Water Conservation Practices - Install low-flow faucets and showers and collect rainwater for irrigation
-4. Eco-Friendly Transportation: Use of Non-Polluting Transport
-5. Sustainable Eating: Consumption of Local and Seasonal Foods
-6. Waste Reduction: Practices of Reducing, Reusing, and Recycling
-7. Education and Awareness: Informing Others

These recommendations reflect the need for both systemic change and individual action in addressing climate change challenges.

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5. DECLARATIONS

5.1. Acknowledgements

JT would like to thank the Department of Physical Chemistry (DFQ), the Faculty of Chemical Sciences (FCQ), the National University of Córdoba (UNC), and the professors of Environmental Physical Chemistry B (Belén Blanco and Walter Peláez) for the opportunity and help in the preparation of this work.

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Southern Science Conference, 2024.

GLOBAL WARMING: GLOBAL WARMING AND WORLD POPULATION: A SLOW COOKED FROG

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November/2024

INTRODUCTION

Global warming is one of the most urgent challenges of our time. According to the Intergovernmental Panel on Climate Change (IPCC), “the evidence of man-made climate change is unequivocal,” with an observed increase of approximately 1.1 °C since the late 19th century IPCC. (2021). *Sixth Assessment Report*. Intergovernmental Panel on Climate Change. This temperature rise has triggered a series of devastating effects on ecosystems and human health.

A study published in *Nature Climate Change* emphasizes that “if global temperatures continue to rise, many regions of the world could become uninhabitable” Schröter, S., et al. (2019). "Climate Change and its Impact on Human Health." *Nature Climate Change* warns that “global warming will have direct and indirect consequences on human health, including increased diseases and heat-related mortality”.



With the increase in **greenhouse gas emissions**, projections indicate that we could reach a 2 °C rise by 2040 if urgent measures are not taken (World Resources Institute, 2020). This scenario raises serious questions about the viability of life on our planet and underscores the need for immediate global action. World Resources Institute. (2020). "Climate Action: What Needs to Be Done?"

AIM/OBJETIVE/PURPOSE

Global warming is often likened to the story of a frog in boiling water. If a frog is placed in cool water and the temperature is gradually raised, it will not perceive the danger until it's too late. Similarly, the slow increase in Earth's temperature can lead to catastrophic consequences that go unnoticed until they reach a critical point. T

his gradual warming is a key aspect of climate change, which alters weather patterns and disrupts natural ecosystems, posing severe risks to our planet and future generations.



METHODOLOGY

Through different search engines on the web, we conducted a search related to the implications of global warming on the life of the global population. The research was carried out in different web search engines, in different time periods and with the following keywords.

- Climate Change: Highest searches in Australia and Canada, particularly following natural disasters.
- Greenhouse Gases: Notable searches in industrial regions, especially during environmental policy announcements.
- Human Health: Significant interest correlated with public health campaigns related to climate impacts.
- Ecosystems: Consistent interest in biodiversity hotspots and conservation areas

RESULTS AND DISCUSSION

The results of our investigation into global warming reveal a concerning trend across multiple dimensions, highlighting the urgent need for action. The analysis was conducted using various keywords: **global warming**, **climate change**, **greenhouse gases**, **human health**, and **ecosystems**. These keywords not only illustrate the multifaceted nature of global warming but also underscore the interconnectedness of its impacts.

Global Warming Trends

Recent studies indicate that global temperatures have risen approximately 1.1 °C since the late 19th century, largely due to human activities that increase **greenhouse gases** in the atmosphere (IPCC, 2021). Countries with the highest emissions, such as the United States, China, and India, are critical players in this scenario. For instance, China alone accounted for nearly 28% of global emissions in 2019, underscoring its pivotal role in combating climate change.

Climate Change and Its Effects

The data we collected shows a notable increase in interest regarding **climate change**, particularly in regions vulnerable to its impacts. For example, coastal areas such as Bangladesh and the Caribbean islands are already experiencing severe flooding, leading to mass displacement. The World Bank estimates that climate change could push over 140 million people to migrate within their countries by 2050 (World Bank, 2021).

As evidenced by our Google Trends analysis, interest in **climate change** peaks during extreme weather events, such as hurricanes and wildfires. This correlation suggests that public concern often spikes in response to immediate threats rather than as a result of gradual changes.

Greenhouse Gases and Human Health

The link between **greenhouse gases** and **human health** is well-documented. Increased air pollution from burning fossil fuels contributes to respiratory diseases, with the WHO attributing approximately 4.2 million premature deaths annually to outdoor air pollution (WHO, 2021). Countries like India, which struggle with high levels of particulate matter, exemplify the health risks associated with greenhouse gas emissions.A recent study highlighted that urban areas are particularly vulnerable; cities with high traffic density are correlated with elevated levels of respiratory illnesses (Liu et al., 2020). This underscores the need for urban planning that prioritizes sustainable transportation options.

Ecosystems at Risk

The impact of global warming on **ecosystems** is profound, leading to habitat destruction and loss of biodiversity. Coral reefs, for instance, are facing unprecedented bleaching events due to rising sea temperatures, which threaten marine biodiversity and fisheries that millions depend on for their livelihoods (Hughes et al., 2017).Our research indicates that regions with rich biodiversity, such as the Amazon rainforest and the Great Barrier Reef, are particularly at risk. The loss of these ecosystems could have cascading effects on global carbon storage, further exacerbating climate change

CONCLUSIONS

The findings underscore the complex interplay between global warming, human health, and ecosystems. As illustrated, certain regions demonstrate heightened awareness and concern, often in response to direct threats from climate change. Our study highlights the urgent need for a global cooperative effort to mitigate the effects of climate change and promote sustainable practices.





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ROSEMARY OIL EXTRACTION THROUGH DIFFERENT METHODS: EXPERIMENTAL AND MATHEMATICAL MODELING

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ABSTRACT

Anxiety and depression are mental disorders that affect many people worldwide, with young people being the most impacted. For pharmacological treatment, anxiolytic and antidepressant medications are used, which trigger different side effects in addition to the risk of dependence. Due to these disadvantages, the adoption of techniques such as aromatherapy has grown to promote relaxation and well-being through essential oils. Among them, rosemary essential oil (*Rosmarinus officinalis L.*) has anxiolytic and antidepressant activities, as well as antioxidant and anti-inflammatory properties. Thus, rosemary essential oil extraction was performed using different techniques: dynamic maceration, soxhlet extraction (hexane), and supercritical extraction. The material underwent pre-treatment, such as grinding, particle size analysis, and drying. Supercritical extraction was carried out at temperatures from 40 to 60 °C and pressures from 100 to 300 bar, with collections every 15 minutes until saturation to construct an extraction kinetic curve. The analysis of the results obtained showed that Soxhlet 1 presented the highest yield, while supercritical extraction performed under conditions of 60 °C and 300 bar obtained the highest yield. The increase in pressure influenced the yield of supercritical extraction, as well as the temperature, which increased the vapor pressure of the components.

Keywords: *Mental disorders, aromatherapy, essential oils, Rosmarinus officinalis L., characterization.*

1. INTRODUCTION

De acordo com dados da Organização Mundial da Saúde, uma em cada oito pessoas no mundo apresentam algum tipo de transtorno mental, e os jovens correspondem ao grupo de maior risco em cerca de um terço dos países no mundo (Tabares *et al.*, 2024). Além disso, segundo o Institut Public de Sondage d'Opinion Secteur, o Brasil se destaca em índices de ansiedade e depressão, havendo uma maior prevalência entre as mulheres e os jovens de 18 a 24 anos (Ipsos, 2024).

Com relação ao tratamento farmacológico, muitos pacientes não atingem a remissão completa dos sintomas devido ao início tardio dos efeitos terapêuticos, altos custos a longo prazo e ampla gama de efeitos colaterais (da Rocha Zurchimitten *et al.*, 2025).

Dessa forma, tem crescido a utilização de aplicações como a aromaterapia, que utiliza óleos essenciais para fins terapêuticos a fim de promover relaxamento e bem-estar. Os óleos essenciais são extratos vegetais concentrados, obtidos por métodos de extração, capazes de estimular seletivamente certas regiões do cérebro e afetar tanto o humor quanto as emoções (Vora *et al.*, 2024). Entre as plantas medicinais e aromáticas, destaca-se o alecrim (*Rosmarinus officinalis L.*) que possui dentre seus empregos os culinários e terapêuticos. Ele se constitui um arbusto perene nativo do Mediterrâneo, com até 2 m de altura e que contém em suas folhas óleo essencial no interior de seus tricomas (Rafya *et al.*, 2024). O óleo essencial de alecrim apresenta propriedades ansiolíticas que são atribuídas à presença de monoterpenos, como o 1,8-Cineol (Mank-Halati *et al.*, 2024). Além disso, polifenóis do alecrim possuem efeitos antidepressivos por meio da inibição de vias inflamatórias.

O objetivo do presente estudo é realizar a extração do óleo de alecrim por diferentes técnicas, determinar o método com maior rendimento e eficiência, assim como, a análise de um modelo matemático para a representação do processo.

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2. MATERIAIS E MÉTODOS

2.1. Métodos

2.1.1. Pré-tratamento

Foi realizada a cominuição do material vegetal em moinho de facas e análise granulométrica em agitador de peneiras, escolhendo a amostra com Mesh 28 (0,595 mm) para as extrações.

Com exceção da maceração dinâmica e da extração supercrítica, as extrações do óleo por Soxhlet foram feitas em triplicata de acordo com os seguintes métodos:

2.1.2. Extração por Maceração Dinâmica

Foram utilizados 20 g de alecrim, que foram secos em estufa por 30 minutos. Posteriormente, foi adicionado ao alecrim seco 200 mL de hexano e colocado sob agitação constante de 100 RPM por 5 dias, onde ocorreu a reposição diária do solvente para maximizar o rendimento. Ao final da extração, a mistura foi vertida em filtro para a remoção de resíduos sólidos e, por último, utilizou-se o aparelho rota-evaporador para realizar a separação do solvente.

2.1.3. Extração por Soxhlet

Foram utilizados 7 g de alecrim, que foram secos em estufa por 30 min. Posteriormente, o material seco foi colocado no cartucho de celulose e foram adicionados 500 mL de hexano no balão aquecido por manta de aquecimento por 6 h. Ao final da extração, utilizou-se o aparelho rota-evaporador para separar o solvente do óleo essencial extraído. Para avaliar o rendimento dos métodos convencionais de extração foi utilizada a equação 1.

$$R = \frac{M_{extraida}}{M_{alimentada}} \qquad \text{(Eq. 1)}$$

sendo $M_{extraida}$ a massa de óleo extraída e $M_{alimentada}$ a massa de planta utilizada.

2.1.4. Extração Supercrítica

Foram utilizados 10 g de alecrim, que foram secos em estufa por 30 min. Posteriormente, foram adicionadas ao alecrim seco, esferas de vidro para evitar a formação de caminhos preferenciais no extrator. As extrações ocorreram a 40, 50 e 60 ºC e em pressões de 100, 200 e 300 bar, respectivamente. A coleta do óleo essencial ocorreu em intervalos de 15 min até a saturação. O mesmo foi recolhido em tubo Falcon, através do processo de despressurização.

A figura 1 mostra o fluxograma da unidade supercrítica utilizada neste trabalho, apresentando uma bomba de alta pressão, extrator de volume de 28 mL e banho termostático.

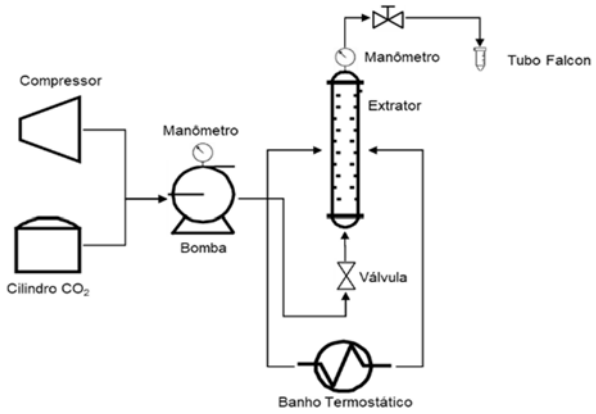


Figura 1. *Diagrama da unidade supercrítica*

2.1.5. Modelo Matemático Esquível (1999)

Dada a importância dos modelos cinéticos para otimização de processos, redução de custos e aumento da eficiência a partir da análise das interações entre os componentes ao longo do tempo, aplicou-se o modelo matemático de Esquível por ser simples e preciso na descrição de curvas cinéticas de extração supercrítica, embora não considere as interações entre o soluto e a matriz sólida. Dessa forma, utilizou-se de uma equação empírica simples para representar o rendimento (*e*) com o tempo predito por esse modelo. A equação 2 apresenta o modelo de Esquível onde t é o tempo de extração, b e e_{lim} (rendimento máximo) são parâmetros do modelo.

$$e = e_{lim}\frac{t}{(b+t)} \qquad \text{(Eq. 2)}$$

O rendimento foi avaliado utilizando as equações 3 e 4.

$$e = \frac{100M_{oe}}{M_{abls}} \qquad \text{(Eq. 3)}$$

$$M_{abls} = \left(\frac{1-M_a}{100}\right)R_{soxhlet} \qquad \text{(Eq. 4)}$$

Sendo M_{oe} a massa de óleo extraída, M_{abls} a massa alimentada em base livre de soluto e $R_{soxhlet}$ o rendimento do Soxhlet, calculado pela equação 1.

Para a validação do quão precisos são os resultados obtidos, realizou-se o cálculo do desvio relativo médio (DRM) entre os rendimentos experimental (exp) e calculado (cal) pelo modelo matemático, utilizando a equação 5, sendo n o número de dados:

$$DRM = \frac{\left(\sum \frac{|exp-calc|}{exp}\right)}{n} \qquad \text{(Eq. 5)}$$

3. RESULTADOS:

Para todas as extrações foi utilizada a amostra referente ao Mesh 28 uma vez que, na literatura,

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recomenda-se que os tamanhos de partículas na extração supercrítica devam variar de 0,25 mm a 1,8 mm devido ao fato de que partículas muito pequenas podem ocasionar o empacotamento do leito.

Na tabela 1 é apresentado o rendimento (%) e a massa extraída para os métodos da maceração e Soxhlet.

Tabela 1. Resultados de rendimento de óleo extraído para os métodos de Soxhlet e maceração

Método	Rendimento (%)	Massa extraída (g)
Soxhlet 1	17,27	1,143
Soxhlet 2	14,54	0,995
Soxhlet 3	9,58	0,656
Maceração	11,47	2,243

Com base nos dados da tabela 1, observa-se que o método de Soxhlet 1 obteve maior rendimento. Embora apresentem rendimentos elevados, essas técnicas não são seletivas quanto à extração de determinadas famílias de compostos presentes na matéria vegetal.

Além disso, o rendimento da extração por Soxhlet 1 resultou em uma massa de 1,1430 g de óleo, utilizada como referência para a determinação da massa livre de soluto, que pode ser considerada como a quantidade total de óleo presente na amostra de alecrim.

Com relação à extração supercrítica, em geral, é importante destacar que a pressão impacta no aumento direto do rendimento, pois o aumento da pressão implica num aumento da densidade do CO_2 e, consequentemente, aumenta o seu poder de solvatação. Assim, são observados rendimentos mais altos nas condições mais elevadas de pressão.

A figura 2 apresenta as três curvas cinéticas de extração nas diferentes condições operacionais que foram empregadas, onde o maior rendimento foi obtido a 300 bar e 60 °C, o que evidencia a maior influência da pressão na solubilidade do óleo, enquanto que obteve-se um baixo rendimento na condição de 100 bar e 40 °C. Ainda, entre as condições de 200 bar e 50 °C e 300 bar e 60 °C, se observa o efeito do *crossover*, o que demonstra as influências da temperatura e da pressão, tornando-se competitivas quanto ao poder de solvatação do dióxido de carbono e ao aumento da pressão de vapor dos componentes que estão sendo extraídos em determinado tempo operacional.

As figuras 3, 4 e 5 mostram as curvas cinéticas experimental e calculada pelo modelo de Esquível (1999), para as condições experimentais de 300 bar e 60 °C, 200 bar e 50 °C e 100 bar e 40 °C, respectivamente. Nesses casos, o modelo descreveu bem melhor os dados experimentais obtidos a 300 bar e 60 °C, mostrando que não há resistência na extração do óleo nos tempos iniciais, porém o modelo indica que o tempo de extração deveria ser maior.

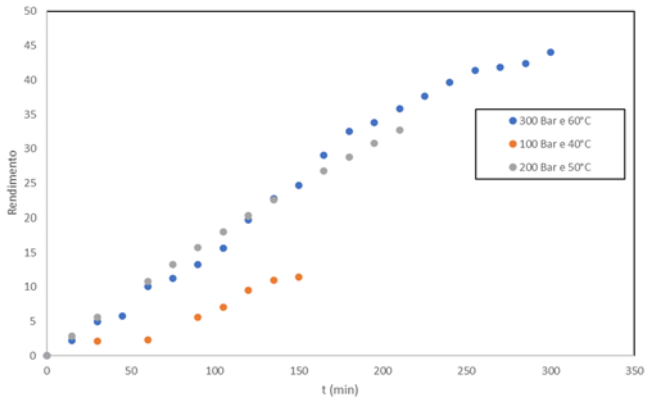


Figura 2. *Curvas cinéticas da extração do óleo usando CO_2 supercrítico nas diferentes condições experimentais*

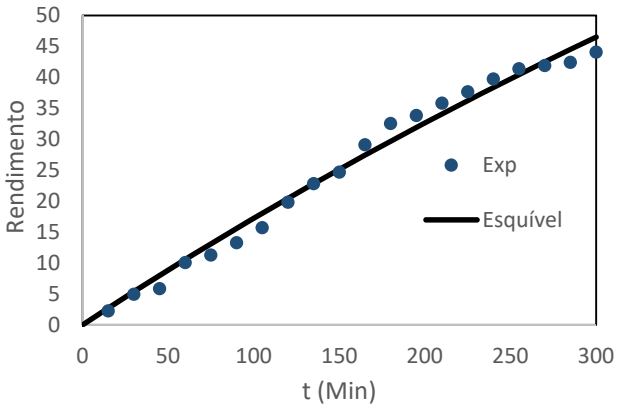


Figura 3. *Curvas cinéticas experimental e calculada pelo modelo de Esquível (1999) na condição de 300 Bar e 60 °C*

Para a condição de 200 bar e 50 °C, o modelo matemático descreveu com menor precisão a fase inicial de extração.

Mais ainda, o modelo matemático não conseguiu representar a curva cinética a 100 bar e 40 °C, visto que o modelo não impõe qualquer resistência à transferência de massa, interpretando a fase inicial de extração como linear, o que não acontece experimentalmente, sendo possível observar o menor rendimento nessa condição experimental.

A tabela 2 apresenta os desvios relativos médio (DRM) e os parâmetros do modelo de Esquível para as condições experimentais de 300 bar e 60 °C, 200 bar e 50 °C e 100 bar e 40 °C, respectivamente. Pode-se observar um alto DRM para a condição de menor temperatura, mostrando que um modelo mais robusto e preciso é necessário para representar as interações entre soluto/solvente, ou seja, grau de afinidade do soluto com o solvente.

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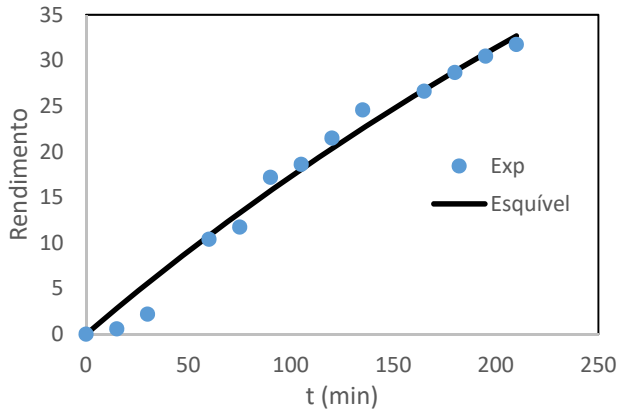


Figura 4. *Curvas cinéticas experimental e calculada pelo modelo de Esquível (1999) na condição de 200 Bar e 50 °C*

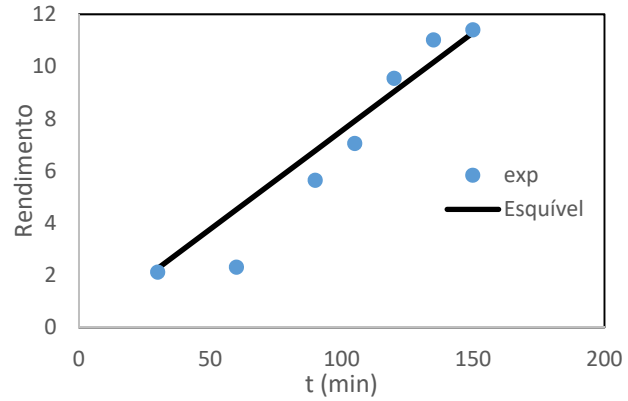


Figure 5. *Curvas cinéticas experimental e calculada pelo modelo de Esquível (1999) na condição de 100 Bar e 40 °C*

Table 2. Desvios relativos médios (DRM) e parâmetros estimados para todas as condições experimentais

DRM (%)	e_{max}	b
300 bar e 60 °C		
8,64	309,26	1695,05
200 bar e 50 °C		
49,59	171,79	893,46
100 bar e 40 °C		
21,31	6233913	82769787,77

4. DISCUSSÃO:

Considerando o estudo de Assumpção (2023), que usou as mesmas extrações, para a *Pereskia aculeata* Miller, com alterações, observou-se maior rendimento na maceração dinâmica em relação ao Soxhlet, respectivamente 8,5% e 7,47%. Quanto à extração supercrítica, o maior rendimento foi nas condições de 456 bar e 74 °C, de 0,23%, ressaltando a influência do aumento das condições de pressão e temperatura no aumento do rendimento na extração supercrítica.

5. CONCLUSÕES:

A partir dos experimentos realizados com diferentes técnicas de extração e da modelagem matemática, pode-se concluir que o Soxhlet 1 obteve o maior rendimento dentre os métodos convencionais de extração. O maior rendimento para a extração supercrítica foi obtido na condição experimental de 300 bar e 60 °C, assim como o que foi melhor representado pelo modelo matemático, evidenciando a maior facilidade de extração do óleo.

Pode-se concluir que o aumento da pressão foi mais evidenciado do que o aumento da temperatura, devido ao aumento do poder de solvatação do dióxido de carbono.

5. DECLARAÇÕES

5.1. Agradecimentos

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EXTRAÇÃO DO ÓLEO DE ALECRIM ATRAVÉS DE DIFERENTES MÉTODOS: EXPERIMENTAL E MODELAGEM MATEMÁTICA

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SUMMARY

EXTRAÇÃO DO ÓLEO DE ALECRIM ATRAVÉS DE DIFERENTES MÉTODOS: EXPERIMENTAL E MODELAGEM MATEMÁTICA

- ✓ Introduction
- ✓ Objectives
- ✓ Methodology
- ✓ Results and Discussion
- ✓ Conclusions
- ✓ Acknowledgements
- ✓ References

INTRODUCTION

- Uma em cada oito pessoas no mundo apresentam algum transtorno mental;
- Os jovens representam o grupo de maior risco em cerca de um terço dos países no mundo;
- Os medicamentos ansiolíticos e antidepressivos são eficientes, porém são relatados diversos efeitos colaterais;
- A utilização de aplicações como a aromaterapia tem crescido visando a elevação do bem-estar e promoção do relaxamento;
- Os óleos essenciais são capazes de estimular certas regiões do cérebro;
- O óleo essencial de alecrim (*Rosmarinus officinalis L.*) apresenta diversas propriedades, incluindo a ansiolítica e a antidepressiva.

OBJETIVES

- Matriz orgânica: Alecrim (*Rosmarinus officinalis L);*

- Propriedades: ansiolíticas e antidepressivas;

- Determinar por meio da extração com diferentes técnicas os compostos presentes no alecrim (*Rosmarinus officinalis L*);

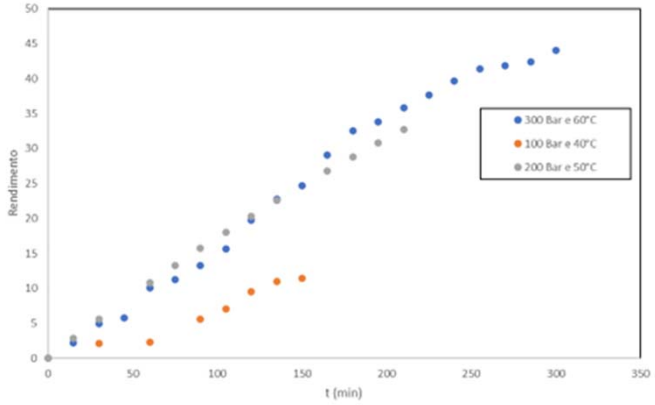
- Determinar o método de extração com maior rendimento e eficiência na obtenção do extrato de alecrim puro;

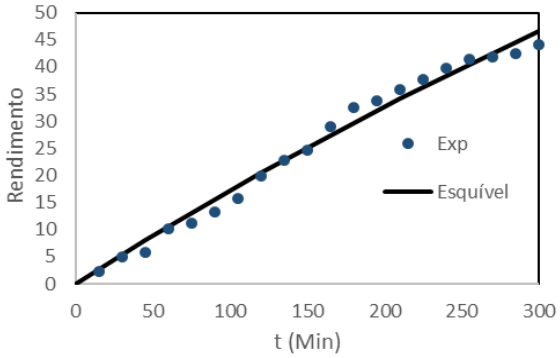
- Determinar quais compostos são extraídos em cada tipo de técnica.

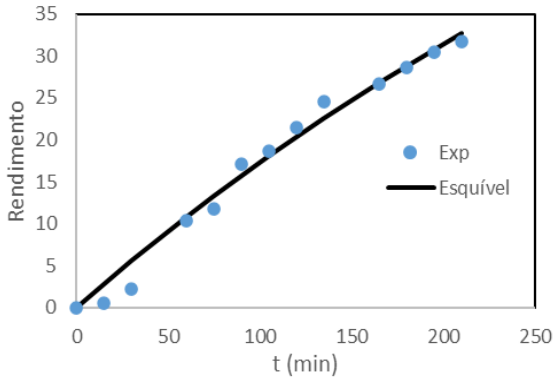
METHODOLOGY

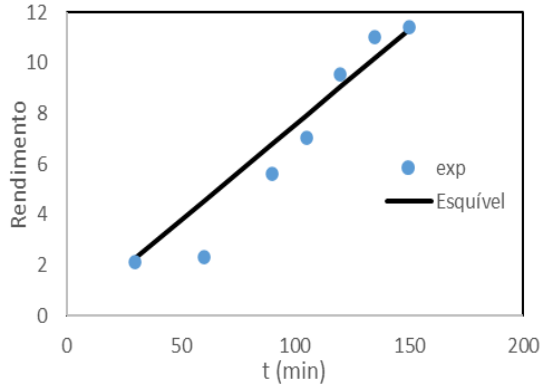
1. *Pré-tratamento*
2. Extração por Maceração Dinâmica
3. *Extração por Soxhlet*
4. Extração supercrítica
5. Modelo Matemático Esquível (1999)

RESULTS AND DISCUSSION









CONCLUSIONS

- O método do Soxhlet obteve o maior rendimento dos métodos convencionais;
- A condição de 300 bar e 60 °C obteve o melhor rendimento;

- O aumento da pressão está diretamente ligada ao aumento do rendimento;
- O aumento da temperatura provocou o aumento na pressão de vapor dos componentes.

ACKNOWLEDGEMENTS

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MANDARIN PEEL WASTE TRANSFORMATION: UNLOCKING HIGH-VALUE PRODUCT GENERATION

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ABSTRACT

The depletion of fossil fuels, the global energy crisis, and environmental pollution have prompted the search for more sustainable energy production alternatives. Biomass has emerged as a promising renewable energy source due to its abundance and the diverse methods available to convert it into fuel, including biochemical and thermochemical processes. Pyrolysis has been adopted as one of the biomass energy conversion techniques. It involves the thermal decomposition of organic matter in an oxygen-free environment, resulting in the production of high-value-added products, including biochar, bio-oil, and non-condensable gases. In this study, fast pyrolysis reactions of mandarin peels were studied at different temperatures (300°C-500°C) using vacuum and atmospheric pressures in a nitrogen atmosphere. The maximum oil yield (23 wt.%) was obtained through vacuum pyrolysis waste mandarin peel at 500 ˚C, producing 2.5 times more than the amount of oil produced from atmospheric pressure pyrolysis at the same temperature. Oxygenated compounds and aromatic derivatives were the principal compounds found in bio-oils under vacuum and atmospheric conditions, respectively. 5-(Hydroxymethyl)furfural (5-HMF) and acid acetic (AcoH) were the main products in vacuum pyrolysis, whereas phenols were predominant compounds in atmospheric pyrolysis. Depending on the pyrolysis pressure conditions, HMF and AcOH concentration was between 11-2 wt.% and 3-15%, respectively, considering the bio-oil mass. Additionally, ^{1}H NMR experiments were carried out as an alternative and simple technique to directly determine the amount of high-value chemicals in bio-oils.

Keywords: *vacuum pyrolysis, waste mandarin peel,5-Hydroxymethyl furfural, acetic acid, NMR experiments*.

1. INTRODUCTION

As the world's population grows unprecedentedly, the energy demand continues to rise. While fossil fuels remain the primary energy source, their environmental impact, decreasing availability, and stricter environmental policies have led researchers and industry to explore and develop affordable renewable energy sources. Biomass has emerged as a promising candidate because of its low cost, environmentally friendly, and abundant sources advantages (He *et al.*,2022). Among the various technologies for the conversion of biomass to energy, pyrolysis has attracted considerable attention as an environment-friendly technique, versatile, and easily scalable (Kim *et al*.,2013). Pyrolisis consists of the thermal degradation of biomass in an inert environment to produce value-added products comprising biochar, bio-oil, and non-condensable gases. The resulting yields and compositions of these remarkable outputs are intricately intertwined with the precise pyrolysis conditions employed, as well as the inherent characteristics of the biomass under consideration.

Citrus is one of the most popular fruits, with a worldwide production of over 88 million tons every year (Zhang *et al*.,2019). Argentina and Brazil stand as the leading citrus fruit producers in Latin America, with mandarins accounting for a significant portion of the production. However, processing and consuming citrus fruits result in significant waste. Current disposal methods, such as composting, landfilling, and open burning, are not entirely effective and may cause

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environmental problems (Lam et al., 2016). As a result, many studies have explored the potential of using citrus peels for bioenergy.

Among the methods for converting mandarin peel into higher value-added products, it can be found bio-transformations (enzymatic hydrolysis, fermentations) (Mahato *et al.*,2021; Jang *et al*.,2022) and thermochemical processes such as torrefaction (Da Silva *et al*. 2020) and pyrolysis (catalytic and non-catalytic). Studies on bio-oils derived from mandarin peels demonstrate their significant potential as renewable sources of industrial chemicals, including furanes, phenols, and terpenes, as well as alternative fuels. To further investigate the utilization of this waste within a circular economy framework, this study compares two pyrolysis methods—vacuum pyrolysis and atmospheric pressure pyrolysis. By analyzing the composition of the resulting bio-oils, the distinct advantages of each method are assessed.

2. MATERIALS AND METHODS

2.1 Raw materials

Mandarin peels (MP) were collected from fruits available in the market in Córdoba, Argentina. The selected MP were washed in distilled water, placed on metallic trays, and put through a drying process at 100 ºC for 24 hours. After, the material was passed through a high-speed grinder to reduce particle size (30-300 mesh). Finally, the samples were stored for subsequent pyrolysis runs.

2.2 . Pyrolysis experiments

The pyrolysis experiments were carried out in a steel tubular reactor under a nitrogen atmosphere. For the vacuum experiments, a vacuum pump reduced pressure was used to reach 1-5 torr in the whole system. Volatile compounds were collected using a liquid nitrogen-cooled trap. The biomass (20 g) was placed in a steel boat, and the reaction time was 1 h. The solid residue was recovered, and bio-oil was extracted with acetone and later evaporated. The gas fraction was determined by subtracting the solid and liquid fractions from the initial biomass mass. The pyrolysis reaction temperatures tested were 300, 400, and 500 °C.

2.3 Bio-oil characterization

Gas Chromatography/Mass Spectroscopy (GC/MS) analyses of the bio-oils were performed in a Shimadzu GC–MS-QP 5050 spectrometer. The peak area of an individual compound was directly proportional to the concentration of such compound in the liquid pyrolysate. Thus, the peak area percentage of a compound was used to compare the change in the relative amount of the bio-oil under different conditions. The identification of chromatographic peaks corresponding to the different compounds was done using the NIST MS library (match > 85 %).

2.4 Quantification of main products in bio-oils

The quantification of HMF and AcOH in pyrolytic bio-oils was carried out by ^{1}H NMR experiments using Presat for water suppression. NMR spectra were recorded with a 400 MHz Bruker spectrometer at room temperature. The samples were prepared weighing 3.0-5.0 mg of oils and 1.0–2.0 mg of pure *NH*-pyrazole as internal standard, and the mixture was then dissolved in DMSO (0.5–1.0 mL) until the solution was transparent.

