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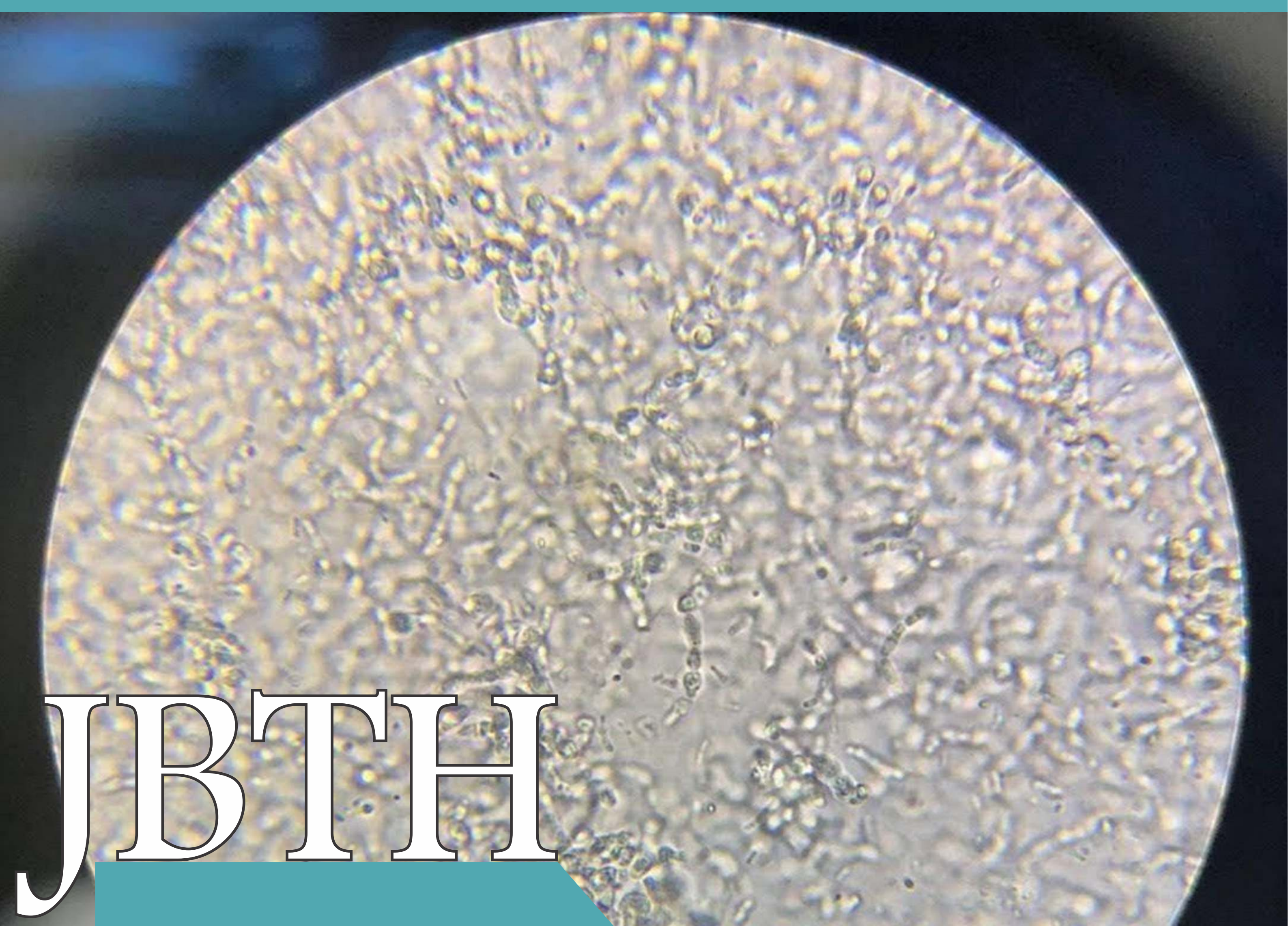

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Volume 8 • Number 2 **SUMMARY** *April 2025*

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COVER: Figure 2. Wet slide: microorganisms prospected on a coverslip being analyzed through microscopy. Bioprospecting Bacteria with Cellulolytic Potential in Cocoa Husks by Davi Ferreira de Oliveira et al. J Bioeng. Tech. Health 2025;8(2):117.

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The Use of Additive Manufacturing was Essential for Creating Customized Components, such as Locks, which Ensur Analysis of Banana Peel (*Musa* spp.) and Agar for Bioplastic Production Enriched with the Citronella (*Cymbopogon winterianus*) Extract with Repellent Action for Use in Waste Disposal

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This study investigates the production of bioplastic from banana peel (*Musa* spp.) and agar enriched with citronella extract (*Cymbopogon winterianus*) for pest-repellent action in waste disposal. In light of the environmental problems caused by conventional plastics, the aim was to develop a biodegradable bioplastic using natural waste materials. The method employed was the casting method with a film-forming aqueous solution. The results demonstrated that the appropriate ratio of banana peel starch and glycerin provided both strength and flexibility to the bioplastic. The developed bioplastic exhibits the potential to protect the environment and reduce the spread of diseases, serving as a sustainable alternative for waste disposal.
Keywords: Agar. Bioplastic. Banana Peel. Citronella. Waste.

The discovery of the Bakelite polymer in 1907 marked the beginning of the plastic era. However, its extensive environmental impact—particularly its resistance to degradation, associated carbon emissions, health risks, and the proliferation of plastic waste—has become a global concern. Improperly discarded plastic contributes to urban pollution and serves as a breeding ground for insects, thereby increasing the spread of disease. In this context, alternatives such as bioplastics derived from starch and agar—sustainable, biodegradable raw materials that offer functional resistance—are essential for reducing dependence on conventional plastics and mitigating the environmental burden of polymeric waste.

The present study seeks to contribute to this effort by exploring viable solutions to reduce reliance on petroleum-based plastics, especially in waste management. One such solution is using citronella oil, derived from *Cymbopogon winterianus*, a plant of the Poaceae family native to Java, Indonesia. Extracted from fresh or partially dried leaves, citronella oil is renowned for its natural repellent properties due to volatile compounds such as citronellal, eugenol, and geraniol. Additionally, its antifungal and antibacterial characteristics enhance its potential for application in waste disposal, particularly in repellent garbage bags.

Agar, derived from red algae (agarophytes), is one of the most widely utilized gelling agents globally. Comprising agarose and agaropectin—responsible for approximately 70% of its gelling properties—agar plays a vital role in structuring biopolymers. Banana peels, meanwhile, represent a major source of organic waste. When properly utilized, they offer significant environmental and social benefits. Researchers have highlighted the potential of bioactive compounds in banana peels, such as phenolics and pectin, in developing biodegradable films, presenting an alternative to petroleum-based materials [1].

Accordingly, this research aims to analyze the viability of using banana peel (*Musa* spp.) and agar to produce bioplastic enriched with citronella extract (*Cymbopogon winterianus*) with repellent properties for waste disposal applications. The objective is to develop a biodegradable bioplastic derived from banana peel starch, agar, and citronella extract to combat insect infestation during waste disposal. The study involves extracting starch from banana peels, employing agar as a gelling [2] and

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film-forming agent, and incorporating citronella to provide repellent efficacy. The effectiveness of the insect-repellent properties is also evaluated, thereby contributing to environmental preservation by proposing a sustainable and functional alternative.

Materials and Methods

The research was designed with quantitative, exploratory, bibliographic, and experimental characteristics. The bioplastic synthesis process was conducted in the Biotechnology Laboratory of the Integrated Campus of Manufacturing and Technology—SENAI CIMATEC. The primary raw material used was banana peel fiber (*Musa* spp.), complemented with agar and enriched with citronella oil to provide insect-repellent properties.

Extraction of Starch from Banana Peel

The bananas used in the experiment were purchased from local vendors in Salvador, Bahia. The banana peels were collected and placed in a 500 mL beaker containing 2 mL of sodium hypochlorite diluted in 250 mL water for 5 minutes to ensure proper disinfection. After disinfection, the peels were thoroughly rinsed with distilled water.

Next, 75 g of banana peel were weighed using an analytical balance and then blended with 225 mL of distilled water until the mixture was homogenized entirely. The resulting pulp was filtered through a fine sieve into a 500 mL beaker using a spatula to facilitate the separation of solids. The filtered material was allowed to rest undisturbed for 1 hour to enable sedimentation. After decantation, the supernatant was carefully transferred to another beaker, leaving the sedimented starch behind. A vacuum pump was employed to remove the remaining supernatant, isolating the decanted starch for bioplastic synthesis to enhance the separation efficiency.

Production of Bioplastic – Casting Method

The bioplastic was produced following the casting method described by Morais and colleagues (2019) [1]. The formulation consisted of 30 mL of distilled water, 10% citronella oil, 2 g of agar, and 10 mL of glycerin. All materials were combined in a 250 mL container. The mixture was heated to 90 °C and maintained at that temperature for 10 minutes under constant stirring.

After boiling, the solution was poured into Petri dishes and dried under two conditions: (1) in a bacteriological incubator with air circulation at 35 °C for 48 hours and (2) via bench drying at room temperature for performance comparison. After drying, the bioplastic films were weighed using a precision balance, and their thickness was measured with a micrometer.

Incorporation of Citronella for Repellent Action

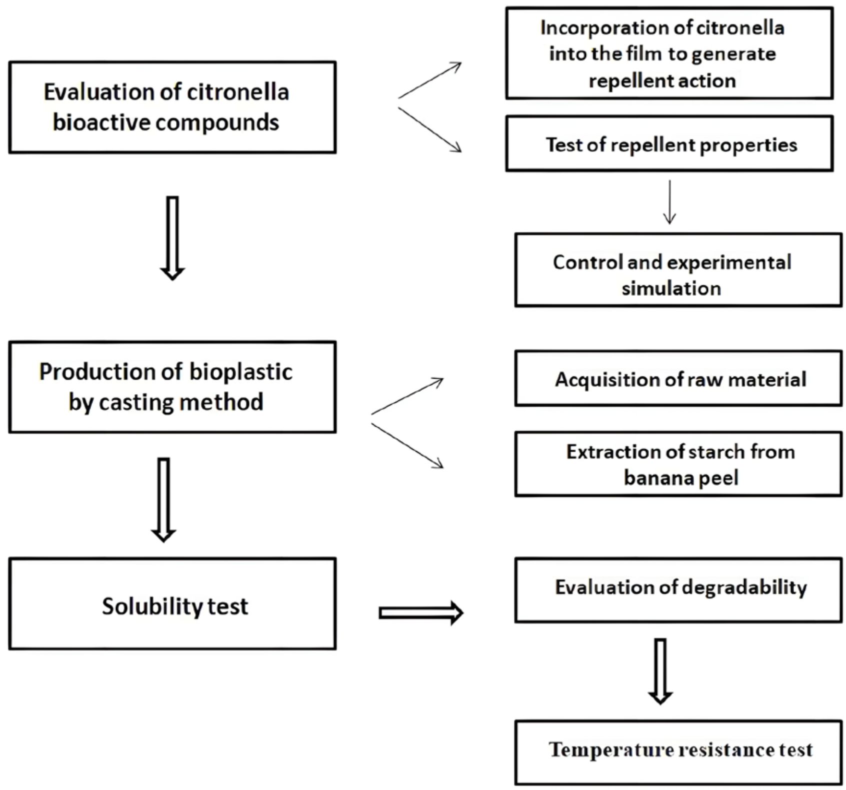
Citronella essential oil (*Cymbopogon winterianus*) with 100% purity (brand: Viaroma) imparted repellent properties to the bioplastic. A 10% citronella oil concentration was incorporated into the bioplastic mixture during the heating process. This concentration was selected to maximize repellent efficacy against insects while ensuring the aroma remained mild enough not to cause discomfort to humans or animals. The selected concentration was also evaluated for its potential antifungal action in the bioplastic matrix derived from banana peel starch. This dual function—repellent and antifungal—was crucial in enhancing the material's practical applications in waste disposal.

Testing and Evaluation Methods

A series of tests were conducted to evaluate the functional properties of the bioplastic—Repellent Activity (repellent efficacy) [3]:

Simulation Test: It was performed using two containers—one containing organic waste covered with the bioplastic and another (control) with only waste. The presence and behavior of insects were observed and compared to evaluate the bioplastic's performance in repelling pests.

Figure 1. Flowchart of the experimental procedure.



Solubility Test: The water solubility of the bioplastic films was determined using the method proposed by Almeida and colleagues (2019) [4]. The films were first dried at 70 °C for 24 hours, then immersed in distilled water and dried again, and their solubility was calculated based on the difference in dry mass before and after immersion.

Biodegradability Test: The degradation rate of bioplastic fragments was assessed following the procedure outlined by Silva and colleagues (2020) [5]. Fragments were incubated in soil for 18 days, after which the remaining dry weight was measured to calculate the biodegradation percentage.

Thermal Resistance Test: This test involved exposing bioplastic samples to a range of temperatures in a greenhouse for 30 minutes. Physical alterations such as cracks and deformations were recorded, with 80 °C being the maximum temperature tested to assess heat tolerance.

Results and Discussion

Evaluation of Bioplastic Formulation

This study investigated the formulation of bioplastics derived from banana peel starch and essential oil, focusing on optimizing the concentrations of citronella and plasticizer to improve the material's physicochemical and functional properties. Initial tests using 50 g of banana peel, 2 g of agar, and 1% citronella oil resulted in thick, brittle bioplastic films with minimal citronella aroma, primarily attributed to excessive glycerin, which interfered with film integrity. Subsequent modifications included increasing the amounts of agar and glycerin and incorporating banana pulp—an ingredient richer in starch—which improved film flexibility. While citronella oil did not significantly alter the material's texture, lower concentrations (below 10%) failed to demonstrate antifungal effectiveness.

Optimizing the composition by increasing the proportion of banana peel and reducing water content led to bioplastics with enhanced malleability, an ideal thickness of 0.7 microns, and a perceptible and pleasant citronella aroma. The optimal citronella oil concentration for both insect-repellent activity and fungal inhibition was determined to be 10%. This concentration also enhanced the overall sensory profile of the film, providing a characteristic fragrance and consistent repellent action.

Improvements in the drying process—particularly through a bacteriological incubator—helped mitigate contamination risks, especially in samples that initially contained banana pulp. Reducing pulp content and fine-tuning component concentrations ultimately resulted in a bioplastic with improved structural integrity, durability, and bioactive properties.

Antifungal Activity of Citronella

Microbiological analyses conducted 48 hours after fabrication revealed fungal and bacterial growth in nearly all bioplastic formulations, necessitating the removal and isolation of contaminated samples. Contributing factors included residue buildup and cross-contamination within the laboratory environment.

Notably, bioplastics embedded with citronella oil exhibited significantly reduced microbial activity compared to control samples, highlighting the antifungal potential of citronella's active compounds, such as citronellal, geraniol, and eugenol. Although a protective paper mask was used to limit exposure to airborne contaminants, it was ineffective against biofilm-forming bacteria. Introducing a bacteriological incubator proved crucial for safeguarding sample integrity and accelerating experimental results by limiting environmental contamination [1,6,7].

Repellent Potential of Citronella

Samples were placed in containers with organic waste to attract insects to assess the repellent properties of citronella-infused bioplastic. Formulations containing 10% citronella oil demonstrated complete repellent activity, with 100% effectiveness observed during exposure. In addition to deterring insects, this concentration inhibited surface-level microbial growth, suggesting synergistic antimicrobial and insect-repellent effects [7].

Lower concentrations of citronella oil were less effective, displaying a rapid decline in fragrance intensity and bioactivity. The 10% citronella bioplastic retained its characteristic aroma and antimicrobial action for approximately 18 days. However, insect activity and microbial colonization resurgence were noted after this period, indicating the gradual loss of volatile compounds responsible for bioactive effects.

Solubility Analysis of Bioplastics

The solubility assessment of bioplastics derived from banana peel revealed a solubility rate of approximately 75%. Despite this significant solubility, the bioplastic did not fully dissolve in water, indicating a structural integrity that resists complete disintegration. This partial solubility can be attributed to the intermolecular interactions among biopolymer constituents—particularly starch—which forms hydrogen bonds that limit water penetration. With its inherent capacity for water absorption and gelatinization,

Banana peel starch contributes to gel-like consistency while retaining mechanical strength. Such findings are critical in evaluating the material's resilience under humid or aqueous conditions, highlighting its potential for applications requiring moderate water resistance. Moreover, incorporating citronella essential oil demonstrated antifungal effects, as evidenced by minimal microbial activity on the film surface. This supports the multifunctionality of the bioplastic for sustainable waste containment.

Biodegradation Analysis

Biodegradability tests used formulations containing 50 g, 30 g, and 20 g of starch to explore the influence of starch concentration on decomposition rates. While the materials exhibited considerable degradation within 15 days, none of the samples fully decomposed. The observed rates are considered promising since bioplastics typically decompose over 3 to 6 months under natural conditions [8].

Notably, thinner films with lower starch content degraded more rapidly, suggesting a direct correlation between material thickness and decomposition time. In contrast, denser films exhibited slower but more consistent degradation, balancing structural durability and environmental degradation. These results support the feasibility of tailoring bioplastic formulations to suit varying degradation timelines, depending on the intended application [9,10].

Thermal Resistance Assessment

The optimized bioplastic's thermal resistance was evaluated across a temperature range of 30°C to 70°C. At ambient conditions (30°C–40°C), the material maintained its integrity and functional properties. However, significant structural alterations were observed at elevated temperatures (60°C and 70°C), with the material becoming viscous and sticky. Although no visible surface cracks were noted, deformation and loss of mechanical strength occurred at higher temperatures, indicating the onset of thermal breakdown. Despite these limitations, the bioplastic's stability at room temperature is sufficient for its proposed use in waste disposal, where exposure to extreme heat is unlikely. This thermal profile confirms its applicability in typical environmental settings.

Conclusion

This study evaluated the feasibility of producing biodegradable and insect-repellent bioplastic from banana peel (*Musa* spp.) and agar enriched with citronella essential oil (*Cymbopogon winterianus*) for waste containment. The experimental results confirmed the achievement of the proposed objectives: the bioplastic exhibited satisfactory physicochemical properties, effective insect-repellent action, and resistance to microbial contamination.

Nonetheless, limitations such as moisture sensitivity and variability in raw material composition were identified, underscoring the need for further optimization. Future research should focus on refining the drying and storage processes, exploring alternative natural additives, and expanding the range of biodegradable sources to enhance product performance and scalability. By offering an eco-friendly solution grounded in circular economy principles, this study contributes to developing sustainable alternatives to conventional plastics. It also reinforces the relevance of biopolymer research in addressing global environmental challenges associated with plastic pollution and public health risks.

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Influence of Biotransformation of *Moringa oleifera* Lam. Oil for Oleochemicals, Food, Pharmaceuthical Applications, and Antimicrobial Activity

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This study explores the biotransformation of *Moringa oleifera* Lam. oil using Eversa® Transform 2.0 (E.T. 2.0) lipase immobilized on an organic support derived from moringa residue. In the first reaction step—hydrolysis—the formation of free fatty acids (FFAs) reached approximately 50%, followed by esterification, which achieved a conversion rate of nearly 90%. The resulting bioproducts (oil, FFAs, and esters) were evaluated for antimicrobial activity, demonstrating efficacy against Gram-positive and Gram-negative bacteria and yeasts. These findings underscore the significance of biocatalysis in enhancing the bioactivity and application potential of oleochemical derivatives obtained from *Moringa oleifera* Lam. oil.
Keywords: *Moringa oleifera* Lam. Lipase. Hydroesterification. Antimicrobial Activity.

Moringa oleifera Lam., a plant native to northwestern India, is well known for its rapid growth, adaptability, and resilience. It thrives in arid soils and adjusts easily to diverse climates, making it suitable for cultivation in several regions, including Brazil [1]. Moringa has a cosmopolitan distribution, primarily found in tropical and subtropical regions. Brazil's cultivation is widespread in the Northeast due to its adaptation to arid and semi-arid conditions [2].

Additionally, *Moringa oleifera* Lam. has gained attention for its high nutritional value, as it contains various secondary metabolites such as vitamins (A, B, E), minerals including calcium and iron, polysaccharides, proteins, polyphenols, and flavonoids (e.g., rutin, quercetin, and kaempferol), along with sterols and fatty acids [3]. These metabolites in multiple plant structures—leaves, bark, stems, and seeds—may exhibit various biological activities, including antimicrobial properties [4].

Oil extracted from the seeds is particularly rich in fatty acids such as oleic acid (C18:1, 70%–76%), stearic acid (C18:0, 5%–8%), and palmitic acid (C16:0, 2%–8%) [5]. Oleic acid, in particular, is noted for its ability to reduce superoxide anions, neutralize hydroxyl radicals, and enhance iron ion reduction, all of which may contribute to its antimicrobial potential [6].

Given these properties, exploring methods capable of biotransforming moringa oil into novel bioproducts with potential biological activity is essential. Biocatalysis is a key technology for the sustainable production of biologically derived chemical and pharmaceutical products [7].

Biocatalysis aligns with 10 of the 12 principles of green chemistry, with the remaining two related to product design rather than processing.

Enzymes used in this process are biodegradable, biocompatible, and derived from renewable resources, making them highly suitable for use in a bioeconomy context [8]. Biocatalysis also avoids using precious metals, eliminates the need for costly post-reaction purification steps, generates less waste, and reduces overall environmental and financial costs [9]. However, using lipases in their free form may pose challenges, especially regarding separation from the reaction medium, which increases operational costs and risks enzyme inactivation [10].

These issues can be mitigated through enzyme immobilization, such as physical adsorption, a reversible technique that requires fewer steps, allows reuse of the support material, and facilitates

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the recovery of the enzyme after use. This approach significantly reduces costs and enables multiple catalytic cycles with the same biocatalyst [11].Effective immobilization requires support materials with specific properties—particularly hydrophobic supports, which promote monomeric enzyme conformation, interfacial activation, purification, and stabilization [8]. Organic supports are especially promising, as they exhibit a high affinity for biomolecules, are biodegradable, and yield non-toxic by-products [10].

Thus, this study aims to evaluate the antimicrobial potential of the by-products obtained from the biotransformation of *Moringa oleifera* Lam. oil through the application of Eversa® Transform 2.0 lipase immobilized by physical adsorption on an organic support, aiming to fill existing gaps in the literature regarding the biological activities of the oil and its derivatives.

Materials and Methods

Reflux Extraction

Crude oil was extracted using 25 mg of M*oringa oleifera* Lam. (MO) seeds and 200 mL of n-hexane in a Soxhlet apparatus at 68 °C for 8 hours. The oil was then separated from the solvent by vacuum distillation using a rotary evaporator [9]. The recovered n-hexane was recycled for subsequent extractions of MO seeds.

Biomass Treatment for Biocatalyst Preparation

After reflux extraction, the biomass was dried at 40 °C for 8 hours to remove residual solvent. Subsequently, it was sieved to obtain particles within the 100–120 mesh range. For biocatalyst synthesis, 1 g of this support material was immersed in 25 mL of ethanol for 24 hours. Afterward, the biomass was vacuum-filtered using a Büchner funnel and Whatman No. 41 filter paper. The filtered support was then prepared for the immobilization process.

Lipase Immobilization by Physical Adsorption

The immobilization of Eversa® Transform 2.0 lipase on the organic support followed the methodology described by Kumar and colleagues [4]. A suspension was prepared using a lipase solution at pH 5.0 (5 mM sodium phosphate buffer) and the support at a 1:19 (w/v) ratio (support: lipase solution), with an initial protein loading of 5 mg/g of support [10].The suspension was stirred at 200 rpm in an orbital shaker for 24 hours. The resulting heterogeneous biocatalyst was vacuum-filtered using a Büchner funnel with Whatman No. 41 filter paper, washed with distilled water, and stored at 4 °C for 24 hours.

Enzymatic Hydrolysis of *Moringa oleifera* Lam. Seed Oil

The enzymatic hydrolysis reaction was conducted to produce free fatty acids (FFAs) from *Moringa oleifera* Lam. seed oil using the immobilized Eversa® Transform 2.0 lipase, with modifications based on the method described by Barbosa (2019). The reaction was carried out at 37 °C, 1000 rpm, for 120 minutes, with the oil comprising 25% of the total reaction volume. For complete FFA conversion in preparation for esterification, Candida rugosa lipase was used under the same temperature and agitation conditions, with 25% oil, 75% water, and an enzyme activity of 550 U/g oil for 60 minutes.

Purification of Free Fatty Acids

Following hydrolysis, the reaction mixture was transferred to a separatory funnel. The upper organic phase was washed five times with boiling distilled water (1:2 v/v). The organic phase (fatty acids) was then separated from the aqueous layer (containing water, glycerol, and biocatalyst) and passed through a column packed with glass wool and anhydrous sodium sulfate to remove residual moisture.

Enzymatic Esterification of Fatty Acids

The purified FFAs were carried out in a reactor containing immobilized enzymes. The FFAs were reacted with isoamyl alcohol at 40 °C and 300 rpm, using a 1:1 molar ratio (oil: alcohol) and a protein concentration of 5% (w/v) relative to the system's total mass. Samples were collected over time and analyzed to determine ester content.

Ester Purification

The purification of esters followed the procedure described by Lage and colleagues (2016) [12]. To eliminate residual fatty acids, the organic phase was neutralized using a 15% (m/v) sodium carbonate (Na_2CO_3) solution at a 1:1 volume ratio. The mixture was then washed five times with distilled water at 40 °C (1:5 v/v). Water was removed using a rotary evaporator under vacuum at 50 °C, followed by incubation at room temperature with 30% (m/v) activated molecular sieves (pre-activated for 24 hours at 250 °C) to eliminate remaining moisture.

Antimicrobial Activity

The antimicrobial and antifungal activities of *Moringa oleifera* Lam. oil, hydrolysis products, and esterification products were assessed using the disk diffusion method according to the guidelines of the National Committee for Clinical Laboratory Standards (NCCLS)[13].

Microbial suspensions (0.5 McFarland standard) containing 1.5×10^8 CFU/mL for bacteria and 1.5×10^6 CFU/mL for fungal strains were prepared. Mueller-Hinton agar (Merck KGaA, Darmstadt, Germany) and Sabouraud dextrose agar were used for bacterial and fungal inoculations, respectively. The test solutions (1:1 dilution in acetone) were applied in 10 µL aliquots onto sterile paper disks placed on the inoculated agar surfaces. The test organisms included *Escherichia coli*, *Candida albicans*, and *Staphylococcus aureus*. Fluconazole (20 and 40 µg/mL) and commercial gentamicin discs were positive controls for antifungal and antibacterial activities, respectively. Discs containing only acetone served as negative controls.

All Petri dishes were incubated at 37 °C for 24 hours (bacteria) or 48 hours (fungi). Antimicrobial susceptibility was evaluated by measuring the diameters of the inhibition zones (in mm) around the disks.