3. RESULTS AND DISCUSSION

The reactions were carried out under vacuum and atmospheric pressure to evaluate how the residence time affected the product composition. The variation of the liquid (bio-oil), solid (biochar), and gaseous (gas) fractions are presented in Figure 1. Regardless of how the pyrolysis of MP was performed, the gaseous fraction was the major product, exceeding 50% yield in all cases evaluated. Biochar formation was also preponderant, especially in the reactions at atmospheric pressure, and was favored at the lowest temperatures evaluated. The bio-oil yields were between 5-23%, lower values than those found in other pyrolysis studies (Sanchez *et al.,* 2016), and an increase was observed when the experiments were carried out at low pressures. This is explained by the fact that when the system is under vacuum, the volatile condensable compounds derived from the different reactions of the biomass components can emerge faster from the hot zone to be condensed in the traps under cryogenic temperatures, avoiding secondary or re-polymerization reactions leading to char formation. The maximum pyrolytic oil formation was obtained at 500°C, as reported by other authors (Kim et al., 2011).

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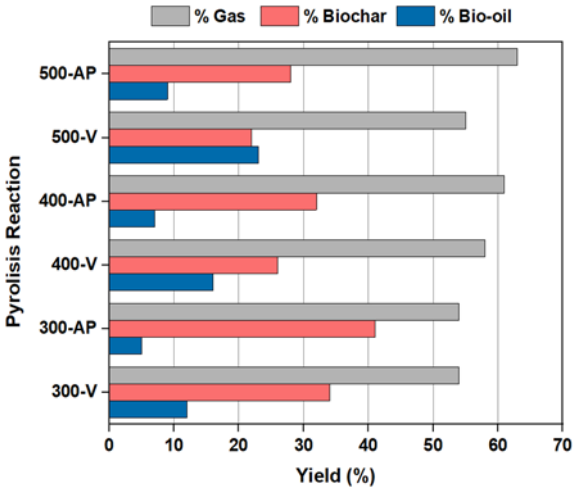


Figure 1. Product distribution in pyrolysis reactions at different temperatures. V denotes vacuum, and AP denotes atmospheric pressure

When the product composition of the bioliquid obtained under different conditions was analyzed, a remarkable change was observed in the products formed in the reactions carried out both in the presence and absence of a vacuum. For a simpler analysis, the compounds were grouped according to their chemical nature in the following families oxygenates (Oxy), aromatic derivatives (Ar), carbohydrates and derivatives (Carb), and others (not included in the previous categories). Figure 2 shows the variation of the areas assessed by GC-MS for each of the families as a function of the type of pyrolysis and the temperature at which the process was carried out.

For the vacuum pyrolysis, 57-70 products were detected in the chromatograms. A preponderance of oxygenated compounds was observed at all the temperatures evaluated, with a higher formation between 300 and 400 °C, and a significant decrease at 500 °C. Aromatics constituted the second most important group of compounds at 400 °C and above, and monosaccharides and derivatives varied between 8-14 % of the total area over the whole temperature range. Within the family of oxygenates, carbonyl derivatives (carboxylic acids, ketones, aldehydes, furans, and alcohols) were detected. The main components of this group were 5-HMF (5-(Hydroxymethyl) furfural and AcOH (acid acetic), followed by C16-C18 fatty acids (FA) as palmitic and linoelaidic acid, 2,3-dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one (DDMP) or maltol, acetol, and pentanal. The formation of acetic acid is mainly attributed to the initial breakdown of acetyl residues in the xylan, a key hemicellulose component. This results in the formation of hexatomic ring intermediates, which undergo a ring-opening process to produce linear carbon chains, like acetic acid and hydroxyacetone, both products detected in considerable quantities in bio-oils derived from MP. These results are in line with the literature, which reports that acetic acid is the predominant carboxylic acid in several bio-oils generated by catalytic and non-catalytic thermal processing of citrus peels (Kim *et al*.,2011).

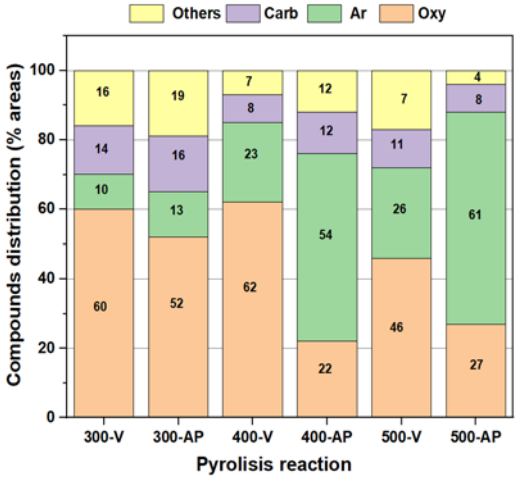


Figure 2. Type of compounds detected in the pyrolytic oils from MP at different conditions

On the other hand, 5-HMF serves as a versatile platform chemical with the potential to produce a range of valuable compounds (2,5-furandicarboxylic acid, dimethylfuran, furan diols, γ-valerolactone, *n*-hexane, 1,6-hexanelol, 2,5-hexanediol, levulinic acid) through various reactions such as esterification, condensation, hydrogenation, rehydration, oxidation, and more (Kostyniuk *et al*., 2024). HMF is formed from the thermal degradation of cellulose and represents a versatile chemical intermediate that can be converted to a variety of interesting molecules such as 2,5-hydroxymethylfuran (DHMF), 5-(hydroxymethyl)-furanoic acid. HMF has been reported as one of the most important furans in different types of pyrolysis of citrus reticulata peel (Gomez Da Silva *et al*., 2019), with a decrease in the proportion of this derivative being observed as the temperature of the process increases (Kim *et al.,* 2011). In the case of aromatics, phenols, and benzoic acid were detected as major contributors. Among the phenols, catechols, unsubstituted-phenol, and 4-vinylguaiacol (4-VG) were the compounds found in all oils in high proportions. Levoglucosan (LG), ethyl-α-d-glucopyranoside (α-EG), and 1,4:3,6-dianhydro-α-d-glucopyranose (DGP) were the

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components of the carbohydrate fraction in the bio-oil.

When the crude oils from the atmospheric pressure reactions were analyzed, a decrease relative in the number of products detected in the bioliquids was observed between 28-37 compared to vacuum pyrolysis. Although the presence of oxygenates predominated at the lowest temperature evaluated, the quantity declined markedly from 400 °C onwards, with aromatic derivatives being the majority. Within the group of oxygenated compounds, the major derivatives, in this case, were firstly FA (mainly palmitic acid and linoelaidic acid), then acetic acid, HMF, and pentanal. It should be noted that the formation of acetic acid and HMF was much lower than that observed in the pyrolysates obtained from the vacuum processes. Catechols (1,2-benzenediol and 3-methyl-1,2-benzenediol), cresols (2-methyl phenol, 3-methyl phenol), and phenol were the major aromatic derivatives in all bio-oils. These results suggest that atmospheric pressure pyrolysis favors the degradation of lignin over cellulose/hemicellulose. It is known that phenolic compounds are mainly derived from the lignin component of lignocellulosic biomass. Concerning the sugars, LG, DGP, and altrosan were detected as the main products, while the formation of α-EG was very small.

Considering the relative amounts of the main oxygenated products, such as AcOH and 5-HMF, determined by GC-MS in the different pyrolytic oils, quantification of each of these compounds was carried out using proton nuclear magnetic resonance (^{1}H NMR). Acetic acid was quantified using the methyl group signal at 1.90 ppm, HMF by the aldehyde proton signal at 9.53 ppm, and *NH*-pyrazole by the vinyl proton signal at 6.25 ppm. These proton signals were chosen because they did not overlap with other signals in the spectrum. Based on the quantification, the bio-oil produced under vacuum conditions showed concentrations between 5-11% for HMF and 9-15% for AcOH. In contrast, the bioliquids obtained under atmospheric pressure conditions had lower concentrations, ranging from less than 2% to 3-9% for these same compounds. Additionally, these results indicate that vacuum pyrolysis promotes higher yields of HMF at low temperatures and AcOH at high temperatures.

4. CONCLUSIONS

This study investigated the pyrolysis of MP waste under vacuum and atmospheric pressure between 300 and 500 °C. Vacuum pyrolysis improved bio-oil yields, reaching 23 wt% at 500 °C, and favored the production of oxygenated compounds, with 5-HMF and AcOH as the main products. Atmospheric pyrolysis, on the other hand, predominantly produced aromatic derivatives. These findings highlight the potential of optimizing pyrolysis conditions, particularly vacuum pyrolysis, to enhance the yield of valuable chemicals like 5-HMF and acetic acid.

5. DECLARATIONS

5.1. Open Access

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MANDARIN PEEL WASTE TRANSFORMATION: UNLOCKING HIGH-VALUE PRODUCT GENERATION

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October/2024

INTRODUCTION

- The cumulative depletion of fossil fuels, the global energy crisis, and environmental pollution have prompted the search for more sustainable energy production alternatives. Biomass has emerged as a promising renewable energy source because of its low cost, environmentally friendly, and abundant source advantages. [1]

- Citrus is one of the most popular fruits with a worldwide production of over 88 million tons annually [2]. Argentina and Brazil are the main citrus fruit producers in Latin America contributing to a yearly output of 1.8 million tonnes, with mandarins accounting for a significant portion [3].

- Pyrolysis has been adopted as one of the biomass energy conversion techniques. It involves the thermal degradation of organic matter in an oxygen-free environment, resulting in the production of high-value-added products, including, biochar, bio-oil, and non-condensable gases.

- The extensive research on pyrolytic bio-oils derived from mandarin peels highlights their great potential as a renewable source of valuable industrial chemicals such as furanes, phenols, and terpenes. Furthermore, these bio-oils can serve as an alternative fuel, adding to their versatility.

OBJETIVE

This study aims to evaluate the valorization of citrus waste within the framework of the circular economy by comparing two pyrolysis methods—vacuum pyrolysis and atmospheric pressure pyrolysis—for the conversion of mandarin peel into value-added products. Through a comprehensive analysis of the resulting bio-oil compositions, this research intends to elucidate the distinct advantages associated with each pyrolysis methodology, thereby providing insights into its potential as a source of value-added chemicals.

METHODOLOGY

- **Raw materials**: Peel mandarin (MP) was washed in distilled water and put through a drying process at 100 ºC for 24 hours. The material was passed through a high-speed grinder to reduce particle size.
- **Pyrolysis experiments:** The experiments were carried out in a steel tubular reactor under a nitrogen atmosphere. Approximately 20 g of biomass were pyrolyzed at 300, 400, and 500 °C for 1 hour. After the reaction, solid residues were recovered and weighed. Likewise, the bio-oil was removed with acetone and later evaporated. Vacuum experiments were conducted at 1-5 Torr with nitrogen flow at 0.1 mL/s, while non-vacuum experiments were performed with nitrogen flow rates of 1.5-8 mL/s.
- **Bio-oil characterization*:*** The bio-oils recollected were analyzed by GC/MS. The peak area of an individual compound was directly proportional to the concentration of such compound in the liquid pyrolysate. The identification of chromatographic peaks corresponding to the different compounds was done using the NIST MS library (match > 85 %).
- **Quantification of the main compounds in bio-oils:** The quantification of acetic acid, HMF, and fatty acids in pyrolytic bio-oils was carried out by ^{1}H NMR experiments at room temperature. The samples were prepared weighing 3.0-5.0 mg of oils and 1.0–2.0 mg of pure NH-pyrazole as internal standard, and the mixture was then dissolved in DMSO (0.5–1.0 mL).

RESULTS AND DISCUSSION

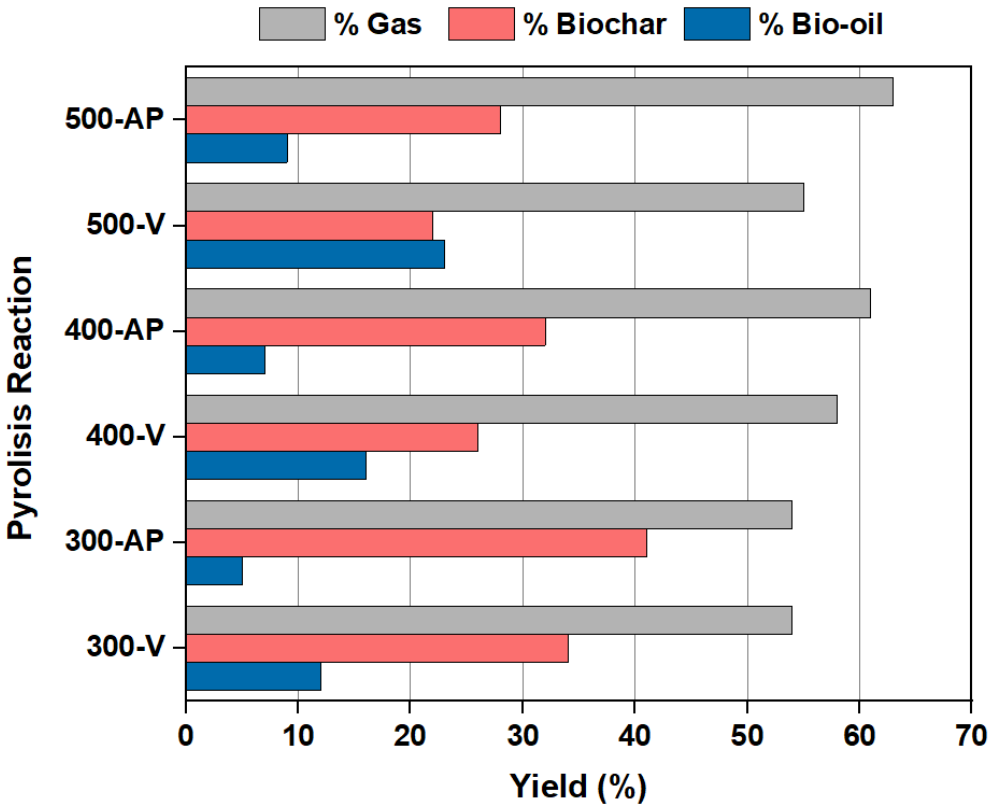


Figure 1. Product distribution in pyrolysis reactions at different temperatures. V denotes vacuum and AP denotes atmospheric pressure.

- The gaseous fraction was the major product, exceeding 50% yield in all cases evaluated.
- Biochar formation was preponderant, especially in atmospheric pressure reactions, and favored at the lowest temperatures evaluated.
- The maximum pyrolytic oil formation was obtained at 500˚C, as reported by other authors (Kim et al., 2011).
- An increase in bio-oil yield was observed for low pressure, due to the vacuum allowing volatile compounds to escape quickly and condense at cryogenic temperatures, reducing secondary reactions that lead to char formation.

RESULTS AND DISCUSSION

For the vacuum pyrolysis :

- A preponderance of oxygenated compounds was observed at all temperatures.
- Aromatics constituted the second most important group of compounds at 400 ˚C and above, and monosaccharides and derivatives varied between 8-14 % of the total area over the whole temperature range.
- The main components of this group were 5-(Hydroxymethyl)furfural(5-HMF) and acid acetic (AcoH), followed by C16-C18 fatty acids (FA) as palmitic and linoelaidic acid, 2,3-dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one (DDMP) or maltol, acetol, and pentanal.

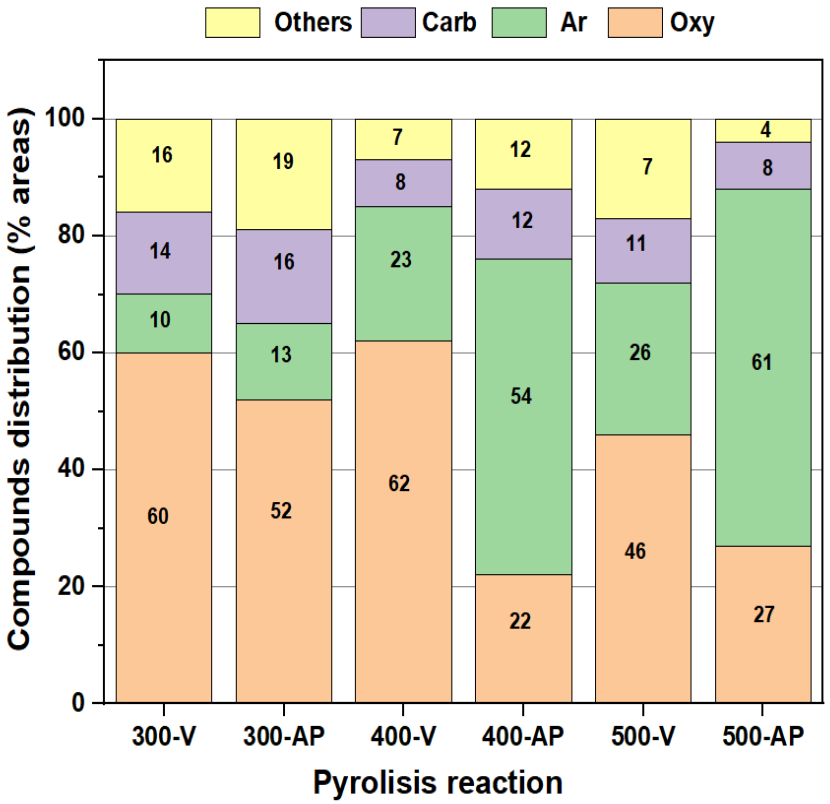


Figure 2. Type of compounds detected in the pyrolytic oils from MP at different conditions (a) Vacuum and (b) atmospheric pressure

Oxygenates (Oxy) **Aromatic derivatives (Ar)**
Carbohydrates and their derivatives (Carb)
Compounds not included in these categories (Others)

RESULTS AND DISCUSSION

For the atmospheric pyrolysis :

- A decrease relative in the number of products detected in the bioliquids was observed between 28-37 compared to vacuum pyrolysis.
- At the lowest temperature, oxygenates were the predominant compounds, however, their quantity significantly decreased at temperatures above 400 °C, where aromatic derivatives became the majority.
- Catechols (1,2-benzenediol and 3-methyl-1,2-benzenediol), cresols (2-methyl phenol, 3-methyl phenol), and phenol were the major aromatic derivatives in all bio-oils.

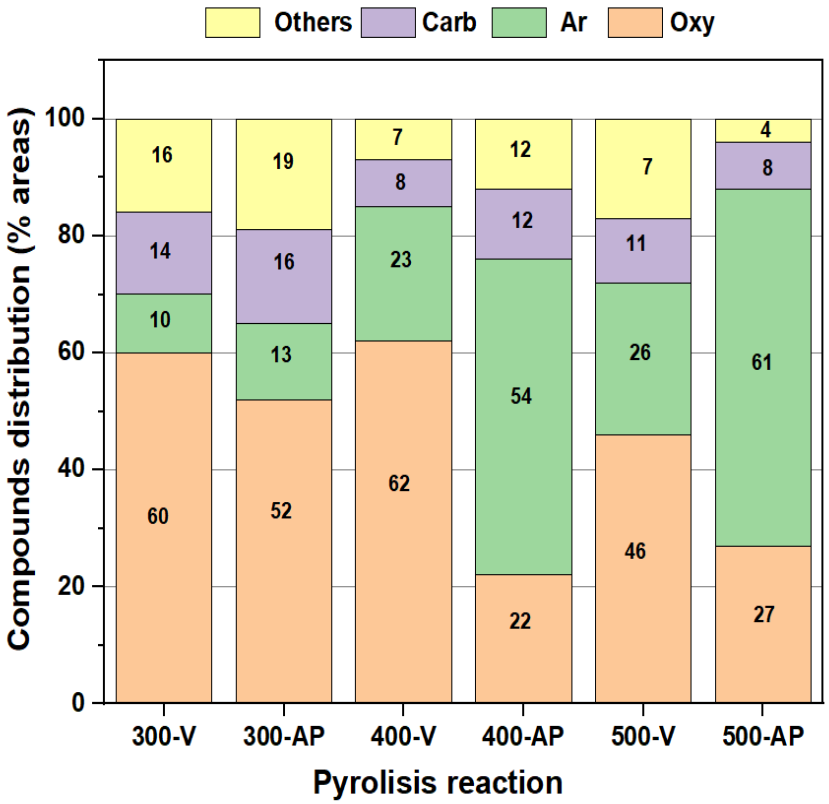


Figure 2. Type of compounds detected in the pyrolytic oils from MP at different conditions (a) Vacuum and (b) atmospheric pressure

Oxygenates (Oxy) **Aromatic derivatives (Ar)**
Carbohydrates and their derivatives (Carb)
Compounds not included in these categories (Others)

RESULTS AND DISCUSSION

The bio-oil produced under vacuum conditions showed concentrations between 5-11% for HMF and 9-15% for AcOH. In contrast, the bioliquids obtained under atmospheric pressure conditions had lower concentrations, ranging from less than 2% to 3-9% for these same compounds.

These findings suggest that vacuum pyrolysis enhances HMF yields at lower temperatures and AcOH yields at higher temperatures.

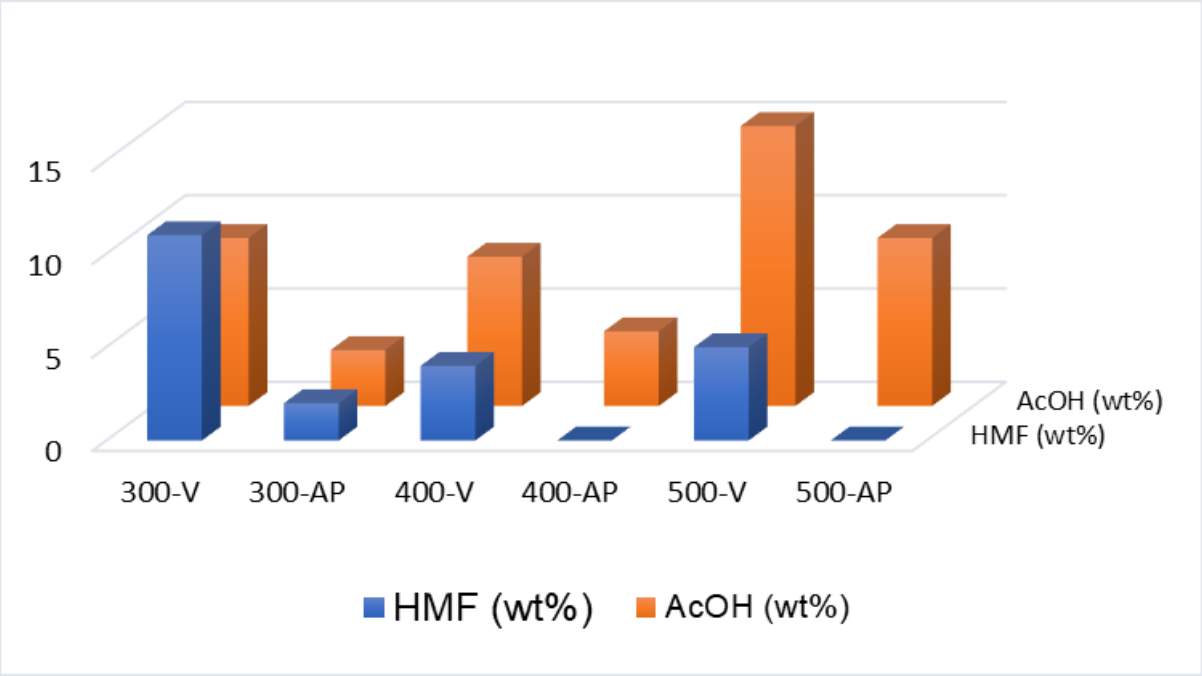


Figure 3. HMF and AcOH yields from MP at different pyrolysis temperatures. *V denotes vacuum and AP denotes atmospheric pressure*

CONCLUSIONS

- The use of vacuum pyrolysis of waste mandarin peel resulted in an improvement in bio-oil yield of up to 23 wt% at 500˚C, producing 2.5 times the amount of oil produced by atmospheric pressure pyrolysis at the same temperature.
- The production of oxygenated compounds was favored under vacuum pyrolysis in all the conditions studied, with HMF and AcOH being the predominant products. In contrast, the aromatic derivatives were the predominant products for atmospheric pyrolysis.
- ^{1}H NMR experiments were carried out as an alternative and simple technique to directly determine the amount of high-value chemicals in bio-oils.
- Vacuum pyrolysis promotes the yield of platform chemicals such as HMF and acetic acid.

ACKNOWLEDGEMENTS

This work was supported by National Research Council of Argentina (CONICET- Proyecto de Unidad Ejecutora-INFIQC) and Secretary of Science and Technology from National University of Cordoba (Projects SECyT-Consolidar 2023-2027).





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INNOVATIVE TECHNIQUE FOR RAPID DETECTION OF ANALYTES IN COMPLEX MATRICES

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ABSTRACT

In this work we present an innovative technique to detect analytes in complex matrices. Thioverbenone was synthesized using verbenone and Curphey's reagent without further purification, and was detected in the mixture reaction using SERS spectroscopý coupled to thin layer chromatography (TLC). Combining both techniques enables the rapid and efficient detection of components in complex matrices without prior purification, thereby saving time and reagents.

Keywords: *thioverbenone, TLC-SERS, Raman SERS.*

1. INTRODUCTION

Verbenone is one of the main components found in the essential oil extracted from *Suico*, a native plant in South America.

This compound has demonstrated significant biological activity against fungi and bacteria, and has been the subject of extensive studies, such as the obtention of derivatives. (Erman, 1966; Hu *et al*., 2017; Ravid *et al*., 1997). Our research group is interested in contributing to the knowledge and application of this substance for specific uses. Therefore, we have proposed and conducted the thionation of verbenone, with the objective of increase its antifungal activity, particularly against phytopathogens that affect maize (Jonathan Roberto Olmo, 2021).

SERS technique (Surface-Enhanced Raman Spectroscopy) is characterized by the enormous enhancement experienced by the Raman spectrum of the molecules when these are in close proximity to certain nanostructured metallic surfaces, thus allowing for the detection and identification of analytes in trace concentrations. Since 2016, applying SERS to systems of varying complexity using different silver-based nanostructured platforms built *ad hoc* has been our main goal. (Díaz-Mirón *et al*., 2018; Alfredo Nicolás Dominguez, 2024). Recently, a contaminants identification in a complex mixture using a coupled TLC-SERS technique was successfully carried out (Qu *et al*., 2018). This involves seeding silver nanoparticles (AgNPs) onto the chromatographic plate containing the already eluted mixture. With this purpose, we used the TLC-SERS technique, incorporating AgNPs sprayed over the sample (Alfredo Nicolás Dominguez, 2024).

We present here the application of the coupled TLC-SERS technique to detect the presence of thioverbenone directly in the mixture reaction. The identification of the thionated molecule was based on the vibrational behavior calculated by quantum mechanical methods at the B3LYP/6-311+G(d,p) level using the Gaussian 16 program (Frisch *et al*., 2016).

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2. MATERIALS AND METHODS

2.1. Chemicals

1S-(-)-verbenone, hexamethyldisiloxane (HMDO), phosphorus pentasulfide (P_2S_5) and silica gel were obtained from Sigma-Aldrich Argentina.

2.2. TLC cromatography

The thionation products were analyzed by thin layer chromatography (TLC) using silica gel as stationary phase and a mixture of hexane and ethyl acetate (2:1) as mobile phase.

2.4. Raman and SERS measurements

A DXR confocal Raman microscope (Thermo Fisher Scientific) was used to acquire spectra in the 3500-50 cm^{-1} range. An excitation wavelength of 780 nm at 24 mW power (spectral resolution of 5 cm^{-1}) and a 50 µm slit aperture were used for spectral collection. Samples were focused with a 50x objective. Each spectrum resulted from the accumulation of 50 scans with an exposure time of 5 s each.

2.4.1. Synthesis of AgNPs.

AgNPs were synthesized by chemical reduction from silver nitrate ($AgNO_3$) and hydroxylamine hydrochloride ($NH_2OH.HCl$). 10 mL of $NH_2OH.HCl$ solution (~1.5 x 10^{-2} M) containing NaOH (~3 x 10^{-2} M) was added dropwise to 90 mL of $AgNO_3$ solution (~1.11 x 10^{-3} M) under vigorous stirring at room temperature. All solutions were prepared with ultrapure water (18.2 MΩ.cm), and all glassware was previously washed with aqua regia and alcoholic potash.

2.5. Computational calculations

The Gaussian 16 software package was used to perform quantum chemical calculations, applying density functional theory (DFT). For this purpose, 6-311+G(df) basis sets was used to optmimize the molecular geometry and perform the vibrational spectrum calculation for the most stable conformer.

The vibrational frequencies obtained were adjusted by a scale factor of 0.9733 for the spectral range (3500-50 cm^{-1}). The identification of the vibrational modes was performed using GaussView 4.1 graphical interface (Dennington II *et al*., 2003).

3. RESULTS AND DISCUSSION:

The structure of verbenone and thioverbenone with the atomic numbering used in this study is shown in Figure 1.

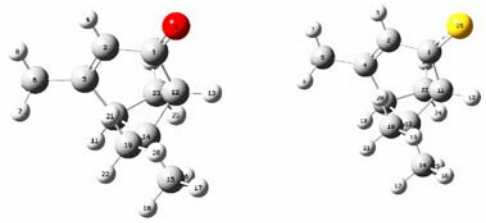


Figure 1. *Optimized structures and atom numbering of verbenone (left) and thioverbenone (right).*

Raman spectra analysis of thioverbenone in a mixture.

Figure 2 shows the calculated spectrum of thioverbenone (a), the experimental of the mixture (b) and the experimental spectrum of pure verbenone in the 1800-50 cm^{-1} region.

The spectrum of verbenone shows two characteristic bands, located at 1671 cm^{-1}, (asigned to the stretching vibration of the carbonyl group, $\nu C_1{=}O_2$), and at 1614 cm^{-1}, corresponding to the stretching vibration of the double bond ($\nu C_3{=}C_5$). The latter was asigned to the band at 1584 cm^{-1} in the mixture spectrum, which is shifted respect to the verbenone counterpart. The signal at 1633 cm^{-1} ($\nu C_1{=}O_2$) in the mixture spectrum suggest an incomplete modification of the terpenoid, indicating the presence of verbenone. This interpretation is supported by the band at 1078 cm^{-1} in both spectra.

Three additional high-intensity bands at 1323, 1090, and 429 cm^{-1} are observed in the mixture spectrum, which are not present in the verbenone spectrum. Their assignment to other contributing by-products is ruled out based on the Raman spectrum calculated for thioverbenone (Figure 2). The remarkable correlation between the experimental vibrational data and the computational results allowed for an accurate assignment of the observed bands and indicated that the presence of thioverbenone is dominant in the mixture. Moreover, the formation of the C-S bond is confirmed by the strong band located at 1090 cm^{-1}, which is confidently assigned to the C_1-S_{25} stretching mode, according to the vibrational visualization in the GaussView program. The remaining two new bands (1323 and 429 cm^{-1}) are predicted as complex vibrational modes, also involving the C-S bond.

TLC results

The chromatographic run of the mixture reaction without purification (a), and the same with

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AgNPs (b) is shown in figure 3. It is possible to note three well-defined spots (Figure 3a), each corresponding to different components of the sample. The spot with the highest front of ratio (Rf) is supposed to be thioverbenone. This assumption is based on a decrease in the compound polarity due to the substitution of oxygen by sulfur in the molecular structure. Since sulfur is less electronegative than oxygen, thioverbenone exhibits less interaction with the polar stationary phase, allowing it to elute more efficiently alongside the mobile phase.

The spots obtained were treated with silver nanoparticles (AgNPs), which are incorporated to intensify the Raman spectra signal. The AgNPs act as signal-amplifying agents, improving the sensitivity and resolution of the Raman spectrum, thus facilitating the identification of the compounds present in the sample.

TLC-SERS results

The TLC technique was used to attempt to separate thioverbenone from the mixture, thus its Raman spectrum could be obtained without interference (residual verbenone and other possible by-products). Subsequent seeding of AgNPs for SERS measurement was also performed.



***Figure 3**. TLC of thioverbenone mixture (a), and thioverbenone mixture + AgNPs (b).*

Figure 3 (b) shows the TLC eluted plates after the addition of AgNPs on the three well-defined spots. SERS spectrum collected from the upper spot is compared with the thioverbenone predicted Raman spectrum (Figure 4). A good correlation between both spectral profiles is observed, specifically the bands located at 1323, 1090, and 429 cm^{-1} are well-defined, confirming the presence of thioverbenone in the upper spot. Additionally, the absence of the band at 1600 cm^{-1} ($\nu C_1{=}O_2$) is evident, indicating that efficient separation from the precursor was accomplished.

4. CONCLUSIONS:

We confirm that the analytical technique coupling TLC chromatographic separation with SERS spectroscopy is efficient for the rapid detection and identification of reaction products that are difficult to purify. Specifically, in this case, we demonstrated that the thionation reaction of verbenone was efficient, although not complete, and that the characterization of the main product can still be performed even if it remains in the complex reaction mixture. Additionally, it promises to be a suitable technique for monitoring a chemical reaction.

5. DECLARATIONS

5.1. Acknowledgements

The authors thank to CONICET, Secyt-UNC, and CIUNT for the financial support.

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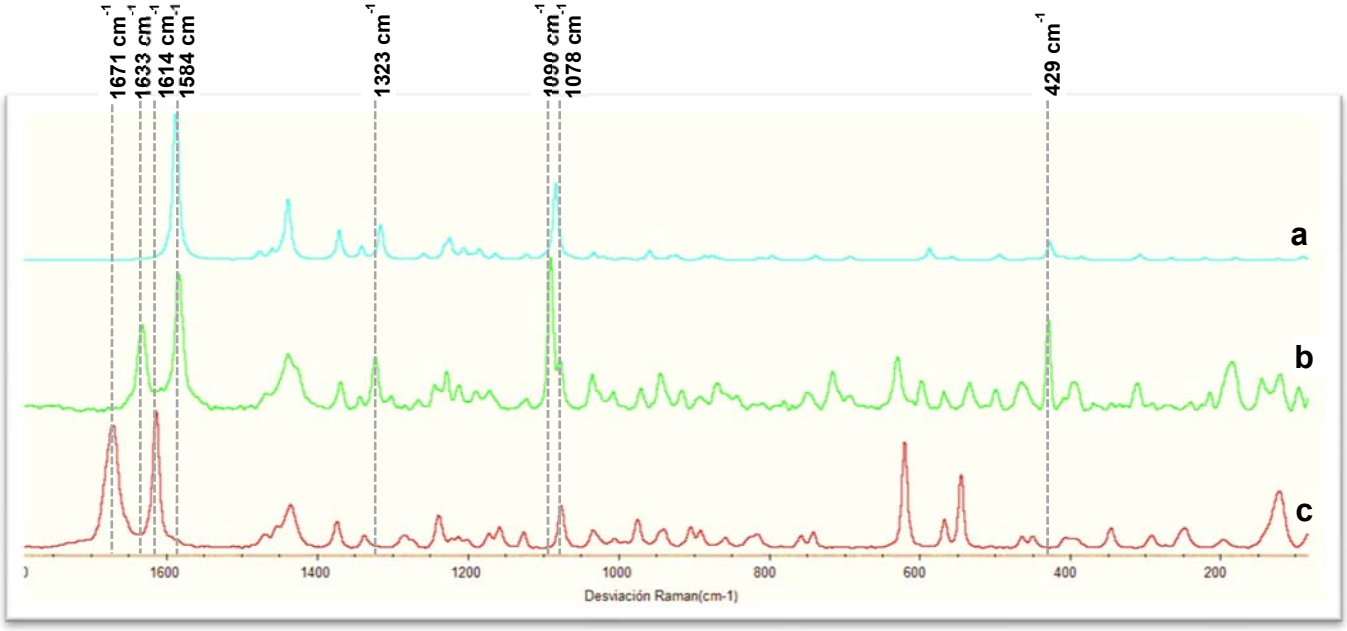


Figure 2. *Calculated spectrum of thioverbenone (a), experimental spectrum of the mixture (b) and experimental spectrum of verbenone (c).*

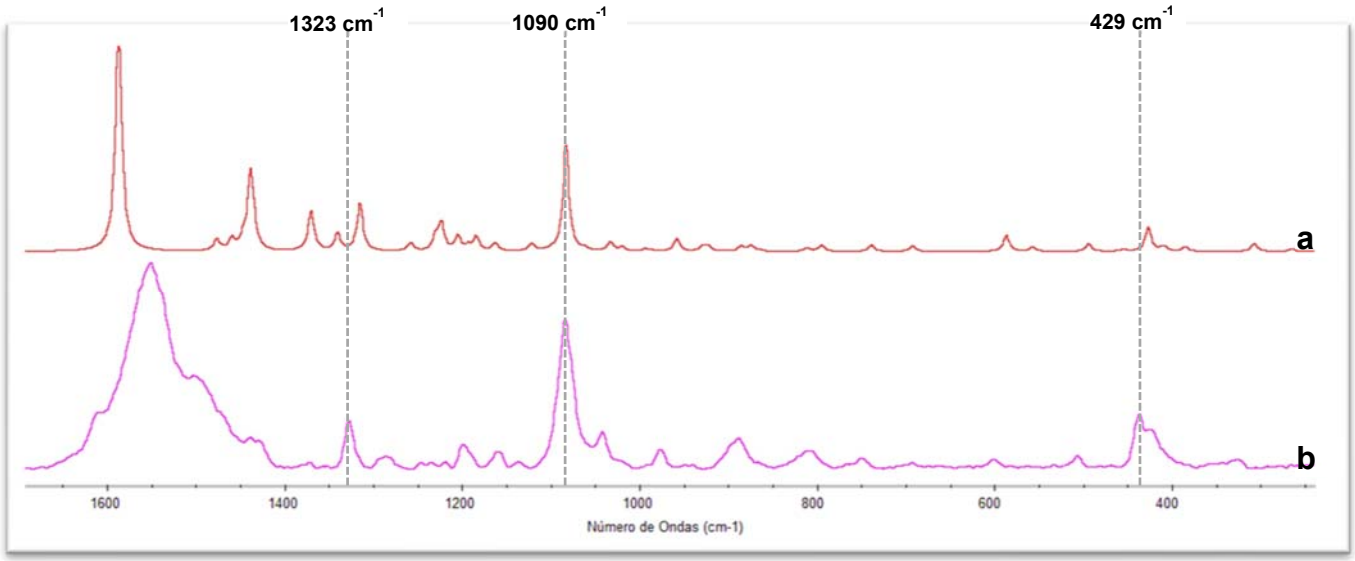


Figure 4. *Calculated SERS Spectra of thioverbenone (a) and SERS Raman spectra of the upper spot of the plate (b).*

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INNOVATIVE TECHNIQUE FOR RAPID DETECTION OF ANALYTES IN COMPLEX MATRICES

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November/2024

INTRODUCTION

- Verbenone is a component of the Suico essential oil, and its biological activity is confirmed against fungi and bacteria.
- A modification of verbenone through thionation reaction could increase its activity.
- A rapid and easy-to-use technique is needed to detect the desired analyte in the reaction mixture.

BACKGROUND

- Raman-SERS technique is a powerful tool for the detection and identification of analytes in trace concentration.
- TLC is a routine technique used in chemical synthesis to determine the purity of a sample.
- TLC-SERS, which involves seeding silver nanoparticles over a chromatographic plate, is used for identified contaminants in a complex mixtures.

AIM/OBJETIVE/PURPOSE

We present the application of the coupled TLC-SERS technique to detect thioverbenone in a mixture.

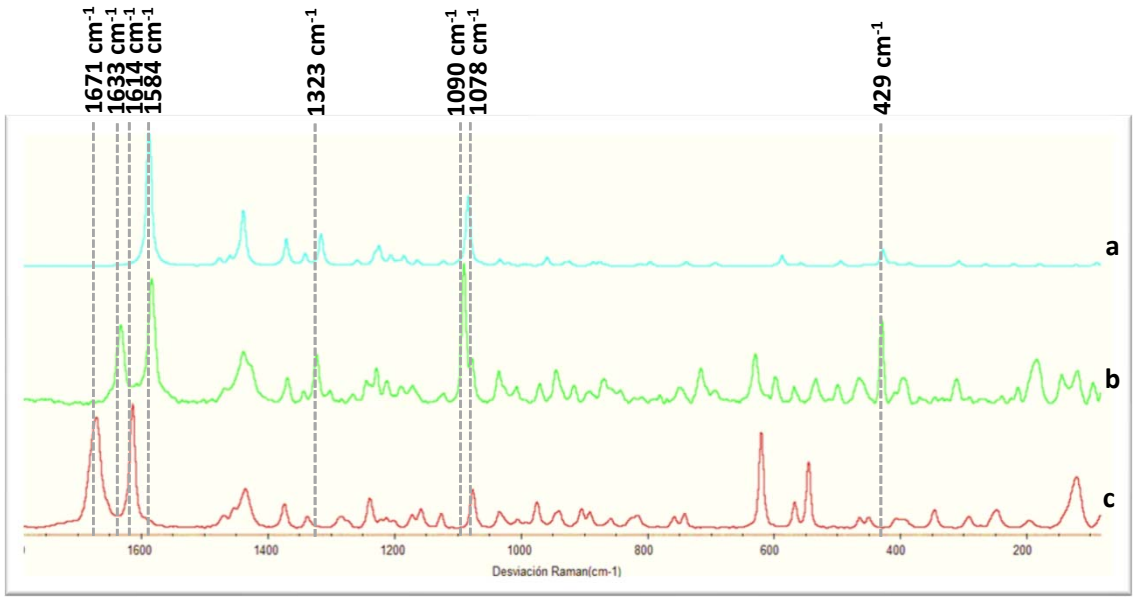
METHODOLOGY

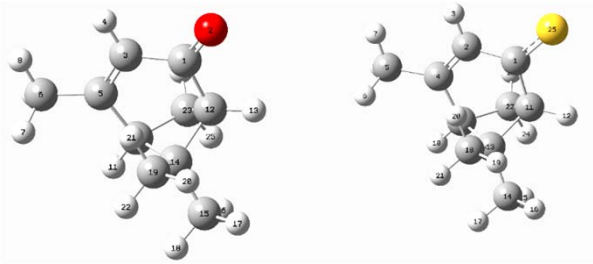
- 1S-(-)-verbenone, hexamethyldisiloxane (HMDO), phosphorus pentasulfide (P_2S_5) were used for the reaction. The thionation products were analyzed by TLC using a mixture of hexane and ethyl acetate (2:1) as mobile phase.
- A DXR confocal Raman microscope was used to acquire spectra in the 3500-50 cm^{-1} range. An excitation wavelength of 780 nm at 24 mW power (spectral resolution of 5 cm^{-1}) and a 50 μm slit aperture were used for spectral collection. (50x objective; 50 scans; 5 s exposure)
- AgNPs were synthesized by chemical reduction of silver nitrate ($AgNO_3$) and hydroxylamine hydrochloride ($NH_2OH.HCl$). 10 mL of $NH_2OH.HCl$ solution (~1.5 x 10^{-2} M) containing NaOH (~3 x 10^{-2} M) was added dropwise to 90 mL of $AgNO_3$ solution (~1.11 x 10^{-3} M) under vigorous stirring at room temperature. All solutions were prepared with ultrapure water, and all glassware was previously washed with aqua regia and alcoholic potash.
- The Gaussian 16 software package was used applying density functional theory (DFT). 6-311+G(d,f) basis sets was used to optimize the molecular geometry and perform the vibrational spectrum calculation for the most stable conformer. The vibrational frequencies obtained were adjusted by a scale factor of 0.9733 for the spectral range (3500-50 cm^{-1}). The identification of the vibrational modes was performed using GaussView 4.1 graphical interface.

RESULTS AND DISCUSSION

Raman spectra analysis of thioverbenone in a mixture.

- The spectrum of verbenone shows two characteristic bands: 1671 cm^{-1} (stretching vibration of the carbonyl group $\nu C_1=O_2$), and 1614 cm^{-1} (stretching vibration of the double bond $\nu C_3=C_5$) (c).
- The stretching vibration of the $\nu C_3=C_5$ was assigned to the band at 1584 cm^{-1} in the mixture spectrum. (b)
- The signal at 1633 cm^{-1} ($\nu C_1=O_2$) in the mixture spectrum suggest the presence of verbenone. This interpretation is supported by the band at 1078 cm^{-1} in both spectra. (c)





Optimized structure of verbenone and thioverbenone.

- Three high-intensity bands at 1323, 1090, and 429 cm^{-1} are observed in the mixture spectrum. Their assignment to other contributing by-products is ruled out based on the Raman spectrum calculated for thioverbenone (a).
- The formation of the C-S bond is confirmed by the strong band at 1090 cm^{-1} (C_1-S_{25} stretching mode). The remaining bands (1323 and 429 cm^{-1}) are predicted as complex vibrational modes, also involving the C-S bond (b).

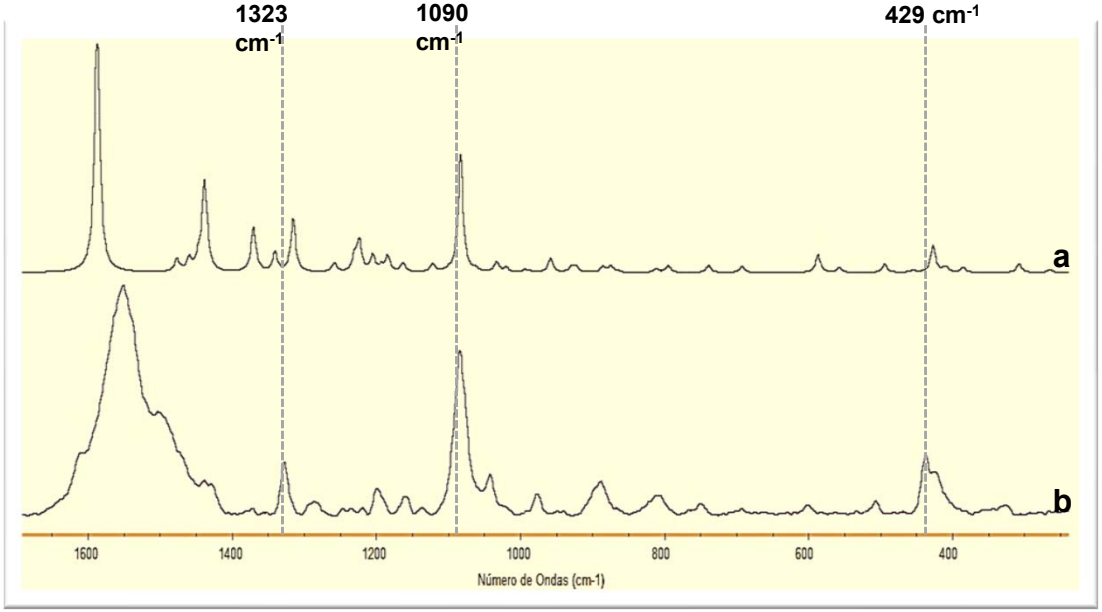
RESULTS AND DISCUSSION

TLC results

- The spot with the highest front of ratio (Rf) is supposed to be thioverbenone (a).



- The spots were treated with AgNPs (b) improving the sensitivity and resolution of the Raman spectrum, thus facilitating the identification of the compounds present in the sample. SERS measurement was also performed.
- SERS spectrum collected from the upper spot (b) is compared with the thioverbenone predicted Raman spectrum (a). A good correlation is observed, specifically the bands located at 1323, 1090, and 429 cm^{-1} are well-defined, confirming the presence of thioverbenone in the upper spot.



- The absence of the band at 1600 cm^{-1} ($\nu C_1{=}O_2$) is indicating that efficient separation from the precursor was accomplished.

CONCLUSIONS

- The analytical technique coupling TLC chromatographic separation with SERS spectroscopy is efficient for the rapid detection and identification of reaction products that are difficult to purify.

- The thionation reaction of verbenone was efficient, although not complete.

- The characterization of the main product can still be performed even if it remains in the complex reaction mixture.

- It promises to be a suitable technique for monitoring a chemical reaction.

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- Secretaría de Ciencia y Tecnica – Universidad Nacional de Córdoba – SeCyT UNC
- Consejo de Investigaciones de la Universidad Nacional de Tucumán - CIUNT

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THERMAL REACTIONS OF 2,2-DIOXO-1H,3H-PYRROLO[1,2-C]THIAZOLES STUDIED FROM GREEN METRICS

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ABSTRACT

The concept of Green Chemistry, introduced 25 years ago by the U.S. Environmental Protection Agency, aims to assess the sustainability of chemical processes. During this time, Dr. Barry Trost developed Atom Economy, which measures how "green" a reaction is using parameters such as Atom Economy (%AE), Mass Intensity (MI), and Reaction Mass Efficiency (RME). Recently, the focus has shifted to evaluating flash vacuum pyrolysis reactions under these principles. This study presents results from evaluating the thermal stability of 2,2-dioxo-1h,3h-pyrrolo[1,2-c]thiazoles, which are of pharmacological interest, through pyrolysis at temperatures between 200-275ºC. The results are compared with traditional yield values and complemented by assessments using multiparametric frameworks like EcoScale and Green Star, aiming to identify the environmental impact of these reactions. This comprehensive approach advances the sustainability of chemical processes, promoting more responsible practices in chemical research and application.

Keywords: Azafulvenium, Pyrolysis, Green Star, Green Parameters, EcoScale.

1. INTRODUCTION

There is a widespread social recognition of the need to develop chemical processes with lower environmental impact. This trend, known as "Green Chemistry," proposes a shift from traditional paradigms that primarily focus on process efficiency based on yield or synthetic perspectives. While the definition of Green Chemistry was established in the early 1990s by the U.S. Environmental Protection Agency (EPA), research in this area had been conducted prior to that time, albeit without the recognition of this specific term. Green Chemistry is defined as "the chemistry that efficiently utilizes raw materials (preferably renewable), eliminates waste, and avoids the use of toxic or hazardous reagents throughout the entire process." Paul Anastas (Anastas *et al.*, 2019), a key pioneer in this field in the U.S., emphasizes that the main focus should be on designing environmentally benign products and processes from the outset. This concept is encapsulated in the 12 principles of Green Chemistry developed by Warner and Anastas. (Anastas and John C. Warner *et al.*, 1998), (Doria *et al.*, 2016).

The synthesis of fluorinated compounds has seen a significant rise in recent years, driven by their broad applications in the pharmaceutical industry, where they are known to enhance metabolic stability, bioavailability, and protein-ligand interactions. (Mei *et al.*, 2020), (Ma, *et al.*, 2020) Leroux, *et al.*, 2020). Despite their growing importance, the synthesis of fluorinated molecules remains challenging from both a technical and environmental perspective (Thayer *et al.*, 2006). The introduction of fluorine atoms or trifluoromethyl groups is known to modify the physicochemical

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properties of organic molecules, improving lipophilicity and stability. (Faillace, *et al.*, 2020)., (Peláez, *et al.*, 2013). However, the sustainability of these processes must be rigorously evaluated to ensure they align with the principles of green chemistry.

A key consideration in this evaluation is atom economy, which measures the proportion of reactants that are incorporated into the final product. The use of fluorinated building blocks, such as 4-ethoxy-1,1,1-trifluorobut-3-en-2-one (ETFBO, 1), is one way to improve atom economy by maximizing the incorporation of fluorine atoms while minimizing the generation of by-products (Sheldon *et al.*, 2020). This approach not only optimizes the efficiency of the synthetic process but also addresses the green chemistry principle of waste prevention by reducing the formation of hazardous or unwanted substances.

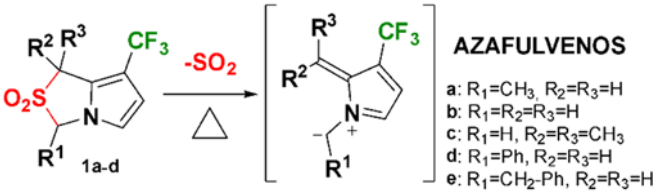
Another critical aspect is the selection of solvents, which can have a substantial impact on the environmental footprint of a chemical process. The use of toxic or non-recyclable solvents increases both environmental and operational burdens. Therefore, it is essential to evaluate the sustainability of solvent choices, opting for greener solvents with lower toxicity higher recyclability, or avoiding solvent use altogether where feasible. This selection impacts the overall eco scale score of the process, a quantitative metric that reflects its environmental performance based on factors such as toxicity, energy consumption, and waste generation.

In addition to solvent choice, the energy efficiency of a synthetic process is a fundamental consideration. Many fluorination reactions require high temperatures or pressures, increasing energy demand and the associated carbon footprint. Designing reactions that proceed under mild conditions—such as ambient temperature and atmospheric pressure—can significantly improve energy efficiency and contribute to greener practices. The assessment of energy consumption is also integral to the Green Star evaluation system, which provides a qualitative measure of sustainability based on compliance with green chemistry principles.

Lastly, the safety of reagents and products is paramount. While fluorinated compounds offer significant benefits in terms of their pharmacological properties, they may pose environmental and safety risks if not properly managed. Evaluating the toxicity, persistence, and potential environmental impact of both intermediates and final products is essential for designing synthetic pathways that are not only efficient but also environmentally responsible. This includes favoring biodegradable products or compounds with a lower ecological footprint.

The synthesis of fluorinated compounds must be evaluated through the lens of green chemistry, applying metrics such as atom economy, solvent sustainability, energy efficiency, and product safety. By integrating these considerations, we can develop processes that are both chemically efficient and environmentally sustainable, supporting the advancement of safer and more eco-friendly products.

The reaction conditions of the 2,2-dioxo-1H,3H-pyrrolo[1,2-c]thiazoles (1a-1e), which are seen in scheme 1, were evaluated by green metrics in vacuum flash pyrolysis reactions.

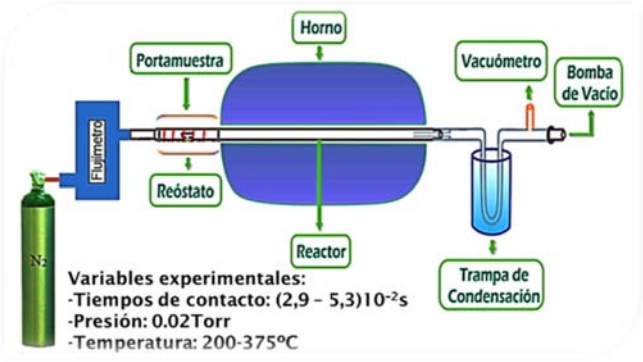


Scheme 1. *compounds evaluated by green metrics.*

2. MATERIALS AND METHODS

2.1. Synthesis of the 2,2-Dioxo-7-(trifluoromethyl)-1H,3H-pyrrolo[1,2-c]thiazoles (3a-e)

The preparation of sulfones **3a-d** was carried out according to scheme 2, FVP reactions were carried out in a Vycor glass reactor using a tube furnace with a temperature-controller device. Oxygen-free dry nitrogen was used as a carrier gas. Approximately 50 mg samples were pyrolyzed. Contact times



Scheme 2. *Reactions conditions*

were around 10-1 s and a pressure of 0.4 torr. Products were trapped at liquid air temperature, extracted with solvent, and subjected to different

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analyses or separation techniques. In all FVP experiments, the recovery of material was >80%.

The products were trapped at the temperature of cryogenic liquid, extracted with solvent and subjected to analysis or separation techniques.

2.2. Evaluation of metrics in green chemistry

The synthesis of fluorinated compounds was conducted following optimized protocols that prioritize sustainability, for which evaluation of green metrics is carried out, such as those presented below.

2.2.1. Atom Economy Evaluation (AE):

The efficiency of each synthetic route was assessed by calculating the atom economy, which is defined as:

$$AE = PM\ product / PM\ reactants\ x\ 100$$

This metric quantifies how well the starting materials are converted into the desired product, thereby minimising waste.

2.2.2. Solvent Selection:

The choice of solvents was guided by their environmental impact. Whenever feasible, solvent-free reactions were conducted. In cases where solvents were necessary, green solvents with low toxicity and high recyclability were chosen.

2.2.3. The E-factor (E):

(waste generated per unit of product) was calculated to evaluate the sustainability of solvent use:

E-factor=Mass of Product Obtained /Total Waste Generated

A lower E-factor indicates a more environmentally friendly process.

2.2.4. Reaction Mass Efficiency (RME)

This parameter considers the real mass values of the product at the end of the reaction in relation to the amount of substrate in it. Therefore, it incorporates the yield and stoichiometric relations of the reaction, the optimal value for this metric is 100 %.(Anastas *et al.*, 2019)

RME=mass product/mass reactants x 100

2.2.5. Mass Intensity (MI)

Those responsible for 80-90% of the mass intensity value in fine chemistry processes are the solvents used. The calculation of mass intensity is defined as follows. (Anastas *et al.*, 2019)

MI=Σ$masa$ total reactants /mass product

To calculate the MI, all reactants and solvents present in the reaction must be taken into account to obtain the product. The optimal value of this metric is 1.

2.2.6. Green Star rating:

Was assigned through qualitative assessments focusing on waste generation, energy consumption, and hazardous materials, aligning with the twelve principles of Green Chemistry. This semi-quantitative metric aids in evaluating sustainability and identifying modifications to enhance environmental performance. The Green Star is represented as a star polygon, with the number of corners corresponding to the assessed principles; each corner's length reflects compliance. Pre-established criteria ensure objectivity in compliance assessment. The area of the Green Star, figure 1, indicates the overall compliance level, with a larger area signifying higher adherence to sustainable practices and a smaller area highlighting potential shortcomings in waste reduction and toxicity. (Andraos *et al.*, 2016), (Ribeiro *et al.*, 2009).

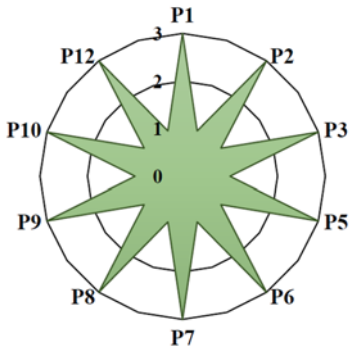


Figure 1. *Green star area*

2.2.7. EcoScale:

Is a metric tool developed in 2006 for the evaluation of the effectiveness of a synthetic reaction. Its simplicity and general applicability characterize it 10 It is a scale based on performance but also takes into account aspects of cost, safety, implementation of technique, energy, and purification. EcoScale gives a score from 0 to 100; subtracting penalty points for non-ideal conditions. These penalty points take into account both the advantages and disadvantages of specific reagents, costs, and technologies. By calculating EcoEscala, a quick evaluation of the "veracity" of the reaction protocols that depend on the analysis

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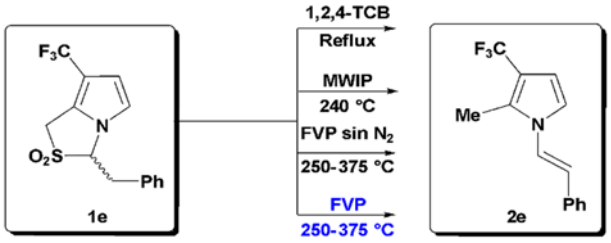
of each process is obtained. In the reaction, figure 2, areas that need further attention are clearly indicated, which can ultimately lead to improvement of reaction conditions.



Figure 2. *Points EcoScale*

3. RESULTS AND DISCUSSION:

The preparation of sulfones 1a-e was carried out by different methodologies recognized as conventional, such as reflux, microwave, and thermolysis or flash vacuum pyrolysis (FVP), Scheme 3. From this last synthesis methodology, the evaluation of GRENN metrics was carried out in order to establish if the process can be considered to follow the principles of green chemistry**.**



Scheme 3. *Methodologies of reactions*

Table 1 presents the yield of the different pyrroles obtained under the different pyrolyzes methodologies. The tendency of complete conversion of the substrate to the product is evident, with the thermolysis system being selective since no by-products are obtained from these systems. Figure 2.

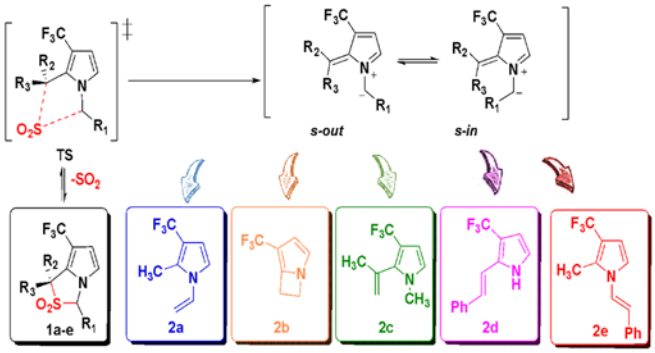


Figure 2. *Sulfone thermolysis reactions*

Table 1. *Thermolysis conditions and yield of obtained pyrroles*

T (°C)	1a	1b	1c	1d	1e
200	100,0	100,0	---	100,0	---
225	88,0	86,0	100,0	95,0	---
250	59,0	71,0	97,0	74,0	100
275	34,0	50,0	79,2	47,7	92,9
300	14,0	10,0	58,3	30,0	55,9
325	0	0	20,8	---	32,4
350	---	---	13,1	---	9,1
375	---	---	0	---	0

The evaluation of the synthetic routes in Table 2, for Substances 1a to 1e, based on key green chemistry metrics, reveals significant disparities in their sustainability and efficiency profiles.

Substance 1e exhibits the highest yield at 98.34%, coupled with a strong Ecoscale score of 82.45 and the highest Reaction Mass Efficiency (RME) of 90. This indicates a highly optimized process that effectively utilizes reagents while minimizing waste generation. The low Material Intensity (MI = 2.5) and E-factor (E = 1.5) further support the conclusion that this route adheres closely to the principles of green chemistry, signifying minimal environmental impact.

Substance 1A follows closely, demonstrating a yield of 89.30% and an Ecoscale score of 81, indicating a strong sustainability profile as well. The RME value of 82 suggests efficient reagent utilization, with an E-factor of 2.0 indicating moderate waste generation. The slightly higher Material Intensity (MI = 2.6) compared to 1e does not significantly detract from its overall favorable evaluation.

Conversely, Substance 1b and 1c present lower yields of 76.78% and 80.56%, respectively. Their Ecoscale scores (58.15 and 58.45) and RME values (45.3 and 40.23) reflect less efficient reagent usage and higher waste production. Both routes exhibit elevated E-factors (E = 2.5 for 1b and E = 3.2 for 1c), indicating a need for improvement in waste management and overall efficiency.

Substance 1d has the lowest yield at 56.45%, while its GSAI score (75.50%) and Ecoscale (77.82) show that it still maintains some degree of sustainability. However, its RME value of 3.20 and E-factor of 2.0 indicate substantial waste generation and suboptimal reagent efficiency. The lower yield and higher waste metrics highlight potential areas for process optimization.

Overall, the analysis reveals that while Substances 1e and 1a are clearly the most efficient and sustainable routes, Substances 1b, 1c, and 1d demonstrate opportunities for enhancement in terms of reagent utilization and waste reduction.

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This evaluation underscores the significance of employing green chemistry metrics in assessing the sustainability of synthetic processes.

Table 2. *Evaluation of green chemistry parameters pyrroles.*

SUST.	YIELD %[A]	GSAI %	E-SCALE	MI	RME	AE	E
1A	89,30	75,50	81	2,6	82	76,62	2,0
1B	76,78	65,00	58,15	3,5	45,3	77,86	2,5
1C	80,56	66,25	58,45	2,3	40,23	79,06	3,2
1D	56,45	75,50	77,82	3,6	3,20	77,67	2,0
1E	98,34	80,78	82,45	2,5	90	77,56	1,5

4. CONCLUSIONS:

The analysis of the evaluated synthetic routes reveals that the processes for Substances 1e and 1a stand out as the most sustainable, combining high yields (98.34% and 89.30%, respectively) with efficient use of reagents and low waste generation. Substance 1e, in particular, shows the best green profile with an Ecoscale of 82.45 and the highest RME (90), positioning it as the most optimized process.

On the other hand, the routes for Substances 1b, 1c, and 1d exhibit areas for improvement, particularly in reaction mass efficiency and waste reduction, suggesting that while they are viable, they require further adjustments to align more closely with green chemistry principles.

In summary, Substances 1e and 1a represent the best synthetic options in terms of sustainability, while the other routes could benefit from additional optimizations to improve their environmental impact.

5. DECLARATIONS

5.1. Acknowledgements

FVM thanks to the Consejo Interuniversitario Nacional (CIN) for the fellowship. This work was supported by Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET-11220200101308CO), Fondo para la Investigación Científica y Tecnológica (FONCYT-PICT-2020-SERIE-A-01862) and Secretaría de Ciencia y Tecnología (SeCyT-UNC-Nº258/23).

5.2. Open Access

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THERMAL REACTIONS OF 2,2-DIOXO-1H,3H-PYRROLO[1,2-C]THIAZOLES STUDIED FROM GREEN METRICS

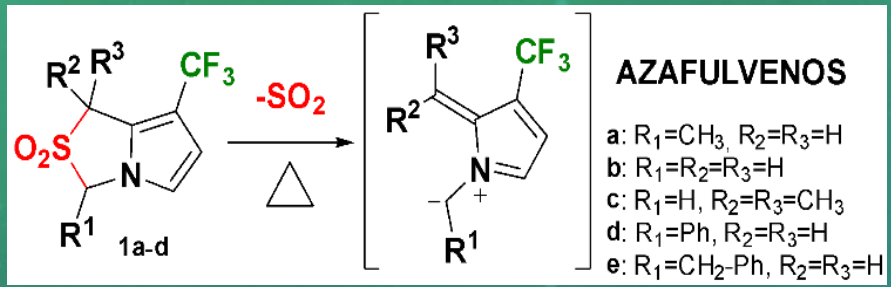
PINILLA PEÑA, DIANA CAROLINA[1]; SOARES, MARÍA ISABEL[2]; PIERELLA, LILIANA BEATRIZ[3], PINHO E MELO, TERESA MARÍA V. D.[2] AND PELÁEZ, WALTER JOSÉ[1,4*].