Results and Discussion

After *Moringa oleifera* seed oil was extracted, a two-step hydroesterification process was carried out. The first step involved the enzymatic hydrolysis of the oil to produce free fatty acids (FFAs), followed by enzymatic esterification to form esters. Both reactions were catalyzed using Eversa® Transform 2.0 lipase immobilized on an organic support. Table 1 presents the results of the hydroesterification reactions—comparing the use of free and immobilized enzymes.

The immobilization of Eversa® Transform 2.0 demonstrated significant advantages in both hydrolysis and esterification reactions. In hydrolysis, the immobilized enzyme increased the conversion rate from approximately 39% (free enzyme) to 46%. During esterification, conversion improved by about 10%, reaching 83%, and the reaction time was notably reduced from 24 hours to just 3 hours. These improvements are consistent with findings in the literature, which highlight the benefits of enzyme immobilization in biocatalytic processes, particularly in esterification reactions involving lipases [4,7]. The enhanced performance observed can be attributed to the physicochemical characteristics of the organic support used for immobilization. The support interacts with the enzyme's polymer matrix, modulating its surface conformation and increasing the accessibility of catalytic sites. This modulation facilitates interfacial activation of the lipase, exposing the active sites and improving the interaction with substrates, thereby enhancing catalytic efficiency [14]. Moreover, the organic support used in this study

Table 1. Performance of Eversa® Transform 2.0 (free and immobilized) in the hydroesterification of *Moringa oleifera* oil.

Lipase form	Hydrolysis (%)	Time of Hydrolysis (min)	Esterification (%)	Time (h)
Free Eversa Transform 2.0	39	45	75	24
Organic support	46,4	180	83	3

offers practical advantages. It is cost-effective, derived from renewable and readily available secondary products, and requires no pre-treatment before immobilization. These features make it a sustainable and scalable option for industrial applications in biocatalysis [14].

Antimicrobial Activity

The oil extracted from *Moringa oleifera* Lam. seeds did not exhibit antimicrobial activity against *Escherichia coli*, *Staphylococcus aureus*, or *Candida albicans* (Figure 1). This finding agrees with previous reports by Özcan (2020) [2], which indicated that extracts from *Moringa oleifera* leaves demonstrated antimicrobial activity against a broad spectrum of microorganisms, while seed extracts generally lacked such effects. The absence of activity may be attributed to seasonal variation in seed composition, which can influence key chemical parameters such as acidity index, iodine content, and the proportions of mono-, di-, and triacylglycerols [15].

In contrast, Figure 2 shows the formation of inhibition zones in areas treated with the fatty acid and ester products obtained from the biotransformation of *Moringa oleifera* seed oil. The fatty acid exhibited an average inhibition zone of 14.04 mm against *E. coli* (A), no inhibition against *S. aureus* (B), and 13.09 mm against *C. albicans* (C). The ester product demonstrated broader antimicrobial effects, with average inhibition zones of 14.44 mm for *E. coli* (D), 9.35 mm for *S. aureus* (E), and 14.56 mm for *C. albicans* (F).

These antimicrobial effects can be attributed to the amphipathic nature of fatty acids and monoglycerides, which are known to disrupt bacterial membranes and increase cell permeability. Such biophysical interactions can lead to loss of cellular integrity and, ultimately, inhibition of microbial growth and proliferation [16].

Notably, the fatty acid and esterified products demonstrated antimicrobial activity, starkly contrasting with the original seed oil. This highlights the potential of enzymatic biotransformation as a strategy to enhance the biological activity of vegetable oils. Although promising, the literature still lacks comprehensive studies evaluating the antimicrobial potential of such biocatalytic derived products, underscoring the relevance and originality of the present work.

Conclusion

Biocatalysis using immobilized Eversa® Transform 2.0 lipase proved effective for operational optimization and enhancing antimicrobial activity. The immobilization of renewable and untreated organic support increased conversion efficiency in hydrolysis and esterification reactions and eliminated the need for chemical pre-treatment during enzyme immobilization.

Notably, the biotransformed products (fatty acids and esters) exhibited antimicrobial activity against *E. coli*, *S. aureus*, and *C. albicans*, suggesting potential applications in developing bioactive formulations. These may include natural deodorants, antiseptic soaps, and vaginal

Figure 1. Average inhibition diameter of *Moringa oleifera* Lam. oil and its products (fatty acid and ester) obtained by hydro esterification reaction with ET 2.0 immobilized on organic support by disk diffusion method, using *Escherichia coli*, *Staphylococcus aureus*, and *Candida albicans*.

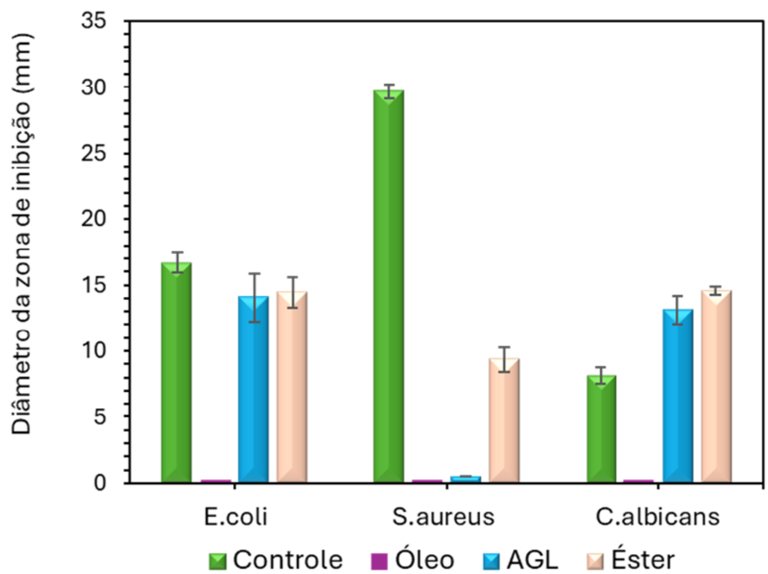
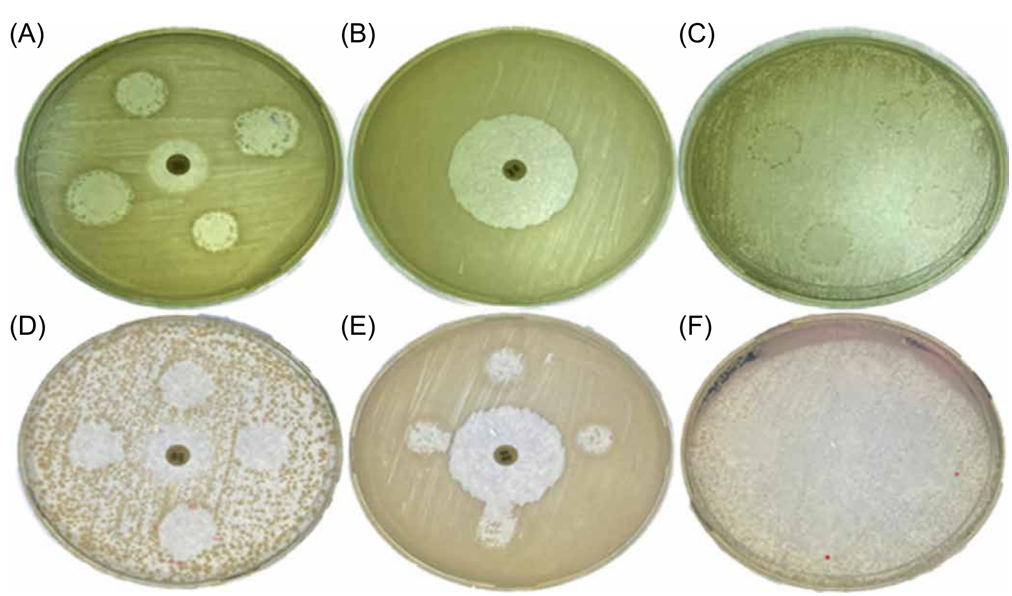


Figure 2. Result of the disk diffusion test with the products of *Moringa oleifera* Lam. oil (fatty acid and ester) obtained by hydroesterification reaction with ET 2.0 immobilized on organic support by disk diffusion method using *Escherichia coli* in A, *Staphylococcus aureus* in B and *Candida albicans* in C, respectively.



creams, positioning enzymatically modified oils as valuable alternatives in pharmaceutical and cosmetic industries.

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Bioprospecting Bacteria with Cellulolytic Potential in Cocoa Husks

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This study aimed to identify bacteria with cellulolytic degradation potential and evaluate their ability to degrade cellulose. Samples of cocoa fruit were collected, treated, and inoculated into a carboxymethylcellulose (CMC) medium, with cellulose as the sole carbon source. After microbial growth, the bacteria were isolated, morphologically characterized, and assessed for their cellulolytic activity. A total of 42 colonies were observed on the initial four plates. The results were promising, with the largest degradation halo measuring approximately 46 mm and an enzymatic index of 3.4. These findings highlight the biotechnological relevance of this research and its contribution to ongoing studies in the field.
Keywords: Cellulolytic Microorganisms. Cellulose. Bioprospecting.

Cellulose is widely used across several industries, including the paper, chemical, textile, food, and pharmaceutical sectors. In Brazil, the pulp and paper industry employs over 175,000 individuals across approximately 4,000 companies, with 32.5% of its production destined for export [1]. As the primary structural component of plant cell walls, cellulose provides rigidity and strength, making it a challenging compound to hydrolyze. However, certain bacteria and fungi produce enzymes capable of degrading cellulose, facilitating its conversion into fermentable sugars [2].

These microorganisms can be found in plant-based environments, such as cocoa residues. Brazil is the seventh largest cocoa producer globally, with an annual output of approximately 265,000 tons. This production generates a substantial amount of plant waste, primarily from cocoa husks, which account for about 80% of the total biomass. When improperly discarded, these residues can pose significant environmental risks [3].

Utilizing cocoa waste offers both economic and environmental benefits. The application of cellulolytic microorganisms has gained attention over chemical catalysts due to advantages such as operational safety, shorter processing time, lower energy consumption, economic feasibility, non-toxicity, and environmental sustainability [4]. Therefore, the main objective of this study was to prospect bacteria with cellulolytic potential in cocoa husks, assess the production of bioactive compounds capable of degrading cellulose, and determine the microbial load of bacteria found in the plant material. Additionally, the study aimed to evaluate the cellulose degradation potential of selected microorganisms with a view toward their industrial applicability and contribution to the development of biotechnological products.

Materials and Methods

Treatment of the Plant Source

Cocoa (*Theobroma cacao*) was selected as the plant source for this study. Aseptic treatment was performed to reduce the microbiota in the cocoa husks. The samples were divided and subjected to two types of surface sterilization: the first was treated with 70% ethanol, and the second was treated sequentially with sodium hypochlorite and 70% ethanol, each for 60 seconds.

Preparation of the Culture Medium

The culture medium was prepared with the

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following composition: 1 g of $(NH_4)_2SO_4$, 1 g of K_2HPO_4, 5 g of $MgSO_4$, 1 mg of NaCl, 15 g of agar, and 10 g of carboxymethylcellulose (used as the sole carbon source) per liter of distilled water [5].

Cultivation and Isolation of Colonies

For microbial cultivation, 1 g of the treated plant material was added to 9 mL of sterile saline solution (0.85% NaCl), shaken for 1 minute, and left to rest at room temperature for 1 hour. Afterward, 0.1 mL aliquots of the suspension were spread on CMC agar plates [6]. Microbial growth was assessed after 24–48 hours. Colonies showing clear zones (indicative of cellulolytic activity) were transferred to new CMC agar plates for enzymatic activity confirmation and colony purification [7].

For isolation, colonies were picked with a platinum loop and serially diluted in microtubes containing 0.9 mL of sterile saline until no turbidity was observed. The diluted samples were inoculated on CMC agar plates and incubated for 24–48 hours. The streaking method was used to reduce microbial density and facilitate the isolation of pure colonies through two sequential streaks on solid media [8]. Pure cultures were subsequently analyzed by Gram staining.

Wet Mount Slide

Wet mount slide observation was performed to differentiate the isolates as bacteria, fungi, or yeasts. Morphological features such as cell size and shape were used as parameters to aid in microbial identification [9].

Gram Staining

The Gram staining technique was employed to analyze bacterial morphology. Microorganisms staining pink or red were classified as Gram-negative, while purple or blue were classified as Gram-positive [10].

Analysis of Cellulolytic Activity

The cellulolytic activity was quantified using the Enzymatic Index (EI), which is calculated as the ratio between the diameter of the degradation halo and the diameter of the bacterial colony. This index was used to select strains with the highest potential for extracellular cellulase production [11].

The presence of cellulolytic activity was confirmed by the formation of orange zones around the colonies following the application of an iodine solution (prepared with 2 g of potassium iodide, 1 g of iodine in 300 mL of distilled water) poured onto the plate surface, and allowed to react for 2 hours, according to Florêncio and colleagues (2012) [12]. The diameter of the halos was measured using a caliper.

Results and Discussion

Isolation of Bacteria

This section discusses the entire methodological process of the present study, which employed a qualitative-quantitative, experimental approach. Through laboratory analyses, the study aimed to prospect for bacteria capable of producing cellulase and to assess their cellulolytic potential based on cellulose degradation in carboxymethylcellulose (CMC) medium, thereby enabling the qualification of the studied microorganisms.

The initial isolation of bacteria from cocoa husks was carried out on four culture plates, categorized according to the aseptic treatment applied to the fruit. The plates treated solely with 70% ethanol yielded 21 colonies, while the plates subjected to both ethanol and sodium hypochlorite treatments produced 22 viable colonies. These colonies were identified and documented in Table 1, with further characterization presented in Tables 2 and 3 to facilitate the tracking and analysis of each microorganism throughout the study.

Table 1. Total number of colonies isolated from cocoa husk samples according to aseptic treatment method.

Aseptic Tratment	Plate Number	Colony Number
Alcohol 70%	A1 or A2	A1-7
Sodium Hypochlorite	H1 or H2	H2-7

Table 2. Characterization of colonies in cocoa husks treated with 70% alcohol.

Colony	Form	Aspect	Colony	Form	Aspect
A1-1	Regular	Opaque	A2-1	Rhizoid	Opaque
A1-2	Irregular	Translucent	A2-2	Irregular	Opaque
A1-3	Regular	Opaque	A2-3	Regular	Opaque
A1-4	Circular	Opaque	A2-4	Regular	Translucent
A1-5	Circular	Opaque	A2-5	Regular	Opaque
A1-6	Irregular	Opaque	A2-6	Regular	Opaque
A1-7	Regular	Opaque	A2-7	Regular	Opaque
A1-8	Regular	Translucent	A2-8	Irregular	Opaque
A1-9	Regular	Opaque	A2-9	Irregular	Opaque
A1-10	Circular	Translucent	A2-10	Regular	Opaque
A1-11	Irregular	Opaque			

Table 3. Characterization of colonies present in cocoa husks treated with hypochlorite and 70% alcohol.

Colony	Form	Aspect	Colony	Form	Aspect
H1-1	Regular	Translulcent	H2-2	Regular	Translulcent
H1-2	Regular	Opaque	H2-3	Irregular	Translucent
H1-3	Regular	Translucent	H2-4	Filamentous	Translucent
H1-4	lrregular	Translucent	H2-5	Irregular	Translucent
H1-5	Irregular	Translucent	H2-6	Filamentous	Translucent
H1-6	Irregular	Opaque	H2-7	lrregular	Opaque
H1-7	Irregular	Opaque	H2-8	Regular	Translucent
H1-8	Irregular	Translucent	H2-9	Regular	Translucent
H1-9	Filamentous	Translucent	H2-10	Regular	Translucent
H1-10	Filamentous	Translucent	H2-11	Regular	Translucent
H2-1	Irregular	Opaque	H2-12	Irregular	Translucent

Plates treated only with 70% ethanol exhibited a predominance of opaque colonies (80.95%), whereas plates treated with sodium hypochlorite and ethanol showed a higher frequency of translucent colonies (77.27%). This discrepancy may be associated with the effectiveness of the aseptic treatments: the ethanol-only procedure appears less effective, resulting in a greater microbial load, which may lead to more visibly opaque colonies due to denser bacterial growth.

Gram Staining

Gram staining was performed to analyze the morphology of the isolated microorganisms. This method allows differentiation based on the structural and chemical properties of the cell wall, classifying the bacteria as either Gram-positive or Gram-negative. The results of this analysis are summarized in Table 4 and visually represented in Figure 1.

Wet Mount Slide

Wet mount slide microscopy was conducted to differentiate between bacteria, fungi, and yeasts (Figure 2). The analysis confirmed the predominance of bacterial structures, characterized by their prokaryotic morphology (absence of a defined nucleus). This distinguishes them from yeasts—which typically exhibit budding—and from filamentous fungi, which present hyphal structures.

Analysis of Cellulolytic Activity

For the degradation test in a solid medium, the colony diameter and the diameter of the CMC degradation halo were measured. The Enzymatic Index (EI) estimated the extracellular enzyme production, calculated as the ratio between the degradation halo diameter and the colony diameter (Table 5).

The isolated bacteria's EI values ranged from 1.07 to 3.4. In a similar study by Behera and colleagues (2014) [13], bacteria incubated aerobically at 37ºC showed EI values ranging from 1.18 to 2.5 under comparable conditions.

The presence of a degradation halo indicates the ability of the microorganism to produce cellulase, as it reflects the breakdown of carboxymethylcellulose. Among the isolates, A1-2 exhibited the largest

Figure 1. Plate A1-3 slide analyzed under the microscope for determination of gram stain, predominantly Gram-negative monococcus.

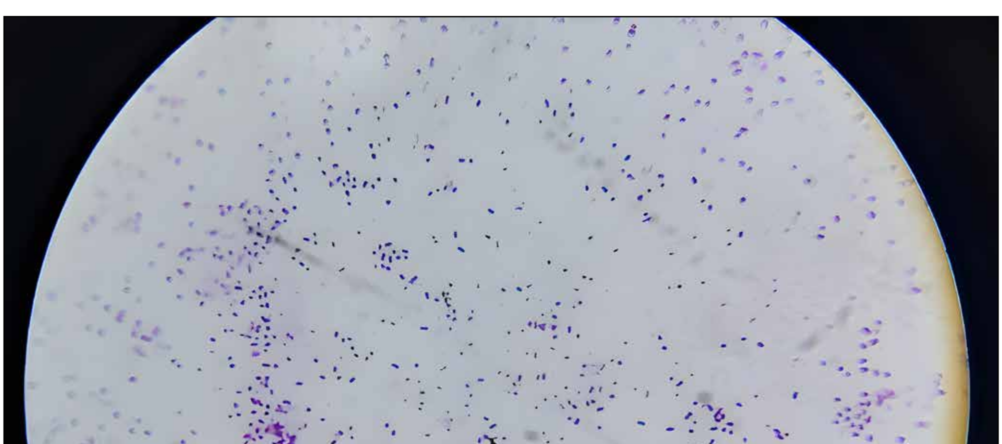


Table 4. Gram tests and morphological characterization of isolated colonies.

Colony	Morphology	Gram	Colony	Morphology	Gram
A1-1	Bacillus	+	A2-2	Monococcus	+
A1-2	Bacillus	+	A2-3	Monococcus	+
A1-3	Monococcus	+	A2-4	Bacillus	+
A1-4	Monococcus	-	H1-1	Monococcus	+
A1-7	Streptococcus	+	H1-3	Monococcus	-
A1-8	Diplococcus	-	H2-2	Streptococcus	+
A1-9	Bacillus	-	H2-5	Diplococcus	+
A1-10	Bacillus	+	H2-6	Bacillus	-
A2-1	Streptococcus	+	H2-7	Monococcus	-

Figure 2. Wet slide: microorganisms prospected on a coverslip being analyzed through microscopy.

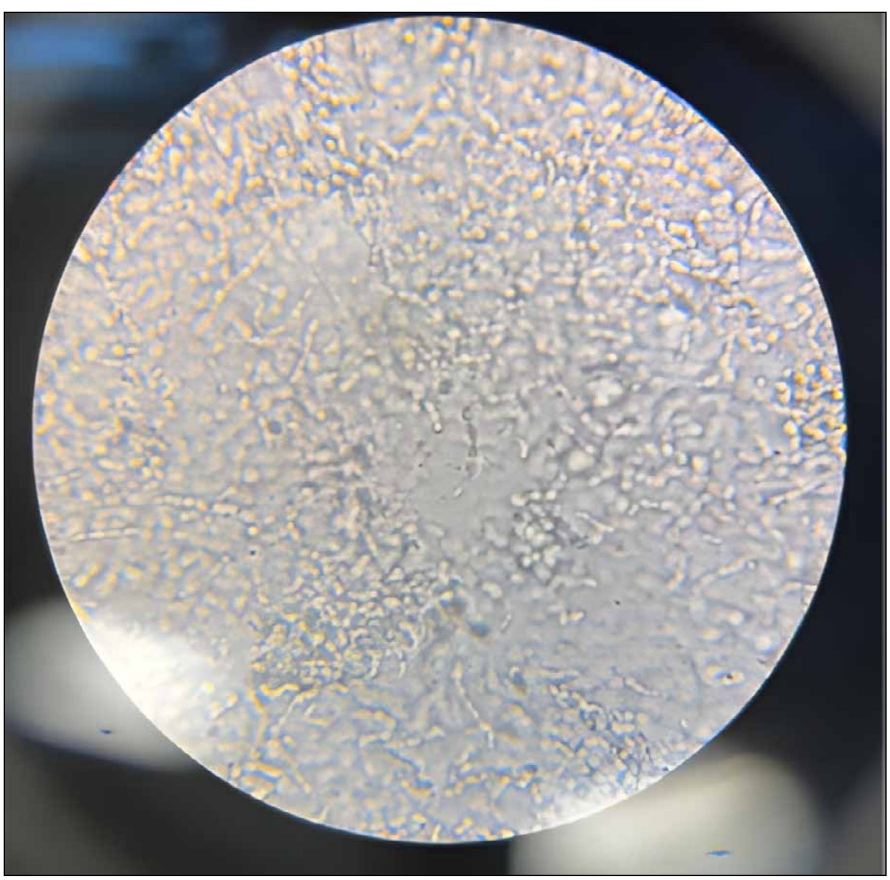
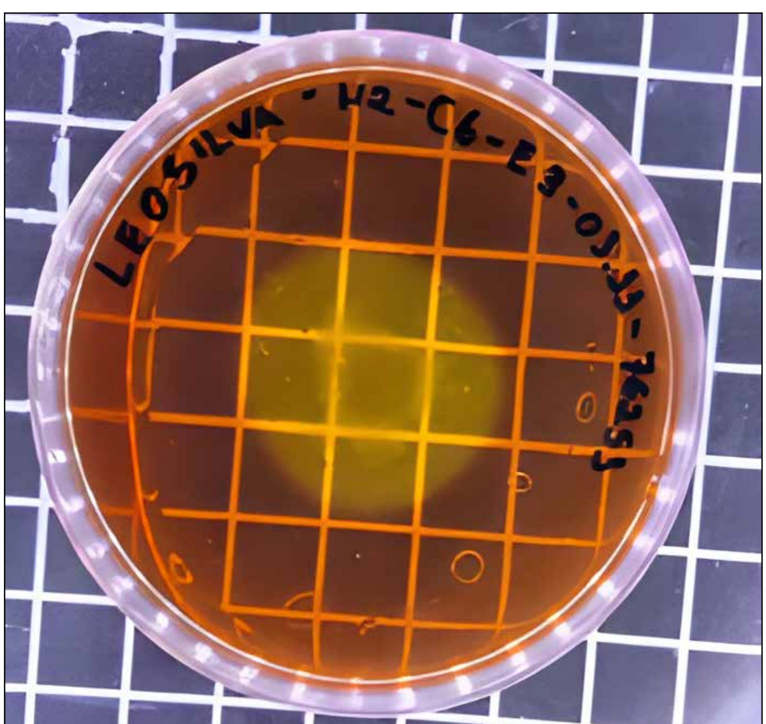


Table 5. Cellulolytic activity of microorganisms isolated from cocoa husks.

Colony	Colony Diameter (mm)	Halo Diameter (mm)	Enzyme Index
A1-1	21	46	2.19
A1-2	27	29	1.07
A1-3	20	44	2.2
A1-5	10	34	3.4
A1-7	22	43	1.95
A1-9	16	32	2
A1-10	26	34	1.3
A2-1	15	32	2.13
A2-4	23	40	1.73
H1-3	17	31	1.82
H2-3	22	36	1.63
H2-5	16	42	2.62
H2-6	22	39	1.77
H2-7	20	34	1.7

Figure 3. Plate H2-6 halo degradation test with the aid of iodin.



colony diameter at 27 mm, followed by A1-10 with 26 mm. In terms of halo size, isolate A1-1 displayed the largest halo at 46 mm, followed by A1-3 at 44 mm (Figure 3).

The highest enzymatic index was observed in colony A1-5 (EI = 3.4), followed by H2-5 (EI = 2.62). Isolates A1-1 (EI = 2.19), A1-3 (EI = 2.2), A2-1 (EI = 2.13), and A1-9 (EI = 2.0) also met the recommended threshold of EI ≥ 2.0, as proposed by Lealem & Gashe (1994) [14], to indicate strong cellulolytic activity. These results suggest that the studied microorganisms possess a high capacity for cellulose degradation, with most colonies producing degradation halos greater than 30 mm.

Conclusion

Based on the results presented in this study, bioprospecting is a promising approach for advancing biotechnology and industrial applications. The successful isolation of cellulolytic bacteria from a natural source—cocoa husks—demonstrated significant degradation potential. Isolate A1-1 achieved the largest halo diameter (46 mm), A1-2 exhibited the largest colony diameter (27 mm), and isolate A1-5 presented the highest enzymatic index (3.4). These findings reinforce the potential use of these microorganisms in developing biotechnological processes focused on cellulose degradation.

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Synthesis of the New Chemical Marker, [Eu(DBM)3(Lap), and Design Via Molecular Docking for Use in Recognition of *Candida auris* Polymerase

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The recent emergence of infections caused by *Candida auris* has raised significant global concern. Efforts to develop structure-based drugs using secondary metabolites from plant species offer promising strategies to reduce the virulence of these fungal pathogens. Lapachol, a member of the 1,4-naphthoquinone family, has shown potential as a metal complex ligand and is a candidate for such therapeutic applications. In the present study, we report the extraction of lapachol using a novel purification process from a natural source—the wood of *Tabebuia impetiginosa* (purple ipê)—and the synthesis of a unique complex of the type [Eu(DBM)3(Lap)]. Additionally, we present a molecular docking simulation of the synthesized lapachol-based complex, evaluating its potential as an inhibitory agent targeting *Candida auris* polymerase.
Keywords: Lapachol. Europium. Naphthoquinone. Lanthanides. Superfungus.

Candida auris and Computational Studies

Candida auris is a yeast species notable for its multidrug resistance, and it has emerged as a significant fungal pathogen due to its capacity to cause invasive infections and outbreaks in healthcare settings that are difficult to manage and treat [1].

Since its emergence, cases of *C. auris* have been reported on five continents as a cause of nosocomial infections, including instances identified in the external auditory canal of patients [2]. Of the nearly 150 *Candida* species described in the literature, only about 10% are known to cause human infections (candidiasis). *Candida* species and other yeasts are part of the human microbiota, commonly found on the skin, mucosal surfaces, the female genital tract, and the gastrointestinal tract [1,3].Infections caused by *C. auris* are associated with high mortality rates and often exhibit resistance to multiple classes of antifungal agents. These infections range from mild and localized conditions (such as vaginitis) to severe and life-threatening systemic infections, including candidemia [4].Despite the rapid global dissemination of *C. auris*, determining the actual burden of infection remains challenging, as standard laboratory identification techniques frequently fail to identify this species [5–8] correctly.

Naphthoquinones: Pharmacological Properties

Lapachol is a naturally occurring organic compound classified as a 1,4-naphthoquinone. It contains a hydroxyl group attached to carbon 2 and a branched 3-methyl-2-butenyl side chain attached to carbon 3. The most stable tautomeric form features carbonyl groups at positions 1 and 4, although a less stable resonance form with carbonyls at positions 1 and 2 also exists (Figures 1a–1b). Lapachol is primarily found in the heartwood of trees belonging to the *Bignoniaceae* family, particularly in the

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Tabebuia genus [9]. These trees, commonly called pau d'arco, are native to the Amazon region.

Pharmacological studies on decoctions made from the sawdust of these trees have identified lapachol as one of the key bioactive components [10]. However, despite its biological potential, lapachol exhibits significant toxicity when ingested in large quantities. To mitigate its cytotoxic effects, several studies have explored the complexation of lapachol with metal ions [11,12], which has been shown to enhance its bioavailability and reduce toxicity.

Lanthanides: General Considerations

The IUPAC Commission on Nomenclature of Inorganic Chemistry recommends using the term "rare earth metals" for the elements Sc, Y, and La–Lu. This designation arises not from their scarcity but because these elements are typically found in nature as mixtures of oxides, or "earth," which require complex separation processes.

Rare earth elements exhibit predominantly ionic chemistry, primarily influenced by the size of the ionic radius. A remarkable phenomenon in this group is the lanthanide contraction, which results from the imperfect shielding effect of the $4f^n$ electrons. This poor shielding increases the effective nuclear charge, reducing the size and volume of the entire $4f^n$ configuration. Consequently, the entire ion or atom contracts - which is significant enough to impact chemical properties such as coordination number, acid strength, and the stability of the 3^+ oxidation state [13–15].

Lanthanides have many applications, including in optical materials, catalysts, magnets, ceramics, and pharmaceuticals [14]. In this study, we synthesized a new material, [Eu(DBM)3(Lap)], using a hydrated europium precursor complex and lapachol extracted from purple ipe sawdust. We investigated this compound's interaction potential and inhibitory activity against *Candida auris* super fungus through *in silico* assays. The objective was to generate new data for this system and explore the potential application of europium complexes as pharmacological agents.

Materials and Methods

Preparation of Lapachol

Approximately 200 g of bow wood sawdust was mixed with 1 L of saturated sodium bicarbonate, producing an intense red solution. The mixture was stirred for 45 minutes and then filtered, discarding the solid residue. Subsequently, approximately 50 mL of hydrochloric acid (37%) was slowly added to the filtrate until the red solution turned yellow, forming a precipitate. The liquid was then vacuum-filtered and discarded.

At this stage, lapachol was obtained, although still containing impurities derived from the sawdust. The crude lapachol was dissolved in ethyl acetate and subjected to a simple filtration. Recrystallization was achieved by allowing the solvent to evaporate at approximately 25 °C (Figure 2).

Figure 1. Lapachol with carbonyls in position for (1,4) (a) and ortho (1,2) (b).

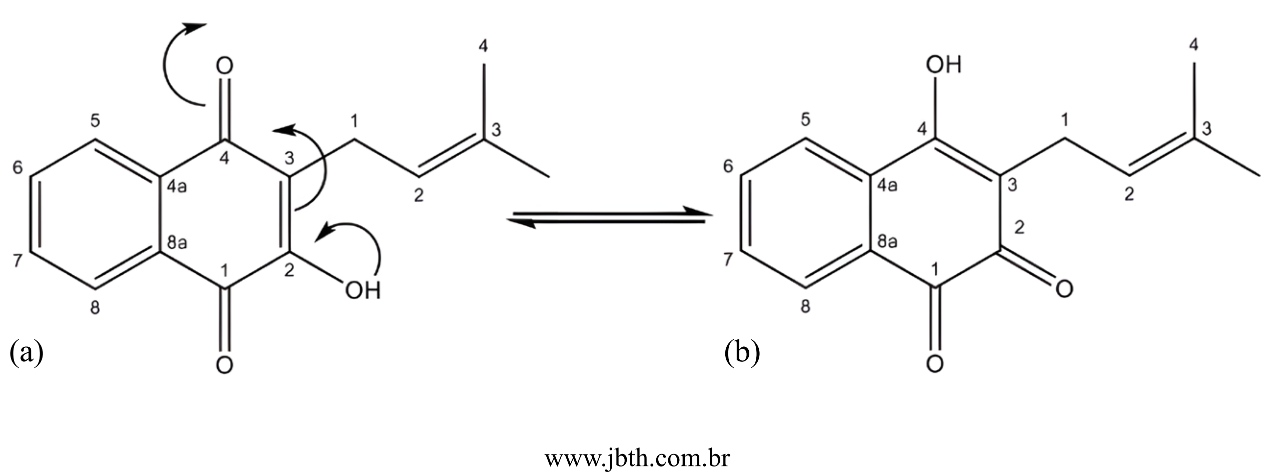
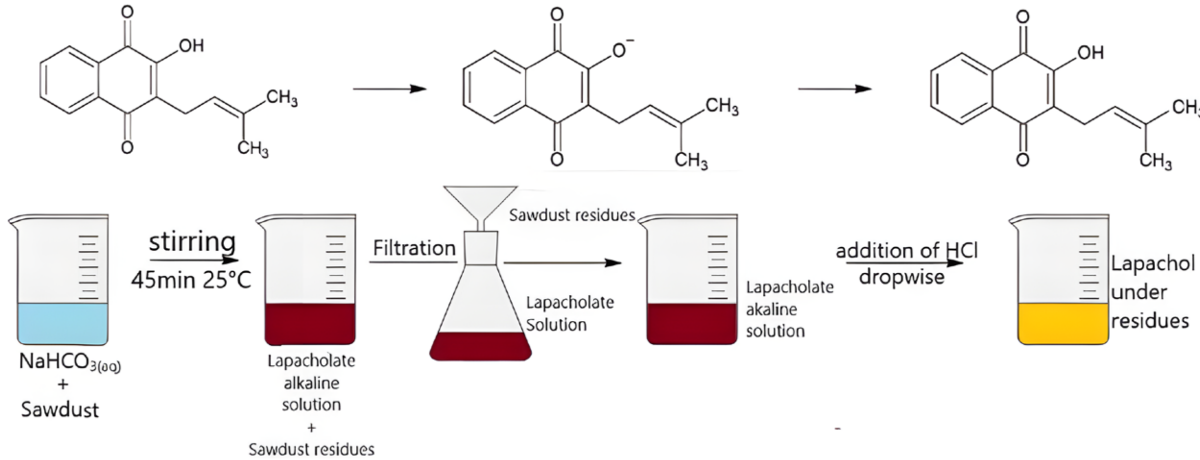


Figure 2. Lapachol extraction process from the sawdust of pau d'arco.



Synthesis of the [Eu(DBM)3(Lap)] Complex

It dissolves about 0.2 mmol of [Eu(DBM)3(Lap)] in approximately 30 mL of ethanol and 0.4 mmol of lapachol. After the salt and ligand dissolve, they are mixed, and agitation begins. The suspension is stored for ten days. Parts of the supernatant are removed, and the crystals are grouped in a well-defined way.

Washing was done using the same solvent as a reaction medium, as shown in Figure 3.

Methods

Melting point data were obtained using a Gehaka fusion point meter, model PF1000, with a temperature accuracy of ±0.3 °C up to 100 °C. For thin-layer chromatography (TLC), chromatoplates with Silica gel 60G F254 (Merck®) were used as the stationary phase. The mobile phase consisted of a mixture of hexane and ethyl acetate in a 3:7 ratio.

Infrared (IR) spectra were recorded on a PerkinElmer Frontier FT-IR spectrometer using KBr pellets. Each sample underwent 32 scans at a resolution of 4 cm^{-1}. Electronic absorption spectroscopy data were collected using a dual-beam UV-VIS spectrophotometer (Thermo Scientific GENESYS 10S) in methanol, with a sample concentration of 0.05 mg/mL.

Molecular Docking

Molecular docking was carried out using AutoDock Vina, applying the Lamarckian genetic algorithm (GA) and a grid-based energy estimation model. Gasteiger partial charges were assigned to the ligands, while Kollman charges were added to the protein. Non-polar hydrogen atoms were merged, and torsional degrees of freedom were assigned to the ligands.

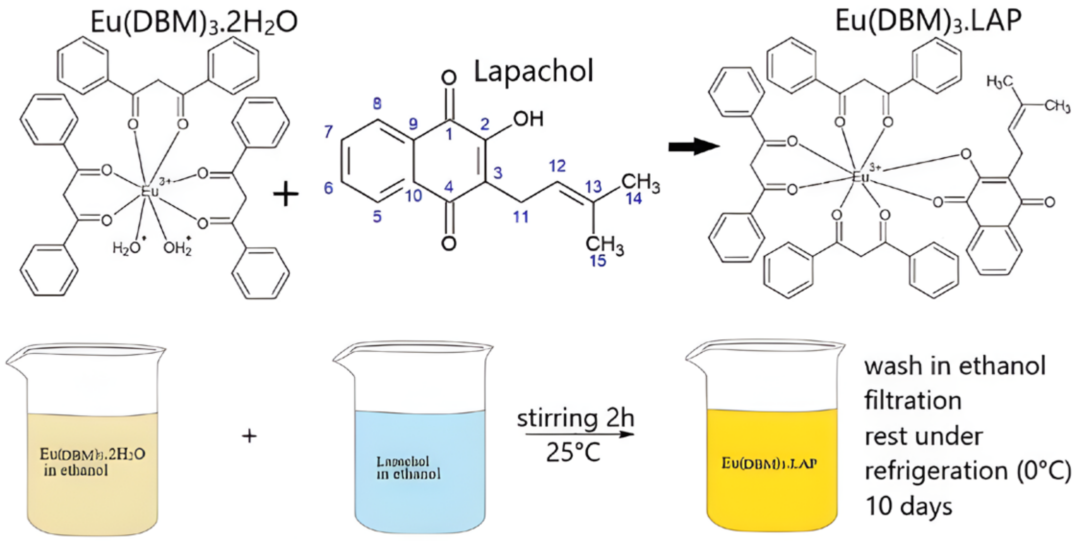
The docking grid box was set to dimensions of 25 Å × 25 Å × 25 Å, centered at x = –28.152, y = 24.208, and z = –1.140. Based on the three-dimensional structure of the target protein, this region, containing residues Leu94 (97) and Phe91 (94), was selected as a potential binding pocket.

Results and Discussion

New Purification Method

The literature typically recommends recrystallization in ethanol for lapachol purification following extraction from sawdust. However, in this study, purification was achieved via dissolution in ethyl acetate. This method proved simpler and more efficient, reducing the steps required to isolate the compound. The resulting lapachol appeared as yellow crystals. Melting point analysis of the purified sample yielded a range of 141 °C–143 °C,

Figure 3. New complex synthesis route of [Eu(dbm)₃.(lap)].



closely aligning with the literature values of 139.5 °C–140.2 °C, confirming the compound's purity.

[Eu(DBM)3(Lap)] Complex

The newly synthesized complex, [Eu(DBM)3(Lap)], was obtained as a dark purple powder, indicating the presence of the naphthoquinone moiety in the form of a lapacholate ion. The complex exhibited good solubility in organic solvents such as ethyl acetate, hexane, and ethanol but limited solubility in water, likely due to the non-polar ligands present in the first coordination sphere of the metal center.

Thin Layer Chromatography

TLC analysis in this study aimed to validate the purity of lapachol synthesized via the new route and to identify the components of the complex [Eu(DBM)3(Lap)]. The TLC analysis of pure lapachol yielded an R_f value of 0.51 (Figure 4a). Comparative TLC (Figure 4b) involving the complex [Eu(DBM)3(Lap)] (C), lapachol (L), and HDBM (D) demonstrated successful complexation. The chromatographic profile of the complex (C) contained signals corresponding to L and D, confirming the incorporation of both constituents into the complex without excess unreacted material.

Infrared Spectroscopy

The infrared spectrum of the complex containing lapachol purified using the new method exhibits an intense broadband corresponding to the O–H stretching vibration, with a maximum of 3427.84 cm^{-1}. In contrast, the IR spectrum of pure lapachol shows a narrower band at 3357 cm^{-1}, which may suggest the presence of more accessible hydroxyl groups in the complex. Upon complexation, several bands characteristic of the free ligand (LAP) are either shifted or absent, indicating successful coordination. The primary coordination sites in LAP are the carbonyl group (C1=O1) and the hydroxyl group. In the IR spectrum of the metal complex (Figure 5), the band attributed to the carbonyl stretch is shifted from 1643 cm^{-1} in free LAP to 1549.47 cm^{-1} in the complex. This shift to a lower frequency suggests coordination of the carbonyl oxygen to the metal center, which weakens the double bond character and is consistent with a reduction in bond order upon coordination.

Figure 4. (a) Lapachol sample (L) in chromate plate after performing TCL; (b) Samples of [Eu(DBM)3(Lap)] (C), Lapachol (L), and Dibenzoilmethane (D), respectively, in Chromate plate after TLC revelation.

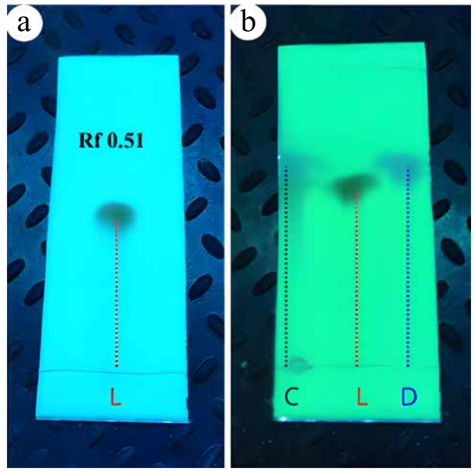


Figure 5. The infrared spectrum of pure lapachol and [Eu(DBM)3(Lap)] complex.

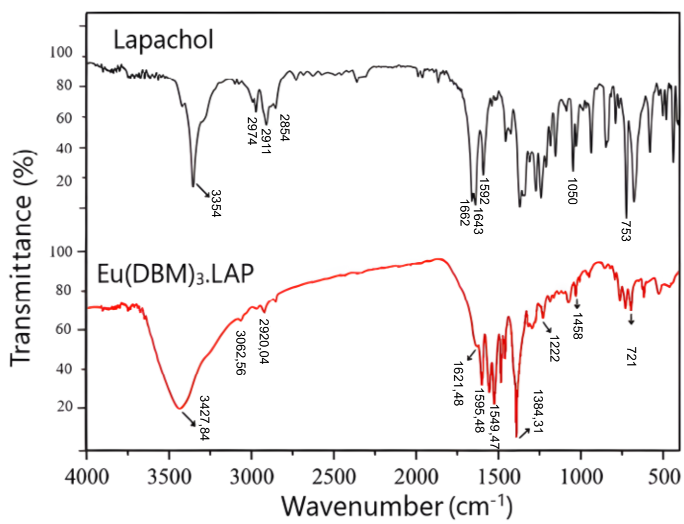
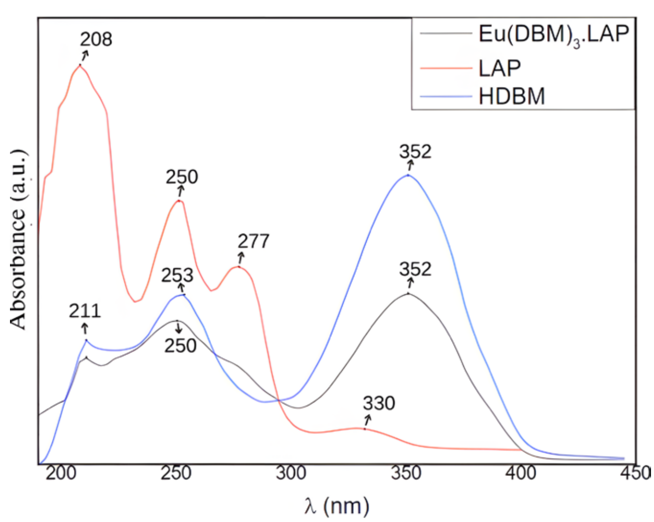


Figure 6. Complex UV-vis Spectrum of [Eu(DBM)3(Lap)], LAP and HDBM.



Furthermore, the IR data suggest that the phenolic oxygen of lapachol may also coordinate with the europium ion. These spectral changes support the forming of a new chemical species through ligand-to-metal complexation.

<u>UV-Vis</u>

Figure 6 shows the ultraviolet absorption curve of free ligands, lapachol (LAP) and dibenzoylmethane (HDBM), and the novel complex, [Eu(DBM)3(Lap)].

Electronic Absorption

In the UV-Vis absorption spectrum of lapachol, the most intense peaks are observed in the 200–280 nm region, a characteristic interval for π→π* electronic transitions. These transitions are associated with the high density of C=C bonds in the molecule's structure, extending from the bicyclic aromatic ring of the naphthoquinone core to the unsaturated side chain. In contrast, the less intense peaks correspond to n→π* transitions, which arise from non-bonding electron pairs on the C=O groups (ketones).

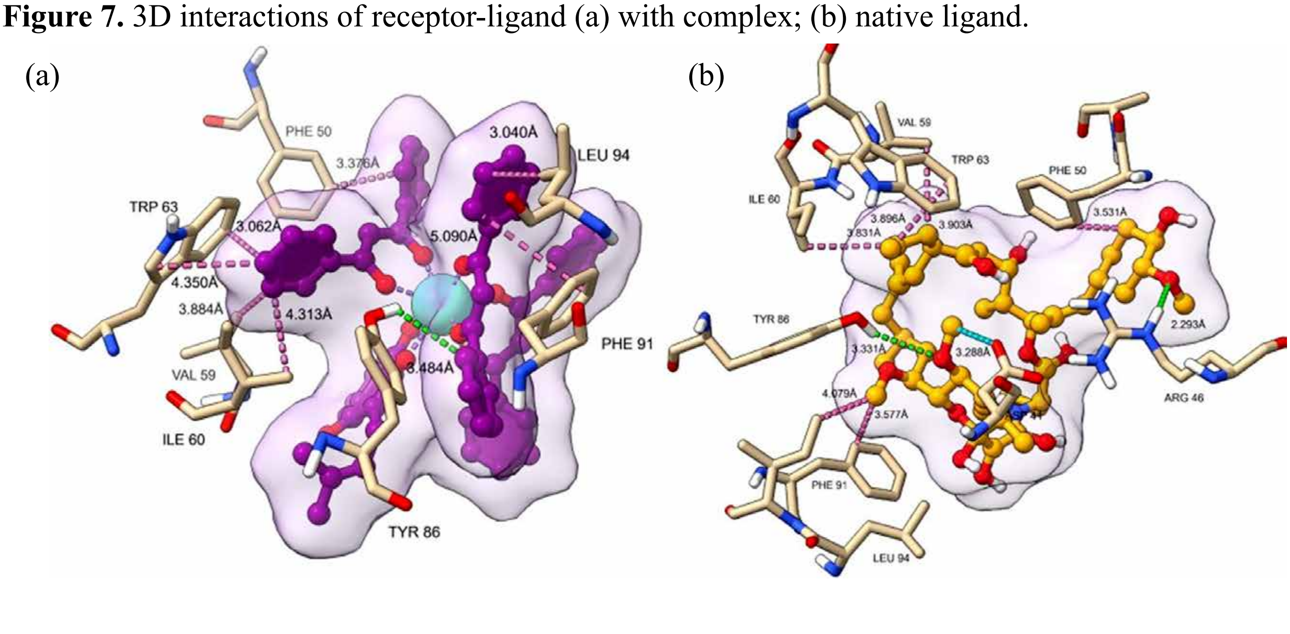
The absorption bands observed at 208, 250, and 277 nm correspond to other chromophoric regions within the LAP molecule. In the absorption spectrum of the novel material [Eu(DBM)3(Lap)], a more substantial influence from HDBM is evident. This is due to HDBM's β-diketone structure, which has a high affinity for europium and is present in greater proportion within the complex relative to lapachol. These spectroscopic findings are consistent with the infrared results, reinforcing the conclusion that both ligands are successfully coordinated to the central metal ion.

Interaction with Protein Residues

The molecular docking analysis revealed that the europium complex [Eu(DBM)3(Lap)] exhibited potential inhibitory activity through hydrophobic interactions within the active site of the target protein. Several amino acid residues were consistently involved in the binding interactions: Phe50, Gly57, Val59, Ile60, Trp63, Tyr86, Phe91, and Leu94.

Figure 7 illustrates the main interactions between [Eu(DBM)3(Lap)] and the protein. All observed interactions were hydrophobic. Among them, two π-alkyl interactions were identified: one with Phe50 (3.37 Å) and another with Val59 (3.88 Å). Previous studies [14,47] have highlighted the importance of Phe91 (5.09 Å) and Leu94 (3.04 Å) in mediating biological activity, particularly when interacting with inhibitory ligands. This study also observed

Figure 7. 3D interactions of receptor-ligand (a) with complex; (b) native ligand.



these interactions involving both the europium complex and the reference compound FK-506.

Additionally, the complex exhibited alkyl interactions with Ile60 (4.31 Å and 4.89 Å) and with Trp63 (3.06 Å and 4.35 Å), as well as a π-donor hydrogen bond with the Tyr86 residue (3.48 Å). These findings suggest a potent and specific binding mode, supporting the potential of the europium complex as a pharmacological agent targeting the protein.

Conclusion

This study presents the novel complex [Eu(DBM)3(Lap)], validated through IR spectroscopy, UV-Vis absorption, melting point determination, and TLC analysis. The data obtained indicate the effective coordination of the ligands HDBM and LAP to the europium ion (Eu^{3+}), confirming the successful synthesis of the complex. The findings suggest that this material holds promise for future applications, particularly as a chemical marker or inhibitor of the multidrug-resistant fungus *Candida auris*, given the known pharmacological potential of lapachol derivatives. This preliminary *in silico* investigation lays the groundwork for future *in vitro* studies to validate the compound's biological activity further.

Acknowledgments

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Application of Activated Carbon Produced from Licuri Bark (*Syagrus coronata*) in Water Filtration

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This work aims to produce activated carbon from the bark of licuri (*Syagrus coronata*) and evaluate its effectiveness in water filtration. The bark was separated from the pulp, and biochar was produced through pyrolysis and chemical activation. The filtration performance was assessed by measuring the optical density using a spectrophotometer and analyzing the samples that passed through the filtration system containing the licuri-based activated carbon. The results confirmed the efficiency of activated carbon derived from licuri bark. Regarding adsorption capacity, the pyrolyzed charcoal alone demonstrated superior performance, yielding results comparable to commercial activated carbon commonly used in drinking water filtration systems.

Keywords: Licuri. Activated Carbon. Filtration.

The Northeast region of Brazil faces significant challenges related to water scarcity and poor water quality, particularly during prolonged drought periods. These issues affect not only the availability of water but also critically impact sectors such as agriculture, public health, and the daily lives of local communities. To mitigate these effects, developing sustainable technologies is essential to ensure reliable access to water in the region.

Activated carbon is currently widely used as an adsorbent in water filtration systems due to its porous structure. This structure enables it to trap and retain contaminant molecules, thereby improving water quality.

Licuri, a native fruit of the semi-arid Northeast region, is harvested from the *Syagrus coronata* palm. It is abundant in various commercial applications, including handicrafts and regional culinary dishes. However, agro-extractivist communities often discard the fruit's bark as agricultural waste agro-extractivist communities often discard. Repurposing this by-product for the production of activated carbon adds both economic and social value to the lecture bark. In this context, two primary methods can be employed to produce activated carbon using simple and effective techniques: pyrolysis, which involves thermal decomposition in the absence of oxygen, and chemical activation, which entails treating the material with chemical agents to enhance porosity and adsorption capacity.

This study's objective is to explore the use of lecture bark (*Syagrus coronata*) in the production of activated carbon for water filtration, with the goal of reducing the concentration of microbial cells in contaminated water samples. Furthermore, the study investigates the microorganism removal potential of samples prepared from pretreated bark subjected to pyrolysis and chemical activation methods.

Materials and Methods

This study is applied as it seeks to apply experimental techniques derived from methodological theory to assess the efficiency of activated carbon produced from licuri bark for removing microorganisms from water. It

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adopts a quantitative approach, analyzing data by measuring optical density in different samples. Additionally, it is classified as exploratory research, based on hypotheses concerning the quality of activated carbon derived from the selected raw material. The research also fits the experimental design category, as it involves subjecting licuri bark to controlled variables to obtain measurable outcomes. Specifically, the study examines the influence of licuri bark–based activated carbon on removing contaminants from water.

Collection and Preparation of Raw Materials

Licuri fruit was obtained from residents of the municipalities of Dias D'Ávila, Alagoinhas, and Salvador, Bahia, during the first quarter of 2023. After collection, 150 g of material was weighed and washed in hot water. The material was then dried in an oven at temperatures ranging from 95°C to 170°C for 1 hour to remove excess moisture. Following this, it was cooled to room temperature. The bark was manually separated from the pulp and fragmented into smaller pieces.

Pyrolysis

The fragmented licuri bark was subjected to pyrolysis, a thermal decomposition process of organic material without oxygen, used to create a porous structure. Five pyrolysis tests were conducted. In each test, 100 g of bark was weighed on an analytical balance and distributed into crucibles. The process was conducted in a muffle furnace with continuous heating up to 700°C. After pyrolysis, the samples were allowed to cool to room temperature.

Chemical Activation

Chemical activation was performed to enhance the porosity of the charcoal. Sulfuric acid (H_2SO_4) was selected for this process. In three activation assays, 20 mL of H_2SO_4 was added to 50 g of charcoal from the pyrolysis stage, with contact time ranging from 12 to 24 hours. After activation, the samples were filtered under vacuum and washed with distilled water until reaching a pH of approximately 5. Subsequently, the samples were dried in an oven at 120°C, yielding chemically activated carbon derived from licuri bark.

Prototype Assembly

A filtration prototype was constructed to test the effectiveness of the produced activated carbon, mimicking the structure of a household water filter. The prototype consisted of a PET bottle, a plastic sheet, and hydrophilic cotton to retain charcoal particles. A cap with a central hole was installed at the top, connected to a siphon tube linked to a drainage pump attached to a larger PET bottle used to store the contaminated sample. The pump facilitated water flow, while the upper bottle held the saline solution inoculated with microorganisms. The contaminated sample was placed in the upper bottle, passing through the siphon and into the charcoal-filled chamber, allowing filtration. The filtered solution was then collected and analyzed using a spectrophotometer to measure optical density.