[1] Universidad Nacional De Córdoba. Facultad De Ciencias Químicas. Departamento De Fisicoquímica, X5000HUA, Córdoba, Argentina. [2] Departamento De Química, Universidad De Coímbra, Coímbra, Portugal. [3] Citeq-conicet, Facultad Regional Córdoba, Universidad Tecnológica Nacional. [4] Consejo Nacional De Investigaciones Científicas Y Técnicas (CONICET), Instituto De Investigaciones En Fisicoquímica De Córdoba (INFIQC), X5000HUA, Córdoba, Argentina.
e-mail: walter.pelaez@unc.edu.ar

INTRODUCTION AND OBJECTIVES

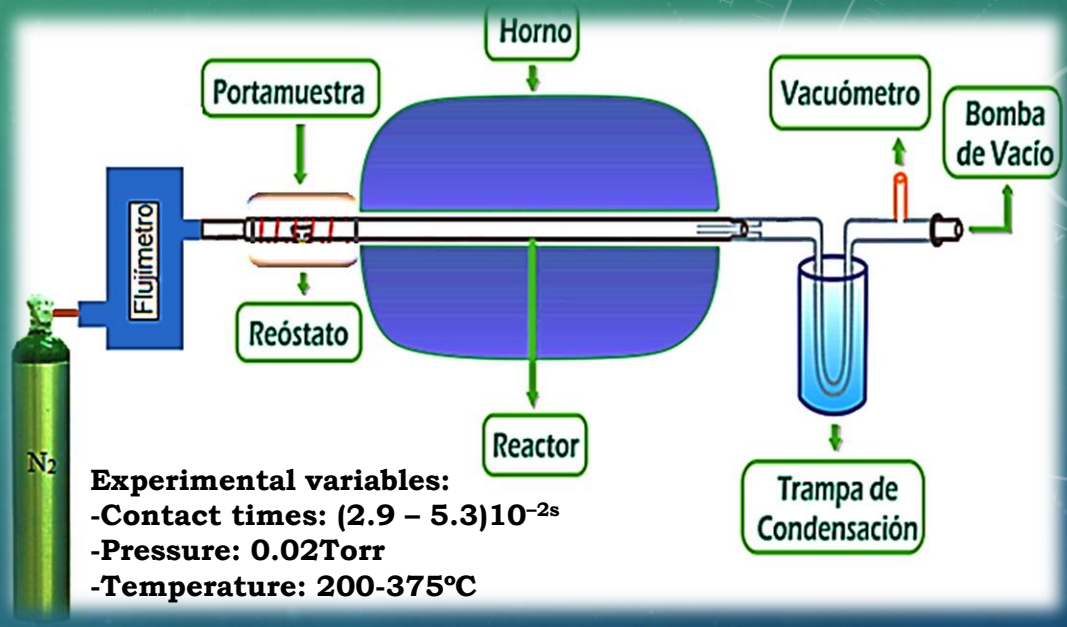
Substrates

Insecticidal action.[1]



CF3 group increases the bioavailability and interactions between these heterocycles and different proteins.[2]

FVP



It is proposed

Evaluate by green metrics the FVP reactions of 2,2-dioxo-1h,3h-pyrrolo[1,2-c]thiazoles.

Recognize green metrics as a tool to design more sustainable methodologies

Green Chemistry [3]

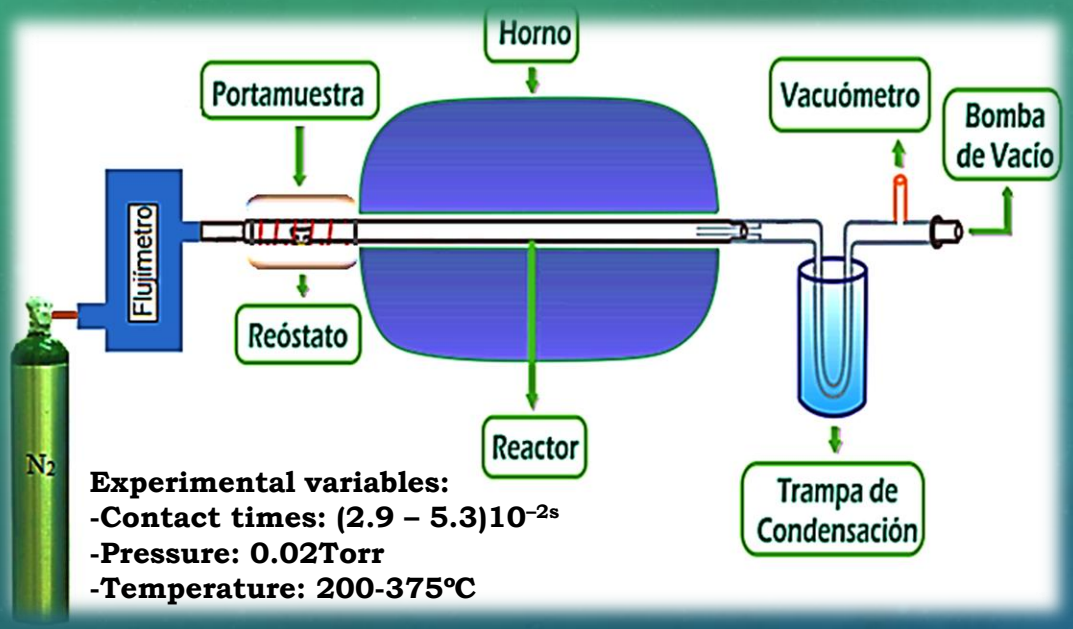
Biodegradability designs at all stages of the chemical product life cycle.

Precisely design chemical products to reduce their risks to human health and the environment.

Coherent system of design principles and criteria.

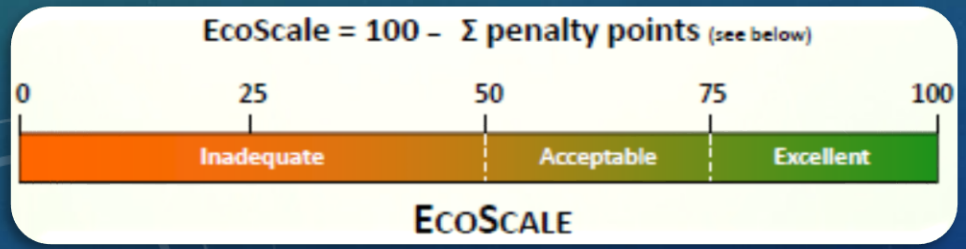
METHODOS

Synthesis of the 2,2-Dioxo-7-(trifluoromethyl)-1H,3H-pyrrolo[1,2-



Experimental variables:
-Contact times: (2.9 – 5.3)10^{-2s}
-Pressure: 0.02Torr
-Temperature: 200-375ºC

EcoScale



Green Metrics

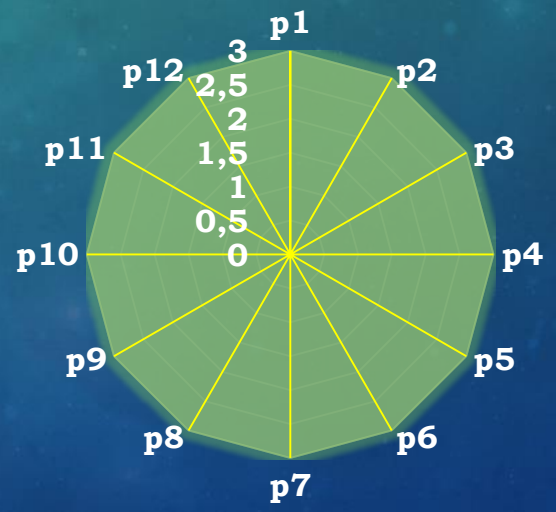
Atomic Economy (AE)

Solvent Selection

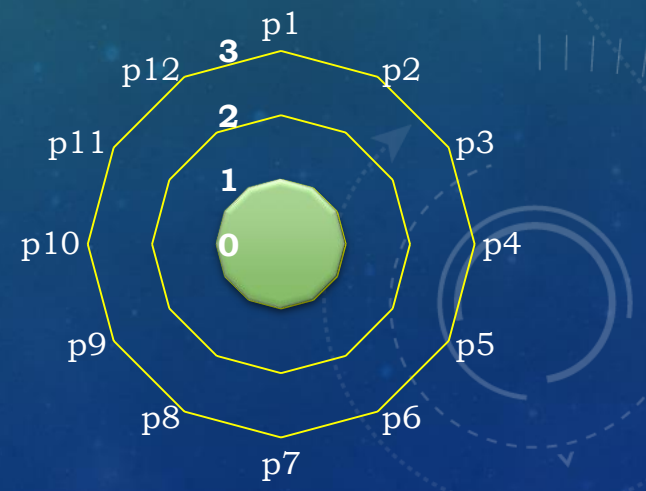
Mass Intensity (MI)

Reaction Mass Efficiency (RME)

Green Star rating



Excellent 100% area



Unacceptable ≤50% area

RESULTS AND DISCUSSION

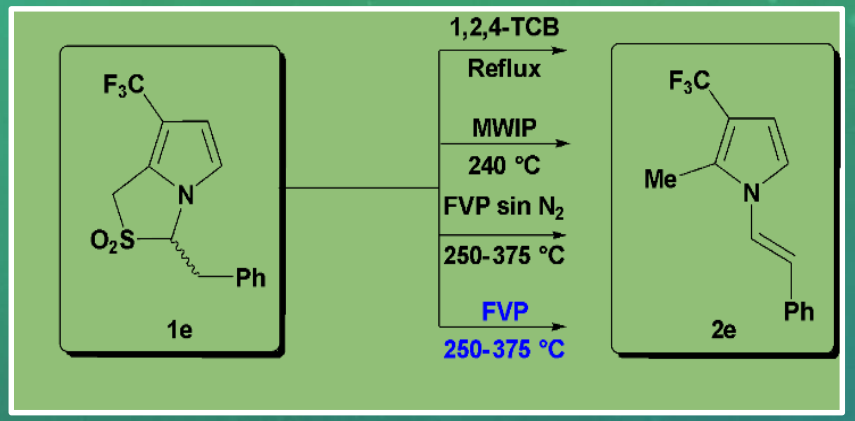


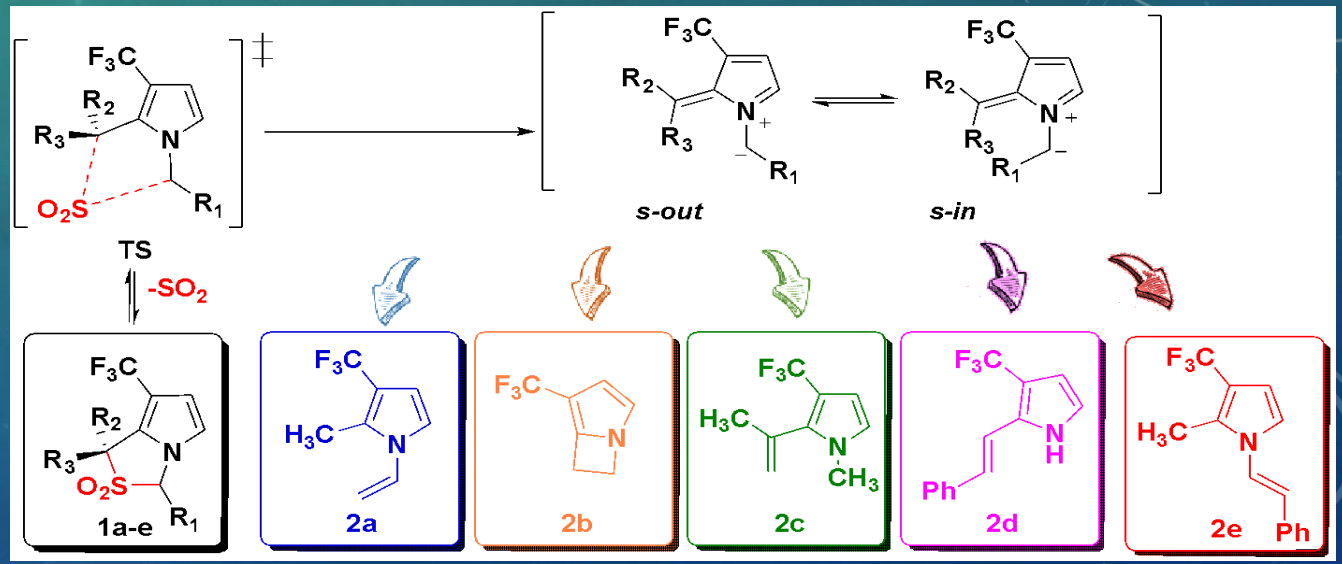
Table 1. *Thermolysis conditions and yield of obtained pyrroles*

T (°C)	1a	1b	1c	1d	1e
200	100,0	100,0	---	100,0	---
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250	59,0	71,0	97,0	74,0	100
275	34,0	50,0	79,2	47,7	92,9
300	14,0	10,0	58,3	30,0	55,9
325	0	0	20,8	---	32,4
350	---	---	13,1	---	9,1
375	---	---	0	---	0

Sulfone preparation methods

Utilized conventional techniques: reflux, microwave, and thermolysis/flash vacuum pyrolysis (FVP).

Sulfone thermolysis reactions



High conversion efficiency

Selective thermolysis system

Evaluating Reactions by Green Metrics

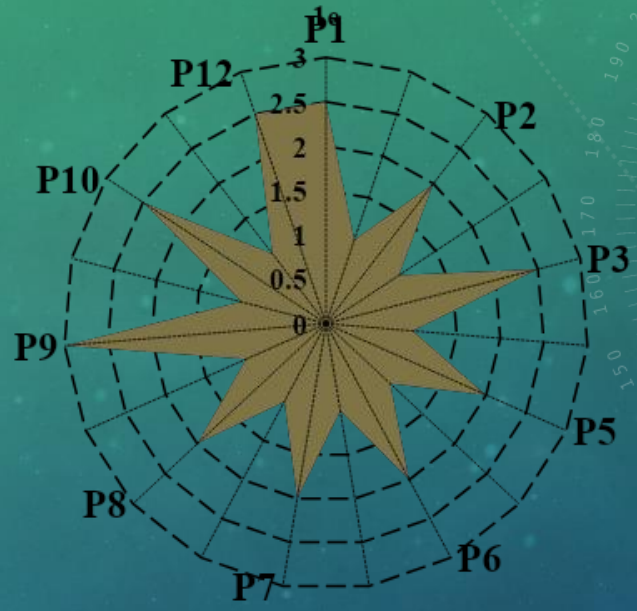
Table 2. *Evaluation of green chemistry parameters pyrroles.*

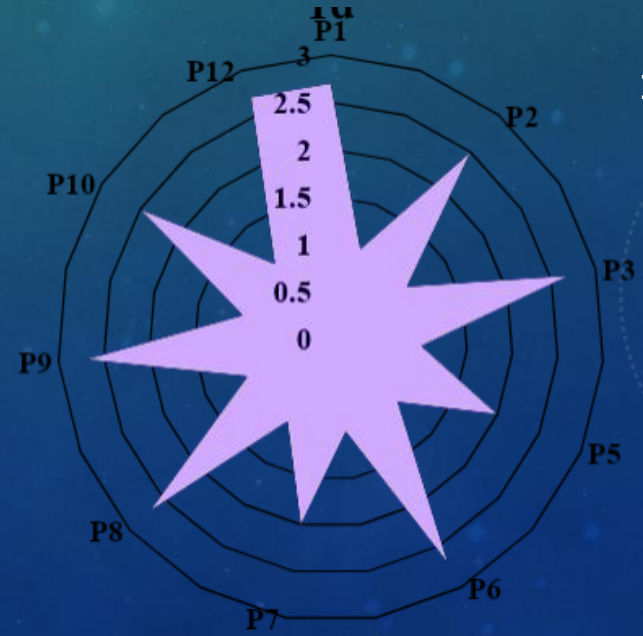
SUST.	YIELD %[A]	GSAI%	E-SCALE	MI	RME	AE	E
1A	89,30	75,50	81	2,6	82	76,62	2,0
1B	76,78	65,00	58,15	3,5	45,3	77,86	2,5
1C	80,56	66,25	58,45	2,3	40,23	79,06	3,2
1D	56,45	75,50	77,82	3,6	3,20	77,67	2,0
1E	98,34	80,78	82,45	2,5	90	77,56	1,5

Substances 1e and 1a are clearly the most efficient and sustainable routes, with 1e leading in all metrics, indicating a highly optimized process.

Substances 1b, 1c, and 1d show significant opportunities for enhancing sustainability through better reagent utilization and waste management.

Employing green chemistry metrics is crucial for enhancing the sustainability of synthetic processes.





CONCLUSIONS

•**Substances 1e** and **1a** represent the best choices for sustainable synthesis, effectively combining high yields and low waste, with **Substance 1e** exemplifying optimal green chemistry practices through pyrolysis.

•**Substances 1b, 1c, and 1d** need focused improvements in reaction mass efficiency and waste management to align better with green chemistry principles.

•The analysis highlights pyrolysis as a crucial green technique that facilitates high efficiency and low environmental impact in synthetic processes, reinforcing its importance in sustainable chemistry.

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EXPLORING TEACHERS' PERSPECTIVES ON INTEGRATING WASTE MANAGEMENT EDUCATION INTO TEACHER TRAINING PROGRAMMES TO PROMOTE ENVIRONMENTAL SUSTAINABILITY IN NIGERIA

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ABSTRACT

This study investigates the integration of waste management education into teacher training programs in Nigeria, addressing the critical need for environmental sustainability in the face of increasing waste generation. A qualitative approach was employed, utilizing thematic analysis to gather and interpret data from teachers regarding their awareness, understanding, and attitudes toward waste management and sustainability concepts. Findings reveal significant gaps in teachers' knowledge and confidence in teaching waste management, with many relying on external resources due to insufficient institutional support. Teachers expressed a strong desire for enhanced professional development opportunities and collaborative partnerships to improve their teaching practices. The study emphasizes the importance of an integrated curriculum that incorporates waste management across various subjects, alongside experiential learning opportunities. Recommendations include the establishment of robust professional development programs to equip educators with the necessary skills and resources to effectively teach sustainability concepts, ultimately fostering a culture of environmental responsibility among students.

Keywords: *Waste Management, Teacher Education, Environmental Sustainability, Curriculum Integration and Knowledge*

1. INTRODUCTION

Environmental sustainability has become an increasingly important global issue, with waste management being a critical component of this challenge. Nigeria, as Africa's most populous nation, faces significant waste management problems, which have severe implications for public health, environmental quality, and overall development. Despite generating over 32 million tons of solid waste annually, more than 70% of this waste is improperly managed, leading to widespread environmental degradation and health risks (World Bank, 2018). In this context, the education system, particularly teacher training programs, plays a crucial role in shaping the environmental consciousness of future generations. This study aims to explore teachers' perspectives on integrating waste management education into teacher training programs to promote environmental sustainability in Nigeria.

The current state of waste management in Nigeria is alarming. According to the United Nations Environment Programme (UNEP, 2020), only a small fraction of the waste generated in Nigerian cities is collected and properly disposed of, with most waste ending up in open dumpsites, rivers, or burned in the open air. These practices contribute to the contamination of water bodies, air pollution, and the spread of diseases such as cholera, dysentery, and respiratory illnesses (National Environmental Standards and Regulations Enforcement Agency [NESREA], 2021). The World Health Organization (WHO, 2019) reported that poor waste management is a significant factor in the spread of communicable diseases in Nigeria, with waste-related diseases contributing to high mortality rates, especially among children under five years old.

Given these challenges, there is an urgent need to enhance waste management practices across the country. Education, particularly at the formative stages of a child's development, is a powerful tool for instilling environmental awareness and promoting sustainable practices. However, the Nigerian education system, especially in teacher training programs, currently lacks a strong focus on environmental education, including waste management. This gap in the

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curriculum has significant implications for the ability of teachers to effectively educate students on the importance of environmental stewardship and sustainable practices. The role of teachers in promoting environmental sustainability cannot be overstated. Teachers are not only responsible for imparting knowledge but also for shaping the values, attitudes, and behaviors of their students. Studies have shown that when teachers are equipped with the necessary knowledge and skills, they can effectively influence their students' understanding and engagement with environmental issues (Oladejo et al., 2021). In this regard, integrating waste management education into teacher training programs is essential for fostering a culture of sustainability among future generations.

Despite the recognized importance of environmental education, there is a paucity of research on the perspectives of teachers regarding the integration of waste management content into teacher training programs in Nigeria. This study seeks to address this gap by exploring the attitudes, beliefs, and experiences of teachers in relation to waste management education. By understanding teachers' perspectives, the study aims to identify the challenges and opportunities associated with integrating waste management into the teacher education curriculum and to provide recommendations for enhancing the effectiveness of environmental education in Nigeria.

The importance of integrating waste management education into teacher training programs is supported by evidence from other countries. For instance, Finland, widely recognized for its high-quality education system, has successfully integrated environmental education, including waste management, into its teacher training programs. Finnish teachers are trained to incorporate sustainability into all aspects of their teaching, resulting in high levels of environmental awareness and engagement among students (Pereira, 2019). Similarly, South Korea has implemented a nationwide program that mandates the inclusion of environmental education in teacher training, leading to significant improvements in waste management practices and environmental consciousness among students (Kim & Chung, 2020).

In contrast, Nigerian teacher training programs have been slow to adopt environmental education, particularly in the area of waste management. This is partly due to a lack of resources, inadequate training materials, and limited awareness among educators about the importance of environmental sustainability (Akintunde & Oloyede, 2020). Furthermore, the curriculum in many teacher training institutions is heavily focused on traditional subjects, leaving little room for the inclusion of contemporary issues such as environmental education.

This study explores the perspectives of teachers who are on the front lines of education in Nigeria. By engaging with teachers through interviews and focus group discussions, the research will seek to uncover their views on the importance of waste management education, the challenges they face in integrating it into their teaching, and the support they need to effectively incorporate environmental sustainability into their classrooms. The qualitative nature of this study will allow for an in-depth exploration of teachers' experiences, providing rich insights into the practical realities of promoting environmental education in Nigeria.

Moreover, this research will contribute to the existing body of knowledge by highlighting the specific needs and concerns of Nigerian teachers regarding environmental education. It will also offer practical recommendations for policymakers, curriculum developers, and teacher training institutions on how to effectively integrate waste management education into teacher training programs. By addressing the gap in the current curriculum, this study aims to empower teachers to become agents of change, capable of fostering a generation of environmentally conscious citizens who are committed to sustainable practices.

Purpose of the problem: The study investigated teachers' perspectives on integrating waste management education into teacher training programs in Nigeria to promote environmental sustainability. Specifically the study:

a. examined teachers' awareness and understanding of waste management and environmental sustainability concepts.
b. explored teachers' attitudes towards the inclusion of waste management content in the teacher training curriculum.
c. assessed the support and resources available to teachers for delivering waste management education.

2. MATERIALS AND METHODS

This study employs a qualitative research design to explore the perspectives of pre-service teacher educators on integrating waste management education into teacher training programmes.

2.1. Population, sample and Sampling Techniqes

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The population of the study was the pre-service teachers educators in North-western Nigeria. Three Federal Colleges of Education were purposively sampled out of eight from the locale. Forty-five pre-service teacher educators were sampled through a simple random sampling procedure from the three selected Colleges in Zamfara, Kano, and Katsina.

2.1.1 Instrumentation

A researcher's design questionnaire was used to gather data. The questionnaire is an unstructured one with psychometric properties of content validity and a reliability index of 0.86. The questionnaire was prepared in an open-ended format in Google form to encourage participants to express their thoughts freely, providing valuable qualitative data.

The data collection process was through Google form, which was sent to pre-service teachers educators platforms, and responses were provided for analysis. Absolute confidentiality was maintained throughout, and participants were assured that their responses will remain anonymous in the reporting of findings.

2.1.1.1 Data Analysis

Once the data was collected, it was analyzed using thematic analysis, a method well-suited for qualitative research. This process involves identifying, analyzing, and interpreting patterns or themes within the data. The researcher carefully examined the responses, coding significant statements and organizing them into coherent themes that reflect the participants' perspectives on waste management education. These themes were then synthesized to provide a comprehensive understanding of the participants' awareness, attitudes, and the challenges they face.

Throughout the study, ethical considerations were rigorously observed. Participants were fully informed about the research's purpose and their rights, including the right to withdraw at any point. Informed consent was obtained, and all data were handled confidentially, with participants' anonymity preserved in the final report.

3. RESULTS AND DISCUSSION:

Results were presented as follows:

Research Question 1:
What is the level of teachers' awareness and understanding of waste management and environmental sustainability concepts?
Research question one was presented in Figure 1



Fig.1: ***A*** *mindmap diagram illustrating teachers' awareness of waste management and sustainability*

Teachers show varying levels of awareness about waste management and environmental sustainability, with many expressing limited knowledge and confidence in teaching these topics. Some, like T1 and T6, understand basic waste practices like recycling but lack depth on environmental impacts. Others, such as T9 and T31, are familiar with segregation but unsure of its sustainability role. Teachers like T3 and T10 struggle to incorporate waste management concepts despite personal knowledge, and T5, T14, and T25 emphasize a need for training on broader sustainability. Many, including T8 and T18, are aware of waste issues but uncertain about effective teaching methods. Teachers such as T20 and T37 know waste practices but question their environmental effects. Overall, while basic waste awareness exists, teachers report a need for additional resources and training to link everyday waste management to broader sustainability topics, enhancing their ability to teach environmental education confidently and comprehensively.

Research Question 2:
What are teachers' attitudes towards the inclusion of waste management content in the teacher training curriculum?
This was presented in Figure 2:

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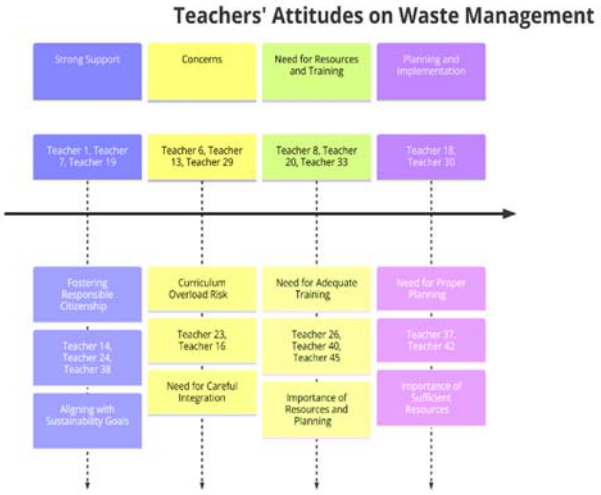


Fig. 2. *A timeline diagram illustrating teachers' attitudes toward waste management content inclusion*

Teachers overwhelmingly support including waste management in the training curriculum, seeing it as vital for fostering environmental responsibility. Teachers like T1, T7, and T19 believe it will prepare students to be eco-conscious citizens, while T14, T24, and T38 view it as aligning with global sustainability goals. However, T6, T13, and T29 express concerns about fitting this content into an already crowded curriculum, emphasizing the need for balance. Teachers such as T8, T20, and T33 stress the importance of adequate training and resources for effective delivery. Overall, teachers agree on the need for well-planned, resource-supported integration.

Research Question 3:
What support and resources are available to teachers for delivering waste management education?
Figure 3:

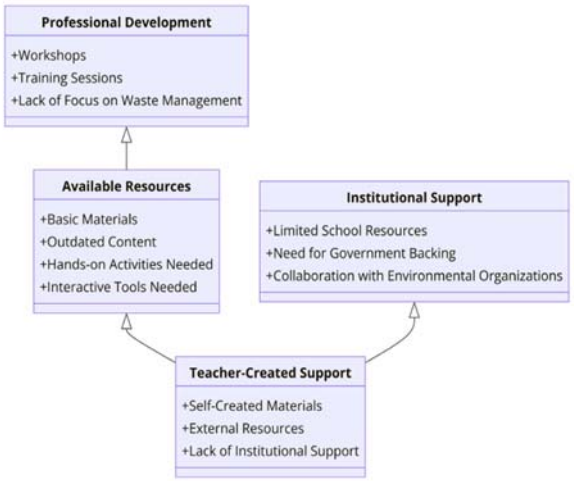


Fig. 3: *A class diagram illustrating the support and resources available for waste management education*

Teachers highlight a significant lack of resources and support for waste management education. Many, like T1 and T42, find existing materials insufficient for effective teaching. T4, T14, and T38 note limited and shallow instructional resources, hampering comprehensive education. Outdated materials concern T7, T26, and T33, who feel they're unsuitable for modern teaching needs. A need for practical, interactive tools is echoed by T6, T17, and T40, who seek hands-on activities to engage students. Teachers such as T5 and T39 often create their resources due to institutional gaps, with T15, T23, and T43 calling for greater government and organizational support.

4. CONCLUSIONS:

The study reveals a gap in teachers' understanding of waste management's link to sustainability, highlighting a need for enhanced education and resources. Recommendations include:

- Prioritizing waste management in teacher training curricula.
- Updating teaching materials with interactive tools and hands-on activities.
- Organizing regular training sessions focused on practical applications.
- Partnering with environmental organizations for support and resource sharing to bridge theory and classroom practice.

5. DECLARATIONS

5.1. Acknowledgements

Appreciation to the Pre-service teachers and educator who participated in this study

5.2. Open Access

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Southern Science Conference, 2024.

Exploring Teachers' Perspectives on Integrating Waste Management Education into Teacher Training Programmes to Promote Environmental Sustainability in Nigeria

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November/2024

INTRODUCTION

- Environmental sustainability has become an increasingly important global issue, with waste management being a critical component of this challenge.

- Nigeria, ------- waste management problems,
- Implications ------
- public health,
- environmental quality, and
- overall development.

- Nigeria is generating over 32 million tons of solid waste annually,
- > 70% ---- is improperly managed, -----leading to widespread environmental degradation and health risks (World Bank, 2018).

BACKGROUND

•The current state of waste management in Nigeria is alarming.

• only a small fraction of the waste generated in Nigerian cities is collected and properly disposed of,

• most waste ending up in

- •open dumpsites,
- • rivers, or
- • burned in the open air, causing environmental

• Urgent need to enhance waste management practices across the country.

• Education, powerful tool for instilling environmental awareness and promoting sustainable practices (at all educational level)

•Teacher education Programme -----Teachers shaping the values and behaviours of young people towards waste management

PURPOSE

The study examined teachers' views on incorporating waste management education into teacher training programs in Nigeria to enhance environmental sustainability. Specifically :

- examined teachers' awareness and understanding of waste management and environmental sustainability concepts.

- explored teachers' attitudes towards the inclusion of waste management content in the teacher training curriculum.

- assessed the support and resources available to teachers for delivering waste management education.

METHODOLOGY

The study's methods are one are as follows:

- **Research Design**: Qualitative research design
- **Population**: pre-service teachers educators in North-western Nigeria
- **Sample and Sampling Techniques**: Three Federal College of Education (Purposive sampling)
  - 45 Pre-service teachers educators
- **Instrumentation**: Researchers designed questionniare in Google form Psychometric Properties of Content validity and 0.86 reliability index
- **Procedure for data Collection**: Self administration and Research Assistants
- **Data Analysis Techniques**: Thematic analysis, Atlas ti statistical tool

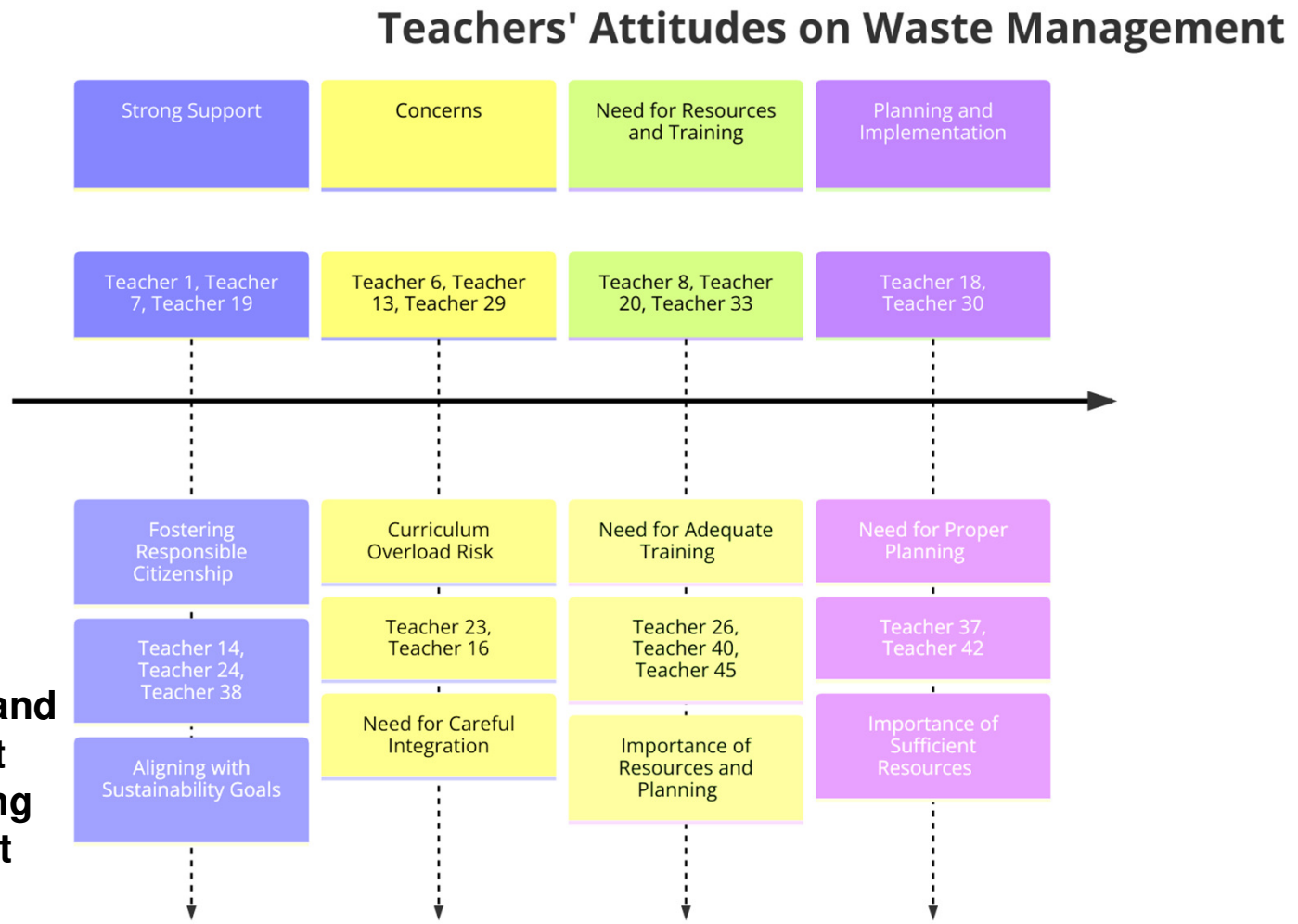
RESULTS AND DISCUSSION

Research Question 1:
What is the level of teachers' awareness and understanding of waste management and environmental sustainability concepts?



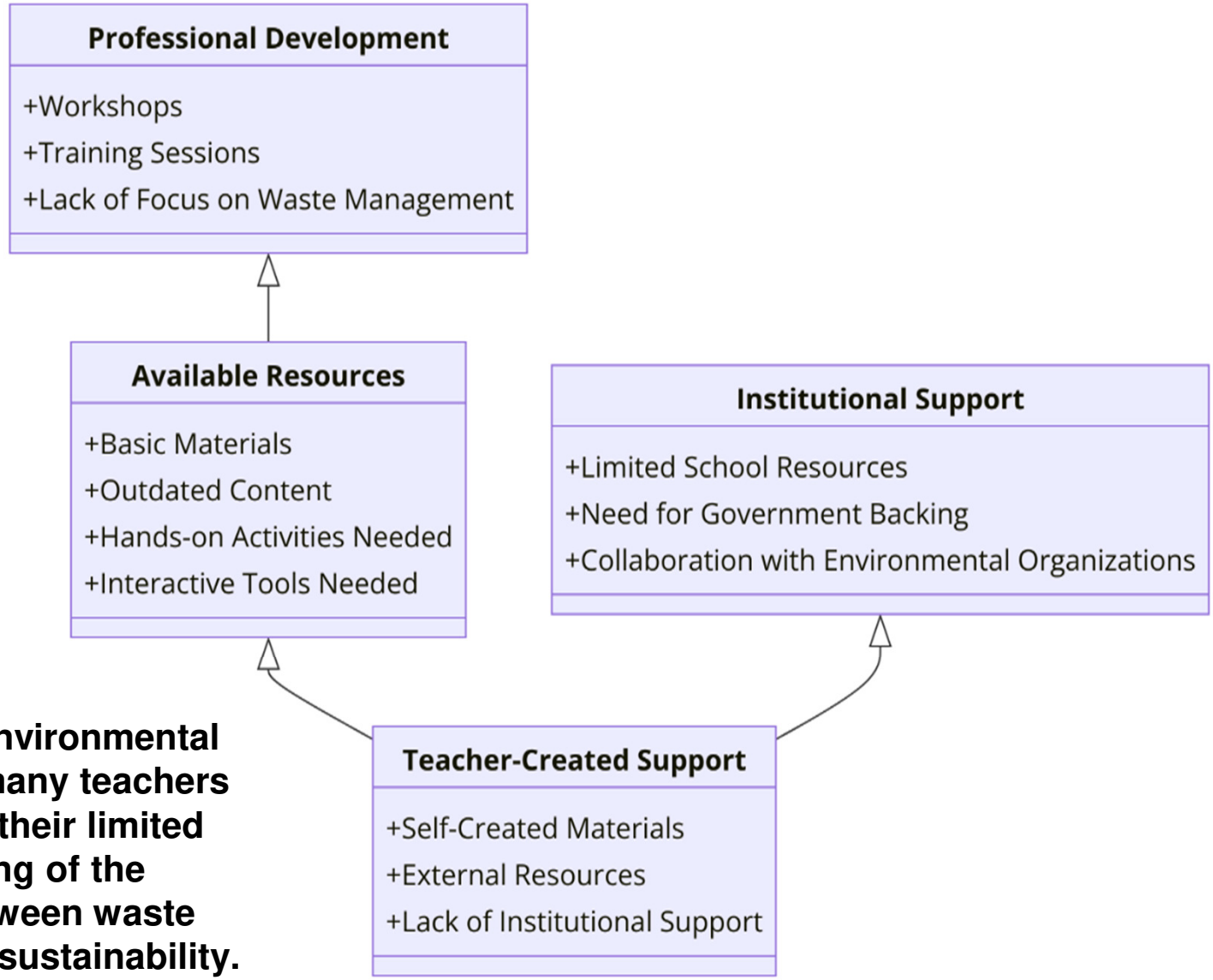
Overwhelming support among teachers for the inclusion of waste management content in the teacher training curriculum.

Research Question 2:
What are teachers' attitudes towards the inclusion of waste management content in the teacher training curriculum?



Critical need for adequate resources and training to support teachers in delivering waste management education.

Research Question 3:
What support and resources are available to teachers for delivering waste management education?



broader gap in environmental education, with many teachers acknowledging their limited understanding of the connection between waste management and sustainability.

CONCLUSIONS

The findings underscore the importance of integrating waste management education into teacher training curricula while providing adequate resources and support to facilitate this process to promote environmental suitability

- Integrate waste management and sustainability into teacher training
- Provide interactive, modern teaching materials.
- Offer regular training on practical waste management
- Partner with environmental groups for support and resources.

ACKNOWLEDGEMENTS

Special appreciation to the pre-service teachers educator who participated in this study

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2024 - VIRTUAL CONFERENCE AND IN PERSON EDITION

DETECTION OF URL PHISHING BASED ON MACHINE LEARNING TECHNIQUES

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ABSTRACT

Phishing URLs continue to pose a significant threat to online security, using sophisticated deception techniques to trick users into revealing sensitive information like passwords and financial data. Our research explores the potential of machine learning, specifically a Multilayer Perceptron (MLP) neural network, to effectively identify and flag these malicious websites. We trained and validated our model using two distinct datasets, focusing on distinguishing legitimate URLs from phishing attempts. To ensure thorough evaluation, we compared the MLP's performance against traditional machine learning approaches, including Decision Tree and Naive Bayes algorithms. Through this research, we aim to strengthen existing cybersecurity measures and provide more reliable protection against increasingly sophisticated phishing attacks. The results demonstrate promising potential for using neural networks in phishing detection, though further refinement may be needed to address emerging attack patterns.

Keywords: *Decision Tree, ANN, Naive Bayes, algorithms*.

1. INTRODUCTION

URL phishing poses a significant threat to web users, necessitating strong responses to evolving tactics used by attackers. This paper explores the intersection of machine learning (ML) and URL phishing detection to enhance security measures against these ongoing threats (Kaur *et al*., 2023).

The widespread use of the internet in daily life highlights the urgent need to combat phishing attempts that deceive users into revealing sensitive information, such as login details and financial data. A proactive approach is essential for tackling these risks, with ML serving as a powerful tool for improving the accuracy of phishing URL detection (Alkhalil *et al*., 2021).

This research focuses on analyzing URL characteristics to differentiate between benign and malicious links. As internet reliance grows, the impact of URL phishing becomes more severe, underscoring the need for effective measures to protect users from potential financial losses. The study aims to contribute to developing robust solutions to address the persistent threat of URL phishing, ultimately enhancing online security for users.

2. METHODOLOGY

1. Data Collection

We collected two datasets from Kaggle. The first dataset has 10,000 samples with 17 features (e.g., NumDots, UrlLength, CLASS_LABEL) indicating if URLs are benign (0) or malicious (1). The second dataset contains 450,175 URLs and their classifications.

2. Data Preprocessing

We extracted features from the second dataset to match the first for training and testing. Duplicate rows were removed using Python's Pandas drop_duplicates(). To address class imbalance, we used the SMOTE

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oversampling method to ensure equal representation of classes.

3. Model Selection and Implementation

We developed a Multi-Layer Perceptron (MLP) architecture. Starting with one hidden layer of 5 neurons, we gradually increased the count to 17, finding no accuracy improvement beyond that. We implemented two additional hidden layers, with the best configuration being three layers with 17, 30, and 10 neurons. The optimizer used was ADAM, and we applied the ReLU activation function for better performance in deep learning.

2.4. Model evaluation

In this research, we adopt a novel approach to demonstrate the effectiveness of our method. We will train and test on a smaller data set (10,000 samples) and validate on a larger one (450,175 samples), contrasting previous studies that train on large datasets and validate on smaller ones.

We utilize a confusion matrix (CM) to evaluate model performance in supervised learning. The CM parameters include:

- TP (True Positive): Correctly classified as positive
- TN (True Negative): Correctly classified as negative
- FP (False Positive): Incorrectly classified as positive
- FN (False Negative): Incorrectly classified as negative

These parameters help calculate:

- Recall: [\text{Recall} = \frac{TP}{TP + FN}]
- Precision: [\text{Precision} = \frac{TP}{TP + FP}]
- Accuracy: [\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}]
- F1 Score: [\text{F1 Score} = \frac{2 \times (\text{Precision} \times \text{Recall})}{\text{Precision} + \text{Recall}}]

This framework provides a comprehensive assessment of our model's performance.

3. RESULTS and DISCUSSION:

This section reviews the training, testing, and validation results of the proposed model, comparing it with Decision Tree (DT) and Naive Bayes (NB) algorithms.

Training and Testing Results

- **Data Sets**: Training on 10,000 samples; validation on 450,175 samples.
- **DT Results**:
  - Correctly predicted: 636 malicious, 944 benign.
  - Incorrectly classified: 63 benign as malicious, 532 malicious as benign.
- **NB Results**:
  - Correctly predicted: 984 malicious, 116 benign.
  - Incorrectly classified: 896 benign as malicious, 4 malicious as benign.
- **Proposed Model Results**:
  - Correctly predicted: 832 malicious, 917 benign.
  - Incorrectly classified: 95 benign as malicious, 156 malicious as benign.

Performance Metrics

- **Precision**: Proposed model: 0.876; highest among the models.
- **Recall**: Proposed model: 0.8741; effectively identifies malicious URLs.
- **F1-Score**: Proposed model: 0.875; best balance between precision and recall.
- **Accuracy**: Proposed model: 87.45%; strong performance overall.

Validation Results

- **DT on Larger Set**:
  - Correctly predicted: 99,672 malicious, 88,275 benign.
  - Significant drop in performance metrics.
- **NB on Larger Set**:
  - Correctly predicted: 201 malicious, 101,691 benign.
  - Notable decrease in performance metrics.
- **Proposed Model on Larger Set**:

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- Correctly predicted: 282,870 malicious, 93,085 benign.
- Maintained high precision, recall, and F1-score.

The proposed model consistently outperforms DT and NB across various metrics, demonstrating robustness and generalizability to larger datasets, while DT and NB show significant performance drops, indicating challenges in handling increased data volume and diversity.

4. CONCLUSIONS:

In conclusion, this paper demonstrates the effectiveness of the proposed machine learning model for detecting URL phishing, achieving commendable accuracy and sensitivity. The results indicate that the model not only performs well on both test and validation datasets but also maintains a low false positive rate, which is crucial for protecting benign websites from being misclassified as malicious. To enhance the model's performance further, future research should focus on adapting to the evolving landscape of phishing attacks by continuously updating the model and exploring feature selection techniques to optimize computational efficiency. Overall, the proposed model stands as a reliable solution for phishing URL detection, with ample opportunities for improvement and adaptation in response to emerging threats.

5. DECLARATIONS

5.1. Open Access

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DETECTION OF URL PHISHING BASED ON MACHINE LEARNING TECHNIQUES

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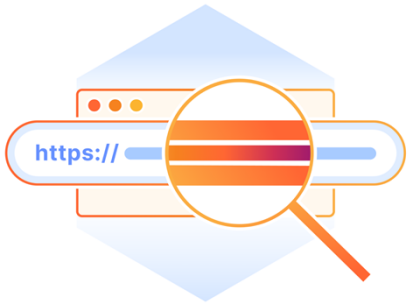
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College of Administration and Economics, University of Misan - Iraq

October 2024

INTRODUCTION



URL phishing is a growing threat to internet users, heightened by widespread use of the web, while traditional detection methods **struggle** to keep up with the evolving attacks.



Machine learning solutions can provide **enhanced security measures** against these threats by analysing URL characteristics



Phishing aims to deceive users into revealing *sensitive information*.
An increased reliance on the internet results in a larger attack area e.g. Banks, ID, etc.

Massive economical consequences of up to millions in damages (Ponemon Institute, 2021)

Literature Review & Background

Early studies explored various anti-phishing techniques, including heuristics, blacklists, and visual similarity (Khonji et al., 2013)

Challenges identified:

- Need for real-time detection
- Maintaining low false positive rates
- Addressing mobile phishing threats (Goel and Jain, 2018)

Recent research focuses on:

- Deep learning applications in cybersecurity (Dixit and Silakari, 2021
- Online algorithms for handling large datasets
- Feature extraction to improve ML model performance



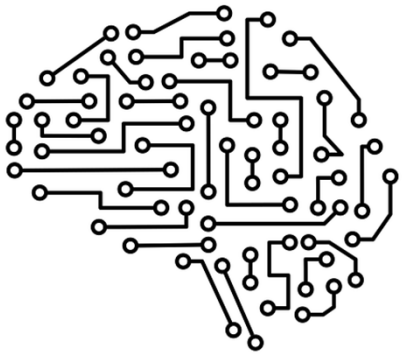


Artificial Neural Networks (ANNs) emerging as powerful tools for phishing
n (Yang et al., 2020)

Ongoing research on optimizing ANN architecture, including activation
functions and hidden layer configuration (Tran-Ngoc et al., 2019)

GOALS

To develop a **robust** machine learning model for detecting URL phishing

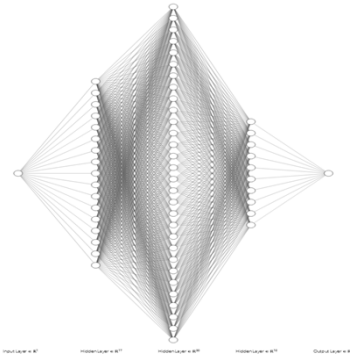


To enhance online security by improving the *accuracy and efficiency* of phishing detection techniques

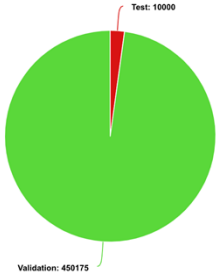


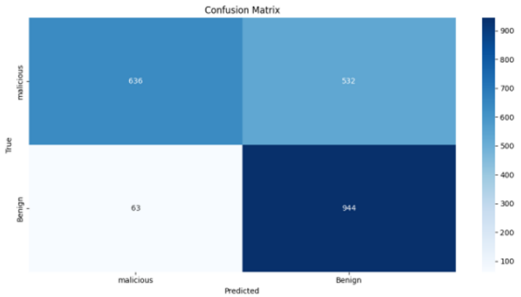
METHODOLOGY

- Data Collection:
  - Two datasets used: 10,000 samples (training/testing) and 450,175 samples (validation)
  - Features include URL characteristics (e.g., NumDots, SubdomainLevel, PathLevel)
- Data Preprocessing:
  - Feature extraction from second dataset
  - Removal of duplicate entries
  - Balancing dataset using SMOTE oversampling technique
- Model Development:
  - Proposed model: Multilayer Perceptron (MLP) neural network
  - Architecture: Three hidden layers (17, 30, 10 neurons)
  - Activation function: ReLU
  - Optimizer: ADAM
- Comparative Analysis:
  - Proposed MLP model compared with Decision Tree (DT) and Naive Bayes (NB) algorithms
- Evaluation Metrics:
  - Confusion matrix
  - Precision, Recall, F1-Score, Accuracy
- Validation:
  - Training/testing on 10,000 sample dataset
  - Validation on larger 450,175 sample dataset





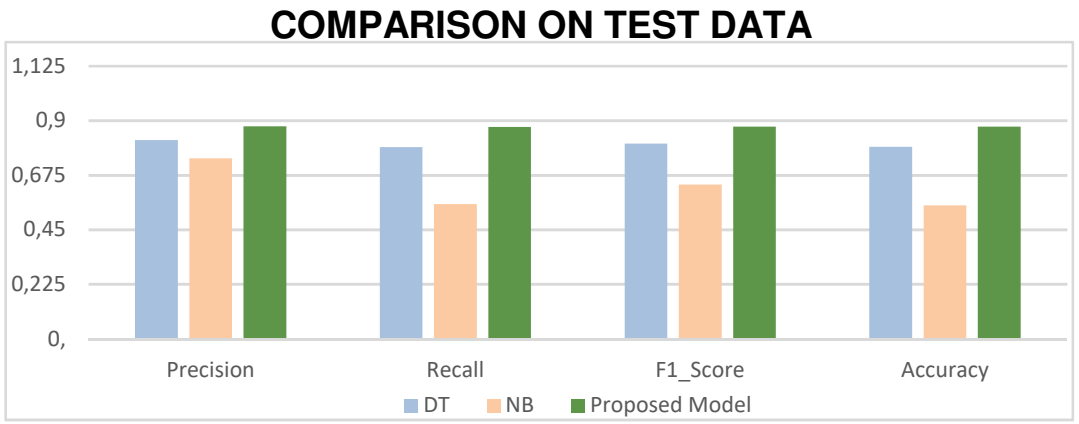


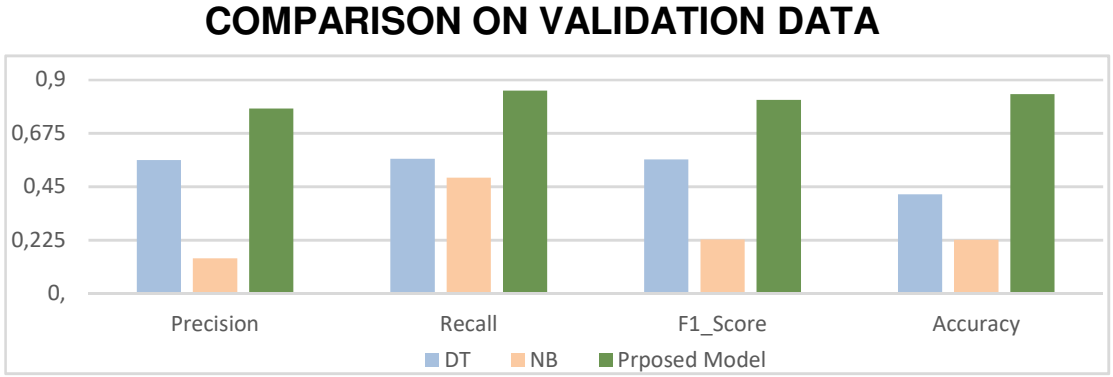


RESULTS AND DISCUSSION

Key Findings:

- Proposed MLP model **outperforms** DT and NB in all metrics
- *High generalizability* demonstrated on large validation dataset
- Consistent performance across both test and validation sets

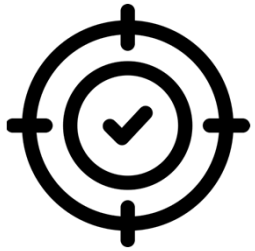




CONCLUSIONS

Proposed MLP model **outperforms** traditional ML algorithms:

- Higher accuracy on both test (87.45%) and validation (84%) datasets
- Better generalization to *unseen data*

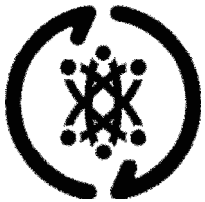


Advancements over previous research:

- Effective handling of large-scale datasets
- Improved balance between precision and recall

Potential impact:

- Enhanced online security through more accurate phishing detection
- Reduced false positives, minimizing disruption to legitimate websites



Future directions:

- Continuous model updating to address evolving phishing techniques
- Exploration of additional features for improved detection
- Potential integration with real-time web browsing security systems





Contribution to the field:

- Demonstrates viability of deep learning for URL phishing detection
- Provides benchmark for future phishing detection models

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II SOUTHERN SCIENCE CONFERENCE
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GLOBAL WARMING: MELTING OF THE ROOF OF AFRICA. MOUNT KILIMANJARO AND THE FOOTPRINT OF CLIMATE CHANGE.

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ABSTRACT

This paper will analyze the social relevance generated by global warming, glacier melting in order to see its impact on society through the importance of topics such as Mount Kilimanjaro in Africa, sea level rise and various vector-borne diseases. Through the use of Google, Google Scholar and Google Trends we will demonstrate the importance and attention that society gives to the topic over time, both in its relevance at a scientific level and in everyday life.

Keywords: *Global warming, Mount Kilimanjaro, Glacier melting, Sea level rise, Vector-borne diseases*.

1. INTRODUCTION

Global warming has been a much-discussed topic over the last decades, numerous organizations and governmental bodies have debated about how it affects the planet and have warned society about the implications for future generations of living in a world where climate cataclysms have no limits.

Global warming occurs due to the accumulation of greenhouse gases in the atmosphere, which cause the infrared radiation reflected by the Earth to be retained, causing an increase in the average surface temperature of the planet. However, due to anthropogenic actions, the concentrations of gases such as water vapor, carbon dioxide, methane, nitrogen oxide, ozone and chlorofluorocarbons (Gov. of Mexico, 2024) have potentially increased, causing imbalances that result in an adjustment of the climate system causing global warming.

Among the numerous consequences of the increase in the earth's average temperature are the melting of the large ice masses that make up the poles and glaciers, the consequent rise in sea level, and the appearance of diseases transmitted by different vectors (Bermúdez-Tamayo et al. 2023).

Mount Kilimanjaro in Africa has been one of the victims of global warming because its ice mass decreased considerably from 1970 to the 2000s as can be seen in Figure 1, where photographs taken thirty years apart show the melting of the glacier at its summit.



***Figure 1**. Mount Kilimanjaro (Africa) in 1970 and 2000.*

UNESCO states: “Its glaciers have endured at their peak for more than 10,000 years. However, climate change and human activities have caused an 80% decrease in the area covered by these glaciers during the 20th century”. UNESCO (2023). World Heritage glaciers: Sentinels of climate change (*UNESCO report No. 383551*).

According to the report launched in 2023 by UNESCO, the great icy mountains of Africa, Kilimanjaro in Tanzania, Kenya and Ruwenzori in the Democratic Republic of Congo, are symbols of global climate change and the first to disappear, and with them, the last remaining snow in Africa.

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This glacial retreat implies the lack of availability of fresh water for consumption, since it generates a great impact on the rivers whose flow depends on the thaw. The consequences on the growing populations living near the mountains and their surroundings have been severe since they depend on the hydrological and ecological functioning of the mountain. Likewise, melting ice does not only affect the vicinity, but also has implications such as an increase in sea level, the release of methane accumulated in the depths of the ice masses and even the slowing and modification of the course of ocean currents (UNRIC, 2023).

Melting glaciers and global warming are causing sea levels to rise, affecting coastlines, flooding and polluting coasts, and contributing to the spread of vector-borne diseases such as dengue fever and malaria. As a result, climate change affects the environment and the health of millions of people.

2. MATERIALS AND METHODS

2.1 Main materials and methods.

In this work a search was carried out using different search engines on global warming taking into account different keywords. For this purpose, five key words were established, Global Warming, Mount Kilimanjaro, Glacier Melting, Sea level rise, Vector-borne diseases; and, depending on the search engine, the number of results obtained was analyzed, whether they were scientific papers, news, or simply searches that included a term from the list. This is important to make a survey about how involved society is with these topics and how much relevance is given to the current climate situation.

2.1.1. Google search engine

First, we went to the main page of the Google search engine (Google, 2024) and searched for these words using the criteria of the number of searches performed in the last week and the last year, as it is shown in Figure 2 and 3, respectively.

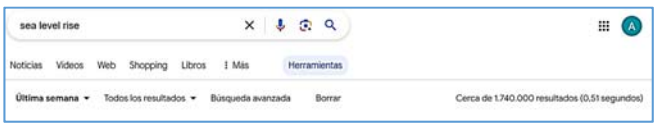


Figure 2. *Google image. Data mining on Sea Level Rise search performed in the last week.*

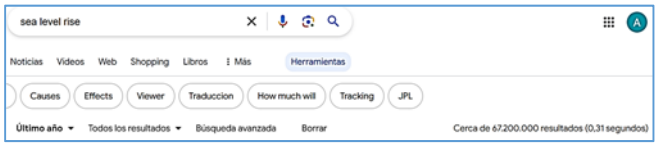


Figure 3. *Google image. Extraction of data on sea level rise search performed in the last year.*

The table of results obtained can be found in the Results and Discussions in the section 3.

2.1.2. Google Trends search Engine

Google Trends is a tool that allows us to analyze the population's interest in different topics through the volume of Google searches. Similarly to the above, the 5 keywords were inserted into the google trends search engine (Google Trends, 2024) and the search trends over a 5-year period were evaluated. Likewise, the geographic trend of searches will be analyzed to see which countries are most interested in the issues raised in order to correlate the results obtained.

2.1.3. Search in Google Scholar

In this search engine, a search for the aforementioned keywords was performed in Google Academic (Google academic, 2024). The search was conducted for the period 2019- 2024, i.e. a period of five years. The results of these searches were evaluated, as an example the following figure is placed below (Figure 4).

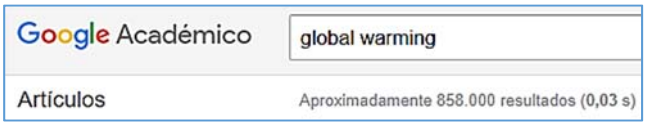


Figure 4*. Extraction of data on the search for global warming, carried out in the period 2019- 2024.*

3. RESULTS AND DISCUSSION:

3.1. Google.

The search results for the keywords were then analyzed using the Google search engine and are attached in Table 1.

Table 1*. Keyword search results.*

Keyword	One-week results	One-year results	Five-year results
Vector-borne diseases	12.100	1.500.000	13.100.000
Global warming	1.850.000	61.500.000	185.000.000
Mount Kilimanjaro	49.100	2.480.000	6.960.000

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Melting glaciers	17.100	292.000	4.510.000
Sea level rise	1.740.000	67.200.000	210.000.000

The table above shows that the word with the highest number of results after one week is global warming. From the one-year-old results it can be seen that the keyword with the highest number of searches is sea level rise, and finally it can be seen that the search with the highest number of results at five years old is again sea level rise.

It could be stated that the word with the highest number of searches is global warming and sea level rise. This may be due to the amount of information found in articles and websites because its effects are becoming more and more visible and urgent at a global level. In addition, the importance of awareness that is generated through the media, social networks and political influences on this topic.

3.2. Google trends.

The same searches performed in Google Trends showed a certain tendency depending on the keyword searched (Graphs 1-5).

When analyzing the phrase “rising sea levels”, countries with sea coasts were among those with the highest percentages of searches. When searching for “Mount Kilimanjaro”, Tanzania, the country where it is located, obviously led the search percentage. When analyzing the phrase “global warming”, if the word was in Spanish, the area of interest was South America and there were several peaks of interest in the months of April-May, since April 22nd is International Earth Day, according to the United Nations (UN). When analyzing the word “Glacier melting”, it is observed that the regions with large ice masses nearby are interested in this issue, such as Iceland, Canada, USA, etc. In addition, Figure 5 presents a summary of the results obtained, taking into account the five keywords as a whole. In this figure it can be seen that the darkest regions are the countries with the highest search peaks for the keywords analyzed.

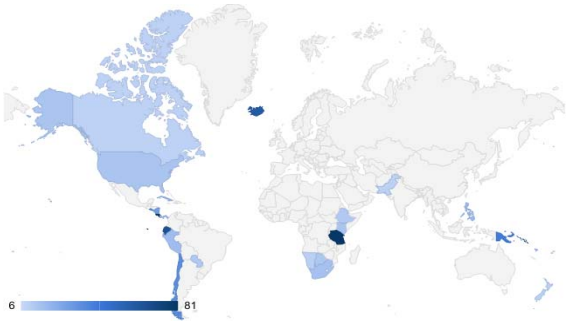
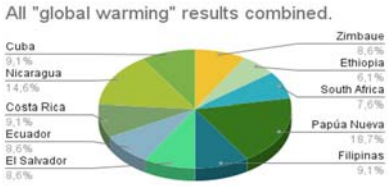
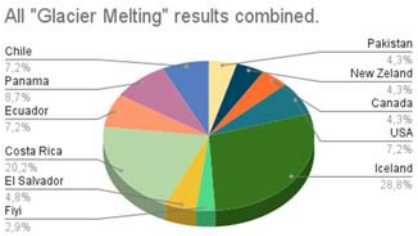


Figure 5. *Summary of the results taking into account the five keywords, the darkest regions are the countries with the highest search peaks.*

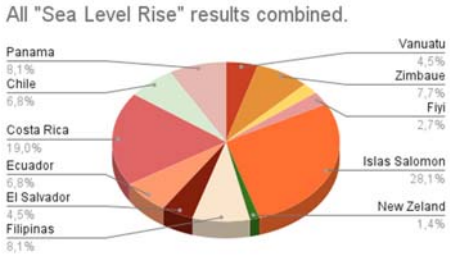
Graphs 1-5. *The graphs indicate the geographic areas that had the highest search interest. The time interval analyzed was 5 years (2019-2024).*



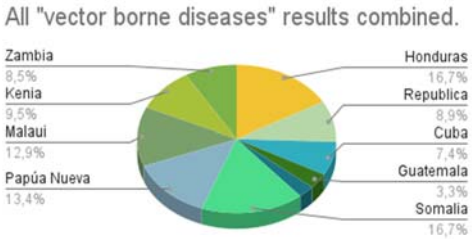
Graph 1. Combined results (English and Spanish) for the word “calentamiento global”.



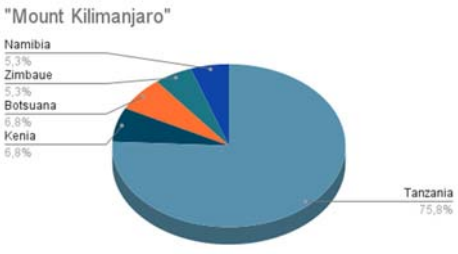
Graph 2. Combined results for “glacier melting”.



Graph 3. Combined results for “Sea level rise”.



Graph 4. Combined results for the word “vector-borne diseases”.



Graph 5. Combined results for the word “mount Kilimanjaro”.

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3.3. Google Scholar:

The results of the search for the different topics in the last five years were as follows and are presented in figures 6-10:

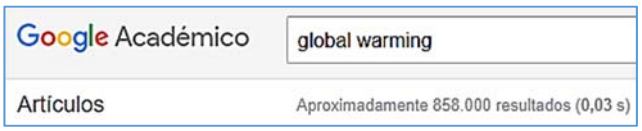


Figure 6. *Extraction of data on the search for Global Warming, carried out in the period 2019- 2024.*

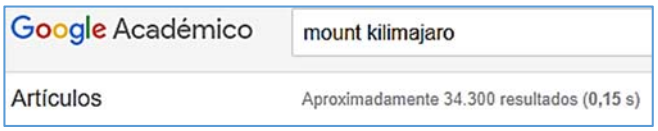


Figure 7. *Extraction of data on the search for Mount Kilimanjaro, conducted in the period 2019- 2024.*

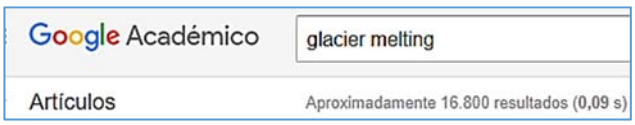


Figure 8. *Extraction of data on the search for glacier melting, carried out in the period 2019- 2024.*

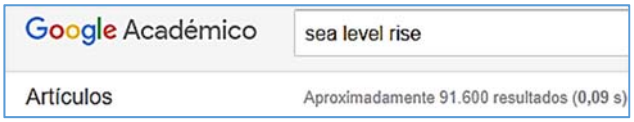


Figure 9. *Extraction of data on the search for Sea Level Rise, conducted in the period 2019- 2024.*

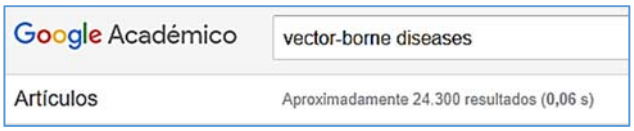


Figure 10. *Extraction of data on the search for Vector Borne Diseases, carried out in the period 2019- 2024.*

According to the results obtained we can see a big difference between the number of articles naming global warming compared to other of the selected words, also when entering many of these articles we can see that not all of them talk about the importance of climate or its consequences, but about recreational activities and other topics that are not important for this analysis.

4. CONCLUSIONS:

According to the results found by analyzing the “searches” for the different keywords, the impact on public opinion and the general interest of the population in general on the issue of climate change and global warming is reflected, being the melting of glaciers, including Mount Kilimanjaro, a clear example of these effects. The loss of these glaciers not only threatens local ecosystems, but also the availability of fresh water for human consumption and the global climate balance. These types of phenomena should motivate us as a society to ask governments in general to take urgent and sustainable measures to mitigate the impact of climate change and protect our natural resources for future generations, the need for change is crucial.

5. DECLARATIONS

5.1. Acknowledgements

The authors GB, HDA, RBL would like to thank the Department of Physical Chemistry (DFQ), the Faculty of Chemical Sciences (FCQ), the National University of Córdoba (UNC), and the professors of Environmental Physical Chemistry B (Belén Blanco and Walter Peláez) for the opportunity and help in the preparation of this work.

5.2. Open Access

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Southern Science Conference, 2024.

GLOBAL WARMING: MELTING OF THE ROOF OF AFRICA. MOUNT KILIMANJARO AND THE FOOTPRINT OF CLIMATE CHANGE.