Microbiological Analysis

Microbiological tests were conducted to evaluate the water quality after filtration with licuri-based charcoal using Bacillus subtilis, a bacterium cultivated under laboratory conditions. The bacteria were grown in tryptic soy broth (TSB) and distributed into Falcon tubes after inoculation. The cultures were centrifuged to sediment the inoculum, which was then resuspended in a sterile saline solution. The resuspended inoculum was transferred to a 1 L beaker, resulting in a contaminated test sample. The optical density of this sample was measured using a spectrophotometer. Filtration tests were then performed using different filtering materials: commercial activated carbon, chemically activated licuri carbon, pyrolyzed licuri carbon, and untreated licuri bark. The performance of each was evaluated by comparing the reduction in optical density of the filtered samples. Figure 1 briefly demonstrates the experimental steps performed in this study.

Results and Discussion

Filtration System

The filtration prototype built to evaluate the retention capacity of the samples—obtained during the experiments and compared with commercial activated carbon—proved to be effective. It successfully allowed the passage of contaminated water through the coals and bark samples without overflow and with a consistent flow rate throughout the filtration process.

Charcoal Yield

Approximately 51.8 g of pyrolyzed charcoal was obtained from 100 g of original biomass. This relatively low yield can be attributed to the absence of a controlled heating ramp during the pyrolysis process. The available muffle furnace allowed only for continuous heating until the final temperature of 700°C was reached. The lack of a gradual temperature increase likely contributed to excessive biomass carbonization, resulting in a substantial amount of ash.

Figure 1. Flowchart of the processes performed during the research.

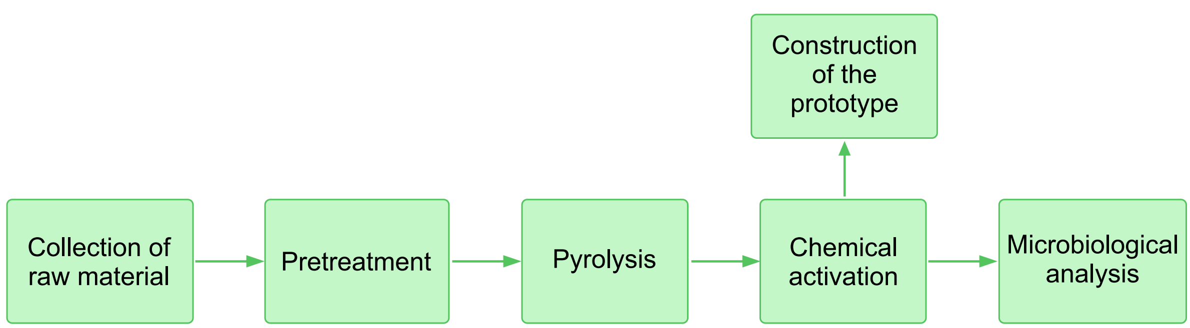

Table 1. Optical density of samples obtained with initial concentration of the contaminated solution of 10^8 cells of microorganisms.

Samples	Optical density (540 nm)			Average
	1° read	2° read	3° read	
Contaminated solution	0.116	0.122	0.111	0.116
Shell pretreated	0.089	0.091	0.090	0.090
Coal pyrolysed	0.058	0.058	0.058	0.058
shell activated	0.070	0.071	0.071	0.070
Coal pyrolysed and actived	0.076	0.075	0.074	0.075
Commercial carbon	0.058	0.056	0.056	0.056

Optical Density

Based on the results presented in Table 1, the following order of efficiency was observed regarding the removal of Bacillus subtilis: Commercial activated carbon > Pyrolyzed licuri charcoal > Activated bark > Chemically activated carbon > Pretreated bark.

This ranking suggests that the pyrolyzed licuri charcoal exhibited promising adsorptive performance, approaching that of commercial activated carbon. Notably, the chemically activated carbon, although processed to increase porosity, did not surpass the performance of the pyrolyzed sample. This may be due to reagent concentration, exposure time, or incomplete pH neutralization during washing. While less efficient, The pretreated and activated bark still demonstrated measurable microbial reduction, indicating the potential for further optimization.

Pyrolyzed and Chemically Activated Carbon

The filtration capacity of the pyrolyzed and chemically activated charcoal was 35.3%. Given the combination of thermal and chemical treatments, this result was lower than expected. One possible explanation for this underperformance is the presence of excess H^+ ions in the medium, which may have influenced the adsorption process. This finding indicates the need for pH correction and stabilization during or after the chemical activation process to optimize filtration efficiency.

Activated Bark

Like the chemically activated and pyrolyzed charcoal, the activated bark demonstrated a lower-than-expected optical density reduction. Although derived from the same biomass (licuri bark), this sample yielded a less satisfactory result. This suggests that proper pH correction could enhance its performance, bringing it closer to that of conventional activated carbon.

Pyrolyzed Charcoal

The pyrolyzed licuri bark exhibited excellent performance, closely approaching commercial activated carbon. The difference in optical density between the two samples was only 0.002. This result reinforces the potential of producing effective adsorbent charcoal from agricultural waste using relatively simple methods with fewer procedural steps. It highlights the viability of pyrolysis as a cost-effective and efficient alternative for water filtration.

Commercial Activated Carbon

As anticipated, the commercial activated carbon—commonly used as an adsorbent—achieved a high adsorption efficiency, removing approximately 51.7% of microorganisms from the contaminated water sample. This result validates the comparative benchmark for the study.

Pretreated Bark

The pretreated bark sample achieved a removal rate of 22.41%, demonstrating a modest yet measurable adsorption capacity. Despite minimal processing, the bark reduced the optical density compared to the unfiltered contaminated sample. This outcome suggests that even raw or lightly processed licuri bark has inherent filtering potential.

Conclusion

This study demonstrates a significant advancement in the environmental field by developing an activated carbon derived from licuri bark—a renewable and widely available agricultural residue. The research not only contributes to sustainability efforts but also encourages the adoption of more environmentally conscious practices.

The comparative analysis of two industrially applicable methods—pyrolysis and chemical activation—revealed that both can yield satisfactory results. Notably, the pyrolyzed licuri bark performed most closely to conventional activated carbon in microorganism removal, confirming the hypothesis that effective adsorbent carbon can be produced from this biomass. In addition to its scientific relevance, the project is of socioeconomic importance due to its low cost of production and its potential to benefit regions with limited access to clean water. Future studies will explore the use of this biochar in soil bioremediation, leveraging its strong adsorptive properties for broader environmental applications.

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The Effect of Acid Addition on Certain Properties of Polyamide 66 Polimeric Membranes

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In this study, four polymeric solutions were prepared to contain 10% of different additives—benzoic, adipic, tartaric, and citric acids—relative to the amount of polyamide 66 (PA66), with the total composition comprising 20% PA66 and 80% hydrochloric acid (HCl). The objective was to analyze these additives' influence on the resulting membranes' microstructure. The polymeric solutions were evaluated for viscosity, and the membranes produced with each additive were characterized in terms of water absorption capacity, porosity, water flux, maximum pore radius, and water vapor permeation. Incorporating acids with varying molecular weights (MW) into the PA66 solutions resulted in a progressive increase in viscosity, corresponding to the increase in molecular weight of the respective additive.

Keywords: Membranes. Polyamide 66. Additives. Microfiltration.

A synthetic membrane is a structure that wholly or partially restricts the transport of one or more chemical species in a mixture [1]. The classification of a membrane as porous or dense is determined by its surface characteristics, which develop upon contact with the solution to be separated. Various materials can be employed in membrane fabrication, directly influencing key properties such as permeability, selectivity, mechanical strength, thermal stability, and chemical resistance. The chemical nature of the membrane material plays a central role in defining the interaction between the polymer and the penetrant species, which is essential in determining separation efficiency and optimal operating conditions [2].

Polyamides, such as PA66, exhibit hygroscopic behavior due to hydrogen bonding between the carbonyl groups of one polymer chain and the amide hydrogen of another. Water molecules can penetrate between the chains, expanding the matrix and integrating into these hydrogen bonds.

The selection of the most appropriate membrane filtration method must consider boundary conditions and the membrane's performance relative to the specific water composition to be treated [3].

Currently, membranes are widely applied in solid-liquid separations and removal of dissolved contaminants. This work aims to investigate the effects of different acidic additives on the structural and functional properties of polyamide 66 (PA66) membranes.

Materials and Methods

Prior to membrane preparation, synthetic PA66 fibers and the selected additives—$C_7H_6O_2$ (benzoic acid), $C_6H_{10}O_4$ (adipic acid), $C_4H_6O_6$ (tartaric acid), and $C_6H_8O_7$ (citric acid)—were dried. These components were then dissolved in hydrochloric acid (HCl) to formulate the solutions. Each of the four solutions contained 10% of the additive relative to the total solids, which comprised 20% of the mixture, with the remaining 80% being solvent (HCl). The additives' molecular weights were accounted for in the formulations: PA66/$C_7H_6O_2$, PA66/$C_6H_{10}O_4$, PA66/$C_4H_6O_6$, and PA66/$C_6H_8O_7$, as summarized in Table 1. These concentrations and ratios were based on previous literature standards for similar membrane systems.

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The prepared polymeric solutions were processed using immersion-precipitation, which involved casting the solution into a non-solvent bath. Each membrane remained immersed until complete precipitation occurred. Following precipitation, the membranes were removed from the bath, rinsed with water, and then submerged in a mixture of 10% hexane and 90% water. Subsequently, the membranes were dried under controlled conditions, with temperature and ambient relative humidity specified. Membranes intended for permeation flux testing were kept submerged in the water-hexane mixture until the test was conducted. Conversely, membranes designated for other characterizations were dried at room temperature (25 ± 2 °C), with relative humidity recorded during drying. This storage protocol aimed to prevent pore collapse due to capillary forces, considering the high surface tension of water.

The polymeric solutions were analyzed for viscosity, and the membranes produced with acidic additives were characterized in terms of viscosity, bubble point, water absorption capacity, porosity, water flux, average pore radius, and water vapor permeation.

Results and Discussion

Viscosity is directly related to the energy required for a fluid to flow and is influenced by the cohesive forces between the liquid's molecules [4]. Figure 1 presents the viscosity measurements of the polymeric solutions containing different acidic additives: PA66/$C_7H_6O_2$, PA66/$C_6H_{10}O_4$, PA66/$C_4H_6O_6$, and PA66/$C_6H_8O_7$. The results revealed that the solution containing benzoic acid exhibited a viscosity of 2841 mPa·s, followed by the adipic acid solution with 2930 mPa·s, tartaric acid with 3000 mPa·s, and citric acid with 3154 mPa·s. These values indicate a gradual increase in viscosity corresponding to the increasing molecular weight of the acids incorporated.

Viscosity during membrane formation increases with the polymer concentration in the polymer-rich phase [1]. As shown in Figure 1, the viscosity of the solutions followed a trend corresponding to the molar mass of the additives. Higher molar mass additives led to higher viscosities—for instance, citric acid ($C_6H_8O_7$), which has the highest molar mass among the four acids studied, resulted in the highest viscosity. Conversely, benzoic acid ($C_7H_6O_2$), the additive with the lowest molar mass, exhibited the lowest viscosity.

Figure 2 presents the porosity results for the membranes: PA66/Benzoic Acid ($C_7H_6O_2$) at 60.8%, PA66/Adipic Acid ($C_6H_{10}O_4$) at 50.5%, PA66/Tartaric Acid ($C_4H_6O_6$) at 45.2%, and PA66/Citric Acid ($C_6H_8O_7$) at 40.4%. These results indicate that porosity varied depending on the additive used due to their distinct chemical structures and interactions with the polymer solution.

During membrane formation, the polymer-poor phase solidifies into pores, while the polymer-rich phase forms the dense matrix of the membrane. An increase in polymer concentration typically reduces the formation of micropores—defined as

Table 1. Composition of PA66 membranes with their additives.

Membranes	HCI (g)	PA66 (g)	Additives (g)	MW ($g.mol^{-1}$)
PA66/ Benzoic Acid ($C_7H_6O_2$)	80.0	20.0	1.0	122.12
PA66/ Adipic Acid ($C_6H_{10}O_4$)	80.0	20.0	1.0	146.14
PA66/Tartaric Acid ($C_4H_6O_6$)	80.0	20.0	1.0	150.10
PA66/Citric Acid ($C_6H_8O_7$)	80.0	20.0	1.0	192.12

Figure 1. Viscosity of the solutions of PA66/$C_7H_6O_2$, PA66/$C_6H_{10}O_4$, PA66/$C_4H_6O_6$, and PA66/$C_6H_8O_7$ membranes.

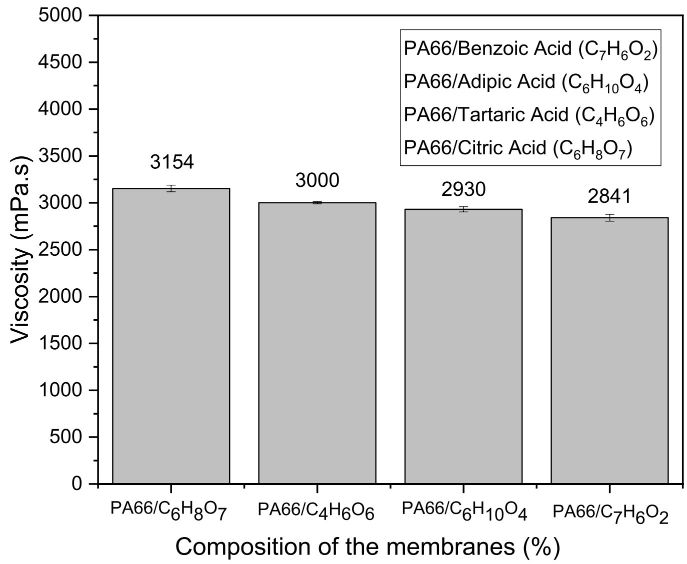
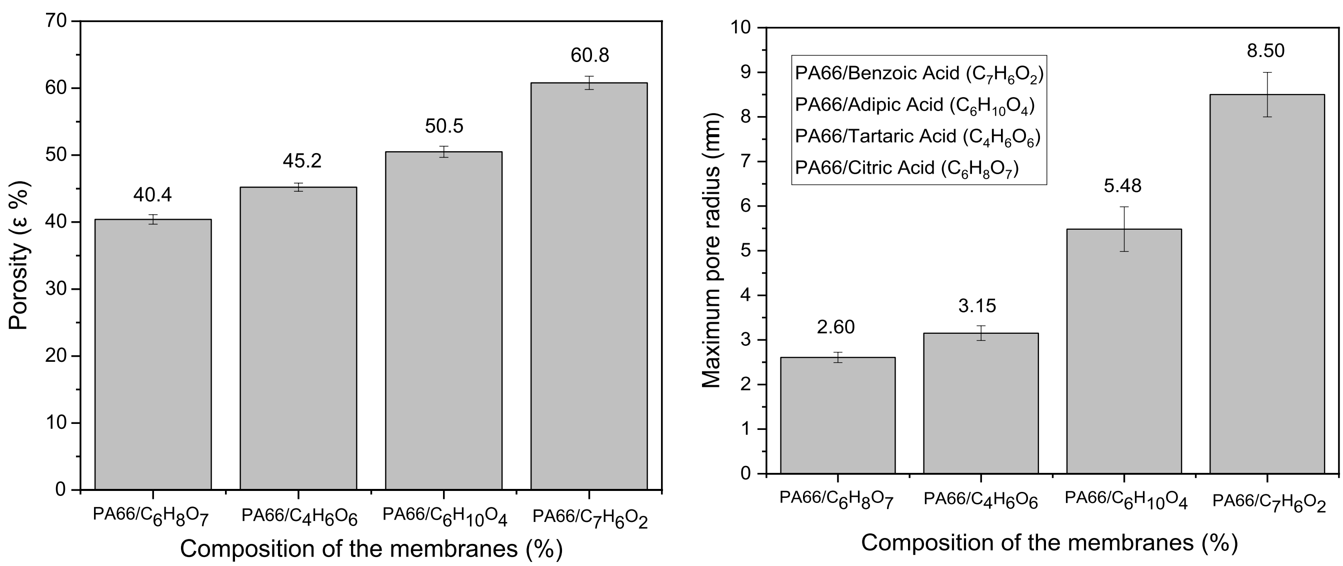


Figure 2. Porosity and Maximum pore radius of the membranes of PA66/C7H_6O_2, PA66/$C_6H_{10}O_4$, PA66/$C_4H_6O_6$, and PA66/$C_6H_8O_7$.



the smallest pore structures—resulting in narrower porous channels. This influences the porosity and the average pore size, often reducing pore diameter while increasing structural integrity [5].

The influence of viscosity on membrane porosity is evident, as higher viscosity solutions tend to form membranes with lower porosity, while lower viscosity solutions promote excellent porosity. Accordingly, the membrane prepared with citric acid—exhibiting the highest viscosity—demonstrated the lowest porosity, whereas the benzoic acid-based membrane, with the lowest viscosity, exhibited the highest porosity.

Porosity directly impacts pore size, as illustrated in Figure 2. The maximum pore radii for the PA66/Benzoic Acid, PA66/Tartaric Acid, PA66/

Adipic Acid, and PA66/Citric Acid membranes were approximately 8.50%, 5.48%, 3.15%, and 2.60%, respectively. The maximum pore radius was determined using the bubble point method, which involves measuring the pressure needed for gas (typically air or nitrogen) to pass through a membrane saturated with liquid [6].

Figure 2 clearly shows that the PA66/Citric Acid ($C_6H_8O_7$) membrane, which had the lowest porosity, also exhibited the smallest maximum pore radius. In contrast, the PA66/Benzoic Acid ($C_7H_6O_2$) membrane presented the largest maximum pore radius, consistent with its lower viscosity and higher porosity. Accurate pore size and distribution knowledge are essential for evaluating and characterizing microfiltration membranes. Smaller pore diameters require higher pressure for water permeation, which enhances filtration performance by increasing selectivity and flow rate [7–8]. Membranes may exhibit microporous, macroporous, or nanoporous structures, with water permeating under applied pressure.

Membrane characterization also includes assessing water absorption capacity, which measures the amount of water absorbed when membranes are immersed in distilled water at room temperature over various time intervals, as well as the total mass loss after immersion. As shown in Figure 3, water absorption capacities for the PA66/Citric Acid, PA66/Tartaric Acid, PA66/Adipic Acid, and PA66/Benzoic Acid membranes were 65.8%, 70.8%, 74.6%, and 81.2%, respectively.

We observed that the PA66/Citric Acid ($C_6H_8O_7$) membrane exhibited the lowest water absorption capacity, approximately 65.8%, compared to the other membranes. In contrast, the PA66/Benzoic Acid ($C_7H_6O_2$) membrane demonstrated the highest absorption rate, at 81.2%. One of the primary factors contributing to increased water absorption is the porous structure of the films, as the presence of pores facilitates the penetration and subsequent retention of water within the polymer matrix [9].

According to the data presented in Figure 4, the water flux under a pressure of 0.5 bar varied over 60 minutes as follows: PA66/Benzoic Acid ($C_7H_6O_2$) ranged from 260 to 85 $L·m^{-2}·h^{-1}$, PA66/Adipic Acid ($C_6H_{10}O_4$) from 90 to 70 $L·m^{-2}·h^{-1}$, PA66/Tartaric Acid ($C_4H_6O_6$) from 75 to 55 $L·m^{-2}·h^{-1}$, and PA66/Citric Acid ($C_6H_8O_7$) from 45 to 40 $L·m^{-2}·h^{-1}$.

The water flux behavior across the four membranes under different pressures revealed notable variations. Due to its porous structure,

Figure 3. Water absorption of the membranes of PA66/$C_7H_6O_2$, PA66/$C_6H_{10}O_4$, PA66/$C_4H_6O_6$, and PA66/$C_6H_8O_7$.

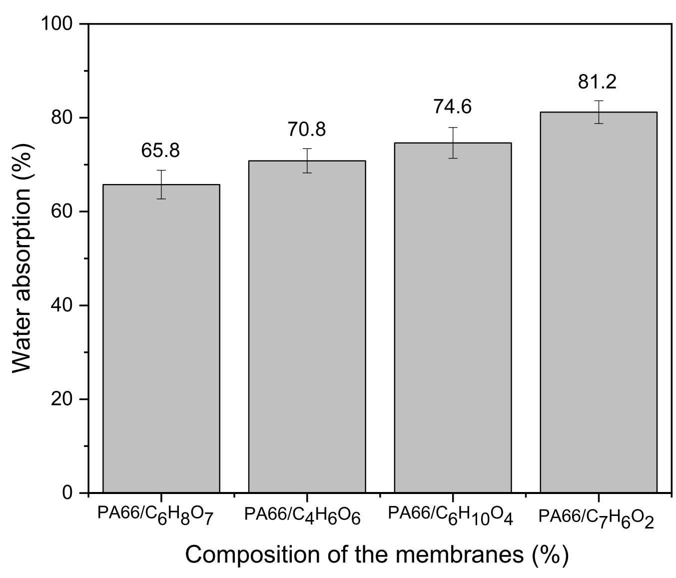
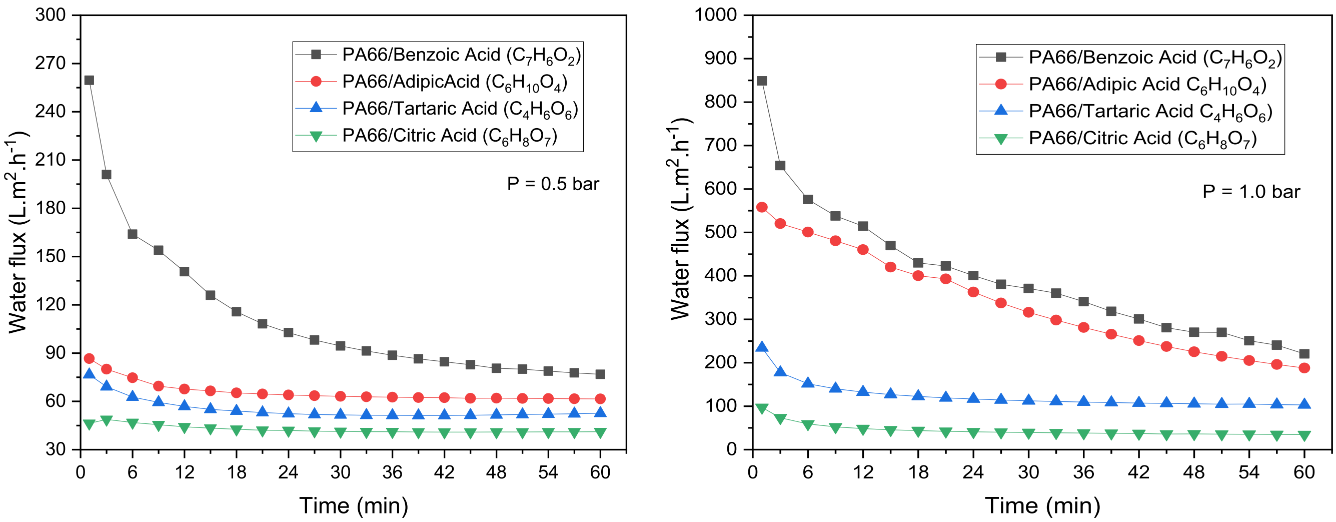


Figure 4. Water flux of the membranes of PA66/$C_7H_6O_2$, PA66/$C_6H_{10}O_4$, PA66/$C_4H_6O_6$, and PA66/$C_6H_8O_7$ at a pressure of 0.5 and 1.0 bar.



PA66 tends to swell upon prolonged immersion in water, which can significantly hinder water passage by narrowing or obstructing pore channels. Consequently, membranes with smaller initial pore sizes exhibit further pore constriction during swelling, drastically reducing permeated flow, although not eliminating it [11].

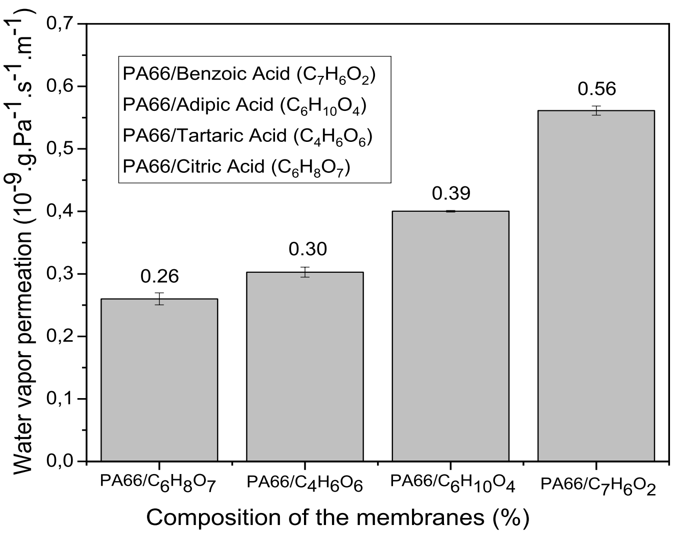
Since additives influence membrane porosity and maximum pore radius, the reduction in flow observed is consistent with structural modifications. The PA66/Benzoic Acid membrane demonstrated higher water flux, though with lower stability at pressures of 0.5 and 1 bar. Conversely, the PA66/Citric Acid membrane exhibited the lowest water flux but showed enhanced flow stability compared to the other membranes. As pressure increases, greater resistance to flow is observed due to the development of a polarization layer and gel layer on the membrane surface, which leads to increased fouling and partial clogging of surface pores [12]. Nonetheless, higher pressures can result in a proportional increase in permeated flow depending on membrane characteristics.

Determining water vapor permeation is necessary to assess the amount of water vapor transferred through the membrane. According to the information in Figure 5, it was observed that the water vapor permeation of the membranes of PA66/Citric Acid, PA66/Tartaric Acid, PA66/Adipic Acid, and PA66/Benzoic Acid were 0.26 x 10^{-9} g.Pa^{-1}.s^{-1}.m^{-1}, 0.30 x 10^{-9} g.Pa^{-1}.s^{-1}.m^{-1}, 0.39 x10^{-9} g.Pa^{-1}.s^{-1}.m^{-1}, and 0.56 x 10^{-9} g.Pa^{-1}.s^{-1}.m^{-1}, respectively.

The PA66/Citric Acid membrane presented fewer but larger pores than the other membranes, increasing water vapor permeation. In contrast, the PA66/Benzoic Acid membrane was primarily composed of smaller pores, which did not allow for effective permeation at a pressure of 1.0 bar. The introduction of acidic additives led to variations in water vapor permeation values. Membranes incorporating lower molecular weight (MW) additives exhibited higher water vapor permeation, whereas those with higher MW additives showed reduced permeability. These variations may be attributed to the incorporation of plasticizing agents, known for their strongly hydrophilic character, which enhance the mobility of water vapor through the membrane matrix [13].