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Aldana Huerta Derrac
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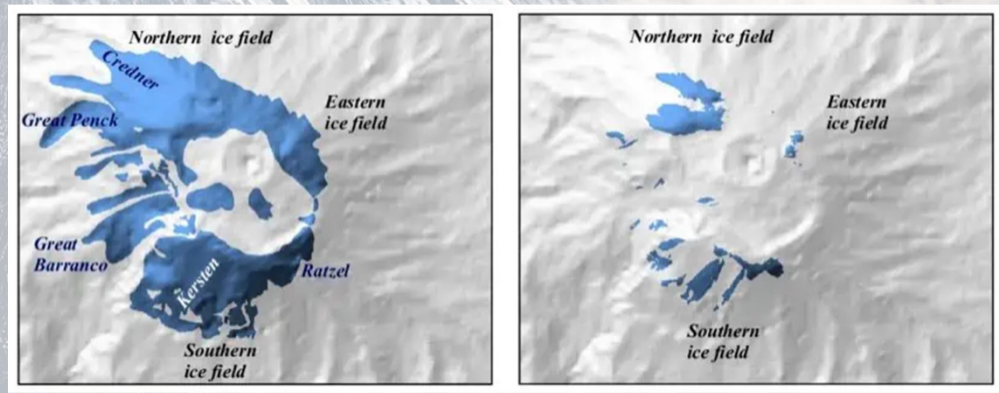
Bianca Lucia Renaudo
Universidad Nacional de Córdoba , Facultad de Ciencias Quimicas - Argentina.

November/2024

INTRODUCTION

Global warming, caused by the increase of greenhouse gases in the atmosphere, retains radiation and raises the surface temperature of the planet. Although beneficial at low levels, human activities have dangerously increased the concentrations of these gases, destabilizing the climate.

The consequences include melting glaciers, rising sea levels and the spread of diseases. Visible examples, such as the reduction of the ice mass on Mount Kilimanjaro, symbolize the effects of climate change, which also impacts the freshwater supply and affects the lives of millions of people and public health.



Comparative image of Kilimanjaro glaciers in 1912 (left) and in 2011 (right).

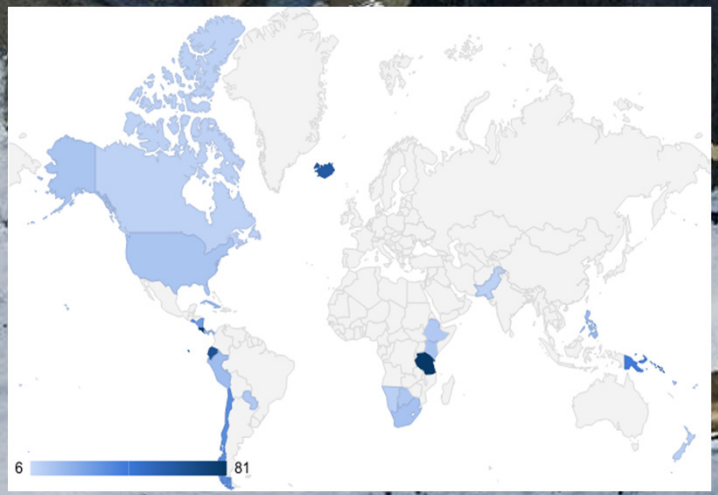
AIM/OBJECTIVE/PURPOSE

- Define key words as a consequence of a given image.
- Evaluate the social impact of global warming and glacier melting.
- Measure public and scientific interest in topics such as Mount Kilimanjaro and sea level rise using different search engines.
- With these data, analyze geographic trends in concern about climate change in different regions.

METHODOLOGY

A crawl was carried out using different search engines where the number of results obtained, scientific papers, news and clicks were analyzed. For which five key words were established:

Summary of the results, where the darkest regions are the countries with the highest search rates.



1. **Global Warming**
2. **Mount Kilimanjaro**
3. **Glacier melting**
4. **Sea level rise**
5. **Vector-borne diseases**

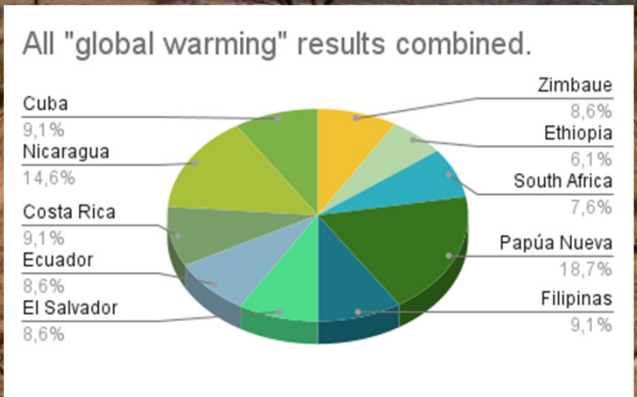
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RESULTS AND DISCUSSION

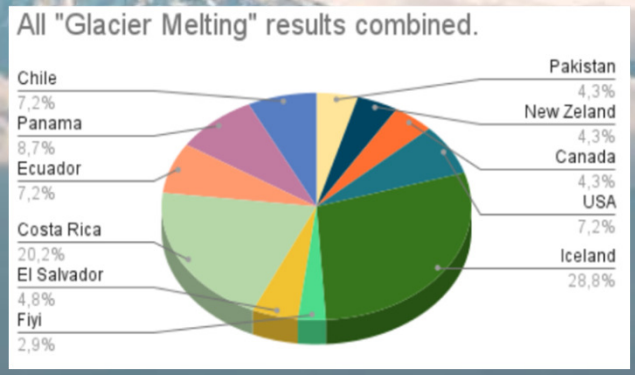
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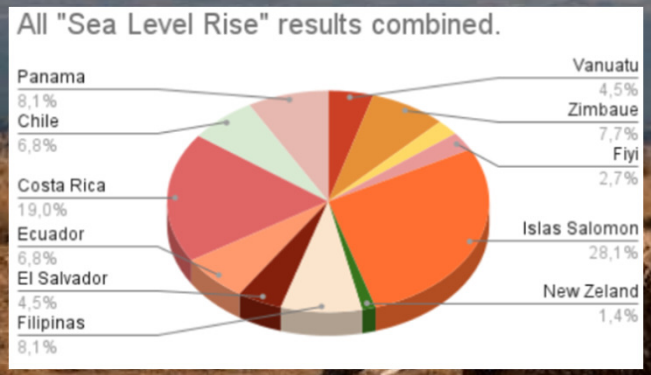
Results obtained through Google for the keywords.



Graph 1. Combined results (English and Spanish) for the word "global warming" obtained in Google Trends.

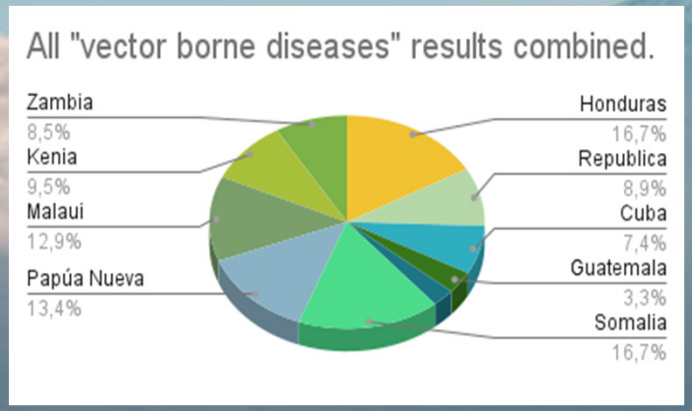


Graph 2. Combined results for "glacier melting" obtained in Google Trends.

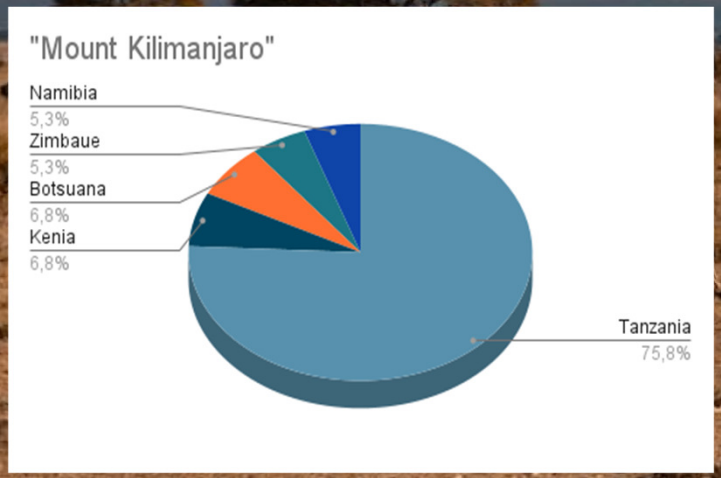


Graph 3. Combined results for "Sea level rise" obtained in Google Trends.

RESULTS AND DISCUSSION



Graph 4. Combined results for the word "vector-borne diseases" via google trends.



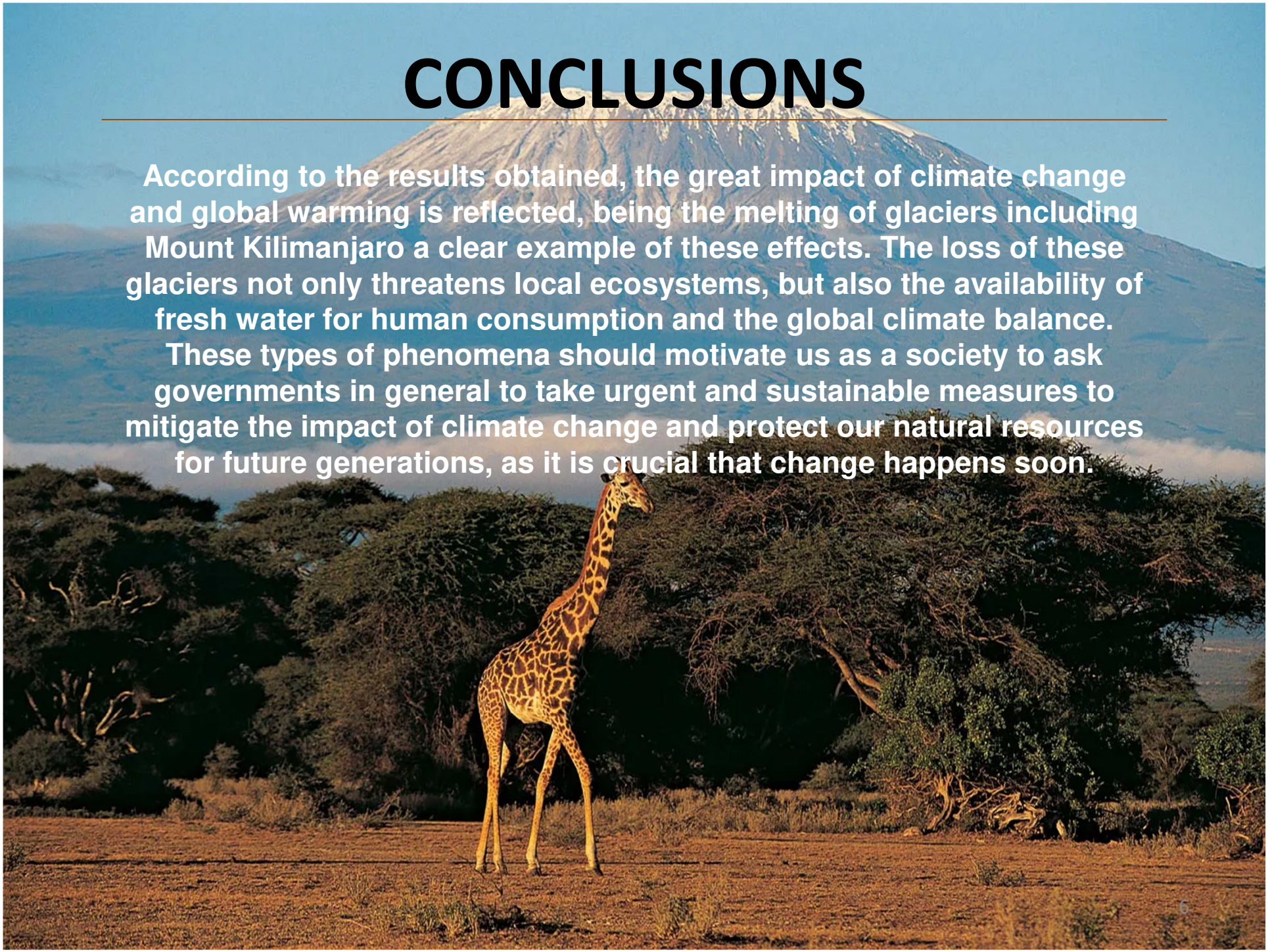
Graph 5. Combined results for the word "mount Kilimanjaro" via google trends

1	Global Warming	858.000
2	Mount Kilimanjaro	34.300
3	Glacier Melting	16.800
4	Sea level rise	91.600
5	Vector-borne diseases	24.300

Search results via google scholar

CONCLUSIONS

According to the results obtained, the great impact of climate change and global warming is reflected, being the melting of glaciers including Mount Kilimanjaro a clear example of these effects. The loss of these glaciers not only threatens local ecosystems, but also the availability of fresh water for human consumption and the global climate balance. These types of phenomena should motivate us as a society to ask governments in general to take urgent and sustainable measures to mitigate the impact of climate change and protect our natural resources for future generations, as it is crucial that change happens soon.



ACKNOWLEDGEMENTS

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EDUCATIONAL MANAGEMENT STRATEGIES TO MITIGATE CLIMATE CHANGE

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ABSTRACT

The study explores educational strategies for climate change mitigation, emphasizing community engagement, infrastructure management, and student involvement in schools. To explore educational strategies for effective climate change mitigation, a quantitative survey will be conducted with school administrators and teachers in Kwara State, analyzed using SmartPLS 3.0 for climate change strategies. Findings highlight key strategies for effective climate change mitigation in education. The study emphasizes the need for integrated strategies in education to foster community engagement and resilience against climate change. Finally, integrated educational strategies are vital for effective climate change mitigation and community resilience. The study underscores the significance of educational institutions in building climate-resilient communities through comprehensive mitigation strategies. These strategies encompass curriculum development, infrastructure adaptation, and community outreach programs. The research methodology employs a systematic approach to data collection and analysis, ensuring robust findings that can inform policy development and implementation. Results indicate that successful climate change mitigation in educational settings requires a multi-faceted approach combining theoretical knowledge with practical applications. The discussion examines the implications of these findings for educational policy and practice, highlighting the potential for schools to serve as catalysts for broader community engagement in climate action. Recommendations include developing targeted training programs for educators, establishing climate action committees within schools, and creating partnerships with environmental organizations. This research contributes to the growing body of knowledge on educational approaches to climate change mitigation, providing practical insights for educators and policymakers working to enhance climate resilience in educational settings.

Keywords*: Climate Change. Community Engagement. Infrastructure Management. Student Involvement. Educational Strategies*

1. INTRODUCTION

Climate change poses a significant global challenge, demanding innovative and collaborative solutions (Borde *et al*., 2022). Education is pivotal in this fight, as it empowers individuals and communities to embrace sustainable practices (Ballew *et al*., 2019). This article explores how community engagement, infrastructure management, and student involvement intersect to mitigate climate change locally. By fostering shared responsibility and equipping future leaders, educational strategies can enhance resilience and promote sustainability (Henderson & Serafeim, 2020; Abdullahi, 2020).

To explore educational strategies that enhance community engagement, infrastructure management, and student involvement in climate action.

2. MATERIALS AND METHODS

2.1. Materials

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The study utilized a standardized questionnaire to gather data from school administrators and teachers in public senior secondary schools in Kwara State, Nigeria. Additionally, SmartPLS 3.0 software was employed for data analysis. Relevant literature on climate change education and community engagement was also reviewed to support the research framework.

2.2. Methods

The study employed a quantitative research design, utilizing a standardized questionnaire distributed to school administrators and teachers in Kwara State, Nigeria. Data collection involved stratified sampling to ensure diverse representation. The collected data was analyzed using SmartPLS 3.0 to assess relationships between educational strategies and climate change mitigation.

2.2.1. Research Design

The study used a quantitative cross-sectional survey design. A standardized questionnaire was distributed to a stratified sample of 300 school administrators and teachers in Kwara State, Nigeria.

2.2.3. Data Analysis

Data was analyzed using SmartPLS 3.0 to assess relationships between educational strategies and climate change mitigation, focusing on path analysis and structural equation modeling for robust insights.

3. RESULTS AND DISCUSSION:

3.1. Results

Key findings revealed that involving communities fostered shared responsibility for sustainable practices (Abdullahi, 2020). Effective infrastructure management enhanced resilience against climate-related disasters (Ballew *et al*., 2019). Student participation in climate initiatives cultivated future leaders equipped to advocate for sustainability. The research, based on a survey of school administrators and teachers in Kwara State, Nigeria, highlighted the interconnectedness of these strategies and their significance in developing educational policies for climate mitigation.

3.2. Discussions

Climate change demanded innovative mitigation strategies. This article examined community engagement, infrastructure management, and student involvement in local climate action. Engaging communities fostered responsibility, while effective infrastructure enhanced sustainability (Unruan *et al*., 2022). A survey in Kwara State, Nigeria, highlighted the importance of these elements in informing educational policies.

4. CONCLUSIONS:

The study underscored the importance of community engagement, sustainable infrastructure, and student involvement in education to effectively mitigate climate change and foster future leaders.

5. DECLARATIONS

5.1. Study Limitations

Study limitations include geographic focus and potential bias in sampling.

5.2. Acknowledgements

The management of the University of Ilorin.

5.3. Funding source

University of Ilorin.

5.4. Competing Interests

No competing interests declared by the author.

5.5. Open Access

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6. HUMAN AND ANIMAL-RELATED STUDIES

6.1. Ethical Approval

The University of Ilorin's University Ethical Review Committee (UERC) has granted full committee approval for a research study titled "Educational Management Strategies to Mitigate Climate Change Issues." The project, led by Principal Investigator ABDULLAHI, Nimota Jibola Kadir from the Department of Educational Management, Faculty of Education, received approval on October 10, 2024 (Protocol ID: UERC/EDU/090, Approval Number: UERC/ESM/2023/2953). The approval period extends from October 10, 2024, to October 9, 2027, during which the investigator must comply with institutional guidelines and report any adverse events to the UERC. The research received full committee review and approval, with the requirement that the committee be informed at the commencement of research activities.

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Southern Science Conference, 2024.

EDUCATIONAL MANAGEMENT STRATEGIES TO MITIGATE CLIMATE CHANGE ISSUES

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November/2024

INTRODUCTION

- Climate change poses a significant global challenge, demanding innovative and collaborative solutions. Education is pivotal in this fight, as it empowers individuals and communities to embrace sustainable practice;
- This article explores how community engagement, infrastructure management, and student involvement intersect to mitigate climate change;
- Numerous research studies have been conducted on education and climate change issues such as Abdullahi (2020), Helen et al. (2021) among others;
- However, it is worth noting that none of the authors cited in this study specifically addressed educational management strategies and mitigation of climate change issues. Additionally, previous studies did not emphasize the importance of community engagement, student involvement, and infrastructure management as critical variables to measure educational management strategies. The great difference in the geographic locations and regions covered by the available studies is another important gap that prompted this investigation.

BACKGROUND

- Educational management strategies refer to the procedures, methods, and approaches that educators, administrators, and teachers use in schools, colleges, and other educational settings to plan, coordinate, lead, and manage the resources, activities, and learning process (Tonwe, 2019).
- Climate change refers to the alteration of weather patterns mostly brought about by an increase in atmospheric carbon pollution (Borde et al., 2022).
- The theoretical background of this study is based on the theory of planned behaviour proposed by Ajzen (1991).

AIM/OBJETIVE/PURPOSE

This purpose of this study is to explores the intersection of community engagement, infrastructure management, and student involvement in addressing climate change.

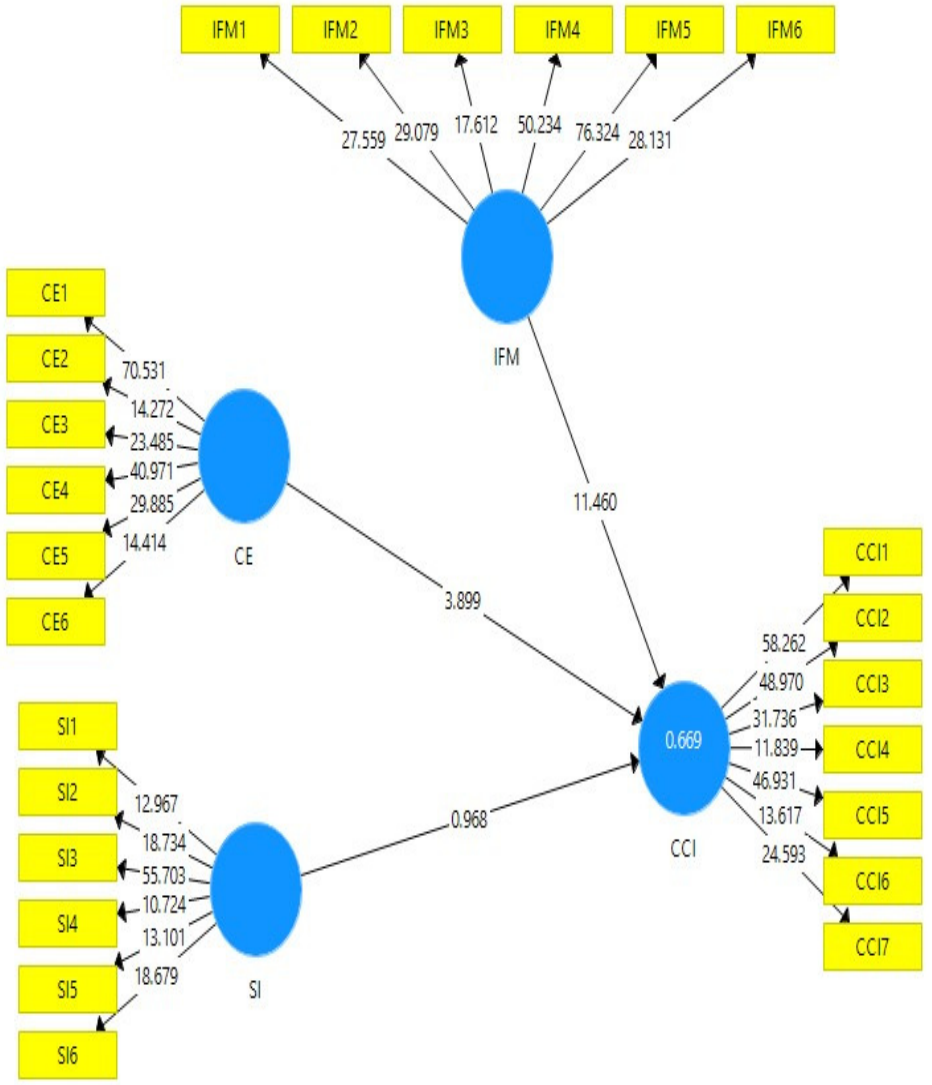
METHODOLOGY

- **Research design**: This research employs a quantitative research design.

- **Population**: A total number of 440 principals and teachers from Kwara State public senior secondary schools were purposively sampled and 430 participants responded to the survey
- **Data Collection**: A structured questionnaire was employed for the target participants to complete over the Internet by filling out a Google Forms survey. There were four variables namely community engagement, infrastructure management, waste management, and climate change issues with 25 items adapted as an instrument.
- **Ethical**: The survey questionnaire includes the ethical consent that the participants have to agree on before proceeding to answer the questionnaire. In this study, participation was completely optional, and participants were allowed to withdraw at any time without giving a reason. The participants' identities remained anonymous because their data was kept secret and confidential..
- **Data Analysis:** SMART PLS 4.0 was employed to analyze the data collected for this study. It was selected because SMART PLS comes with a wide range of tools and subroutines for formative and reflective assessments as well as structural models, like goodness of fit, bootstrap-based significance testing, PLS prediction, and the heterotrait-monotrait (HTMT) criterion.

RESULTS AND DISCUSSION

- **FINDINGS**- The findings revealed that two indicators of leveraging AI (community engagement and infrastructural management) have a positive relationship with mitigation of climate change. H2 (student involvement) is not supported

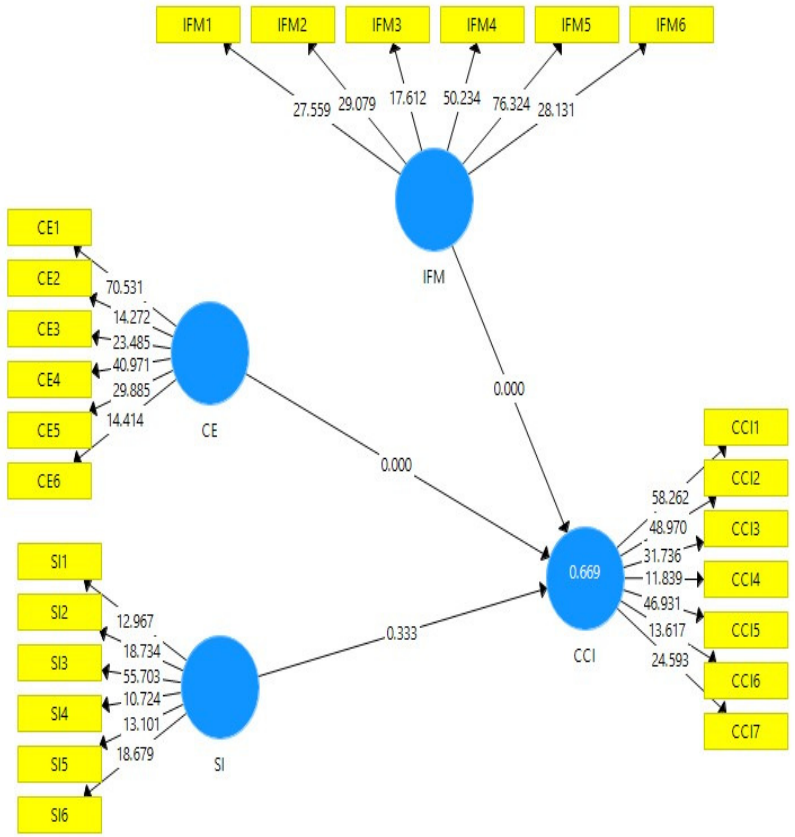


RESULTS AND DISCUSSION

.

Table 5: *Result of Structural Model (Path Coefficient)*

	Hypotheses	Original sample (Beta)	Standard Deviation (STDEV)	t-Value	P Value	Decision
	CE -> CCI	0.275	0.065	4.220	0.000	Supported
	SI -> CCI	-0.047	0.057	0.825	0.410	Not Supported
	IFM -> CCI	0.628	0.057	10.982	0.000	Supported



CONCLUSIONS

- The findings of this study show that effective educational management strategies can enhance the mitigation of climate change issues;
- Hypotheses 1 and 3 were shown to have a significant impact on the mitigation of climate change issues, however, hypothesis 2 had no significant impact on mitigation of climate change issues. ;
- **NOVELTY/VALUE:** This study provides evidence that educational management strategies (community engagement and infrastructure management) has a positive relationship with mitigation of climate change. Also, this study sheds light on how student involvement can improve the effective mitigation of climate issues.

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- Appreciation
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SOIL FERTILITY ANALYSIS" REFERS TO THE ASSESSMENT OF SOIL'S CAPACITY TO PROVIDE ESSENTIAL NUTRIENTS FOR PLANT GROWTH

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ABSTRACT

Understanding soil fertility variability in cultivated areas provides important insights for the rational use of soil amendments and fertilizers. This study aims to evaluate changes in the spatial variability of soil chemical properties resulting from intensive vegetable cultivation over more than 50 years in mountain agroecosystems in Nova Friburgo, Rio de Janeiro. The creation of maps for each attribute allowed visualization of its spatial distribution in the area, which is not possible when using only descriptive statistical analysis. The soil's chemical and physical attributes showed spatial variation, with P, K^+, Mg^{+2}, Al^{+3}, base saturation (V%), and silt displaying high variability, while Ca^{+2}, Ca+Mg, H+Al, organic carbon, CEC, sand, and clay showed medium variability. However, pH demonstrated low variability. Two main sources of variation in fertility spatial distribution were identified: one characterized by topography and another associated with agricultural activities, which, through intensive use of agricultural inputs, are contributing to increased soil fertility. Another factor is associated with inadequate soil management and topography, which cause the transport of finer soil particles and their accumulation in lower parts of the terrain, where enrichment in P, K^+, Ca^{+2}, Mg^{+2}, and organic carbon levels is observed. The evident acidity in agricultural soils is due to high natural acidity and farmers' infrequent use of liming. The soils showed values considered high or very high for P (88%) and K^+ (65%) in the study area. These values are directly associated with excessive use of poultry litter and soluble phosphate and potassium fertilizers during vegetable production.

Keywords: *Spatial variability; Geostatistics; Ordinary kriging; Soil fertility.*

1. INTRODUÇÃO

Em uma paisagem natural, o solo apresenta variabilidade espacial de seus atributos, resultante da interação de processos que comandam os fatores responsáveis por sua formação e fatores intrínsecos. Somado a esse efeito, tem-se que nos solos agrícolas, os fatores extrínsecos, normalmente, relacionados com as práticas de manejo são fontes adicionais de heterogeneidade (CARVALHO et al., 2003). A variação dos atributos químicos do solo é mais acentuada em áreas com cultivo intensivo do que em paisagem natural. A microbacia de Barracão dos Mendes, Nova Friburgo – RJ vem sendo explorada para produção de hortaliças por, aproximadamente, 50 anos. Nesse período, o sistema intensivo de produção adotado nessa região, em solos de baixa fertilidade natural, levou a aplicação de quantidades massivas de adubos orgânicos e fertilizantes minerais. O adequado manejo da fertilidade do solo, incluindo a análise química do solo é a chave para o aumento da produtividade agrícola. Através da interpretação dos resultados é possível realizar manejo químico do solo de maneira eficiente e econômica (RAIJ, 1991). A convencional aplicação de insumos agrícolas é baseada em teores médios de fertilidade do solo, podendo subestimar ou superestimar esses teores no solo, em consequência pode acarretar excessos ou déficit nutricionais em determinadas áreas. No entanto,

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segundo Bernardi et al. (2015), a gestão da fertilidade do solo, sem levar em consideração a variabilidade espacial pode afetar, diretamente, a produtividade e a qualidade ambiental. No entanto, a modernização da agricultura tem como ênfase o desenvolvimento sustentado, em que a otimização dos recursos de produção, minimização dos efeitos indesejáveis ao meio ambiente e aumento de produtividade são os objetivos finalísticos deste processo. Dessa forma, o conhecimento detalhado da variabilidade espacial dos atributos da fertilidade pode otimizar a aplicação localizada de fertilizantes, melhorando, dessa maneira, o controle do sistema de produção das culturas. O objetivo do presente trabalho é identificar os fatores responsáveis pela as alterações na variabilidade espacial ocorridas nos atributos químicos do solo decorrentes do cultivo intensivo de hortaliças, há mais de 50 anos, em agroecossistemas de montanha em Nova Friburgo - RJ.

2. MATERIAIS E MÉTODOS

A pesquisa foi realizada em área selecionada de exploração intensiva de hortaliças em região de montanha, localizada no município de Nova Friburgo-RJ, em área de amortecimento do Parque Estadual dos Três Picos. Usualmente, os agricultores da área de estudo utilizam o preparo convencional do solo, caracterizado por aração, seguida de gradagem, realizadas no sentido da pendente, comumente conhecida como “morro abaixo” e não utilizam práticas conservacionistas. O preparo do solo sempre é realizado antes da implantação da cultura objetivando o revolvimento de camadas superficiais para reduzir a compactação, ou visando a incorporação de corretivos. Foram coletadas 498 amostras de solo na profundidade de 0-20 cm, distribuídos pelas áreas cultivadas com hortaliças. Todas as amostras foram georreferenciadas, com a utilização de um GPS topográfico (Garmin, modelo Montana TM 650). Posteriormente, as amostras coletadas foram submetidas à determinação da fertilidade do solo e análise granulométrica, ambas as análises foram feitas conforme o Manual de Análise de Solo da Embrapa (DONAGEMMA et al. 2011). Os atributos químicos do solo avaliados foram: pH em H_2O (acidez ativa); fósforo assimilável (P); potássio trocável (K^+); cálcio trocável (Ca^{+2}); magnésio trocável (Mg^{+2}); alumínio trocável (Al^{3+}); H+Al (acidez potencial); carbono orgânico (Corg); capacidade de troca catiônica (CTC), e saturação por base (V%). Foi também realizada a análise granulométrica (teores de areia, silte e argila). Para cada atributo estudado, efetuou-se a análise descritiva clássica, com auxílio do software estatístico R, em que foram calculados a média, mediana, valores mínimo e máximo, desvio padrão, coeficiente de variação, assimetria e curtose. Para testar a hipótese da normalidade dos dados, os mesmos foram submetidos ao teste de Shapiro e Wilk (1965) a 5%.