Moreover, increasing the percentage of titanium dioxide (TiO_2) in the polymeric matrix led to a progressive enhancement in water vapor permeability. Membranes containing 1%, 3%, and 5% TiO_2 exhibited permeability values of 0.18 × 10^{-9}, 0.21 × 10^{-9}, and 0.23 × 10^{-9} g·Pa^{-1}·s^{-1}·m^{-1}, respectively. This increase is likely due to the hydrophilic nature of TiO_2 and its physical

Figure 5. Water vapor permeation (WVP) of the membranes of PA66/$C_7H_6O_2$, PA66/$C_6H_{10}O_4$, PA66/$C_4H_6O_6$, and PA66/$C_6H_8O_7$.



interaction with the polymer chains, acting as a porogenic agent and facilitating vapor transport through the membrane [14]. Incorporating hydrophilic additives into the polymeric solution generally enhances water vapor permeation compared to membranes prepared without such additives.

Conclusion

Flat membranes were successfully fabricated from industrial polyamide 66 (PA66) fiber waste with acidic additives using the immersion-precipitation method via the phase inversion technique. The results demonstrated that incorporating additives with different molecular weights into the PA66 solutions led to a progressive increase in viscosity, following the order of benzoic acid < adipic acid < tartaric acid < citric acid. Among the membranes evaluated, the PA66/Benzoic Acid membrane exhibited superior performance, showing the highest values for water absorption capacity, porosity, water flux, maximum pore radius, and water vapor permeation. These findings indicate that this membrane's microstructural properties are particularly favorable for microfiltration applications, especially in treating industrial effluents.

Acknowledgments

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Aluminum Dross Recycling by Melting: Effect of Particle Size and Flux Salt Quantity on Recorvered Aluminum Yield

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In recent years, aluminum recycling has significantly increased, particularly in Brazil, where the recycling rate of aluminum cans exceeds 95%. Aluminum dross is generated as a byproduct during the melting and recycling processes. The composition and morphology of this dross vary according to its metallic aluminum content. This study analyzed the recovery of aluminum from secondary dross, focusing on particle size and the amount of flux salt used. The results showed that particles larger than 7.5 mm yielded an aluminum recovery rate of 73.99% with 15% salt. The melting of larger particles improved aluminum recovery, suggesting greater process efficiency when targeting particles above 3.0 mm.
Keywords: Aluminum Dross. Recycling. Melting.

Aluminum is widely used due to its advantageous properties, such as low density and high corrosion resistance. Its production can be either primary, using bauxite as the raw material, or secondary, based on recycling scrap. Primary production involves bauxite extraction and processing and is highly energy-intensive, generating dross that can cause environmental harm. In contrast, secondary production uses aluminum scrap and consumes significantly less energy [1,2]. As a result, secondary aluminum production has gained prominence due to its economic benefits and alignment with sustainable development goals [3].

However, it is estimated that approximately 8–15% of the total mass of raw material used in the melting process is converted into solid waste considered environmentally hazardous. A significant portion of this waste is disposed of in landfills without proper treatment, contributing to severe environmental impacts [2].

Aluminum recycling has grown substantially, increasing its share in global aluminum production. Brazil has emerged as a global leader in secondary production, with a recycling rate for aluminum cans exceeding 95%. As production increases, hazardous waste generation is also expected to rise [4].

According to Mahinroosta and Allahverdi (2018) [5], the main wastes generated in the aluminum industry include red mud, produced during bauxite beneficiation; primary dross, generated during the electrolysis of alumina; secondary dross, produced during scrap melting; skimming, produced during the remelting of aluminum ingots without coatings and salts; and salt dross, generated during the melting of secondary dross using large quantities of salts for metallic aluminum recovery.

Secondary Aluminum Dross and Treatment Techniques

Secondary aluminum dross is an unavoidable byproduct of aluminum melting and recycling and is formed through multiple sequential processes. Oxidation occurs at the molten bath surface, where oxide particles decompose, sink, or float due to the bath's agitation. These particles coalesce, forming voids later filled with metallic aluminum. As these oxidized particles are removed from the bath surface, dross forms. Contact of hot dross with the atmosphere triggers chemical reactions that produce hazardous waste, including reactive compounds such as aluminum nitride, aluminum carbide, and leachable salts [5].

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Treatment of secondary dross can be performed using pyrometallurgical or hydrometallurgical methods, depending on the aluminum content. Dross with high metallic aluminum content is typically processed pyrometallurgically, while low-content dross is treated hydrometallurgically [1]. Salt fluxes are commonly used to aid the recovery of aluminum trapped in the dross; however, their use generates salt dross waste, which must be appropriately managed to prevent environmental contamination. Improper disposal can lead to soil and groundwater pollution and the emission of toxic gases such as ammonia and methane caused by the reactions of aluminum nitride and aluminum carbide with moisture [3].

Conventional methods for extracting metallic content from dross involve using salt flux and melting in reverberatory furnaces. Emerging technologies include plasma arc rotary furnaces [6] and rotary furnaces with salt flux. Plasma arc furnaces eliminate the need for flux salts, thus reducing waste generation. Rotary furnaces using salt flux can use up to 50% of the dross weight in flux to enhance aluminum recovery efficiency [7]. The rotational dynamics of these furnaces improve the interaction between the flux and oxides in the dross, promoting aluminum droplet coalescence.

Another critical factor influencing recovery efficiency is the viscosity of the dross, which increases with higher non-metallic content, complicating the separation of high-purity aluminum. Hazar and colleagues (2005) recommend melting high-aluminum-content dross, particularly with particle sizes above 125 µm, at temperatures between 800 and 850°C to maximize recovery efficiency. In non-rotary furnaces, increased melting temperatures lower the molten metal's viscosity, enhancing droplet coalescence.

The literature indicates that dross composition and morphology vary with metallic aluminum content. Dross with high aluminum content exhibits a compact, granular morphology, while dross with lower content—composed mainly of salts and oxides—results in finer particles. Particle size significantly affects process efficiency, with larger particles typically containing more metallic aluminum [2,7,8]. This study aimed to evaluate the aluminum recovery yield from secondary dross generated during the melting process. It also examined the effects of particle size and the quantity of flux salt used on the recovery rate.

Materials and Methods

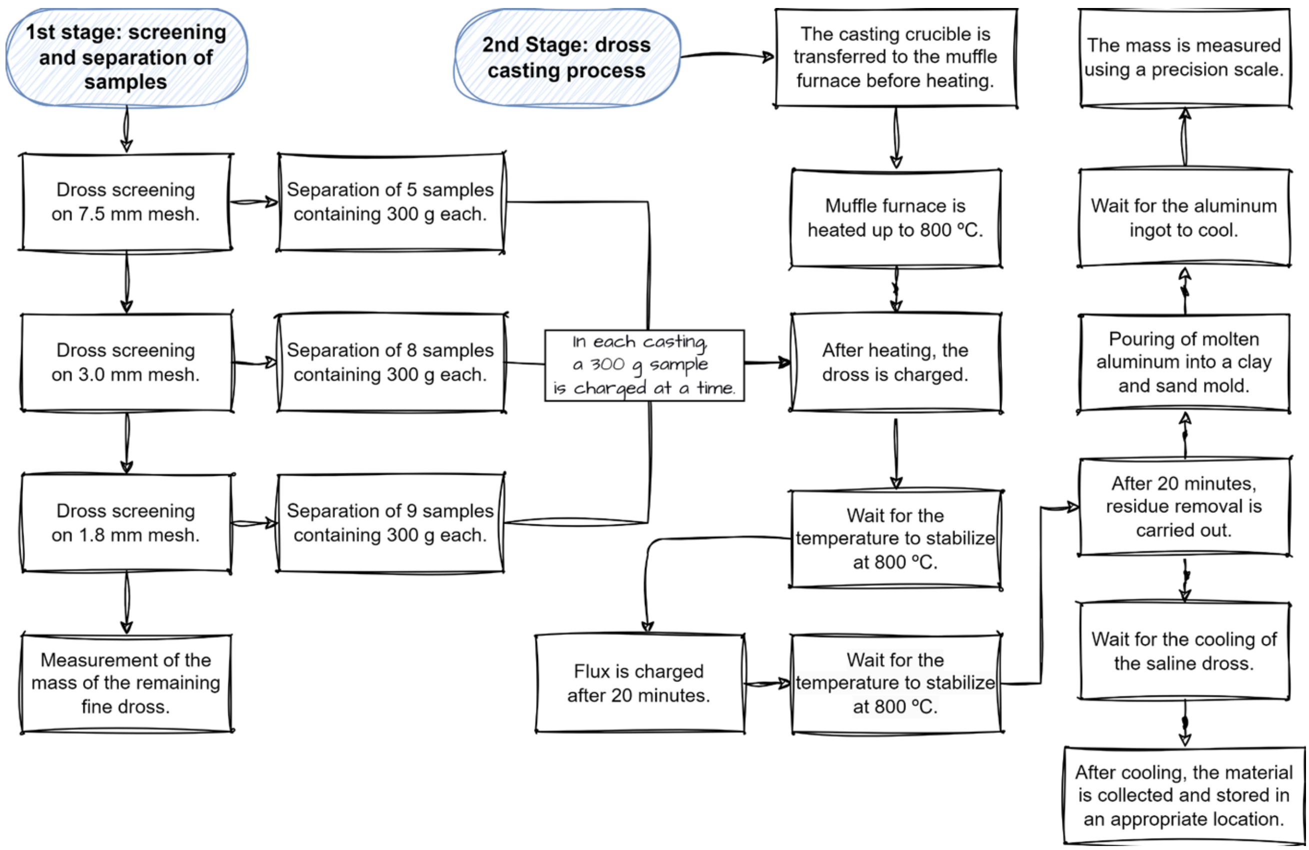
The materials used in this study included secondary aluminum dross supplied by RSA Fundições de Alumínio LTDA, located in Feira de Santana, Bahia, Brazil. Approximately 10 kg of dross was provided and used in its original state without pretreatment. The flux employed was ESCORIMIL AL LP/20, supplied by COMIL COVER SAND Produtos. This flux was selected for its cleaning, deoxidizing, and refining grain structure properties during melting.

A cordierite crucible manufactured by Up Brasil was used in the melting operations. The crucible had a capacity of 600 mL and could withstand temperatures up to 2000°C. Its external dimensions were 128 mm in depth, 130 mm in height, and 115 mm in width. An EVEN precision balance, model BL-4200AS-BI, with a maximum capacity of 4200 g, was used to record the mass of the recovered aluminum ingots.

The melting processes were carried out in a muffle furnace (model LF7013) manufactured by Fornos Jung LTDA. This equipment has a power rating of 6.8 kW and a maximum operating temperature of 1300°C. It is installed at the Advanced Manufacturing Laboratory (LAMAv-CETENS), part of the Center for Science and Technology in Energy and Sustainability (CETENS), Federal University of Recôncavo da Bahia (UFRB).

Figure 1 presents a flowchart of the experimental procedure, which was divided into two stages. The first stage involved screening the aluminum dross by particle size, followed by dividing the screened

Figure 1. Experimental procedure.



material into 300 g samples. A total of 22 samples were prepared: 9 samples with particle sizes between 1.8 mm and 3.0 mm, 8 samples between 3.0 mm and 7.5 mm, and 5 samples larger than 7.5 mm.

The fraction with particles smaller than 1.8 mm was excluded from the melting stage and weighed separately using the precision balance. The mass of this excluded fraction was recorded as 3,341.33 g to quantify the proportion of material not used in the experimental trials. The second stage involved melting the prepared samples, varying the particle size and percentage of added flux salt. All experiments were conducted at a fixed temperature of 800°C. The data collected from these experiments are presented in Table 1.

The aluminum recovery yield (ρ) from the melting process was calculated using Equation (1), where m_{Al} represents the mass of recovered aluminum and m is the initial mass of the dross sample:

Equation (1):

$$\rho = \frac{m_{Al}}{m} \times 100\% \tag{1}$$

The average recovery yield (η) for each condition was determined using Equation (2), where n is the number of replicates under the same experimental parameters:

Equation (2):

$$\eta = \frac{\sum \rho}{n} \tag{2}$$

Results and Discussion

As described in the experimental procedure, the first stage involved screening the dross by particle size. In Figure 2.C, particles larger than 7.5 mm contain large aluminum sheets resembling skimmings formed by oxidation of the metallic surface. These skimmings are typically removed

Table 1. Data obtained from the experiments.

ID	Replicates	Particle size (mm)	m(g)	Q_{flux} (wt%)
S1.10	3	1,8 < d < 3,0	300	10
S1.20	3	1,8 < d < 3,0	300	20
S1.30	3	1,8 < d < 3,0	300	30
S2.05	3	3,0 < d < 7,5	300	5
S2.15	3	3,0 < d < 7,5	300	15
S2.30	2	3,0 < d < 7,5	300	30
S3.05	2	d > 7,5	300	5
S3.15	2	d > 7,5	300	15
S3.30	1	d > 7,5	300	30

ID = experimental test identifier, coded based on particle size range and flux salt concentration; replicates = independent repetitions performed under each experimental condition; particle size (mm) = the range of aluminum dross particle diameters in millimeters (m (g) denotes the total mass of the sample subjected to the melting process, expressed in grams); Q_{flux} (wt%) = the percentage by weight of fluxing salt added during the melting process.

during the extraction of dross from molten metal, resulting in metal loss due to partial removal of the metallic phase and the dross [5].

In Figures 2.A and 2.B, the presence of non-metallic compounds dispersed among metallic aluminum grains is evident. These darker, non-metallic regions are attributed to impurities in the recycled scrap, such as coatings and aluminum pot handles.

Table 2 presents the experimental data. The results indicate a clear dependence of aluminum yield (η) on particle size and the quantity of flux salts used. For the tiniest particles (1.8 < 3.0 mm), the aluminum yield ranged from 41.39% to 47.12% as the flux salt content increased from 10% to 30%. The associated standard deviation (σ) was relatively low, indicating moderate variability among replicates.

For intermediate-sized particles (3.0 < 7.5 mm), aluminum yield increased substantially, ranging from 58.24% to 72.42%, as flux salt content increased from 5% to 30%. The standard deviation was higher for lower salt percentages. However, it decreased as the salt content increased, suggesting that greater amounts of flux improve the process's recovery and consistency. The maximum aluminum yield achieved for particles larger than 7.5 mm was 73.99% with 15% flux salt. This group also exhibited the lowest standard deviation, especially at the 15% flux level, indicating highly consistent results. Due to the limited number of experiments with 30% salts in this particle size range, no definitive conclusion could be drawn for that specific condition. Figure 3 illustrates the yield behavior as a function of particle size and flux salt content (Q_{Flux}).

The results show that the quantity of flux salt considerably impacts yield across all particle sizes. At 5% flux salt, aluminum yield is comparatively low but increases notably with higher flux quantities. An intermediate flux concentration (15%) significantly boosts yield, especially for larger particles, while reducing variability.

At 30% flux, yields continue to increase but show signs of saturation, implying that further increases in flux salt content do not proportionally enhance recovery. Excess salt may diminish returns, increasing operational costs without additional benefits.

Figure 2. Aluminum dross (A) particle size 1.8 - 3.0 mm; (B) particle size 3.0 - 7.5 mm; (C) particle size greater than 7.5 mm.

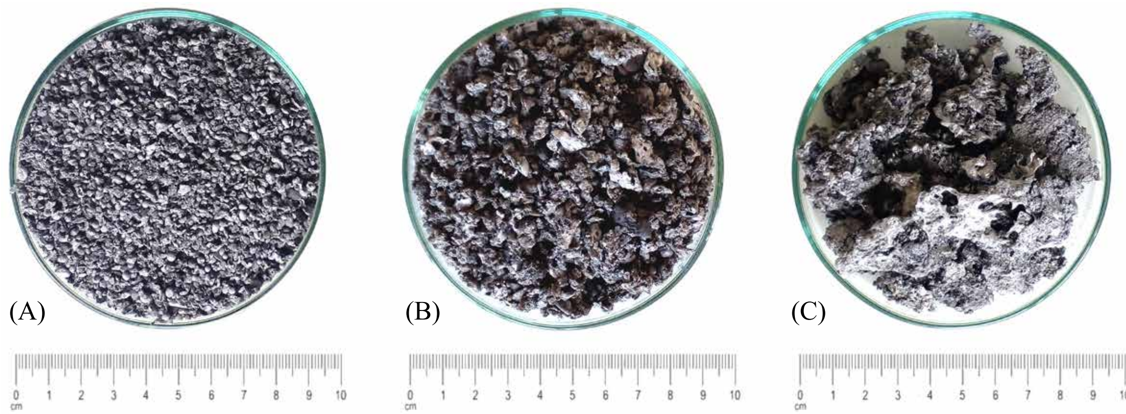


Table 2. Average yield (η) of aluminum recovered.

ID	$\bar{m}Al(g)$	$\eta\ (wt\%)$	σ
S1.10	125.90	41.39	2.66
S1.20	141.35	47.12	6.05
S1.30	133.64	43.37	5.35
S2.05	174.72	58.24	7.09
S2.15	191.82	63.94	4.63
S2.30	217.25	72.42	2.66
S3.05	192.67	64.22	2.20
S3.15	221.97	73.99	0.58
S3.30	216.98	72.33	-

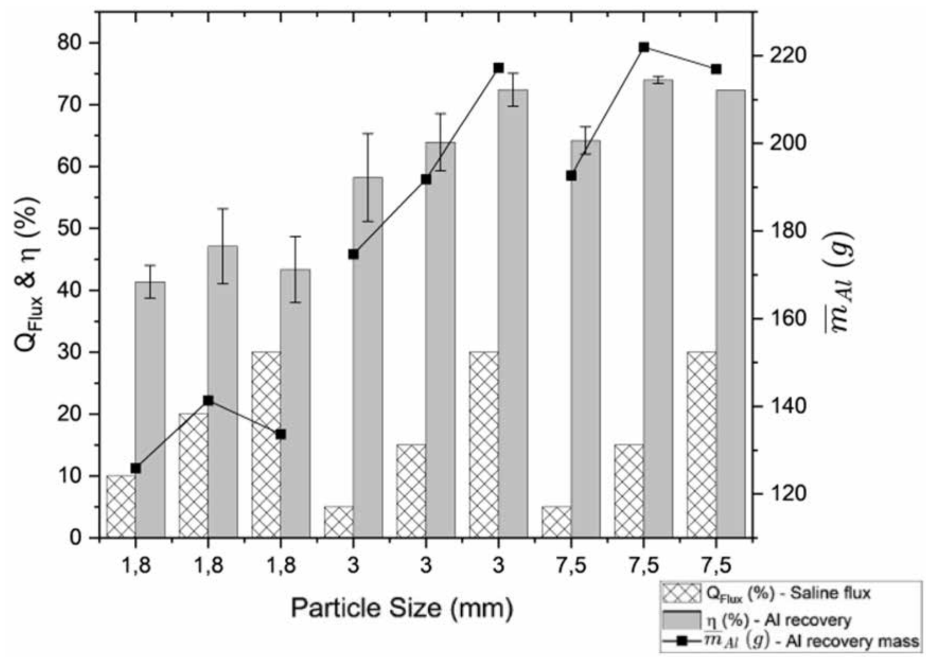
Overall, the data in Table 2 indicate that the highest recovery yields were associated with particles larger than 7.5 mm (average yield of 69.75%), followed by particles between 3.0 and 7.5 mm (average yield of 63.92%). The lowest yields were observed for the smallest particle group (1.8 < 3.0 mm), with an average yield of 44.54%.

Conclusion

This study evaluated the aluminum recovery yield from dross melting, focusing on varying flux salt concentrations and implementing particle size-based separation to optimize metal recovery. The results demonstrated that particle size and flux salt quantity significantly influence the yield of metallic aluminum. Particles larger than 7.5 mm achieved the highest yield, reaching 73.99% when treated with 15% flux salts. This high performance is attributed to the greater presence of metallic aluminum in these skimmings, which are primarily composed of metal and whose efficient recovery is crucial for minimizing losses.

The findings suggest maximizing aluminum yield is best achieved by targeting the recovery of particles larger than 3.0 mm. This approach

Figure 3. Aluminum recovery yield (η) as a function of dross particle size and flux salt content (Q_{Flux}).



results in more efficient extraction processes and enhances the overall recovery rate, contributing to more sustainable and cost-effective aluminum recycling operations.

Acknowledgments

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Cyber-Physical Systems for Predictive Maintenance Monitoring of Legacy CNC Machine Tools Toward Industry 4.0 Environment

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CNC machine tools are essential equipment in modern industry, and maintaining their operational condition is critical to ensuring production efficiency and product quality. Traditionally, maintenance strategies have relied on corrective and preventive actions. However, predictive maintenance is gaining importance with the advent of new technologies and the Industry 4.0 paradigm. Despite its advantages, the high costs associated with predictive maintenance still limit its widespread adoption. This study proposes a Cyber-Physical System (CPS) model for monitoring CNC machine tools. To this end, critical subsystems and related variables were identified, appropriate sensors were selected, and a hardware monitoring system was designed. Implementing the CPS will enable early fault detection, reducing downtime and maintenance costs.
Keywords: CNC Machine Tools. Predictive Maintenance. Monitoring. Cyber-Physical System.

Computer Numerical Control (CNC) machines are among the most critical equipment in the manufacturing industry. Their reliability, productivity, and robustness make them integral to industrial operations. A primary goal in modern manufacturing is to enhance productivity and quality by applying strategic maintenance practices—particularly for CNC machines—to improve production rates and product quality [1,2].

CNC machines are complex systems composed of electromechanical and hydraulic components, including mechanically movable parts and precision control systems. Issues such as wear, malfunction, and component failure may occur during manufacturing processes [3,4]. The absence of effective maintenance methodologies often exacerbates these issues. In many industrial settings, the prevailing maintenance approaches are either corrective or preventive, which can lead to unexpected downtimes, loss of productivity, and waste of resources [2,5].

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While appropriate maintenance strategies significantly enhance equipment reliability—and consequently, the entire manufacturing process—predictive maintenance remains challenging to implement, primarily due to its high cost and complexity [2].

The rise of Industry 4.0 and enabling technologies such as sensors, simulation, big data analytics, and artificial intelligence (AI) have begun to transform industrial practices [4,6,7]. Among the most promising applications of these technologies is the deployment of predictive maintenance strategies for CNC machines [2]. Predictive maintenance allows for continuous monitoring of machine components, enabling early fault detection and intervention before failures disrupt operations. This approach is superior to corrective and preventive maintenance as it minimizes idle time and reduces unnecessary interventions and associated costs [8].Despite these advantages, the high investment costs associated with predictive maintenance—such as those required for sensors and data analysis algorithms—have hindered its broader adoption in the manufacturing industry [8]. To make implementation more feasible, it is crucial to identify the most critical machine subsystems and their respective failure modes, focusing monitoring efforts where they are most impactful [2].

However, identifying and defining the variables to be monitored presents challenges, as it requires sensor integration and network connectivity—features not commonly present in legacy CNC machines [9]. These limitations hinder the application of predictive maintenance and make real-time monitoring difficult.

This study aims to identify and define the key variables for implementing predictive maintenance in CNC machines and propose a prototype Cyber-Physical System (CPS) for real-time data acquisition and monitoring.

This article is organized as follows: The current section introduces the context, problem statement, research objectives, and the relevance of the study. Section 2 details the structure of CNC machines, highlights critical components, and describes standard failure modes. Section 3 outlines the hardware development process, including the components used. Section 4 discusses the expected outcomes of the proposed monitoring system. Finally, Section 5 presents concluding remarks and outlines future steps.

CNC Machine Tools

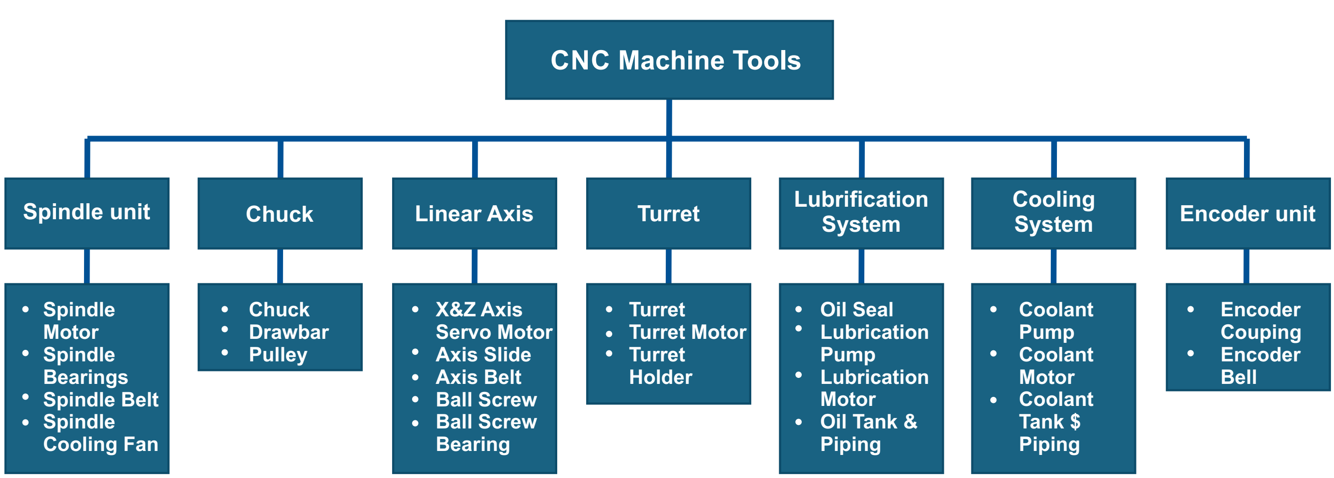
CNC machines are integrated electromechanical and hydraulic systems comprising various interdependent components [4]. While electronic and electrical subsystems may experience sensor failures, relay malfunctions, or blown fuses [2,10–13], these failures are generally less critical than mechanical subsystem failures. In most cases, electronic faults do not directly compromise product quality [8]. Therefore, the maintenance strategy for CNC machines can be optimized by focusing primarily on their mechanical subsystems, which are illustrated and analyzed in Figure 1.

Critical Components

Identifying critical subsystems and their associated failure modes is essential for selecting appropriate sensors for condition monitoring and implementing predictive maintenance strategies. According to Thoppil and colleagues [2], the existing literature provides only a superficial treatment of methods for analyzing the criticality of components in CNC lathes, particularly in prioritizing components for predictive maintenance. A literature review reveals that the monitoring of CNC machine subsystems and components can generally be classified into two categories: the machine tool and the machining process [14].

Within the machine tool category, the primary critical components that require monitoring include the spindle bearings, X- and Z-axis servo motors, ball screw bearings, the turret, the spindle, and the coolant system [2,15]. In the machining process category, monitoring typically focuses on the

Figure 1. CNC machine components.



Source: Thoppil and colleagues (2020) [2].

cutting tool, the machining table, and spindle wear [4,9,14–16].