3. RESULTADOS E DISCUSSÕES:

Os resultados da análise descritiva para os atributos químicos: pH em H_2O; teores de fósforo; potássio; cálcio; magnésio; sódio, e alumínio trocáveis; acidez potencial; carbono orgânico; capacidade de troca catiônica, e saturação por bases; e atributos granulométricos: areia; silte, e argila, são apresentados na Tabela 1. Os valores médios dos atributos químicos na camada de 0-20 cm apresentaram-se baixos para pH (moderadamente ácido, pH = 5,4), para Al^{+3} (0,2 $cmol_c\ dm^{-3}$), baixos para V% (35,2 $cmol_c\ dm^{-3}$); médios para Corg (15,5 g kg^{-1}) e Ca+Mg (4,5 $cmol_c\ dm^{-3}$); bom para Ca^{+2} (3,5 $cmol_c\ dm^{-3}$) e Mg^{+2} (1,0 $cmol_c\ dm^{-3}$); muito bom para CTC (12,5 $cmol_c\ dm^{-3}$); alto para H+Al (7,1 $cmol_c\ dm^{-3}$); e muito alto para P (204,9 mg dm^{-3}) e para K^+ (275,6 mg dm^{-3}). Observou-se o maior coeficiente de variação para o Al^{+3} e P (154,87% e 78,67%) e o menor para pH (9,51%). Segundo Frogbrook et al. (2002) valores elevados de CV podem ser considerados como os primeiros indicadores da existência de heterogeneidade nos dados. Estes resultados demonstram que existe uma grande variabilidade natural que pode ser decorrente de fatores como: material de origem, geomorfologia, uso do solo e tipo de solo, que será discutido com mais detalhes mais à frente. A classificação da variabilidade de um atributo pode ser classificada segundo a magnitude de seu CV, onde classifica-se como baixo: (CV ≤ 12%); médio (12% < CV < 60%), e alto (CV ≥ 60%) (WARRICK E NIELSEN, 1980). Nesse sentido, tem-se que o atributo pH apresentou baixa variabilidade; os atributos Ca^{+2}, Ca+Mg, H+Al, Corg, CTC, areia e argila apresentaram média variabilidade; e os atributos P, K^+, Mg^{+2}, Al^{+3}, V% e silte apresentaram alta variabilidade. Quando comparado aos resultados em solos sem atividade antrópica o mesmo padrão de classificação foi observado, com exceção de Ca^{+2} e silte, que em áreas naturais apresentaram variabilidade alta e média, respectivamente. Os valores de média e mediana da maioria dos atributos químicos do solo na profundidade de 0-20 cm estão próximos, mostrando assim, a tendência para concentração

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de valores menores que a média, apesar de terem valores mínimos muito baixos e máximos muito altos, relativamente, as classes de fertilidade adotadas. Os dados não apresentam distribuição simétrica, pois os coeficientes de assimetria e curtose não se encontram próximos a zero.

4. CONCLUSÕES:

Foi evidenciada duas fontes principais de variabilidade na distribuição espacial da fertilidade: uma associada às atividades agrícolas, através do uso massivo de agroquímicos, principalmente, adubos fosfatados, potássicos e cama de aviário, e o manejo inadequado do solo (preparo no sentido da pendente), estão contribuindo para o aumento dos teores de nutrientes do solo. E a segunda associada pelo relevo local. Onde, esses dois fatores em conjunto determinam maior acumulação de P, K^{+}, Ca^{+2}, Mg^{+2} e Corg nas partes mais baixas do relevo.

O uso intensivo do solo com hortaliças promoveu aumento nos teores P, K^{+}, Ca^{+2}, Mg^{+2} e Corg, quando comparado com as áreas de vegetação natural sem atividade antrópica.

A acidez evidenciada dos solos agrícolas, se deve a baixa frequência de uso da calagem pelos agricultores.

5. DECLARATIONS

5.1. Open Access

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Tabela 1. *Análise descritiva dos atributos químicos e granulométricos na profundidade de 0-20 cm*

Atributos[(a)]	Média	Mediana	Valores		Desvio Padrão	Coeficiente			W[(b)]
			Mínimo	Máximo		Variação	Assimetria	Curtose	
pH (H_2O)	5.4	5.4	4.1	6.9	0.52	9.51	0.1	-0.4	0.992
P (mg dm^{-3})	204.9	156	11.1	1060.3	161.23	78.67	1.7	3.4	0.842
K^+ (mg dm^{-3})	275.6	228.2	3.9	1362	185.39	67.27	2	6.2	0.83
Ca^{+2} ($cmol_c$ dm^{-3})	3.5	3.1	0	10.9	1.88	53.63	1.2	1.8	0.912
Mg^+ ($cmol_c$ dm^{-3})	1	0.9	0	4.2	0.68	66.37	0.9	1.1	0.943
Ca+Mg ($cmol_c$ dm^{-3})	4.5	4	1.1	12.2	2.1	46.24	1.2	1.2	0.912
Al+3 ($cmol_c$ dm^{-3})	0.2	0.1	0	2.1	0.35	154.87	2.5	6.9	0.675
H+Al ($cmol_c$ dm^{-3})	7.1	6.4	0.3	27.7	3.57	50.56	1.4	4.1	0.923
Corg (g kg^{-1})	15.5	14.9	0	80.6	8.37	53.89	2.1	11.4	0.876
CTC (cmo_{lc} dm^{-3})	12.5	11.8	3.9	36	4.45	35.62	1.5	4.6	0.906
V% ($cmol_c$ dm^{-3})	35.2	37.3	0	96	21.38	60.76	0	-0.5	0.964
Areia (g kg^{-1})	404.7	469.6	35.7	920	191.38	47.29	-0.2	-0.9	0.906
Silte (g kg^{-1})	210.4	169.5	0	570	131.74	62.62	0.5	-0.9	0.929
Argila (g kg^{-1})	384.6	396	54.7	794.7	110.39	28.7	-0.1	1.1	0.978

[(a)]pH, P, K^+, Ca^{+2}, Mg^{+2}, Al^{+3}, H+Al, Na, Corg, CTC e V% são respectivamente potencial hidrogeniônico, fósforo, potássio, cálcio, magnésio, alumínio, acidez potencial, sódio, carbono orgânico, capacidade de troca catiônica e saturação por bases; [(b)]teste de Shapiro e Wilk.

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Southern Science Conference, 2024.

ANÁLISE DA FERTILIDADE DO SOLO E SUA DISTRIBUIÇÃO ESPACIAL: IMPACTOS NO MANEJO DE SISTEMAS AGRÍCOLAS SUSTENTÁVEIS

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Nelson Moura Brasil do Amaral Sobrinho
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Universidade Federal Rural do Rio de Janeiro, Instituto de Agronomia - Brasil.

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INTRODUÇÃO

- A variação dos atributos químicos do solo é mais acentuada em áreas com cultivo intensivo do que em paisagem natural;
- O adequado manejo da fertilidade do solo, incluindo a análise química do solo, é a chave para o aumento da produtividade agrícola;
- A gestão da fertilidade do solo, sem levar em consideração a variabilidade espacial pode afetar produtividade e a qualidade ambiental;
- O conhecimento detalhado da variabilidade espacial dos atributos da fertilidade pode otimizar a aplicação localizada de fertilizantes, melhorando, dessa maneira, o controle do sistema de produção das culturas.

OBJETIVO

O objetivo do presente trabalho é identificar os fatores responsáveis pela as alterações na variabilidade espacial ocorridas nos atributos químicos do solo decorrentes do cultivo intensivo de hortaliças, há mais de 50 anos, em agroecossistemas de montanha em Nova Friburgo - RJ.

MATERIAIS E MÉTODOS

- A pesquisa foi realizada em área selecionada de exploração intensiva de hortaliças em região de montanha, localizada no município de Nova Friburgo-RJ;

- Foram coletadas 498 amostras de solo na profundidade de 0-20 cm, distribuídos pelas áreas cultivadas com hortaliças;

- Todas as amostras foram georreferenciadas, com a utilização de um GPS e as amostras coletadas foram submetidas à determinação da fertilidade do solo e análise granulométrica, ambas as análises foram feitas conforme o Manual de Análise de Solo da Embrapa;

- Os atributos químicos do solo avaliados foram: pH em H2O (acidez ativa); fósforo assimilável (P); potássio trocável (K+); cálcio trocável (Ca+2); magnésio trocável (Mg+2); alumínio trocável (Al3+); H+Al (acidez potencial); carbono orgânico (Corg); capacidade de troca catiônica (CTC), e saturação por base (V%).

RESULTADOS E DISCUSSÃO

Os resultados da análise descritiva para os atributos químicos: pH em H2O; teores de fósforo; potássio; cálcio; magnésio; sódio, e alumínio trocáveis; acidez potencial; carbono orgânico; capacidade de troca catiônica, e saturação por bases; e atributos granulométricos: areia; silte, e argila, são apresentados na Tabela 1.

Tabela 1. *Análise descritiva dos atributos químicos e granulométricos na profundidade de 0-20 cm*

Atributos[a]	Média	Mediana	Valores		Desvio Padrão	Coeficiente			W[b]
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[a]pH, P, K^+, Ca^{+2}, Mg^{+2}, Al^{+3}, H+Al, Na, Corg, CTC e V% são respectivamente potencial hidrogeniônico, fósforo, potássio, cálcio, magnésio, alumínio, acidez potencial, sódio, carbono orgânico, capacidade de troca catiônica e saturação por bases; [b]teste de Shapiro e Wilk.

RESULTADOS E DISCUSSÃO

Os valores elevados de CV podem ser considerados como os primeiros indicadores da existência de heterogeneidade nos dados.
Estes resultados demonstram que existe uma grande variabilidade natural que pode ser decorrente de fatores como: material de origem, geomorfologia, uso do solo e tipo de solo.

Tabela 1. *Análise descritiva dos atributos químicos e granulométricos na profundidade de 0-20 cm*

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RESULTADOS E DISCUSSÃO

Nesse sentido, tem-se que o atributo pH apresentou baixa variabilidade; os atributos Ca+2, Ca+Mg, H+Al, Corg, CTC, areia e argila apresentaram média variabilidade; e os atributos P, K+, Mg+2, Al+3, V% e silte apresentaram alta variabilidade.

Quando comparado aos resultados em solos sem atividade antrópica o mesmo padrão de classificação foi observado, com exceção de Ca+2 e silte, que em áreas naturais apresentaram variabilidade alta e média, respectivamente.

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CONCLUSÕES

- Atividades agrícolas, através do uso massivo de agroquímicos, principalmente, adubos fosfatados, potássicos e cama de aviário, e o manejo inadequado do solo estão contribuindo para o aumento dos teores de nutrientes do solo.

- Associada pelo relevo local, esses dois fatores em conjunto determinam maior acumulação de P, K+ , Ca+2, Mg+2 e Corg nas partes mais baixas do relevo.

CONCLUSÕES

- O uso intensivo do solo com hortaliças promoveu aumento nos teores P, K+, Ca+2, Mg+2 e Corg, quando comparado com as áreas de vegetação natural sem atividade antrópica.

- A acidez evidenciada dos solos agrícolas, se deve a baixa frequência de uso da calagem pelos agricultores.

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Southern Science Conference – Speakers



Mayná Coutinho is a seasoned Environmental Engineer, currently serving as the Environmental/Sustainability Coordinator (ESG) at Companhia Estadual de Águas e Esgotos (CEDAE) in Rio de Janeiro, Brazil. Additionally, she holds the prestigious positions of President of the Guandu River Basin Water Committee and President of the State Water Resources Council of Rio de Janeiro, where she has driven significant environmental policy development and management. With a strong academic background, including a Bachelor of Science in Environmental Engineering from Universidade Federal Fluminense and an Associate Degree in Environment from Colégio Federal Pedro II, Mayná has been instrumental in implementing sustainability practices and pioneering environmental projects. Her notable work includes leading the Forest Restoration Programme of Tingua-Bocaina, in partnership with the State Government of Rio de Janeiro and The Nature Conservancy Brazil, aimed at reforesting 30,000 hectares in the state's most crucial water supply basin. Complementing her professional endeavors, Mayná is currently enhancing her expertise through online specializations in Climate Solutions at the University of Edinburgh and Sustainable Cities at Johns Hopkins University.



Dr. Miguel Walter Fornes, MD PhD, conducts primary research at the National Research Council of Argentina (CONICET) and the Institute of Histology and Embryology in Mendoza (IHEM). He oversees the Mendoza Andrological Research Laboratory (LIAM), focusing on sperm physiology. The laboratory is committed to unraveling the intricacies of sperm formation and physiology within the seminiferous tubule. Our investigations highlight the significant influence of diet on various parameters such as morphology, spermatic capacitation, and ejaculated sperm count. We particularly explore the effects of dietary fat content, with a keen interest in supplementing unhealthy diets with olive oil. Our research has shown promising results in reversing sperm failure induced by high-fat diets. The LIAM team delves into the underlying mechanisms, both positive and negative, to provide comprehensive insights into sperm health and function.



Bhavna Ambudkar is a seasoned professional with expertise in electronics, telecommunications, research, teaching, entrepreneurship, and innovation. With over 25 years of experience in Electronics & Telecommunication, she excels in Computer Networks, Digital Electronics, Healthcare, Innovation, and Educational Technology. Bhavna holds a Doctor of Science (D.Sc.) degree in Engineering, along with a Ph.D. and Masters in Electronics & Telecommunication Engineering. She has authored over 50 research publications and holds 10 patents, showcasing her ability to bridge academic research with practical applications. In addition to her academic achievements, Bhavna has been instrumental in nurturing entrepreneurship and innovation. She has mentored numerous start-ups and entrepreneurs, facilitating idea development and funding acquisition. Bhavna's contributions have earned her recognition at national and international levels, bolstering her extensive networks and collaborations across various domains. Certified by Cambridge International and Dale Carnegie, she is adept at building and fostering professional relationships. Bhavna's multifaceted expertise and commitment to innovation continue to shape her impactful contributions to academia and industry alike.



Juliana Gracieli Rezende de Oliveira. Graduated in Biological Sciences from de the State University of Montes Claros – UNIMONTES – (2004-2008), Master in Rural Studies from Federal University of Vales do Jequitinhonha and Mucuri – UFVJM (2023). Mastering in Professional Master's Degree in National Network in Water Resources Management and Regulation – ProfÁgua (2023). Specialist in Biotechnology from Federal University of Lavras – UFLA (2010). Specialist in Management and Educational Environmental from the Federal University of Maranhão UFMA – (2023). Specializing in Conciliation and Conflict Mediation – Mediator Center (2022). She is currently the owner of the environmental consultancy company, Ipê Environmental Solutions, at Unaí/MG and she has worked with a great focus on managing and mediating conflicts in river basins where there is conflict over the use of water resources through Local Management Committees.



Dr. Fernando Pelegrini holds a degree in Chemical Engineering from the Federal University of Bahia (1981), a specialization in Petrochemical Engineering (CENPEQ-PETROBRAS/UFBA), a specialization in Equilibrium Separation Processes (COFIC / UFBA), a master's degree in Chemical Engineering from the Federal University of Rio de Janeiro (1987) and a PhD in Chemical Engineering from the Federal University of Rio de Janeiro and Lyngby University (Denmark) (1992). He worked at the Federal University of Bahia as a researcher (4 years), at the Camaçari Petrochemical Complex - Bahia (6 years) and at the School of Chemistry of UFRJ for 27 years, where he became a Full Professor. He is currently a Volunteer Professor at EQ/UFRJ and a Full Professor at the SENAI CIMATEC University Center. He was awarded as Researcher 1A (CNPq) and Scientist of the State of Rio de Janeiro. He has about 250 papers published in national and international journals, 600 papers in national and international congresses, and more than 155 students graduated in master's and/or doctoral degrees. Translator of Van Ness (Thermodynamics), Incropera (Mass and Heat Transfer) and Reactor Calculus (Roberts). Coordinator of several projects with companies and government institutions. Coordinator of the Competence Center for Process Intensification at SENAI-CIMATEC. He has experience in the area of Chemical Engineering, with emphasis on Applied Thermodynamics and Process Engineering, working mainly on the following topics: PETROLEUM, PETROCHEMICALS, biofuels, natural products, supercritical fluid, phase balance, intensification and optimization of processes, circular economy and green H_2.



Dr. Nancy F. Ferreyra completed her PhD in 2002, followed by postdoctoral research at various prestigious institutions. She conducted research at the Laboratory of Organic Electrochemistry and Redox Photochemistry of Joseph Fourier University in Grenoble, France, the Laboratory of Biophysical Chemistry and Molecular Oncology at the Institute of Biophysics Brno, Czech Republic, and the Bioelectrochemistry Laboratory of the Faculty of Chemical and Pharmaceutical Sciences at the University of Chile, Santiago de Chile. In 2005, she joined the Scientific and Technical Research Council of Argentina, CONICET. Currently, Nancy holds the position of Associate Professor at the Faculty of Chemical Sciences at the University of Córdoba. She also serves as an Independent Researcher at INFIQC- CONICET. Nancy's research focuses on the design, synthesis, characterization, and application of biofunctionalized nanomaterials for the development of electrochemical biosensors.



Dr. Ramon Loureiro Pimenta graduated in Veterinary Medicine from the Federal Rural University of Rio de Janeiro (UFRRJ) in 2009, PhD in Science, Technology and Innovation in Agriculture from the Federal Rural University of Rio de Janeiro (UFRRJ) in 2018. He has been working in the poultry industry for 14 years, slaughtering, processing and recycling of butcher animals in various industries in Brazil and 6 years as a university professor, currently linked to the Department of Public Health at the Federal Rural University of Rio de Janeiro teaching the subject Poultry Health. Participates as a collaborator in research groups at UFRRJ, Fiocruz and University of Vassouras in the areas of antimicrobial resistance in poultry farming, aquaculture and slaughterhouse effluents. He has been part of the Rio de Janeiro Poultry Health Committee for 6 years, in addition to having carried out several works together with the Ministry of Agriculture, Livestock and Supply (MAPA) and EMBRAPA.



Dr. Paloma Martins Mendonçais Bachelor in Biological Sciences in Universidade Santa Úrsula (2004). Specialist in Medical Entomology from the Oswaldo Cruz Institute - IOC/FIOCRUZ (2006). Training Course in Studies on Muscoid Diptera of Forensic and Public Health Importance, held at the Oswaldo Cruz Institute. Master in Parasitic Biology from the Oswaldo Cruz Institute, Fiocruz. PhD in Veterinary Sciences (Veterinary Parasitology) from UFRRJ where she was a CNPq scholarship holder. He has a Post-Doctorate in Biodiversity and Health at Fundaçõo Oswaldo Cruz (2015-2017), with a scholarship from CNPq. He has experience in the area of Parasitology, with an emphasis onEntomology of Parasites and Vectors and Forensic Entomology, working mainly on the following topics: Bionomy of muscoid dipterans, morphology, scanning electron microscopy, human and animal myiasis, alternative control of arthropods of medical importance-veterinary, molecular taxonomy of muscoid dipterans. She was a scholarship holder of the Bolsa Nota 10-FAPERJ Program from March 2009 to February 2010. She served as Municipal Secretary for the Environment and Urbanism of Itaboraí (2017-2020). She works as an Environmental Consultant at the company Contact Soluções Ambientais. Vice Coordinator of the Professional Master's Degree in Environmental Sciences at the University of Vassouras (04/2021 to 08/2023). Adjunct Professor of the Professional Master's Degree in Environmental Studies at the University of Vassouras. Executive Editor of Revista da Saúde - UV (2017-2024).



André Dantas Martins serves as the Environment Secretary for the Municipal City Hall of Paty do Alferes, leveraging expertise in General Biology with a focus on Environmental Management, Clinical Analysis, Forest Restoration, Recovery of Degraded Areas, Environmental Licensing, Environmental Education, Waste Management, and Conservation Unit Management. With demonstrated experience in public leadership and management, he specializes in Environmental Management of Hydrographic Basins, Environmental Expertise and Audit. Currently pursuing a master's degree in Environmental Sciences at the University of Vassouras, Martins is actively engaged as a member of the Municipal Environmental Council, REBIO ARARAS Advisory Council, and the Executive Board of the Pirabanhas Committee. He also holds the position of President at ANAMMA-RJ.



Daniela Alejandra Quinteros is a pharmacist with a Ph.D. in chemical sciences from the National University of Córdoba (UNC), Argentina. She is currently an Adjunct Professor (by competition) at the same University and an Independent researcher at the National Scientific and Technical Research Council (CONICET). She completed her postdoctoral study at the Complutense University - Madrid (2010), Bioforge (Biomaterials, Biomimetics, Nanobiotechnology) - Universidad De Valladolid - Spain - 2013 and University of Campinas - Brasil - 2018. Her research project is related to the development of pharmaceutical systems for the improvement in pharmacotherapy of pathologies of high prevalence, on this opportunity, we focused in for the treatment of neurodegenerative eye pathologies. She has expertise in neuroprotective pharmaceutical systems applied topically and intravitreally in different models in vivo to improve ocular pharmacotherapy. Within this framework, She has directed master's degrees, doctoral theses, and postdoctoral fellows. In addition, has received awards from The Association for Research in Vision Ophthalmology, the Ministry of Industry and Mining of the province of Córdoba, and awards in congresses. Has published 30 scientific articles in journals 6 book chapters, and is the author of 1 Invention Patent. She is a full member of the Argentine Society of Experimental Pharmacology (AAFE), part of the CONICET-CCT- CORDOBA, is a member of the board of directors of the Institute Research and Development in Pharmaceutical Technology (UNITEFA) and co-founder of 3DFarmic.



Ana Karine Furtado de Carvalho is a Food Engineer graduated from the Federal University of Ceará-Brazil (UFC) and earned both a master's and doctoral degree from the Graduate Program in Chemical Engineering at the Lorena School of Engineering - University of São Paulo-Brazil (EEL-USP). Specialized in Bioprocesses, renewable energy matrix development, and biosystems, contributes to projects of biorefinery systems. With expertise in chemical reactors and bioreactors, the professional also works on the reuse of agro-industrial waste for fine chemistry and material characterization. Currently serving as a faculty member at the University of São Paulo in the Department of Basic and Environmental Sciences at EEL-USP, the engineer continues to make significant contributions to the field of Engineering.



Paulo Wilton Camara is a highly accomplished academic and professional with extensive experience in various fields. He holds a Post-Doctorate in Military Sciences and a Doctorate in Political Science, among other degrees. With over 33 years of experience in teaching and academic management, he has worked in multiple institutions in Rio de Janeiro and Goiás. Throughout his career, he has been involved in creating and managing educational programs, such as the Soma Business Incubator. He currently holds several leadership positions at the University of Vassouras, including General Coordinator of Postgraduate Studies and Deputy Coordinator of the Master's Degree in Environmental Sciences. Additionally, he is actively involved in research projects related to renewable energy, environmental monitoring, and circular economy. In the business realm, he founded PW/TARGET Consulting and Services Ltd., specializing in strategic business management and innovation. He is also a member of professional associations and has served as a consultant and instructor for organizations like Sebrae/RJ. With expertise in public policy, planning, sales, marketing, operations, and logistics, Paulo Wilton Camara is a respected figure in academia and business, contributing significantly to both fields.



Ernesto García graduated in Industrial Engineering from the Universidad Autónoma Metropolitana – Azcapotzalco (UAM-A), obtained a Master's degree in Manufacturing Engineering with a specialization in control and automation from the Escuela Superior de Ingeniería Mecánica y Eléctrica - Azcapotzalco (SEP-ESIME Azc), and completed a Doctorate in the Science of Mechanical Engineering with a specialization in Tribology and surface studies. He is a member of "Investigadoras e Investigadores por México" in CONACYT, having been assigned from 2016 to 2022 to the University of Guadalajara at CUCEI, and since 2022 to the present at the Universidad Politécnica del Valle de México- Tultitlán (UPVM). He has extensive experience in the study, modification, and application of surfaces, including establishing a laboratory at UPVM dedicated to modifying and studying surface properties. He has designed and built several tribometers with sliding contact configurations. Similarly, he has experience in surface modification, including the deposition of metallic, ceramic, polymeric, and composite films on various material substrates using physical and chemical techniques. Currently, he is involved in several projects aimed at improving the tribological properties used in the medical, energy, and food industries.



Dr. Maximiliano Rossa carried out under-graduate and doctoral studies at the Facultad de Ciencias Químicas of the Universidad Nacional de Córdoba, earning a Ph.D. in Chemical Sciencies in 2005. He held post-doctoral positions at INFIQC (Córdoba, Argentina) in 2007-2009, and at the Laboratoire de Chimie Physique/Université Paris-Sud 11 (Orsay, France) in 2010. As well, he performed short research stays at the Departamento de Química Física I/Universidad Complutense de Madrid (Spain) in 2008, and jointly at the Centre Laser Infrarouge d´Orsay (France) and at the Centre Physique des Interactions Ioniques et Molculaires/Université Aix-Marseille (France) in 2017 and 2019. His main research field is Physical Chemistry, with focus on Molecular Reaction Dynamics for studying a variety of gas-phase physical and chemical processes (involving metal-containing species and clusters, as well as s-heptazine derivatives), and on Laser Chemistry, especially in pulsed laser ablation/desorption of solids and its applications to laser processing of (bio)materials.



Dr. McCullough is an internist, cardiologist, epidemiologist holding degrees from Baylor University, University of Texas Southwestern Medical School, University of Michigan, and Southern Methodist University. He manages common infectious diseases as well as the cardiovascular complications of both the viral infection and the injuries developing after the COVID-19 vaccine in Dallas TX, USA. Dr. McCullough has broadly published on a range of topics in medicine with > 1000 publications and > 685 citations in the National Library of Medicine. His works include “Pathophysiological Basis and Rationale for Early Outpatient Treatment of SARS-CoV-2 (COVID-19) Infection” the first widely utilized treatment regimen for ambulatory patients infected with SARS-CoV-2 in the American Journal of Medicine and subsequently updated in Reviews in Cardiovascular Medicine. Subsequently he published the first detoxification approach titled “Clinical Rationale for SARS-CoV-2 Base Spike Protein Detoxification in Post COVID-19 and Vaccine Injury Syndromes” in the Journal of American Physicians and Surgeons. He has dozens of peer-reviewed publications on the infection and has commented extensively on the medical response to the COVID-19 crisis in TheHill, America Out Loud, and on FOX NEWS Channel. Dr. McCullough testified multiple times in

the US Senate, European Parliament, Texas Senate Committee on Health and Human Services, Arizona Senate and House of Representatives, Colorado General Assembly, New Hampshire Senate, Pennsylvania Senate, and South Carolina Senate concerning many aspects of the pandemic response. Dr. McCullough has had years of dedicated academic and clinical efforts in combating the SARS-CoV-2 virus and in doing so, has reviewed thousands of reports, participated in scientific congresses, group discussions, press releases, and has been considered among the world's experts on COVID-19



Master's degree in Applied Health Sciences from Severino Sombra University (2019), Postgraduate in Eating Behavior and Nutritional Coaching from Educamais College (2022), Nutrition and Nephrology from Cristina Martins Institute (2022), and Nutritional Therapy and Clinical Nutrition from Anhembi Morumbi University (2017). Graduated in Nutrition from Leonardo da Vinci University Center - Blumenau/SC (2010). With over 9 years of experience in the hospital field (clinical and kitchen (UAN)), focusing on nutritional therapy, particularly in the following areas: Enteral nutritional therapy, the elderly, intensive care, clinical nutrition, and pediatric nutrition. Engaged in patient care, guidance, and training with the kitchen team, also serving as a member of the Multidisciplinary Nutritional Therapy Team during this period. Providing services in clinical, surgical, oncology, and hemodialysis areas. For the past 6 years, working in the maternal and child hospital area, providing care, participating in support groups for postpartum women, and giving lectures for pregnant women and nursing mothers. Currently, I am the manager of the Nutrition course at the University of Vassouras (Vassouras Campus) and a lecturer teaching the Technical Dietetics course in the Nutrition program at the University of Vassouras.



Dr. Atolani, Olubunmi is an Associate Professor of Organic Chemistry with extensive experience in teaching and research. He obtained his PhD from the University of Ilorin, Nigeria, where he studied the anticancer and antioxidant properties of bioactive compounds from African medicinal plants. His current research focuses on organic synthesis, cheminformatics applications for drug discovery in diseases like cancer and malaria, and exploring green cosmeceuticals from tropical seeds. He also conducts research in scientometrics, analyzing global institutional rankings. Dr. Atolani has received postdoctoral training abroad and secured numerous prestigious research grants. He has authored over 100 peer-reviewed publications, delivered keynote addresses globally, and served as a reviewer for reputable journals. He is a member of professional bodies like the American Chemical Society, European Association of Cancer Researcher, and Nigerian Young Academy. At the University of Ilorin, he supervises undergraduate and postgraduate students. Previously, Dr. Atolani held leadership roles as Assistant Director at the Centre for International Education and Deputy Director (Research) at the Centre for Research Development and In- House Training.



Cristiane Chaché is a Lawyer and Adjunct Professor in the Professional Master's Program in Environmental Sciences at Vassouras University, Rio de Janeiro, Brazil. She holds a PhD and Master's degree in Sociology and Law from the Graduate Program at the Fluminense Federal University, Rio de Janeiro, Brazil, with a research focus on Socio-environmental, Rural, and Urban Conflicts. She works as a researcher at the INCT-Institute of Comparative Studies in Institutional Conflict Management (INCT-InEAC) at Fluminense Federal University, Rio de Janeiro, Brazil. She holds a Bachelor's degree in Law, also from Fluminense Federal University, and initially graduated as a Technician in Environment from the Federal Institute of Education, Science, and Technology of Rio de Janeiro (IFRJ), Brazil. She has worked at the Marine Biology Institute of the Federal University of Rio de Janeiro (UFRJ), Brazil, at the Municipal Secretariat of Environment and Urbanism of Itaboraí, Rio de Janeiro, Brazil, and at the State Institute of Environment (INEA), in the Environmental Licensing Directorate, Rio de Janeiro, Brazil, having passed a public competition. Her research and interests are particularly focused on Environmental and Urban Law, Environmental and Social Sciences, with an emphasis on rural and urban socio-environmental conflicts.



PhD Student in Informatics from the Pontifical Catholic University of Rio de Janeiro (PUC-Rio), Master in Computer Science from the Federal University of Juiz de Fora (UFJF), Executive MBA in Project Management, postgraduate degree in Systems Engineering and degree in Information systems. He works as a University Professor, Coordinator of the Undergraduate Course in Systems Analysis and Development and General Coordinator of Digital Education at the University of Vassouras. Community Manager at Google Developers Group (GDG Vassouras) and Leader in the Google Educators Group (GEG Vassouras). INEP/MEC Higher Education Course Evaluator. He has published and presented at national and international symposiums and conferences. Associate member of the Brazilian Computing Society (SBC) and the Brazilian Health Informatics Society (SBIS).



Patricia S. Romano is a Pharmacist (1993), Biochemist (1997), and PhD in Biological Sciences from the National University of Cuyo (2003). She has served as an Independent Researcher from the National Council of Scientific Research and Technology (CONICET) since 2017. Dr. Romano is an Associate professor at the Cellular and Molecular Biology Department at the National University of Cuyo (2023) and is the Head of the Laboratory "Biology of Trypanosoma cruzi and the host cell" at the Institute of Histology and Embryology of Mendoza in the National University of Cuyo (IHEM-CONICET-UNCUYO). Her main research interests are the study of the actions of virulence factors of T. cruzi on the host cell with a special focus on the search for new targets for the therapy of Chagas disease. Her laboratory works in different infection models (in vitro and in vivo), applying cellular and molecular biology, biochemistry, pharmacology, and optical and electron microscopy methods to analyze promising molecules as targets for chemotherapeutic action.



Cecilia G. Cuffini is a Biochemist (1991), Magister (1998) and PhD in Medical Sciences from the National University of Córdoba (2005). She has served as an Adjunct Clinical Researcher from the National Council of Scientific Research and Technology (CONICET) since 2015. Dr. Cuffini is an Adjunct Professor at the Medical Faculty of the National University of Córdoba (2005) and serves as the Head of the Laboratory for Chlamydias and Human Papilloma Virus at the Institute of Virology Dr. J.M. Vanella of Córdoba within the National University of Córdoba. Her laboratory conducts surveillance of Chlamydia psittaci and the research findings of her team contributed to the enactment of the law on the ownership and commercialization of birds in the province of Cordoba. Her main research interests lie in the field of molecular epidemiology of the two globally prevalent sexually transmitted infections: viral (Human Papilloma Virus) and bacterial (Chlamydia trachomatis) in asymptomatic youth, infertile couples, and vulnerable populations. Currently, her team is researching sexually transmitted infections in extragenital mucosa and exploring their potential synergistic effects in “in vitro” models as well as in patients with cervical cancer and oral cancer.



Dr. Andrew Lindsay is a Senior Lecturer in the School of Biochemistry and Cell Biology in University College Cork, Ireland. Andrew has 20 years’ experience of teaching and research in Biochemistry, Genetics and Biotechnology, and he is the director of the of BSc Genetics degree programme in UCC. He is an editor for the European Journal of Human Genetics. He serves on the Senior Council of the Irish Association for Cancer Research and is a member of the National Research Ethics Committee, Ireland. Andrew is an active researcher, and his laboratory seeks to identify new therapies for treating drug resistant cancers. He also has an interest in studying the role of dysregulated membrane trafficking pathways in neurodegenerative disorders. He holds a Bachelor’s degree in Genetics from Trinity College Dublin and a PhD from UCC. He has obtained substantial research funding and has published over 30 research articles. He has worked in labs in Ireland, the United States and France.



Dr. Myriam R. Laconi is a biologist from the National University of Cordoba and received her PhD from the National University of Cuyo, Argentina. She completed internships in Belgium, Chile and at the National Institute of Health in Washington, learning neurobiology techniques. She is a professor of Biology and Physiology and Biology in the Bioengineering program at UM. Dr. Laconi is the founder of the Clinical Research Specialist Program at the UM School of Medical Sciences. She received her doctoral training from the National Council for Scientific and Technical Research (CONICET-Argentina) and acquires her post doctoral expertise in the Instituto de Medicina y Biologia Experimetal de Cuyo (IMBECU-CONICET). She worked for the pharmaceutical industry for several years, being involved in quality control processes and regulatory aspects of various clinical protocols. As a permanent researcher from CONICET, Dr Laconi has metored several undergraduate and graduate students. Dr Laconi is currently member of National and Local Committee on Research Ethics and Director of Research in Science and Technology of the Ministry of Health of Mendoza. She also directs the Ovarian Pathophysiology Laboratory of IMBECU where several lines of basic and preclinical research on ovarian pathophysiology are developed in different in vitro and ex vivo models.Her team has received local and international recognition for its scientific productions (Italy 2024, Duplin 2024). The lines of research are based on the study of the neuroendocrine actions of neurosteroids on different reproductive parameters in murine, bovine and human models. Recently, a doctoral thesis is being developed on the effects of these substances on ovarian cancer. Another area of development of Dr. Laconi addresses the development of image analysis software with artificial intelligence tools for the study of ovarian structures. .



Dr. Jesse Marques Pavão. Graduated in Agronomy from the Federal University of Alagoas (2006), Master's in Agronomy/Plant Physiology from the Federal University of Lavras (2007), and Ph.D. in Agronomy/Plant Physiology from the same institution (2009). During his master's degree, he studied and developed methodologies for the degradation (breakdown) of the cell wall in monocots using protoplasts. During his Ph.D., he studied the activity of the enzyme Phenylalanine Ammonia Lyase (PAL) related to the lignification processes of the cell wall. He completed his postdoctoral research at the Seed Conservation Department, Royal Botanic Gardens, Kew, Wakehurst Place, West Sussex - England, where he conducted research to understand the basis of desiccation tolerance in seeds of native species. He is currently a professor and researcher at Cesmac University Center, working in the courses of Agronomy, Biomedicine, Nutrition, Physiotherapy, Pharmacy, and Biology. He coordinates the "Oceanos de Plástico" project, approved by the National Council for Scientific and Technological Development (CNPq) under the call: CNPq/MCTI-FNDCT CT-Petro No.43/2022, Process 405449/2022-4, endorsed by the United Nations (UN). Since 2018, he has been the Coordinator of the Graduate Program in Environmental Systems Analysis (PPGASA), rated 4 by CAPES, where he teaches courses in Plant Physiology and Biochemistry, PlantEcology, Structural and Quantitative Plant Anatomy, and Scanning and Transmission Electron Microscopy. Since 2021, he has been a professor in the Professional Graduate Program in Biotechnology in Human and Animal Health (PPGBiotec). Chief Researcher at the Laboratory of Emergetics and Ecosystem Resilience (LERE). Leader of the Socio-Eco-Economy Research Group of the Northeast. He was a Municipal Science, Innovation, and Technology Councilor (2019-2021). Since 2021, he has been a Councilor of the Committee for Non-Patrimonial Damages. Currently, he is a member of the Environment and Sustainability Nucleus (NUMAS/CESMAC). Associate of the Advances in Cleaner Production Network (ACPN) and CEO of the startup Policoncret. He is a researcher in the field of soilless cultivation, where he focuses on strawberry cultivation and its adaptation in the Northeast region



Dr. Melina M. Musri is a Biochemist from the National University of Córdoba, Argentina, and received her PhD from the University of Barcelona, Spain, working on the Epigenetics regulation of adipocyte differentiation with the technical support of Dr. Marcelina Párrizas. Then, she continued working in the Hospital Clinic of Barcelona, Spain, in the differentiation of endothelial progenitor cells under the direction of the physiologist Dr. Victor Peinado. After that, with a Sara Borrell Fellowship from the Spanish Ministry of Science and Technology, she continued her work studying smooth muscle phenotypic switch and RNA biology in both the Hospital Clinic of Barcelona and the Department of Biochemistry I, University of Regensburg, Germany, under the direction of Prof. Dr. Gunter Meister. Nowadays, Dr. Musri is an Independent Researcher from the National Council for Scientific and Technical Research (CONICET). She has directed several undergraduate and PhD theses and obtained national and international Grants and Fellowships for her or the members of her laboratory. The focus of Dr. Musri research is the epigenetic regulation of smooth muscle differentiation in vitro and in in vivo models of vascular remodeling



Dra. Anna Cláudia Santos. PhD in Environmental Sciences/Remote Sensing from the Federal University of Goiás, Master's in Ecology from the Federal University of Rio Grande do Norte, specialist in geoprocessing from the Federal Institute of Goiás, and Bachelor's degree in Biological Sciences from the Federal University of Goiás. She is an associate researcher at the Image Processing and Geoprocessing Laboratory of the Federal University of Goiás (LAPIG), one of the main references in the country for the processing and analysis of moderate spatial resolution satellite data applied to biophysical-environmental monitoring and territorial governance. She serves as a scientific consultant for the Fellowship Cerrado Program, where she is a Senior evaluator of startups focused on life cycle and geotechnologies. She was a member of the Working Group (WG) that developed the Agriculture Sector Plan and participated in the State Management Groups of the ABC Plan, under the leadership of Embrapa, with representatives from various Brazilian Universities. She was a scientific consultant in land use changes and life cycle, where she worked on projects related to energy transition, family farming, decarbonization, ESG trends, and climate change for the three largest biofuel associations in Brazil (UBRABIO, ABIOVE, and APROBIO). She was an associate researcher of the MapBiomas group and a technical consultant in the Terra Class Cerrado Project INPE/MCTI. Recently, she has also worked with the NGO EcoDATA in monitoring springs in the Cerrado.



Dr. Cristián Andrés Quintero is a chemist with a Ph.D. in Chemical Sciences from the National University of Córdoba (UNC), Argentina. He completed postdoctoral research at Institut Curie in Paris, France, and at IHEM-CONICET in Mendoza, Argentina, specializing in cell and molecular biology with a particular focus on vesicular trafficking. Dr. Quintero is currently a tenured professor at the School of Biochemistry and Pharmacy at Maza University and also teaches at the School of Medical Sciences at Mendoza University. In addition to his academic roles, he serves as the director of the Biomedical Sciences Institute (INBIOMED-UM) at Mendoza University and the Cell and Molecular Laboratory (BioCyM) at Maza University. With over 20 years of experience in molecular and cellular biology research, Dr. Quintero's primary research focuses on developing new treatments for gonorrhea by investigating synthetic organic molecules and natural extracts. His secondary research involves studying the prevalence of rickettsioses in ticks in the Mendoza region through molecular methods, in collaboration with the Regional Parasitology Research Center (CIPaR) at Maza University.



Denise Alves Fungaro is a researcher at the Nuclear and Energy Research Institute (IPEN-CNEN/SP) in Brazil, with a Ph.D. in Chemistry from the University of São Paulo (1993) and post-doctoral experience at the University of Coimbra, Portugal, specializing in electrochemistry applied to the environment. Dr. Fungaro leads research projects that focus on converting waste into value-added materials like adsorbent materials, zeolites, biochar, nanosilica, and activated carbon. She also explores the use of waste in green roofs and cementitious matrices. As an academic advisor, she supervises students at various levels, including undergraduate, master's, doctoral, and post-doctoral fellows. Her research addresses the development and environmental application of materials derived from waste, including coal combustion by-products, sugarcane ash, agricultural waste, and aluminum industry waste. These materials are characterized and applied in areas such as wastewater treatment, carbon capture and sequestration, green roof substrates, and cement additives. Dr. Fungaro is a prolific author, with over 80 peer- reviewed journal articles and more than 240 citations in the Web of Science. She has an h-index of 9, reflecting the impact of her work. In summary, Denise Alves Fungaro is an expert in developing sustainable solutions for waste management through the synthesis of innovative materials. Her research transforms industrial and agricultural waste into valuable products for environmental remediation.



Graduated in Pharmacy with a specialization in Industrial Pharmacy from UFC (Federal University of Ceará), holding a Master's and PhD in Pharmaceutical Sciences from UFPE (Federal University of Pernambuco), and completed a post-doctoral fellowship in Pharmaceutical Technology at the University of Coimbra, Portugal. Currently an Associate Professor in the Pharmacy Course at UFPI (Federal University of Piauí), and a member of the Graduate Programs in Pharmaceutical Sciences and Materials Science - Master's/PhD (UFPI), the Graduate Program in Biotechnology - PhD (UFPI/RENORBIO), and the professional master's program in Intellectual Property and Technology Transfer (PROFNIT). Recipient of a Productivity Scholarship in Technological Development and Innovative Extension (DT). Coordinator of the Laboratory of Technological Innovation and Entrepreneurship (LITE). Co-founder of Fitofit– Supplements and Natural Products and Buriti Bioespuma–Solutions in thermal and acoustic comfort. Experienced in pharmaceutical technology and product development, with emphasis on the production and control of medicines and related products. Main areas of expertise include technological development of medicines and related products, entrepreneurship, and intellectual property.



"Understanding the university's R&D infrastructure. Designing the future." is a key initiative by Vassouras University, led by Sandra Regina Alves Confort and Renan Rodrigues Moreira da Silva, who oversee the institution's laboratories. This event showcases the university's cutting-edge research facilities and ongoing innovative projects, providing valuable insights for students, faculty, and industry partners.



A highlight of this initiative is the spotlight on the Chemical Engineering program and the Professional Master's in Environmental Sciences. The Chemical Engineering department, known for its state-of-the-art laboratories and industry partnerships, prepares students to tackle complex industrial challenges with innovative solutions. Meanwhile, the Professional Master's in Environmental Sciences program emphasizes the integration of environmental sustainability with technological advancement, addressing critical global issues.

These advanced facilities serve as hubs for groundbreaking research and practical, industry-relevant education. By highlighting its state-of-the-art R&D infrastructure, particularly in these key areas, Vassouras University demonstrates its commitment to fostering innovation, enhancing educational programs, and preparing students for future challenges in their fields.

This initiative not only reflects the institution's dedication to excellence in research and education but also emphasizes its proactive approach in shaping the future through advanced technology and collaborative efforts. Through programs like Chemical Engineering and Environmental Sciences, supported by these diverse and specialized laboratories, Vassouras University is at the forefront of developing solutions for industrial efficiency and environmental sustainability, ensuring its graduates are well-equipped to lead in their respective fields.

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Dr. Élcio Jeronimo de Oliveira holds a postdoctoral degree in Aerospace Engineering from the University of Rome - La Sapienza (2014), a PhD in Space Engineering and Technology from the National Institute for Space Research - INPE (2011), a master's degree in Ocean Engineering with an emphasis on Submarine Engineering from COPPE (2001), an MBA in Public Management from the Air Force University (2012), a degree in Physics from the Federal University of Rio de Janeiro - UFRJ (1999), and a Technology degree in Aeronautical Communications from the Brazilian Air Force (2001).
He is a retired officer of the Brazilian Air Force, having held the positions of Deputy Chief of the Space Subdirectorate, Head of the Space Systems Division, Manager of the SARA Project (Atmospheric Reentry Satellite), and Coordinator of the Critical Technologies Action (20VB - AEB) at the Institute of Aeronautics and Space - DCTA. He also worked as Flight Test Coordinator for the 14-X Project at the Institute for Advanced Studies - DCTA, carrying out the technical and operational planning of the Scramjet engine (14-X S) flight test mission. Dr. Oliveira is an Academician of the International Academy of Astronautics (IAA), a member of the Space Materials and Structures and Space Transportation Committees of the IAF (International Astronautical Federation), a former Professor in the area of Space Systems at Luleå University of Technology - Sweden, and a former Business Director of Innospace do Brasil, responsible for planning and executing the first private rocket launch operation of a foreign company at the Alcântara Launch Center. Currently, he is CEO/Founder of KVANTUM Tecnologia e Serviços LTDA. He conducts research in the areas of flight dynamics and trajectory optimization of space vehicles, inertial sensors, GNC, and dynamic modeling of flexible vehicles. Dr. Oliveira has experience in Submarine and Aerospace Engineering, having worked mainly on the following topics: Optimization of launch vehicle trajectories, post-flight analysis of suborbital vehicles, inertial navigation, antennas, electromagnetism, sonar, underwater acoustics, signal processing, radio navigation, and control systems.



Mariana Guadalupe Vallejo holds a degree in Pharmacy and a PhD in Chemical Sciences (Facultad de Ciencias Químicas, Universidad Nacional de Córdoba, FCQ-UNC). She completed her postdoctoral training at Universidad Nacional de San Luis (Argentina), Universidad de Santiago de Chile (Chile) and the University of Patras (Greece). She is currently Adjunct Professor of Botany, at the Department of Pharmaceutical Sciences (FCQ-UNC) and Pharmacognosy (Universidad Nacional de La Rioja, UNLaR). Also, she is an Adjunct Researcher at the National Scientific and Technical Research Council (CONICET). She leads Neurogreen, a research team that studies native medicinal plants with nootropic, anxiolytic and antidepressant activity, which includes isolation and identification of active principles, by classical pathways and through metabolomic strategies, and in vitro and in vivo tests for evaluation in animal models of anxiety, depression and memory impairment.



Dr. Anahí Bignante is a Pharmacist with a PhD in Chemical Sciences from the National University of Córdoba (UNC), Argentina. She is currently an Adjunct Researcher at the National Council for Scientific and Technical Research (CONICET), an adjunct professor at the Instituto Universitario de Ciencias Biomédicas de Córdoba (IUCBC), and an assistant professor at UNC. Dr. Bignante has supervised several undergraduate and PhD theses and has obtained both national and international grants and fellowships for herself and members of her laboratory. Her research focuses on the neurobiology and neurochemistry of Alzheimer's disease, particularly in studying the modulation of cellular processes involved in amyloid-beta generation and developing new therapeutic approaches for the treatment of Alzheimer's disease.



Professional with solid academic background and extensive experience in Agronomy and Environmental Engineering, began his career as an Agricultural Technician (1992), followed by a degree in Agronomic Engineering (UFRRJ, 1997), Master's (2001) and Ph.D. in Agronomy/Soil Sciences (UFRRJ, 2005), including research at the University of Évora, Portugal. Currently serves as Deputy Undersecretary at SEAPPA-RJ and Visiting Researcher at PESAGRO-RIO, while also teaching in MBA programs at IBMEC Agro, FIA-SP, and FGV. In the private sector, he manages Costa Brasil Engineering and Embarque Cultural Academic Tourism, providing consulting through Eco4solutions Brazil-Paraguay. His experience includes positions as Advisor at CREA-RJ, Council Member of CECA and CONEMA-RJ, and Research Dean at Severino Sombra University. Specialist in Corporate Environmental Management, Environmental Licensing, and Soil and Water Conservation and Management, he contributes significantly to sustainable development and environmental management in Bra.



Dr. Ricardo Cabrera graduated in Biochemistry from the School of Chemical Sciences of the Faculty of Chemical Sciences of the National University of Cordoba in 1985. D. in Biochemistry from the Faculty of Chemistry, Biochemistry and Pharmacy of the National University of San Luis in 1990. He performed his postdoctoral training in the Reproductive Biology Training Program, Pontificia Universidad Católica de Chile, Rockefeller Foundation, Grant R.F. 88077-B. (1990-1992) and as a Junior Researcher in the Division of Medical Pharmacology, University of Leiden, The Netherlands (1995-1997). He was the Regional Representative for Argentina for the National Institute for Child Health and Development/Fogarty Fellowship Program (NICHD/FOGARTY) - Oregon National Research Primate Center - Oregon Health Sciences University. USA (2002-2003). He started his career as a scientific researcher (CIC) of CONICET in 1993 and is currently the Principal Investigator of the CIC at INBIOMED-IMBECU-CONICET. University of Mendoza. He is a Full Professor of the Department of Biochemistry.
Faculty of Medicine. Faculty of Medical Sciences. The University of Mendoza and Professor of Psychology, with responsibilities in General and Human Biology, Neurobiology 1, Neurobiology 2, and Psychopharmacology. School of Health Sciences. University of Mendoza. He has published more than 60 scientific papers in international peer-reviewed journals. He has presented over 200 papers at national and international congresses and conferences. His lines of research interest include neuromodulation within the area of neuroscience, with a particular interest in neuroprotection and neurorepair in animal models of neurodegenerative pathologies.



Dr. Juan Pablo Mackern-Oberti currently works at IMBECU (Institute of Medicine and Experimental Biology of Cuyo) in CONICET CCT Mendoza. We does research in Fundamental Immunology, physiology and autoimmunity. T cell and inflammation are the main targets of our studies. Flow cytometry, primary cell cultures, Real Time PCR, immunohistochemistry and histology, ELISA and RIA are routinely techniques used in the lab. We are always willing to welcome new students and initiating challenging collaborations. Now, we are working in: 1. the role of prolactin and glucocorticoid receptors in T cell physiology, stess and autoimmunity. 2. Hyperthyroidism in immuneregulation during gestation and lactation. 3. Desmoglein and inflammation.



Dr. Eduardo Goldani completed Bachelor of Science (BSc) in Chemistry (2005), Bachelor of Pharmacy (BPharm) (2018), Master's in Environmental Analytical Chemistry (2007), Ph.D. in Medicine and Health Sciences (2014), and a 4-year Post-Doctoral Fellow in Regenerative Medicine with an emphasis on peripheral nerve injuries (2015-2018). Worked as a Visiting Scientist at the University College London - School of Pharmacy, researching within the Spirogen Ltd project focused on the studies of Drug Discovery, Drug Design, Anticancer Drugs, Medicinal Chemistry, and Organic Synthesis (2009- 2010). Active in scientific publishing since 2002, I joined Springer Nature in 2022, leveraging over 20 years of publishing expertise to manage a portfolio of 13 engineering and applied sciences journals.



Dr. Zura Javakhishvili is one of Georgia's leading academicians and wild life conservationists, with 25 years of experience in wildlife conservation and management and over 15 years as a researcher and lecturer of ecology at Ilia State University. His career began at the Georgian Center for the Conservation of Wildlife (GCCW) in 1997, where he researched and mapped raptor and owl distribution in Georgia, leading to the publication of Georgia's first bird identification books: "Raptors of Georgia" (1999) and "Raptors and Owls of Georgia" (2005). After volunteering at Hawk Mountain Sanctuary in Pennsylvania and participating in American kestrel research, he coordinated the Important Bird Areas project in Georgia with BirdLife International from 2004 to 2006. Javakhishvili earned his Master's degree in Biology and Zoology from Ivane Javakhishvili Tbilisi State University in 2003, studying griffon vulture nest site selection. He served as GCCW's Conservation Program Manager before joining Ilia State University as a lecturer and PhD student, where he focused on seasonal bird movement in the Caucasus and its role in A-type Avian Influenza Virus spread. His expertise expanded through training in satellite telemetry at the University of Idaho and data analysis at the University of Cambridge, leading to ongoing collaborations with prestigious institutions including Erasmus University Medical Center, the University of Cambridge, and Royal Veterinary College, while continuing to build capacity for wildlife conservation and research in Georgia through his teaching.



Dr. Lilian Paiva works at Customer Success Manager for Academic and Government in Brazil. At Elsevier our mission is to help academic and government communities to accelerate knowledge for a better world, we do this by facilitating insights and critical decisions for customers across the global research and health ecosystems.
Graduated in Business with an emphasis in Systems Analysis from Paulista University and an Executive MBA in Services Marketing from Paulista School of Advertising and Marketing.



Dr. Sergio Bontti is a Biochemist from the Universidad Nacional del Sur and a Specialist in Microbiology with a Parasitology Orientation. He works at the Reference Laboratory for Communicable Diseases (LRET) in Mendoza, as a Referrer in the diagnosis of Chagas, Toxoplasmosis, Malaria (Microscopist certified by PAHO/WHO), Leishmaniasis, Enteroparasitosis, Tick-Borne Diseases, and Myiasis. He is a Research Professor and Director of the Microbiology and Parasitology Research Laboratory LIMyP INBIOMED-UM. He has published articles in the area of parasitology. He is a Professor of Microbiology in the Medicine and Dentistry programs at the University of Mendoza (UM) and Secretary of Postgraduate and Continuing Education, and represents the UM in the Provincial Committee on Ethics in Health Research (CoPEIS), Ministry of Health and Sports of Mendoza. Specialist in Engineering in Quality from the National Technological University. Develops training activities in the area of laboratory equipment management. Professor of the postgraduate course Specializing in Clinical Chemistry, Faculty of Chemical and Technological Sciences, Catholic University of Cuyo, San Juan Campus. Member of the Argentine Association of Zoonoses, Cuyo Branch, and the Argentine Parasitological Association.



Franck Perez currently leads the Cell Biology and Cancer Unit at Institut Curie in Paris as Research Director at CNRS. His work has revolutionized the field of cell biology through significant methodological innovations, including an automated cell screening platform (BioPhenics) and the development of an antibody library based on humanized nanobodies.

His academic background includes a Ph.D. from Ecole Normale Supérieure in Paris, where he studied neuroendocrine regulation and cell internalization peptides. He later contributed important research on microtubule dynamics and intracellular trafficking at the University of Geneva.

As an EMBO member and prolific researcher, his scientific output exceeds one hundred papers and ten patents. His entrepreneurial spirit has led him to co-found three biotech companies, including Honing Biosciences, a spin-off from Institut Curie dedicated to developing next-generation cell-based therapies.

II Southern Science Conference Schedule

Important Notes, and last update: 06/11/2024 @ 07:10h Argentine local time zone.

- [HYBRID] - Sessions available both in-person and virtually
- [VIRTUAL] - Online-only sessions
- [IN-PERSON] - Physical attendance required
- All times are in AR (Argentina) time zone
- Virtual sessions require registration

- **Room A**: https://us06web.zoom.us/j/86141137103?pwd=6WkZpHGD4XwjerbzNsPCJhG1J0VxxM.1
- **Room B**: https://us04web.zoom.us/j/76299635848?pwd=3Inz1ElpCjfjQI4c658fbjIpiPEkLs.1

November 7th, 2024

Time	Room	Title & Access Details	Speaker	Language
09:30-10:00	Main Halls AR/BR Virtual ROOM B	International Conference Opening Ceremony [HYBRID]	Opening with the authorities-Organizer Universities Authorities of SSCON Presented by: Dr. Cristián Quintero	EN
10:10-10:40	Virtual Room B	Intracellular Transport : Engineering and Mechanisms [HYBRID]	Dr. Perez Franck. France Presented by: Dr. Cristián Quintero	EN
11:00-12:00	Laboratory BR	Chemical Engineering Lab Tour [IN-PERSON] No virtual transmission.	Sandra Reginal A. C., and Reana R.MOreirada da Silva	PT
11:00-11:50	Virtual Room B	Scopus Indexation Criteria. [VIRTUAL]	Lilian Paiva - ELSEVIER	EN
12:00-13:30	*Lunch Break*			
13:30 **AR**	Virtual Room **C** **Google Meet**	Meeting with the international relations departments of each involved university. Objectives, new agreements, and international conventions.	International departments of the Institutions. Proper staff. Presented by Dr. Cristiane Siqueira	EN/PT/ES

13:30 **AR**	Virtual Room **D**	Institutional Journals Summit. Objective: Discuss strategies to enhance the quality, visibility, and impact of institutional journals. Topics may include: - Best practices in journal management and publishing; - Indexing and citation metrics; - Open access initiatives, policies, and risks; - Collaboration opportunities among journals; - Leveraging digital technologies for dissemination	Journal Editors, Editorial Boards, and University Representatives Editors can prepare a 3 min presentation of the journals Presented by Dr. Luis de Boni	EN/PT/ES
13:30-14:00	Virtual Room **A**	Materials surface modification by pulsed laser techniques [VIRTUAL]	Dr. Maximiliano Rossa. Argentine Presented by: Dr. Walter Pelaez	EN
14:00-14:30	Virtual Room **A**	Development of biofunctionalized hybrid nanomaterials for their application in enzymatic biosensors and glycobiosensors [VIRTUAL]	Dr. Nancy Fabiana Ferreyra. Argentine Presented by: Dr. Walter Pelaez	EN
14:30-15:00	Virtual Room **A**	PRODUÇÃO DE BIODIESEL: UMA VISÃO DA ENGENHARIA VERDE [VIRTUAL]	Dr. Fernando Pelegrini. Brazil Presented by: Dr. Walter Pelaez	PT
15:00-15:30	Virtual Room **A**	Utilizing geotechnology for monitoring raw materials in the production of biofuels [VIRTUAL]	Dr. Anna Cláudia Santos. Brazil Presented by: Dr. Walter Pelaez	PT
15:30-16:00	Virtual Room **A**	Síntese de Sílica a partir de Biomassa: Uso Sustentável de Resíduos Agroindustriais. [VIRTUAL]	Dra. Denise Fungaro. IPEN. Brazil Presented by: Dr. Walter Pelaez	PT
16:00-16:30	Virtual Room **A**	Coating for Tribological applications. .[VIRTUAL]	Dr. Ernesto Garcia. Mexico. Mexico Presented by: Dr. Walter Pelaez	EN
16:30 – 17:00	Virtual Room **A**	Green Valorization of Highly Underutilized Tropical Seeds as Nutricosmeceutics and Dermocosmeceutics. [VIRTUAL]	Dr. ATOLANI, Olubunmi. Nigeria. Presented by: Dr. Walter Pelaez	EN
13:30-14:00	Virtual Room B	Contamination by Sanitary Pads in the Environment. [VIRTUAL]	Bhavna Ambudkar. India Presented by: Dr. Cristián Quintero	EN
14:00-14:30	Virtual Room B	A hypercholesterolemic diet affects sperm cell physiology which could be recovered by adding olive oil. IN-PERSON] / VIRTUAL	Dr. Miguel Walter Fornes, Argentine Presented by: Dr. Cristián Quintero	EN
14:30-15:00	Virtual Room B	Exosome-Like Vesicles as Vectors of Metronidazole Resistance in Giardia lamblia: Insights into Genotype-Specific Mechanisms [VIRTUAL]	Dr. María Carolina Touz, Argentine Presented by: Dr. Cristián Quintero	EN
15:00-15:30	Virtual Room B	Neuroactive Steroids: neuromodulators of neuronal systems under Neurodegeneration. IN-PERSON] / VIRTUAL	Dr. Ricardo Cabrera, Argentine Presented by: Dr. Cristián Quintero	EN

15:30 – 16:00	Virtual Room B	The role of KCTD15 in neural crest development. IN-PERSON] / VIRTUAL	Dr. Valeria Zarelli. Argentine Presented by: Dr. Cristián Quintero	EN
16:00-16:30	Virtual Room B	Impact of HPV and Chlamydia trachomatis Infections on Male Infertility: Interactions, Immune Responses, and Sperm [VIRTUAL]	Dr. Cecilia Cuffini. Argentine Presented by: Dr. Cristián Quintero	EN

November 8th, 2024

Time	Room	Title & Access Details	Speaker	Language
08:00-08:30	Virtual Room **A**	A Atuação das Comissões Gestoras Locais nas Bacias Hidrográficas de Conflito pelo Uso da Água. [VIRTUAL]	Juliana Gracieli Resende. Brazil Presented by Dr. Cristiane Siqueira	PT
08:30-09:00	Virtual Room A	Nutrição e Prevenção de Doenças Crônicas: Abordagens Integrativas para Reduzir o Ônus Global. [VIRTUAL]	Dra. Luciana de Souza Marques. Brazil. by Dr. Cristiane Siqueira	PT
09:30-10:00	Virtual **Room A**	NBS and Water Security [VIRTUAL]	Mayná Coutinho. Brazil Presented by Dr. Cristiane Siqueira	PT
10:00-10:30	Virtual **Room A**	Lab in Space: Chemical Experiments in Low Earth Orbit (LEO) and Suborbital Flights. [VIRTUAL]	Dr. Élcio Jeronimo. Brazil Presented by Dr. Cristiane Siqueira	EN
10:30-11:00	Virtual **Room A**	Changes and Progress in Brazil's Environmental Policies in times of Climate Crisis. IN-PERSON] / VIRTUAL	Cristiane Borborema Chaché. Brazil Presented by Dr. Cristiane Siqueira	PT
11:00-11:30	Virtual **Room A**	Scientific Writing and Publishing. Springer-Nature [VIRTUAL]	Dr. Eduardo Goldani. UK Presented by: Dr. Luis de Boni	EN/PT
08:00-08:30	Virtual Room B	The m6A reader YTHDF2 and DAGAR regulate smooth muscle cell phenotypic plasticity [VIRTUAL]	Dr. Melina M. Musri. Argentine Presented by: Dr. Cristián Quintero	EN
08:30-09:00	Virtual Room B	Neurosteroid Signaling from Brain to Ovary: In Vivo and In Vitro Insights from Diverse Experimental Models [VIRTUAL]	Dr. Myriam R. Laconi. Argentine Presented by: Dr. Cristián Quintero	EN
09:00-09:30	Virtual Room B	Melatonin carrier systems as neuroprotection in an in vivo retinal degeneration model for the treatment of ocular neurodegenerative pathologies. IN-PERSON] / VIRTUAL	Dr. Daniela Quinteros. Argentine Presented by: Dr. Cristián Quintero	EN

09:30-10:00	Virtual Room B	The Endosomal Recycling Pathway: A Novel Target in Cancer? [VIRTUAL]	Dr. Andrew Lindsay. UK Presented by: Dr. Cristián Quintero	EN
10:00-10:30	Main Auditorium Room B	The impact of legal regulation on the monitoring and control of antimicrobial resistance. [IN-PERSON] / VIRTUAL	Dr. Ramon Loureiro Pimenta. Brazil Presented by: Dr. Cristián Quintero	PT
10:30-11:00	Virtual Room B	Bird Migration and Climate. [VIRTUAL]	Dr. Zura Javakhishvili. Georgia Presented by: Dr. Cristián Quintero	EN
Time	**Room**	**Title & Access Details**	**Speaker**	**Language**
11:30-14:00	*Extended Lunch Break*			
14:00-14:30	Virtual **Room A**	AI: Humans and Machines Shaping Tomorrow. [VIRTUAL]	Anrafel Fernandes Pereira. Brazil Presented by Dr. Cristiane Siqueira	PT/EN
14:30-15:00	Virtual **Room A**	Challenges of selective collection: analysis of the implementation of the National Solid Waste Policy. [VIRTUAL]	André Dantas and Paloma Martins. Brazil Presented by Dr. Cristiane Siqueira	PT
15:00-15:30	Virtual **Room A**	Enzymatic approaches in a fungal lipid biorefinery based in agroindustry waste. [VIRTUAL]	Dra. Ana Karine Furtado. Brazil Presented by Dr. Cristiane Siqueira	PT
15:30-16:00	Virtual **Room A**	Production of Bioenergy - Biodiesel. [VIRTUAL]	Dr. Cristiane de Souza Siqueira Pereira. Brazil Presented by: Dr. Luis de Boni	PT
16:00-16:30	Virtual **Room A**	Inovação e oportunidades na Bioeconomia: um novo paradigma econômico. [HYBRID]	Paulo Wilton Camara. Brazil Presented by Dr. Cristiane Siqueira	PT
16:30 – 17:00	Virtual **Room A**	Environmental Management Systems [VIRTUAL]	Dr. Felipe Brasil. Brazil Presented by Dr. Cristiane Siqueira	PT
14:00-14:30	Virtual	Drug Repurposing for Neglected Diseases IN-PERSON] / VIRTUAL	Dra. Patricia Romano. Argentine	EN

	Room B		Presented by: Dr. Cristián Quintero	
14:30-15:00	Virtual Room B	COVID-19 Vaccine Myocarditis [VIRTUAL]	Dr. Peter Andrew McCullough. USA Presented by: Dr. Cristián Quintero	EN
15:00-15:30	Virtual Room B	Multivariate analysis of chemical and biological data oriented to the identification of bioactive compounds in native plants. [VIRTUAL]	Dra. Mariana G. Vallejo. Argentine Presented by: Dr. Cristián Quintero	EN
15:30-16:00	Virtual Room B	Gallein-Loaded Nanoparticles of Human Albumin Are Effective in Avoiding the Toxic Effects of Aβ in In Vitro Models of Alzheimer's Disease. Note: 30-40 min of duration. [VIRTUAL]	Dra. Anahi Bignante. Argentine Presented by: Dr. Cristián Quintero	EN

November 9th, 2024

Time	Room	Title & Access Details	Speaker	Language
09:00-09:30	Virtual Room B	Academic Entrepreneurship: From Idea to Market [VIRTUAL]	Dr. Lívio César Cunha Nunes. Brazil Presented by Dr. Luis de Boni	PT
09:30-10:00	Virtual Room B	Immune function of desmoglein 4. IN-PERSON] / VIRTUAL	Dr. Juan Pablo Mackern-Oberti. Argentine. Presented by: Dr. Cristián Quintero	EN
10:00-10:30	Virtual Room B	Diphyllobothriosis in Mendoza: Three-year experience in a non-endemic area. IN-PERSON] / VIRTUAL	Esp. Bioq. Sergio Bontti Presented by: Dr. Cristián Quintero	EN
10:30-11:30	All Venues Room B	International Conference Closing Ceremony Joint announcement for next edition. [HYBRID]	Cristián Andrés; Cristiane de Souza Siqueira Pereira and all organizing committee	EN/PT

Remember that we may experience last-minute changes in the schedule or changes that are beyond our control. For this reason, please visit the conference website landing page and look for notes in the schedule.

https://www.sscon.org

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