Table 1 presents the components monitored in each group, their associated failure modes, and the measurable variables that can be used to detect and diagnose failures.

Based on the definition of the components to be monitored and the quantities to be measured, the sensors to be used for monitoring and their placement on the machine can be determined.

Materials and Methods

The methodology is based on identifying the most critical subsystems that can be applied with predictive maintenance to evaluate better solutions and propose a prototype of a CPS integrated with a CNC architecture for real-time data acquisition of the machine and its environment on the shop floor. The architecture model integration is viewed in Figure 2.

Initially, sensors will be installed in locations that do not interfere with the machine's operational workflow. The next step involves collecting data from these sensors and transmitting it to a Programmable Logic Controller (PLC) responsible for initial data processing. In the case of vibration data, a Fourier Transform will be applied to obtain the frequency spectrum and identify characteristic frequency peaks corresponding to specific failure modes. For deformation monitoring, the maximum deformation will be calculated using formulas derived from Mohr's Circle for strain analysis. Once the data is processed, the variables will be transmitted from the PLC to a computer database via industrial wireless communication or Ethernet cable. These values will then be compared with the components' reference values. This analysis process is critical for detecting anomalies and generating actionable insights for predictive maintenance. For example, the system may trigger an alert to notify the operator of abnormal operating conditions, thereby improving process safety and extending the machine's service life.

Hardware Components

Appropriate sensors were selected after identifying the critical subsystems and measurable variables, and a hardware configuration for data acquisition and processing was proposed. Table 2 lists the components suggested for building the system.

Hardware Components

PLC Controller

The XP 340 is a cost-effective programmable logic controller (PLC) featuring a compact design

Table 1. Critical components.

Group	Component	Failure mode	Variable
Machine tool	Spindle bearing	Bearing deformation	Deformation
	X and Z axis servo motor	Bearing wear	Vibration
	Ball screw bearing	Unsmooth operation	Vibration
	Turret	Indexing error	Vibration
	Chuck	Worn out	Vibration
	Cutting fluid	Leakage	Fluid level
Process	Tool	Tool wear	Vibration
	Spindle	Spindle wear	Vibration

Figure 2. Architecture for integration.

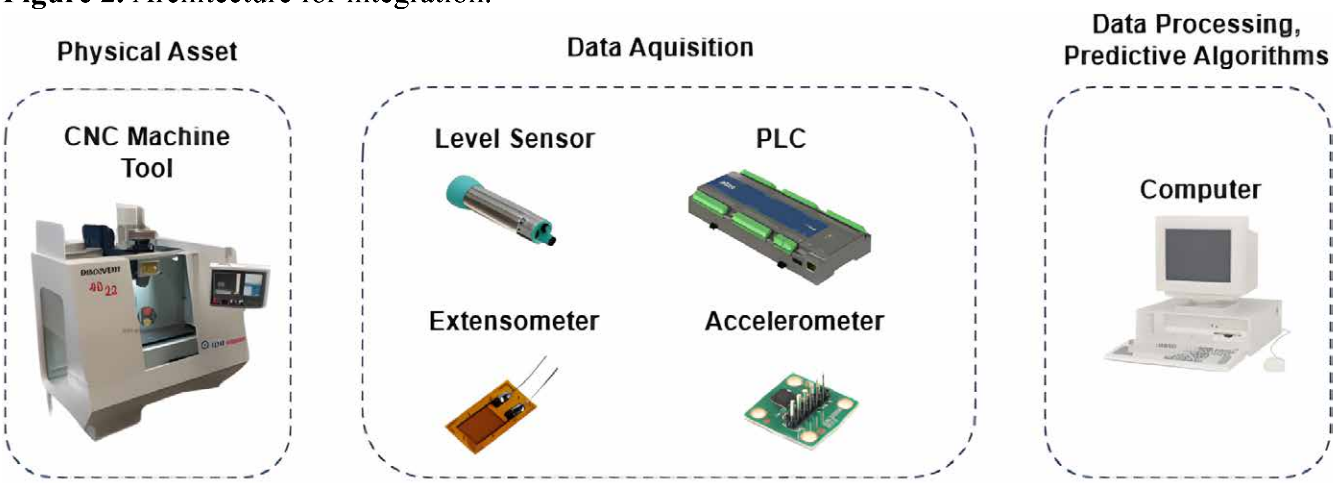


Table 2. Hardware components.

Component	Quantity	Description
Programmable logic controller	1	CLP Altus XP 340
Extensometer	1	CEA-06-250UW-350
Accelerometer	6	Analog Devices ADXL335
Level sensor	1	Pepperl+Fuchs UC4000-30GM-IUR2-V15
Ethernet cable	1	UTP or ScTP, category 5
Connector RJ-45	1	Armored female

and a 32-bit ARM processor. It includes 16 digital inputs, 16 transistor digital outputs, 5 analog voltage/current inputs, 2 three-wire analog inputs, 4 analog outputs, one Ethernet port, and one RS-485 serial port. The device supports a Webserver tool for creating supervisory screens without needing a SCADA system. Additionally, it is compatible with major industrial communication protocols, including MQTT, OPC UA, MODBUS, and PROFINET.

Strain Gauge Sensor

The CEA-06-250UW-350 strain gauge sensor measures mechanical deformation. It operates by varying its electrical resistance when subjected to force. This sensor features compact dimensions, a resistance of 350 ohms, and a tolerance of ±0.3%.

Accelerometer Sensor

Accelerometers are widely employed to measure acceleration or vibration. These devices typically rely on a mass-spring system, where the deformation of a piezoelectric material produces an electric signal proportional to the force applied. The selected Analog Devices ADXL335 operates with a supply voltage of 1.8 to 3.6 V and enables tri-axial (x, y, z) measurement.

Level Sensor

The Pepperl+Fuchs UC4000-30GM-IUR2-V15 ultrasonic level sensor determines fluid levels by calculating the time delay between emitted and received pulses. It offers a measurement range from

350 to 4000 mm, a resolution of 0.5 mm, and an accuracy of ±0.2% of full scale.

Results and Discussion

The proposed cyber-physical system was developed based on the principles outlined in Sections 1 and 2, which enabled the identification of critical subsystems and measurable variables relevant to CNC machine tool performance.

The appropriate sensors were selected based on this foundation, and a hardware prototype for data acquisition and processing was developed. Once implemented, the CPS will enable real-time monitoring of the CNC machine. The collected data will be instrumental in identifying existing faults or potential future failures through predictive algorithms. Monitoring subsystems related to the machine, such as the spindle, motor, and structural components, and tool condition monitoring will ensure greater machine availability and efficiency. Ultimately, this contributes to increased productivity, improved maintenance planning, and higher product quality.

Conclusion

Identifying critical CNC machine subsystems and their failure modes enables the selection of targeted sensors for real-time monitoring. This information significantly contributes to the effective implementation of predictive maintenance, helping to reduce related costs and operational disruptions. The data collected by these sensors can be processed to predict future failures, thereby reducing downtime, minimizing losses, and ensuring consistent product quality.

The proposed hardware will be validated by being deployed on a CNC machine at SENAI CIMATEC's Advanced Manufacturing Plant (PMA). Suitable communication protocols will be defined to integrate the machine, hardware, and management system. Subsequently, sensor-collected data will be processed by the PLC and transmitted to a centralized computer for health condition analysis of the machine components.

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Development of a System for Demonstration of Maintenance 4.0 Technologies in an Advanced Manufacturing Didatic Plant

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Industry 4.0 has introduced new maintenance management paradigms, demanding innovative training and implementation solutions. This article proposes a system architecture integrating sensors, IoT devices, data analysis, and condition-based maintenance techniques to serve as a demonstration and learning platform. The proposed methodology involved four steps, culminating in the system's prototyping. The system enables the visualization of how Maintenance 4.0 technologies impact performance, cost, and compliance indicators. The study concludes that the developed system effectively demonstrates these technologies, supporting the training of professionals in a controlled environment where the benefits of applying Maintenance 4.0 solutions can be observed.
Keywords: Industry 4.0. Maintenance 4.0. Predictive Maintenance. Maintenance Education.

In the era of Industry 4.0, the latest technological advancements are increasingly integrated into industrial systems [1]. According to Shaheen and Németh, maintenance management within industrial manufacturing is significantly shaped by technologies such as the Internet of Things (IoT), cloud computing, big data, artificial intelligence (AI), and cyber-physical systems. In this context, Miguel and colleagues (2022) emphasize that Maintenance 4.0 applies Industry 4.0 tools and resources to enhance the industrial maintenance process. On one hand, it leverages interconnectivity through connected sensors, programmable logic controllers (PLCs), and machines as data sources; on the other hand, it utilizes data processing capabilities to detect trends and support maintenance decision-making [2].

Cachada and colleagues (2018) argue that most current industrial maintenance strategies remain largely reactive or preventive, with predictive approaches limited to critical systems. This is despite the increasing volume of data generated on the shop floor and the availability of emerging information and communication technologies (ICTs), such as IoT, big data, advanced analytics, cloud computing, and augmented reality [3]. However, the maintenance paradigm is shifting. Maintenance is now recognized as a strategic activity and a key contributor to productivity in industrial systems.

Condition-based maintenance (CBM) has emerged as a crucial management strategy within this evolving landscape. CBM focuses on forecasting equipment degradation, operating under the principle that most failures follow a progressive path from normal operation to malfunction rather than occurring instantaneously [4].

Maintenance 4.0 utilizes advanced sensors and data analytics to monitor equipment health and predict failures, enabling proactive and well-planned interventions. To ensure that professionals and students fully understand and apply these concepts and technologies, providing systems that demonstrate the shift from traditional reactive and preventive strategies to data-driven, predictive approaches is essential. This paper presents a system developed and implemented at the SENAI CIMATEC Advanced Manufacturing Plant (AMP), featuring a communication and operational architecture designed to align with Industry 4.0 tools and methods.

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Figure 1 presents the method for developing the system.

Literature Review

The literature review identified three key studies illustrating systems development for demonstrating or experimenting with maintenance technologies aligned with Industry 4.0.

The first study [2] proposes a testbed designed to translate the Maintenance 4.0 paradigm into an educational context using the Project-Based Learning (PBL) approach. This testbed focuses on the maintenance of machines and robots, collecting data from a network of interconnected equipment to support condition monitoring and maintenance decision-making via machine learning. To ensure Industry 4.0 connectivity, the system employs industrial communication protocols (e.g., ProfiNet, ProfiBus, EtherCat) and conventional networking technologies (e.g., Ethernet, WiFi 802.11, Bluetooth). A supervisory control and data acquisition (SCADA) system is utilized for data visualization.

The second study [5] describes a testbed developed to demonstrate maintenance technologies using a FESTO didactic production system. It incorporates an Industrial Internet of Things (IIoT) platform that generates work orders, dispatches maintenance resources via an autonomous robot, and delivers step-by-step instructions for executing maintenance tasks. Built on a cyber-physical production system, the testbed features advanced communication protocols, including OPC-UA, Modbus, WebSockets, IIoT gateways, and application programming interfaces (APIs). Data visualization and analysis are managed through a cloud-based Computerized Maintenance Management System (CMMS) supported by AI-driven analytics.

The third study [6] presents an educational platform developed for remote training in Maintenance 4.0. It leverages the Open System Architecture for Condition-Based Maintenance (OSA-CBM) framework, developed by MIMOSA, to structure data flow. This modular platform comprises three main components: (1) Maintenance 4.0 and CBM; (2) Failure diagnostics and prognostics; and (3) Data-driven maintenance management. The system is designed for integration with external platforms such as CMMS and ERP via Layer 2 or 3 network connectivity (e.g., database or server layer). Additionally, a remote interface was developed to configure data acquisition systems.

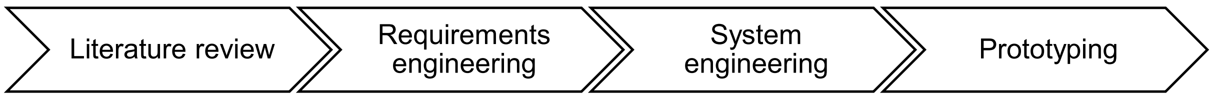
Requirements Engineering

System requirements define what a system should accomplish and how it operates [7]. According to Valente (2020), requirements are generally functional or non-functional. Functional requirements specify the system's expected services and functionalities, while non-functional requirements outline operational constraints and quality of service attributes.

Requirements were identified based on the literature to guide the development of the proposed system. These requirements informed both the functional capabilities and operational characteristics of the system. Mirka and colleagues (2020) emphasize that laboratory environments should adhere to industrial standards in architecture, database schema, and component design.

Accordingly, the system considers the requirements outlined in Institute of Asset Management [8], particularly those related to asset management training, awareness, and competence. At SENAI CIMATEC's Advanced Manufacturing Plant (AMP), maintenance procedures and

Figure 1. The method used for the system development.



competencies were structured according to standard processes.

The primary functional requirements identified include:

- Continuous monitoring of equipment through real-time data collection, a fundamental aspect of CBM;
- Insight generation based on the collected data;
- Support for planning and scheduling maintenance tasks using condition-monitoring techniques.

Maintenance actions may be triggered by either online data (enabled by machine learning) or on-site measurements using portable devices.

The non-functional requirements include:

- Data security, achieved through the use of encrypted communication protocols;
- System scalability, allowing support for a growing number of users and devices;
- Adaptability and flexibility, ensuring compatibility with various test configurations, usage scenarios, and IoT devices;
- Responsiveness, with near-instantaneous updates, even under high data loads.

System Engineering

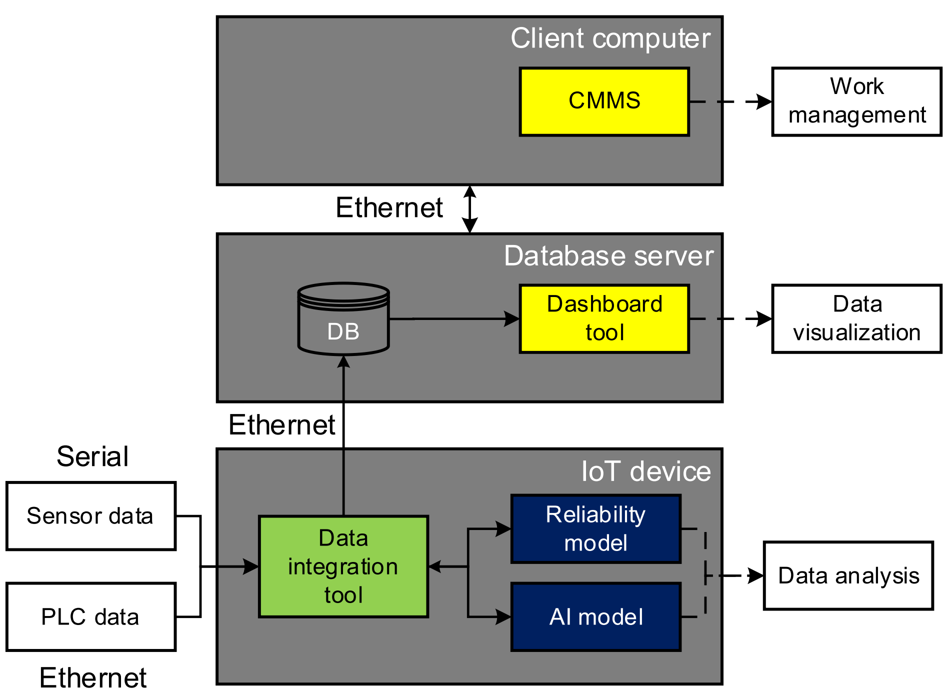
Wasson (2015) notes that the definition of systems engineering varies across disciplines. In this work, systems engineering refers to the interdisciplinary approach encompassing requirement interpretation, architectural design, and prototype development.

The two main focuses of this study—justifying the use of systems engineering—are the integration of Industry 4.0 ICTs (i.e., information technologies [IT] and operational technologies [OT]) and the delivery of maintenance operations such as planning, scheduling, and execution [9].

The system's communication architecture, illustrated in Figure 2, includes sensors, programmable logic controllers (PLCs), an IoT device, a database server, and a client computer. To determine the critical parameters for monitoring an induction motor's performance, a Failure Mode and Effects Analysis (FMEA) was conducted. This analysis played a key role in identifying the variables essential for assessing the motor's operational condition.

The Maintenance 4.0 operational system architecture, depicted in Figure 3, comprises two types

Figure 2. Communication architecture of the system.



of monitoring: online and offline. Online monitoring utilizes mathematical models and AI algorithms to remotely visualize alarms, alerts, anomaly detection, failure diagnostics, and prognostics. Offline monitoring involves periodic on-site analysis scheduled through the CMMS for predictive maintenance. This is achieved by identifying faults using the frequency spectrum of the induction motor and its temperature. The latter activity is facilitated by portable instruments and sensitive inspections following established procedures.

Prototyping

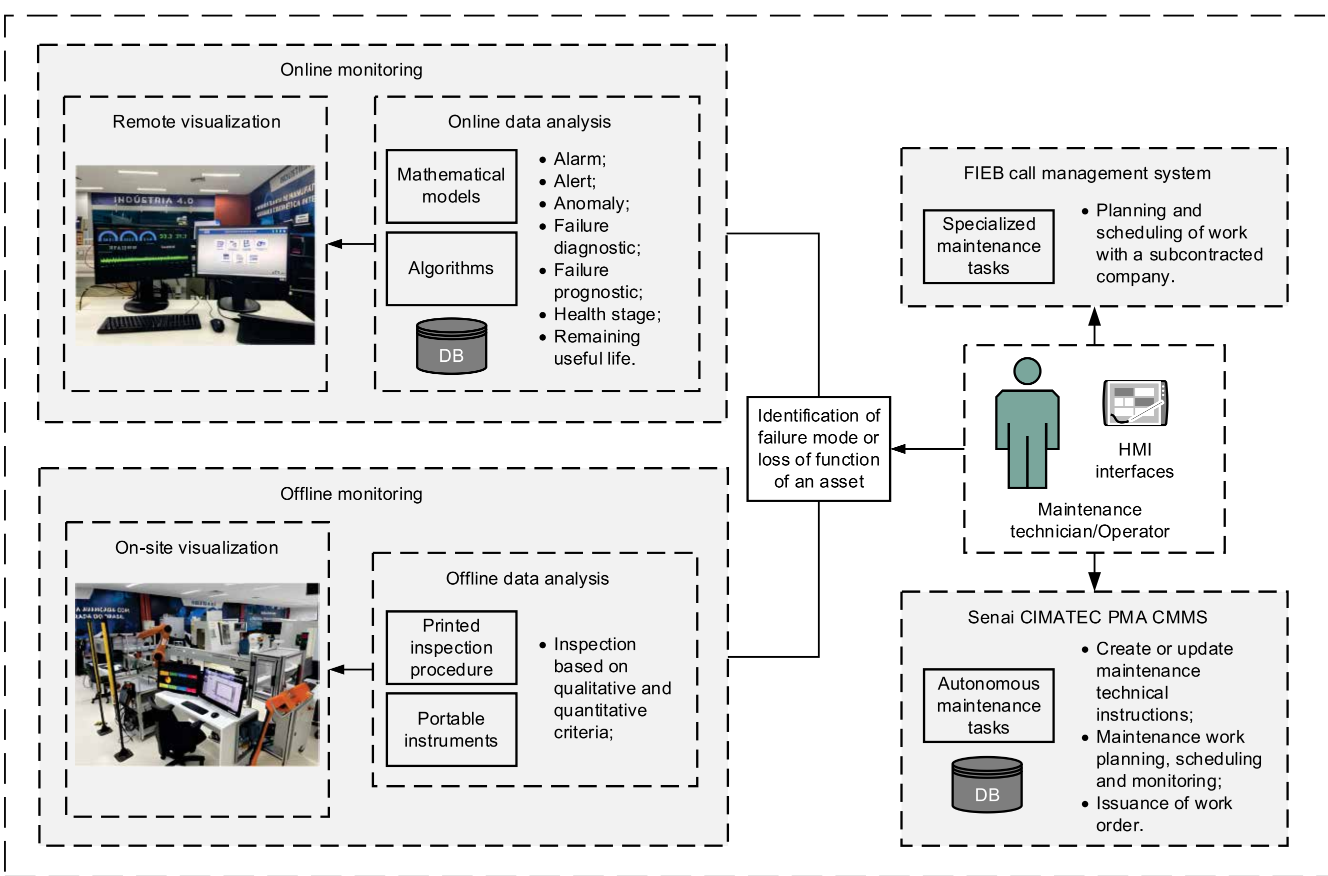
This phase involved implementing the system's communication architecture and developing the scripts required to initiate the monitoring and maintenance of an induction motor. The system was designed to monitor the conveyor belt induction motor located at the SENAI CIMATEC Advanced Manufacturing Plant (AMP) transport station. This motor—specifically a VEMAT 0.5 hp single-phase asynchronous motor, model 7HB 71B—is critical to operations, as its failure results in a complete halt of the AMP system.

Sensor selection considered factors such as maximum vibration levels and the need for physical contact with the motor. The ADXL345 accelerometer was selected for vibration monitoring based on its sampling rate compatibility with the motor's low rotational speed and expected signal frequency. To measure the motor's surface temperature, a GY-906 infrared temperature sensor was used.

Ambient conditions—specifically temperature and humidity—were collected using a DHT22 sensor. Due to budget constraints, voltage and current sensors were not acquired, although their inclusion was recommended during the FMEA analysis.

The selected sensors transmitted data to a Raspberry Pi 4 Model B (RASPi) IoT device using

Figure 3. Maintenance 4.0 operational system architecture.



I2C and SPI communication interfaces, chosen based on the available input pins. However, the I2C interface presented limitations related to cable length when connecting the vibration and temperature sensors. To address this, two P82B715P I2C bus extenders were installed. Additionally, operational data from the Rockwell CompactLogix L18ERM PLC—such as the motor's on/off status and frequency from the inverter—was transmitted to the RASPi via Modbus TCP.

Data analysis models and algorithms were developed once all devices were configured and tested. The RASPi utilized Node-RED to integrate data from sensors and PLCs and feed it into the analysis models. Two analytical models were implemented: a reliability model and an artificial intelligence (AI) model. The reliability model, based on a proportional hazard model [11], used operational time and temperature data to estimate the motor's Remaining Useful Life (RUL). In the absence of historical failure data, expert elicitation generated synthetic data for estimating covariate parameters.

The AI model used a Multilayer Perceptron (MLP) algorithm to classify the motor's condition into four categories: healthy, light deterioration, moderate deterioration, and severe deterioration. Inputs included motor speed, vibration, and temperature. The model employed Adaptive Moment Estimation (Adam) [12] as its optimizer and was trained using real healthy-state data and synthetically generated degradation data. Vibration data was created using a modified sinusoidal function, while temperature data followed a modified sigmoid pattern, both implemented in Python.

Processed data—including sensor readings, PLC values, and model outputs—were transmitted via Ethernet to a Microsoft SQL Server Express database. Grafana was employed for data visualization due to its compatibility with SQL databases and capacity for creating clear and interactive dashboards. This setup gave operators real-time insights to support proactive maintenance and minimize unplanned downtime. Finally, a client computer connected to a Computerized Maintenance Management System (CMMS)—developed by SENAI CIMATEC—was used to manage maintenance activities and integrate real-time monitoring information.

Results and Discussion

Implementing the Maintenance 4.0 system at the AMP represents a significant advancement from traditional reactive and preventive approaches toward a predictive and proactive maintenance strategy. By integrating advanced data analytics, reliability engineering, and AI-driven diagnostics, the system demonstrated the potential to optimize maintenance planning, improve asset availability, and reduce operational costs.

Integration with SENAI CIMATEC's CMMS enabled dynamic planning and scheduling of maintenance activities based on actual equipment conditions rather than relying solely on fixed intervals. This real-time alignment of maintenance tasks with machine health supports greater efficiency and reliability.

The system architecture emphasized scalability, flexibility, and data security. Although Modbus TCP was implemented without encryption for prototyping purposes, the use of IoT gateways to convert insecure protocols into secure communication is strongly recommended for real-world industrial applications.

Despite the unavailability of real-world failure data, the AI and reliability models enhanced visibility into motor health, providing insights previously dependent on expert intuition. The capability to visualize and analyze real-time data also contributed to user education by demonstrating practical applications of predictive maintenance techniques.

Conclusion

This paper presented the development of a system designed to demonstrate Maintenance 4.0 technologies within a didactic Advanced Manufacturing Plant (AMP). Integrating information and communication technologies for real-time data collection and analysis and automated maintenance management creates a robust educational tool for professionals and students alike.

The results indicate that the system significantly enhances the teaching and application of modern maintenance strategies aligned with Industry 4.0 principles. It fosters technical and strategic skill development, preparing users to meet the demands of contemporary industrial environments.

Further assessment of the system's educational effectiveness should be conducted using it in actual classroom and training settings. At SENAI CIMATEC, the system is expected to be adopted in undergraduate, technical, and continuing education programs across industries of various scales. Future work may include evaluating student satisfaction and learning outcomes to refine system architecture, procedures, and educational materials.

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Cloud Data Sharing for the Integration of Heterogeneous Systems for Personalized Production

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The increasing demand for customized products poses significant challenges for companies aiming to optimize logistics and manufacturing operations. Multiple companies within a supply network—each using distinct information systems—must be coordinated from order negotiation to the end of the product life cycle. This challenge involves the integration of heterogeneous systems and the harmonization of data across all sectors of the manufacturing chain. This study proposes cloud-based data sharing to establish seamless communication among distributed information systems. The proposed approach was implemented in two pilot plants supported by advanced Industry 4.0 systems. The analysis indicates that this method facilitates effective data sharing in customer-supplier relationships, thereby improving the coordination and scheduling of production activities.
Keywords: Discrete Manufacturing. Integration of Heterogeneous Systems. Cloud Computing. Distributed Manufacturing. Industry 4.0.

The growing demand for personalized products is driven by increasingly discerning consumers seeking items tailored to their specific preferences and needs. This trend spans several sectors, including fashion, electronics, and automotive industries [1,2]. Consequently, discrete manufacturing companies are under pressure to swiftly adapt factory operations to meet the demand for customized products and navigate volatile market conditions [3].

Personalized production requires integrated systems that facilitate data flow across the various stages and components of a globally distributed production process. Data integration enables seamless communication among heterogeneous systems companies to use in different geographic locations. Data from diverse sources must be shared, processed, and analyzed in real-time to ensure adequate production planning and management.

Beyond enabling integration, sharing information throughout the manufacturing chain enhances collaboration among systems, equipment, and devices. This creates opportunities to coordinate and fine-tune operations in response to shifting market demands. However, integrating distributed systems remains a significant challenge due to a lack of practical tools for managing distributed manufacturing chains [4].

This article proposes a solution for integrating information and process flows across different production chain segments. This approach is essential for addressing the challenges of discrete manufacturing companies in today's dynamic environment. The paper is structured as follows: Section 2 presents the literature review, Section 3 details the methodology and implementation, Section 4 discusses the results, and Section 5 provides the conclusions.

Literature Review

Discrete manufacturing—focused on producing distinct, individual units—has gained renewed importance due to the Industry 4.0 paradigm, which promotes a shift from centralized to more flexible and globally distributed operations [1]. Although implementing this global model remains in progress, companies must contend with increasing product complexity, stricter quality standards, and greater variety in unit products [5].

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The evolving manufacturing profile reflects a more substantial consumer influence, necessitating ongoing adaptation to shifting demands. This includes integrating and sharing data among distributed organizations involved in product development and delivery [4]. The need for newer and more personalized products intensifies the demand for efficient integration and seamless information exchange throughout the production chain.

Nonetheless, the literature offers limited tools for achieving this goal, as synchronous data integration among companies remains uncommon. Integrating heterogeneous systems—facilitated through cloud-based data sharing—is essential for preparing and managing information and process flows, ultimately supporting efficient production planning.

Cloud Data Sharing for Heterogeneous Systems Integration

Extensive research has been devoted to enhancing manufacturing systems' intelligence, flexibility, and service orientation to support collaborative discrete production within distributed networks. Cloud manufacturing stands out for its ability to deliver on-demand services, aggregating manufacturing resources into a network accessible via the cloud. These services can be configured and integrated rapidly to fulfill distributed production orders [6]

According to Ren and colleagues [7], cloud computing comprises three primary service models. Infrastructure as a Service (IaaS) provides hardware resources such as computing power, storage, and networks—via physical or virtual machines—enabling users to customize their IT infrastructure. Platform as a Service (PaaS) offers a development environment for cloud services, while Software as a Service (SaaS) allows users to access applications directly over the Internet.

Lu, Xu, and Wang [8] emphasize that cloud-based equipment-as-a-service can be integrated directly into digital manufacturing networks. In this context, physical assets are connected to cyber-physical systems (CPS) using standardized communication protocols such as OPC UA and MTConnect. Application Programming Interfaces (APIs) are pivotal in ensuring secure and standardized communication between components.

OPC UA was selected as the communication protocol for this work due to its security, stability, and widespread industrial adoption. Furthermore, CPS can be integrated directly into Manufacturing Execution Systems (MES), enabling more effective coordination and scheduling of production activities [8]. The cloud-based data-sharing approach proposed in this study is predicated on developing a cloud communication infrastructure that ensures the reliable and efficient exchange of information between diverse production systems.

MES 4.0

The MES manages production information from order placement to product completion [5]. In discrete manufacturing, such information must be acquired through integrating heterogeneous systems, real-time data sharing, and analysis from distributed companies. MES plays a central role in transforming industrial processes to meet the demands of Industry 4.0.

Shojaeinasab and colleagues [9] argue that an MES designed with Industry 4.0 capabilities can handle large volumes of data (big data) and extract valuable insights about various production dimensions. These insights can be used to identify patterns and trends and support decision-making regarding production tasks. NoSQL databases perform exceptionally well with real-time data, such as quality checks requiring continuous updates [10]. In this study, data sharing between distributed companies forms the basis for an enhanced version of MES, which can deliver personalized analyses and insights into manufacturing operations.

Materials and Methods

The key elements and gaps in the existing literature were identified to formulate a coherent research hypothesis. According to Gil [11], a systematic review must address hypothesis formulation and problem familiarization to enhance clarity. The method adopted in this work also aligns with the guidelines of Gerhardt and Silveira [12], who emphasize generating specific knowledge applicable to practical scenarios. Accordingly, this study aims to implement cloud-based data sharing for heterogeneous systems to improve personalized production services. This work's development leveraged the infrastructure of the Advanced Manufacturing Plant (AMP) and Model Factory (MF) laboratories located at SENAI CIMATEC in Salvador. The MF focuses on producing pneumatic cylinders, while the AMP supports customized base-part production for the MF. The proposed cloud-based integration aims to facilitate real-time information exchange between these two environments, enhancing the responsiveness and coordination of production services.

Figure 1 illustrates the architecture of the proposed integration framework. The data flow outlined in this architecture is incorporated into MES 4.0 to ensure efficient production process management.

API Middleware Architecture

An API middleware architecture was developed to enable the integration of heterogeneous systems. This software architecture is illustrated in Figure 2. The application logic is divided into three main components:

- **AmpFacadeAPI:** This component acts as a wrapper for the AMP MES API routes and leverages the functionalities of MES 4.0. Its primary role is to receive customer order requests, validate their integrity, forward them to the AMP system, and relay the responses to the MF system.
- **SecurityController:** This module verifies whether the user submitting the order request has the appropriate authorization to interact with the AMP system.
- **LogHandler:** Responsible for logging all relevant activities within the API process, ensuring traceability and system observability.

The middleware was developed using Node.js in conjunction with the TypeScript programming language. The Express.js framework was utilized to build the RESTful API endpoints, while the Winston library was adopted for structured logging. All logs are stored in a Cassandra NoSQL database, which includes a dedicated table for log entries.

A key aspect of the logging strategy is using log levels, which support the classification and prioritization of recorded events for troubleshooting

Figure 1. Integration AMP and MF.

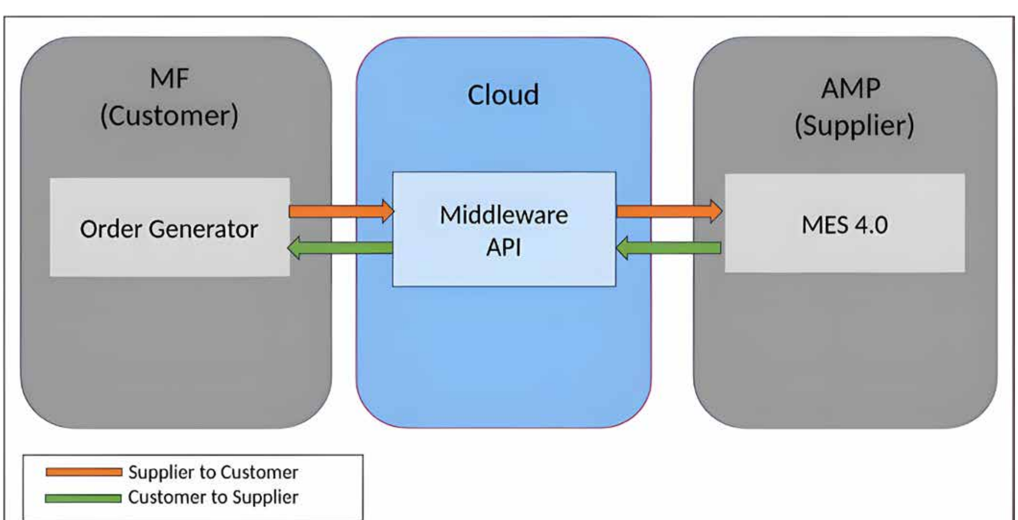
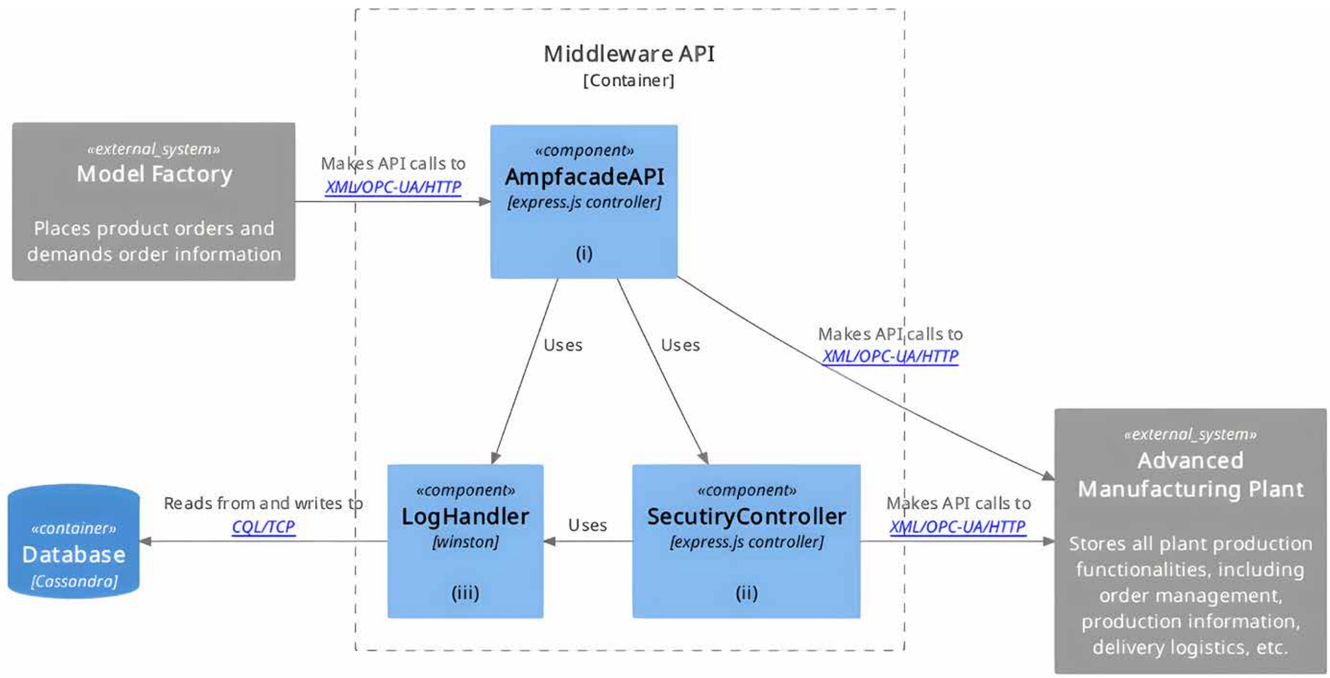


Figure 2. Integration API architecture.



and performance analysis. The three defined levels are:

- **Info:** Used for logging routine operations and process outcomes.
- **Error:** Records issues that impact application performance or flow.
- **Fatal:** Captures critical failures that may interrupt or halt the application.

Each log level is associated with a distinct data retention policy, ensuring that only relevant information is preserved long-term for audit trails and quality assessments.

Results and Discussion

The effectiveness of the cloud-based integration using the middleware was validated by successfully transferring customer orders. The order generator system sent customer requests to the supplier, which were successfully received and registered in the AMP production queue, as shown in Figures 3 and 5. In contrast, Figure 4 illustrates a failed order request due to the absence of valid user credentials, a controlled scenario designed to test system robustness.

These results confirm the expected behavior of the AmpFacadeAPI and SecurityController components under both normal and exception conditions. The integration architecture enables improved digital traceability and real-time monitoring capabilities, enhancing responsiveness and operational efficiency in customer order processing and production management.

The LogHandler component also met the expected behavior by recording transaction information between systems and all interactions involving other components in the Cassandra database, as illustrated in Figure 6. This robust data capture facilitates AI's use for predictive analytics and decision-making and enhances demand forecasting capabilities.These insights enable a deeper understanding of production patterns and trends, supporting strategic planning and operational efficiency.

Conclusion

This work presents a state-of-the-art approach to data sharing and integrating heterogeneous systems in distributed personalized production.

Figure 3. Order Request successful - Code 200.

Figure 4. Order Request unsuccessful - Code 403.

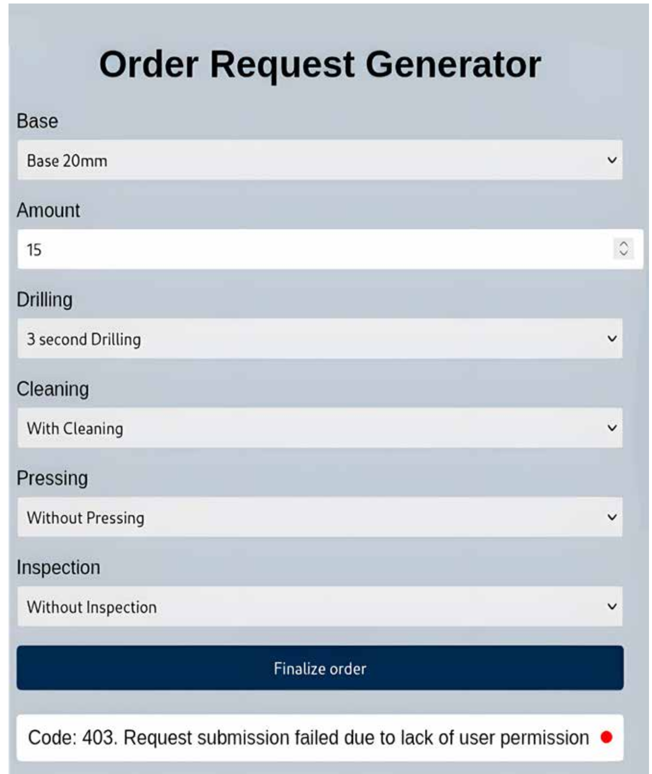
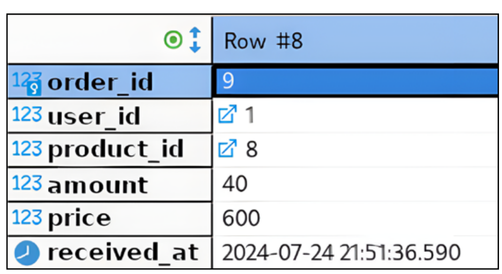
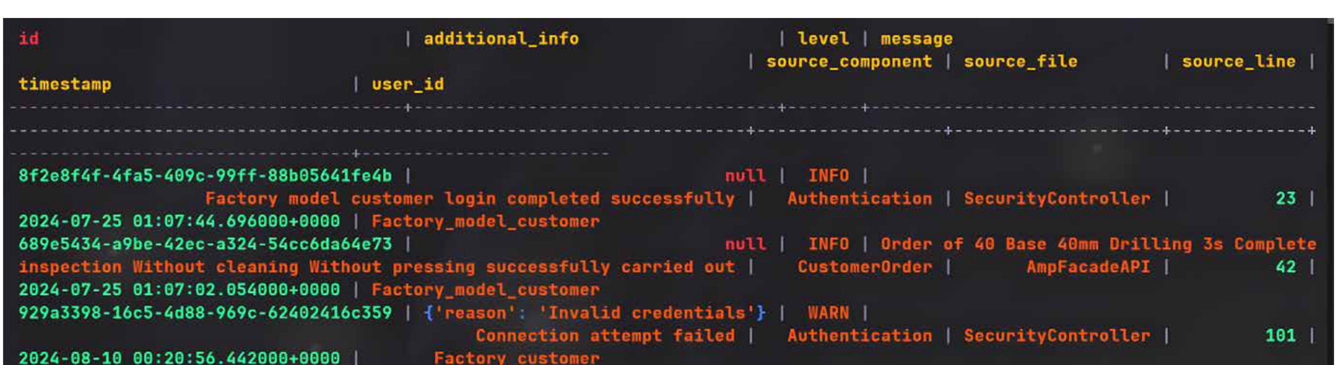


Figure 5. Registration of the requested order in AMP's internal database.



	Row #8
order_id	9
user_id	1
product_id	8
amount	40
price	600
received_at	2024-07-24 21:51:36.590

Figure 6. Result of integration into AMP's MES.



```
id                                   | additional_info                    | level | message
                                                                 | source_component | source_file         | source_line |
timestamp                        | user_id
8f2e8f4f-4fa5-409c-99ff-88b05641fe4b |                               null |  INFO |
                  Factory model customer login completed successfully |   Authentication | SecurityController |          23 |
2024-07-25 01:07:44.696000+0000 | Factory_model_customer
689e5434-a9be-42ec-a324-54cc6da64e73 |                               null |  INFO | Order of 40 Base 40mm Drilling 3s Complete
inspection Without cleaning Without pressing successfully carried out |    CustomerOrder |        AmpFacadeAPI |          42 |
2024-07-25 01:07:02.054000+0000 | Factory_model_customer
929a3398-16c5-4d88-969c-62402416c359 | {'reason': 'Invalid credentials'} |  WARN |
                                           Connection attempt failed |   Authentication | SecurityController |         101 |
2024-08-10 00:20:56.442000+0000 |       Factory_customer
```

Key challenges addressed include the lack of effective tools for integrating and synchronizing data across geographically dispersed enterprises and the need to ensure data harmonization throughout the production chain.

The proposed method involves cloud-based data sharing, from customer order intake through supplier integration, enabling seamless information flow across the various stages of production. This flow is integrated into a new iteration of the Manufacturing Execution System (MES), designed to support the requirements of Industry 4.0. The solution was validated in two educational pilot plants simulating a pneumatic cylinder production scenario: the Advanced Manufacturing Plant (AMP), responsible for the customized production of bases and covers, and the Model Factory (MF), which performs final cylinder assembly.

The results demonstrate that the developed approach supports the efficient management of a discrete manufacturing chain by maintaining consistent and reliable data flow in a customer-supplier context. Despite these positive outcomes, further research is necessary, particularly to address challenges such as system latency due to high transaction volumes and cybersecurity concerns related to handling sensitive production data.

Acknowledgments

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Evaluation of FDM-Printed Soft Pneumatic Actuators in TPU

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This work investigates the mechanical performance of soft pneumatic actuators fabricated using TPU 95A material via Fused Deposition Modeling (FDM) for industrial applications. The study focuses on the influence of wall thickness and infill density on the pressure resistance of the actuators. Nine pneumatic chambers with varying wall thicknesses (1 mm, 2 mm, and 3 mm) and infill densities (30%, 50%, and 100%) were tested under high-pressure conditions. The experimental results indicate that increasing the wall thickness generally enhances pressure resistance; however, lower infill densities (30%) surprisingly demonstrated the highest resistance. Computational simulations using the Finite Element Method (FEM) corroborated these findings, revealing that increased wall thickness significantly improves structural integrity. At the same time, the influence of higher infill density diminishes near the 100% threshold. These results provide valuable insights into optimizing FDM-printed pneumatic components for industrial use, contributing to the advancement of soft robotics.
Keywords: 3D Printing. Pneumatics. Actuators. FDM. TPU.

Soft robotics is a growing field focused on developing actuators, sensors, and technologies that deviate from traditional rigid structures. Its key advantages include high adaptability to complex environments, reduced manufacturing time and cost, and enhanced mechanical resilience [1][2]. Realizing soft robotics requires ongoing materials science research to identify flexible yet durable materials capable of executing mechanical functions effectively—especially actuators, which are crucial to the performance of soft robotic systems.

Soft robotic actuation is generally achieved through two main approaches: (i) the use of innovative materials such as electroactive polymers, shape memory alloys, magnetorheological elastomers, and electrorheological fluids; and (ii) fluidic actuation using hydraulic or pneumatic systems [3].

Pneumatic actuators, in particular, are widely adopted in robotics and automation due to their ability to deliver substantial power, cost-effectiveness, and versatile motion [4].

Nevertheless, achieving flexibility and extension with pneumatic systems can pose significant design and material challenges [5].

Soft pneumatic actuators are essential to mobile robotics and can operate in one, two, or three dimensions. One-dimensional actuators extend and expand, two-dimensional systems enable bending, and three-dimensional actuators can rotate or perform more complex motions [6].

Among various manufacturing methods, 3D printing—especially Fused Deposition Modeling (FDM)—has become a key technique in fabricating soft pneumatic actuators. FDM enables rapid prototyping and design customization, making it highly accessible for research and industrial applications [7]. This technique extrudes thermoplastic material layer by layer, allowing for precise control over parameters such as wall thickness, print speed, and infill density, significantly affecting the actuator's mechanical performance [8]. Additionally, FDM offers significant advantages in cost and design iteration, eliminating the need for specialized molds or tooling [9,10].

This study evaluates the mechanical performance of soft pneumatic actuators fabricated

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using FDM with TPU 95A material. The analysis focuses on the impact of wall thickness and infill density on the actuator's pressure resistance. By combining experimental testing and finite element simulations, this work aims to better understand the structural behavior of 3D-printed pneumatic components under pressure, offering design insights for future industrial applications [11].

Materials and Methods

Nine pneumatic chambers with the same external volume were designed and manufactured using TPU 95A material through FDM 3D printing. The primary printer configuration parameters are presented in Table 1. The chambers were categorized based on their wall thickness (1 mm, 2 mm, and 3 mm) and infill density (30%, 50%, and 100%). The chamber design, with dimensions in millimeters, is shown in Figure 1.

Each chamber was subjected to a gradually increasing internal pressure via a pneumatic valve until failure occurred, defined as the point at which air leakage was observed. The pressure at the moment of failure was recorded for analysis. A comparative assessment was conducted to evaluate the pressure resistance of each chamber configuration. Additionally, this study examined the relationship between wall thickness and infill density, aiming to identify optimal design parameters for maximizing structural integrity in soft pneumatic actuators.

Table 1. Parameters used for print pneumatics chambers.

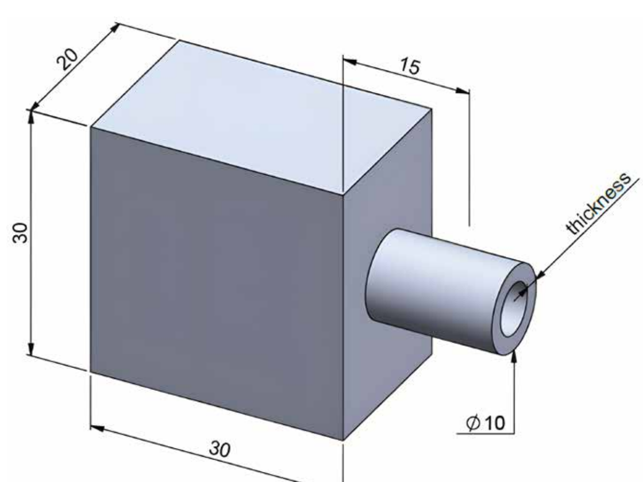
Parameters print	Values
Layer height	0.2 mm
Infill pattern	cross 3D
Retraction amount	4 mm
Retraction speed	40.0 mm/s
Print speed	30.0 mm/s
Wall thickness	1.2 mm

The chamber was simulated considering an infill density of 100%. The models were developed using Finite Element Method (FEM) with a linear isotropic analysis approach imputing symmetry boundary conditions to save processing time. We can see only ¼ of the model in the analysis figures. The fixed boundary condition was applied at the top face of the nodal, while the pressure loading was applied at all the internal faces of the model. The analysis was done using Ansys Mechanical software. The TPU chosen has the following properties shown in Table 2. The internal pressure was gradually increased from 0 to 2MPa (20 bar), happening in 10s, and the failure time was observed, which was when the Von Mises tension got close to the Tensile Ultimate Strength.

Table 2. TPU properties.

Properties	Values
Tensile Yield Strength	38.88MPa
Tensile Ultimate Strength	43.84MPa
Young’s Module	1.6 GPa
Poisson’s Ratio	0.4
Density	1.17 x 10-6 kg/mm³

Figure 1. Main dimensions.



Results and Discussion

Table 3 illustrates the pressure values that caused rupture in pneumatic chambers with varying thicknesses and filling percentages. Three different chamber thicknesses were tested: 1 mm, 2 mm, and 3 mm, under three filling percentages: 30%, 50%, and 100%. For the 1 mm thick chambers, rupture occurred consistently at 1.0 Bar for 30% and 100% filling, increasing to 1.1 at 50%. In contrast, the 2 mm thick chambers exhibited a higher rupture pressure, with values of 7.62 Bar, 6.97 Bar, and 7.25 Bar for 30%, 50%, and 100% filling, respectively. The 3 mm thick chambers showed the highest resistance to pressure, rupturing at 7.9 Bar for 30% filling, 7.81 Bar for 50% filling, and 7.2 Bar for 100% filling

The data suggest that increasing the wall thickness of pneumatic chambers enhances their ability to withstand higher pressures before rupturing, with variations in performance depending on the infill percentage. While this finding may appear intuitive, a surprising observation emerged: increasing the infill density does not necessarily correlate with higher pressure resistance. Chambers with lower infill levels (30%) demonstrated the highest resistance—particularly among those with 3 mm wall thickness—where the low infill significantly influenced rupture pressure. The mechanical behavior associated with infill density was further analyzed using computational simulations. As illustrated in Figure 2, simulations modeled chambers with a 100% infill density and corroborated the experimental observations. The results revealed that the maximum von Mises stress occurred near stress concentration regions, specifically at the corners and the interface between the infill and the chamber's outer wall. These stress distributions aligned well with the rupture points observed during physical testing.

Moreover, the simulations indicated that although a higher infill density generally improves pressure resistance, the benefit diminishes significantly at densities approaching 100%. This plateau effect suggests that additional material beyond a certain point offers marginal structural reinforcement, potentially due to limitations in interlayer adhesion or the inherent mechanical characteristics of TPU.

Figure 3 presents the von Mises equivalent stress as a function of applied pressure for chambers with wall thicknesses of 1 mm, 2 mm, and 3 mm. The red dashed line represents the Ultimate Tensile Strength (Sut) of TPU, fixed at 43.84 MPa, which marks the material's failure threshold.

For chambers with 1 mm wall thickness, the von Mises stress increases rapidly with pressure, reaching the ultimate tensile strength at approximately 0.2 MPa. Beyond this point, material failure is expected. This indicates that 1 mm chambers have the lowest pressure tolerance, consistent with their limited structural integrity. For 2 mm thick chambers, the von Mises stress increases gradually, reaching the ultimate tensile strength at approximately 0.65 MPa. This demonstrates improved pressure resistance, which is attributed to the enhanced support provided by thicker walls.

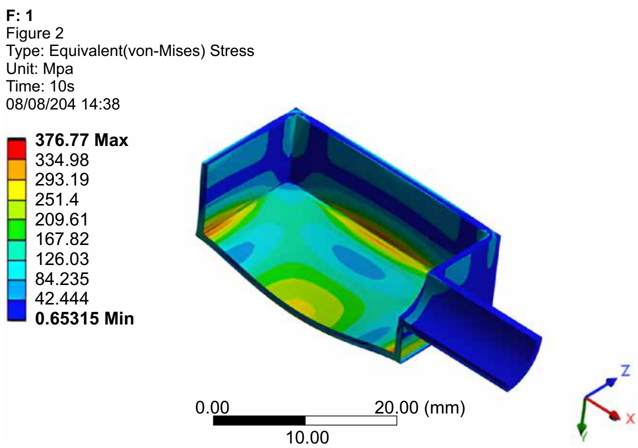
Chambers with 3 mm wall thickness displayed the highest resistance to internal pressure. Even at

Table 3. Pressure values that ruptured the pneumatic chambers.

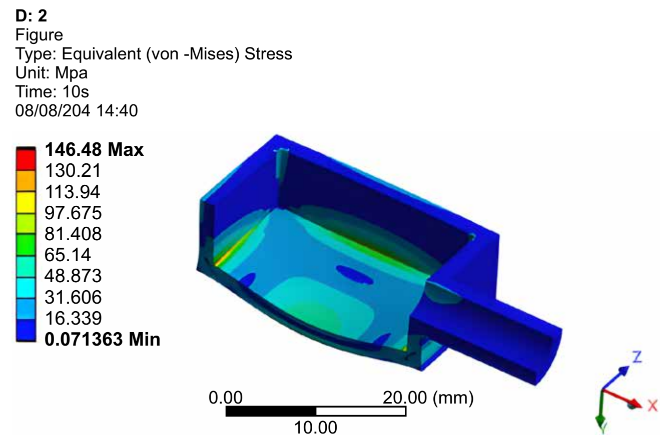
Filling (%)	Thickness 1 1 mm	Thickness 2 2 mm	Thickness 3 3 mm
30%	1.0 Bar	7.62 Bar	7.9 Bar
50%	1.1 Bar	6.97 Bar	7.81 Bar
100%	1.0 Bar	7.25 Bar	7.2 Bar

Figure 2. Distribution of Von-Misis stress at different thickness bodies.

a) *1 mm wall thickness body*



b) *2 mm wall thickness body*



c) *3 mm wall thickness body*

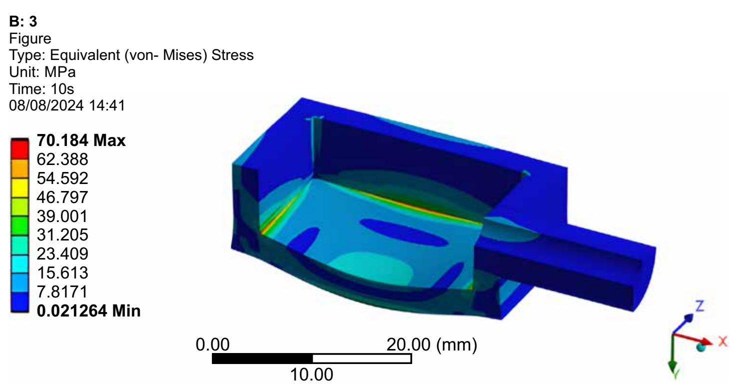
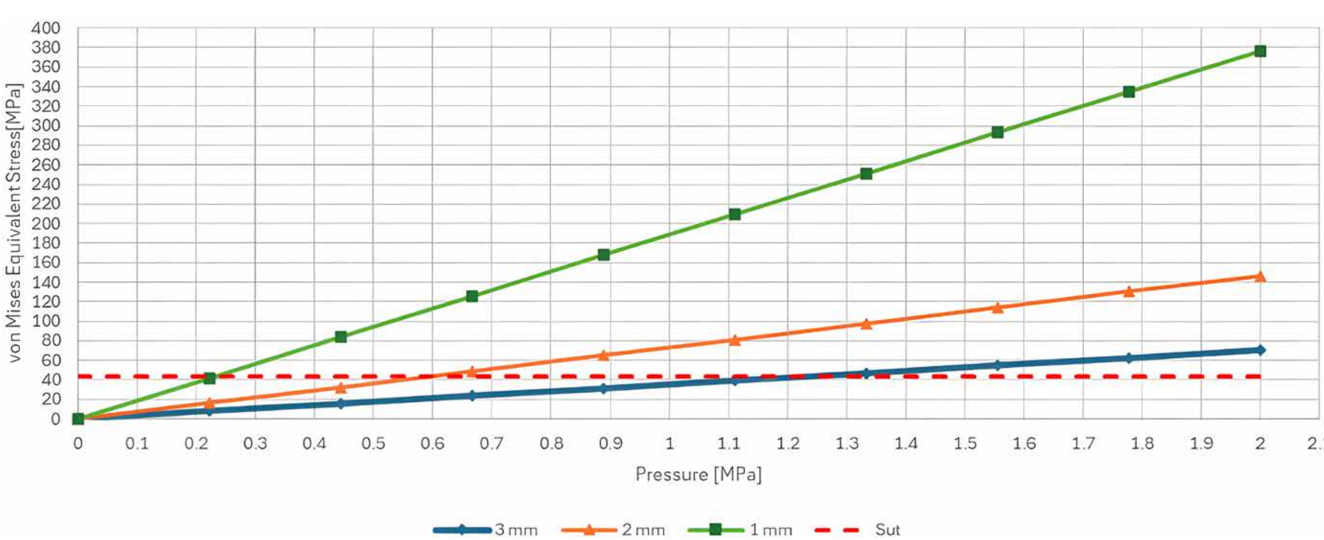


Figure 3. Simulated results of the pneumatic chambers rupture pressures.



1.3 MPa, the simulated von Mises stress remained below the ultimate tensile strength, indicating that no material failure would occur within the tested pressure range. These results underscore the superior structural integrity of thicker chambers. Comparing simulation and experimental data reveals reasonable consistency. For the 1 mm chambers, the experimental rupture pressure was approximately 1.0 bar (0.1 MPa), which aligns with the simulation prediction of failure at around 0.2 MPa. Minor discrepancies are likely due to material inconsistencies or real-world factors not fully represented in the model.

For 2 mm chambers, experimental rupture pressures ranged from 6.97 bar (0.697 MPa) to 7.62 bar (0.762 MPa), whereas the simulation predicted failure at 0.65 MPa. This suggests that the computational model may be conservative, slightly underestimating real-world performance.

For 3 mm chambers, experimental failure occurred between 7.2 bar (0.72 MPa) and 7.9 bar (0.79 MPa). However, simulations showed no failure even at 1.3 MPa, implying that these chambers could likely endure even greater pressures than those tested. The discrepancy highlights the simulation's conservative nature or possible model simplifications. The simulation results provided a reliable predictive framework, particularly for the 1 mm and 2 mm configurations. The 3 mm chambers exhibited higher real-world pressure resistance than predicted, emphasizing their potential for demanding industrial applications.

Conclusion

This study assessed the mechanical performance of soft pneumatic actuators manufactured via FDM using TPU 95A, with varying wall thicknesses and infill densities. Experimental results, supported by computational simulations, confirmed that wall thickness is a primary factor influencing the chambers' pressure resistance.

Thicker walls significantly enhance structural integrity, allowing for higher operating pressures. Among the samples, 1 mm thick chambers failed at the lowest pressures, while 2 mm and 3 mm chambers showed progressively greater resilience. Notably, 3 mm chambers withstood the highest pressures, showing no failure within the tested limits. Surprisingly, lower infill densities, especially 30%, resulted in greater pressure resistance. This counterintuitive finding underscores the importance of not assuming linear improvement with increased infill density.

The results suggest that increasing wall thickness is a practical design strategy for high-pressure applications, while optimizing infill density is equally crucial to balance material efficiency and structural performance. These insights are particularly relevant to designing and developing soft robotic actuators for industrial environments where durability and efficiency are essential.

Acknowledgments

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Luminotechnical Calculation Algorithm for Public Lighting in VBA

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Public lighting is essential for urban quality of life and safety. With the advent of LED technology and increasing energy efficiency directives, its modernization has become increasingly important. This study developed a VBA algorithm to optimize the technological transition of public lighting, focusing on reducing simulation time and installed power. Using the lighting projects from Teresina/PI's Public-Private Partnership (PPP) as a reference, the algorithm was validated through comparisons with DIALux 4.13 software. The results demonstrated that the algorithm achieved a Mean Absolute Percentage Error (MAPE) below 8% for luminance and illuminance calculations, indicating high accuracy. Furthermore, it significantly reduced simulation time, completing 13,161 simulations in 37 hours, compared to 2,121 simulations in 140 hours using DIALux. These results highlight the algorithm's efficiency and effectiveness.
Keywords: Public Lighting. Energy Efficiency. Luminotechnical Simulation.

Public lighting (IP) is fundamental to urban quality of life, directly influencing safety, traffic flow, and nighttime activities. Although public lighting was adopted in Brazil as early as the 18th century, formal standardization only emerged in 1992 with the publication of ABNT NBR 5101.

This standard ensures efficient, safe, long-lasting lighting systems [1].

Brazil has over 18 million lighting points, which consume approximately 14.3 TWh—around 4.5% of the country's total electricity consumption. Most of these points rely on outdated technologies such as fluorescent, sodium vapor, and mercury vapor lamps, which are energy-inefficient and require extensive maintenance. In contrast, LED technology presents a more sustainable solution, offering energy savings of up to 85% compared to incandescent lamps and 65% compared to compact fluorescents. In addition, Public-Private Partnerships (PPPs) have emerged as a strategic model for modernizing public lighting systems, enabling municipalities to outsource their management while ensuring technical and financial viability [2].

The number of lighting simulations required for a given project varies depending on several factors, including the current conditions of each road and the adjustments needed to comply with applicable standards. A single street may demand multiple simulations due to sections with differing lighting characteristics. Furthermore, the quantity and variety of luminaires increase the number of required simulations. For bidding companies, testing a larger number of luminaires enhances the chances of identifying a lower-power option that still complies with standards—thereby reducing implementation costs and maximizing energy savings in PPP projects.

In this context, luminotechnical modeling using specialized software is essential in modernizing public lighting through PPPs. However, this process is often labor-intensive and time-consuming due to the large volume of required simulations and their inherent complexity. To address this challenge, this study presents a tool developed in Visual Basic for Applications (VBA) capable of conducting luminotechnical simulations based on Brazilian standards and public lighting characteristics. The primary objective is significantly reducing simulation time compared to commercially available software. To validate the tool's

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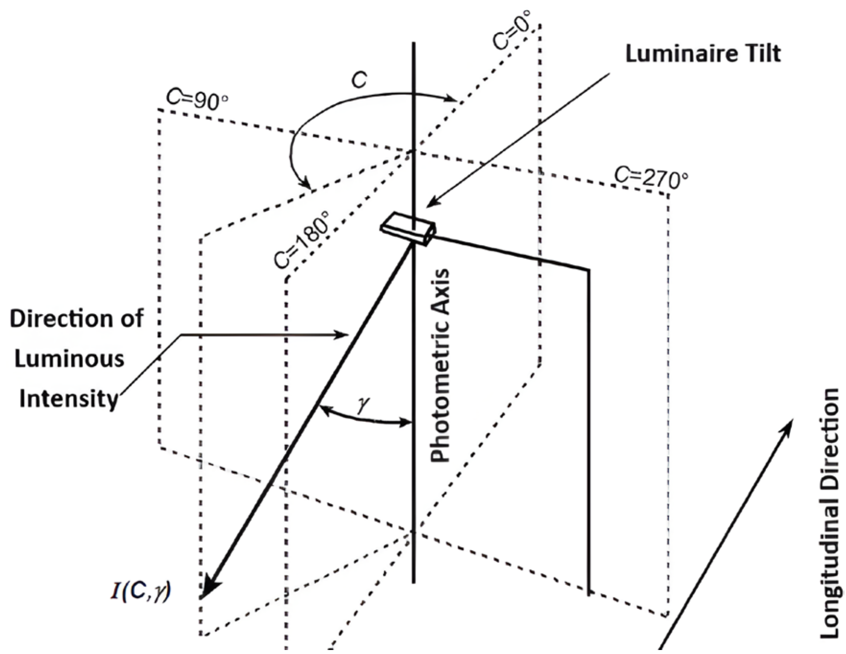
Figure 1. Luminous intensity as a function of angles C and γ [1].



accuracy, the Mean Absolute Percentage Error (MAPE) was employed to compare results for luminance and illuminance obtained using the proposed algorithm with those from DIALux 4.13 simulations [1].

Materials and Methods

The algorithm is based on the Technical Report Road Lighting Calculations CIE 140 - 2000, which defines the necessary variables and formulations to compute the luminotechnical parameters established by NBR 5101:2018 [1–3].

The coordinate system used for road lighting luminaires is typically the I (C,γ) system. This system defines the luminous intensity of a luminaire—usually provided by manufacturers in the IES (Illuminating Engineering Society) format—according to the IES LM-63-1991 standard. The luminous intensity is expressed in candelas per kilolumen (cd/KLM) for all light sources within the luminaire [4].

To determine the luminous intensity emitted by a luminaire toward a specific point on the road, the vertical photometric angle (γ) and the photometric azimuth angle (C) must be calculated. These angles define the light's trajectory from the luminaire to the target point, as illustrated in Figure 1. The calculations must account for the luminaire's orientation, tilt, and rotation in their application. Therefore, mathematical conventions are required to measure distances along the road and to rotate the luminaire around its axes.

Calculation Grid

To calculate the photometric angles C and γ, it is necessary to define the points at which the luminous intensity will be calculated. The calculation grid is established in the NBR 5101:2018 standard, which specifies the sizing and spacing of calculation points according to the characteristics of the road under study. The standard provides guidelines for defining these points on a road with three lanes and a specific spacing between poles [1].

Based on this standard, luminotechnical variables should be calculated at intervals of 6.25% of the spacing between poles along the length of the road, known as the longitudinal spacing. A new calculation line should also be created for every 20% fraction of the lane width, referred to as the transverse spacing.

The resulting calculation grid matrix consists of 17 columns of points evenly distributed along the longitudinal direction and five rows of points within each lane. The NBR 5101:2018 standard also specifies that the width of the road lanes should be considered between 2.7 and 3 meters [1].

Luminous Intensity

Luminous intensity values are determined based on the angles C and γ, which are provided in curves by manufacturers for luminotechnical studies. These curves are typically delivered in the IES (Illuminating Engineering Society) format, allowing for standardized data representation. To obtain the luminous intensity at a specific point, it is essential to calculate the angles C and γ. This calculation calculates the luminous intensity distribution influenced by each luminaire within the system [4].

Once the necessary adjustments are made, such as accounting for the spacing between poles, the installation height of the luminaires, and the coordinates within the rotated system (x', y', z'), the angles C and γ can be accurately calculated for each point, as shown as Figure 2.a. This step is critical in ensuring that the luminous intensity values reflect the actual lighting conditions on the ground, considering the geometric and spatial arrangements of the luminaires [1-3].

In cases where a luminous intensity value is required in a direction that falls between the measured directions in the I-Table, interpolation becomes necessary. The interpolation process involves calculating between the four nearest intensity values in the direction of the azimuth angle C and the elevation angle γ. Due to the lack of more robust statistical modules in Visual Basic, quadratic interpolation was chosen as the method for this task. This method involves interpolating three adjacent columns in the I-Table, allowing for determining intensity values in γ. The interpolation is then performed across the table to find the required value at the specific combination of (C, γ) [3].

Road surface reflection (R-table)

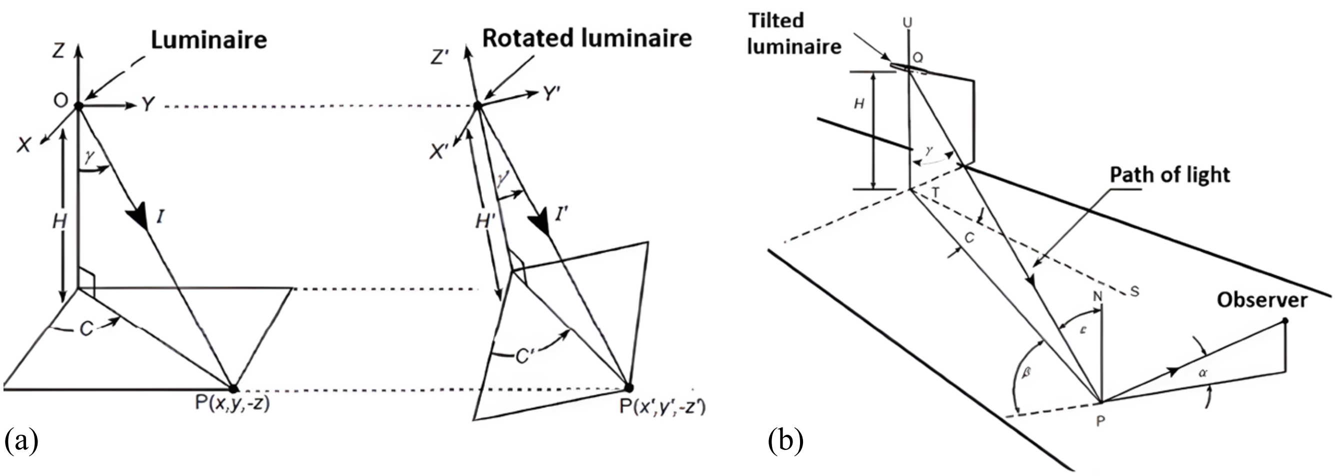
The R-table is a reference table containing data on the road surface's luminous reflection according to the angles β and ε. These data are conventionally expressed in terms of the luminance reduction coefficient multiplied by 10,000 [1]. The data in this table vary depending on the type of road surface, such as asphalt or sand. As illustrated in Figure 2.b, β is the complementary angle between the vertical plane through the luminaire at point Q and the observation point P and the vertical plane through the observer and point P. The angle α represents the angle between the observer's line of sight and the road surface, which is fixed at 1°.

The observer moves along the longitudinal centerline of the calculation grid for each lane. The angle ε is the incidence angle at point P, ST represents the longitudinal direction, Q is the photometric center of the luminaire, UQT is the vertical axis of the luminaire, and PN is normal to the surface.

When an R-value is required for tangent values of ε that fall between the data points in the R-table, quadratic interpolation must be used. This interpolation process requires three values from the R-table for each interpolated value. If an R-value is needed at a specific point (tan ε, β), the interpolation is first performed using three adjacent columns in the R-table that encompass the point. This allows for calculating three R values at the given tan ε. The interpolation is then carried out across the table to find the required value at the specific (tan ε, β) combination.

The R-table model used in this project is the R3, corresponding to the luminous reflection on asphalt-paved roads. The data in this table are consistent with the model used in the OpenEI algorithm. The initial goal was to use the same data utilized in the DIALux 4.13 software; however, the company responsible for developing the software does not disclose such information [5].

Figure 2. (a) Coordinate system with luminaire rotation. (b) Lighting scheme at a specific point on the road [1].



2.6 Luminance, Illuminance, and Uniformities

Given the definitions of the calculation grid, I(C,γ), and R(β, tan ε.), we can define the variables that measure the lighting performance on the road. It is important to note that it is not necessary to calculate these variables at every point on the grid due to the influence of each luminaire. In the transverse direction, the calculation should encompass the entire width of the lane on roads without a central median and the width of a single lane on roads with a central median. [1 – 3]. So, luminance (L) measures the density of light intensity reflected in each direction, with the unit being candela per square meter. Considering the perimeter of influence of the luminaires, the luminance at each point is calculated by:

$$L = \frac{I(C,\gamma).R(\beta, tg\ \varepsilon).MF}{H^2.10000} \quad (1)$$

Where MF corresponds to the maintenance factor of the luminaire, L is the luminance at the calculated point. Additionally, horizontal illuminance was considered the method for calculating the illumination intensity (E), with the unit of measurement being lux (lx). The horizontal illuminance at a specific point is calculated by:

$$E_H = \sum \frac{I(C,\gamma).cos^3\varepsilon.\Phi.MF}{H^2} \quad (2)$$

Where EH is the horizontal illuminance at the point, measured in lux; Φ is the initial luminous flux of the luminaires in kilolumens (klm).

The average illuminance and luminance are calculated as the arithmetic mean of the values obtained at the designated calculation points. The factors used to evaluate luminance distribution along the road include the global minimum uniformity (U_0) and the longitudinal uniformity (UL). Global minimum uniformity assesses the lowest luminance levels on the road by dividing the minimum luminance by the average luminance. In contrast, longitudinal uniformity reflects the consistency of luminance distribution along the calculation grid and is calculated by dividing the minimum luminance by the maximum luminance. Similarly, minimum illuminance uniformity (U) evaluates the lowest level across the road, calculated as the ratio of the minimum illuminance to the average illuminance.

Evaluation

A comparative analysis was conducted using DIALux 4.13, a widely adopted commercial lighting simulation software, to validate the algorithm's performance. The comparison maintained identical simulation parameters, and accuracy was evaluated using the Mean Absolute Percentage Error (MAPE) method. MAPE quantifies the percentage deviation between the algorithm's results and those obtained from DIALux, thereby providing an objective measure of accuracy for luminance, illuminance, and uniformity parameters as required by NBR 5101:2018.

Simulations were carried out for roads with one to four lanes, with lane widths varying from 3 to 12 meters. A depreciation factor of 0.8 was consistently applied across all simulations. Luminaire installation heights ranged from 7 to 10 meters, and tilt angles were incrementally adjusted by 5° up to a maximum of 15°, which aligns with standard recommendations.

Case Study

A case study was conducted using Teresina's public lighting concession, which involved modernizing 92,800 lighting points. The initiative focused on transitioning to LED technology to achieve substantial energy savings. The algorithm executed 13,161 simulations in only 37 hours, compared to 2,121 simulations in 140 hours using DIALux, demonstrating significantly higher computational efficiency.

Results and Discussion

The results of the accuracy evaluation were promising: the MAPE for illuminance (E) was 3.87%, for luminance (L) 3.63%, for illuminance uniformity (U) 5.96%, for global minimum uniformity (U_0) 9.22%, and for longitudinal uniformity (UL) 13.28%. However, longitudinal and global minimum uniformity values exhibited deviations beyond ideal thresholds. These discrepancies can be attributed primarily to differences in the road surface reflectance data (R-Table), significantly affecting luminance and uniformity calculations. The developed algorithm relies on a set of reflectance values that may not correspond precisely to those used in DIALux, as the latter's reflectance database is proprietary and not publicly disclosed. Consequently, discrepancies arise, particularly in parameters that depend on extreme luminance values.

Another contributing factor is the algorithm's interpolation method. Due to the limitations of the VBA platform, quadratic interpolation was used instead of more sophisticated techniques, which may have affected the precision of the luminance calculations.

In terms of efficiency, the algorithm consistently outperformed DIALux 4.13 across all road classes by achieving a lower average power per lighting point, as shown in Table 1. For instance, in V1-class roads, the algorithm reduced the average power per point by over 50W. When these savings are extrapolated across the complete set of road classes in the simulations, the algorithm's predicted reduced installed load following the technology transition was more substantial than that of DIALux—66% compared to 58%, translating to an additional 1.2 MW reduction.

Furthermore, under the Energy Bill Bonus (BCE) incentive, which allows financial benefits from energy savings exceeding a 50% efficiency target to be shared, the algorithm could yield approximately R$1,274,886.30 in additional annual profits for the concessionaire and R$318,722.32 for the municipality (Table 1).

Conclusion

The results demonstrated that the algorithm achieved a Mean Absolute Percentage Error (MAPE) of less than 5% for illuminance and luminance, while uniformity-related errors ranged from 5% to 14%. Regarding computational efficiency, the algorithm proved significantly superior, completing 13,161 simulations in just 37 hours—compared to only 2,121 simulations performed in approximately 140 hours by DIALux 4.13. In the case study involving the municipality of Teresina, the algorithm outperformed DIALux by proposing lighting solutions that achieved a 66% reduction in energy consumption—well above the 50% minimum requirement established by the municipality and the 58% reduction achieved by DIALux. This additional energy savings translates into approximately R$ 1.3 million in annual

Table 1. Calculation basis for the expected load reduction comparison.

Municipality		Algorithm		DIALux 4.13	
Lighting class	**Quantity of Luminaires**	**Medium Power per Luminares (W)**	**% of Savings**	**Medium Power per Luminares (W)**	**% of Savings**
V1	7,401	111,9	75	166,7	63
V2	5,709	90,5	67	116,4	58
V3	8,233	75,1	65	87,5	60
V4	15,122	40,6	76	55,0	68
V5	56,335	34,5	62	40,3	55
TOTAL	92,800	48,71	66	61,65	58

revenue for the concessionaire, thus improving the public lighting project's technical and financial viability.

For future research, it is recommended that alternatives be explored to reduce computational errors in various parameters further. One potential avenue is adopting more versatile programming languages, such as Python, allowing advanced interpolation techniques beyond quadratic interpolation. Moreover, integrating machine learning strategies, such as the Extreme Learning Machine (ELM) in a hybrid grey-box modeling approach, could further minimize discrepancies—particularly those arising from limitations in R-table data [6].

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Prototype of an Automatic Pothole Repair System for Public Roads

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This paper presents the development of equipment designed to support emergency corrective maintenance on public roads, guided by a product development methodology. The central issue addressed is the formation of potholes, which can cause accidents, damage vehicles, slow traffic, and create legal liabilities for public authorities. Potholes result from various factors, including poor-quality asphalt, heavy traffic loads, adverse weather conditions, and a lack of preventive maintenance. The proposed solution investigates efficient methods for rapid pothole repair to enhance road safety, reduce maintenance costs, contribute to environmental sustainability, and improve urban quality of life.
Keywords: Public Roads. Maintenance. Product Development. Potholes.

Public roads are vital components of urban infrastructure, enabling the movement of people and goods and fostering cities' social and economic integration. However, poor road conditions—particularly the prevalence of potholes—pose a persistent challenge in Brazil, leading to a wide array of negative social and economic consequences. Potholes arise from a complex interplay of factors, including intense traffic, unfavorable weather, and using substandard materials in road construction and repair. These issues complicate the timely and effective detection and remediation of surface damage [1]. Figure 1 illustrates the type of pothole targeted by the proposed equipment.

This situation goes beyond mere inconvenience for road users—it also entails significant economic losses and safety risks. Increased travel time, accelerated vehicle wear, and the heightened risk of traffic accidents are among the key consequences. These outcomes can lead to material damage, serious injuries, and even fatalities.

The core issue is the frequent occurrence of potholes on public roads, which, according to Silva [2], may incur legal liability for the responsible authorities. Therefore, enhancing the methods and materials used for road maintenance is of considerable importance to public agencies. According to Romeiro and colleagues [3], the knowledge to generate ideas, assess concepts, and structure the design process are essential components for successful project development. Furthermore, as emphasized in [3,4], project development can be viewed as a progression of sequential phases in which abstract ideas evolve into detailed product specifications. This study seeks to develop a solution to address the pothole problem by applying early-stage product development tools, such as QFD (Quality Function Deployment), morphological matrices, and TRIZ (Theory of Inventive Problem Solving).These tools are essential for professionals engaged in product design, providing opportunities to refine both practical and theoretical competencies.

If further developed and validated, the implementation of the solution proposed in this work could generate significant societal benefits. These include substantially reducing pothole occurrence, improved road safety and user comfort, lower maintenance costs for public infrastructure, enhanced environmental sustainability, and a better quality of life for the general population.

Materials and Methods

This study adopted a systematic approach to developing an innovative machine capable of

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Figure 1. Public road pothole representation.

repairing potholes more rapidly, efficiently, and with superior quality tailored to the specific conditions of Brazilian public roads. The methodology followed is outlined in Figure 2, which illustrates the sequential steps taken to achieve the project's objectives.

The method was structured in two phases. In the first phase, the problem targeted by the project, stakeholder needs, and the technical requirements necessary to meet those needs were defined. This phase also included an analysis of the market, end users, lifecycle considerations for pothole maintenance solutions, and a review of existing patents and business models. Due to challenges involving public administrators, the design team identified stakeholder needs based on official reports and accumulated experience and then independently prioritized them.

The second phase focused on creating and selecting the optimal machine concept. The design team translated user needs into technical specifications and applied the Quality Function Deployment (QFD) method for analysis. Subsequently, the machine's primary functions were defined, potential solutions were generated using a morphological matrix, and the most suitable concept was selected using the Pugh decision matrix method [5,6].

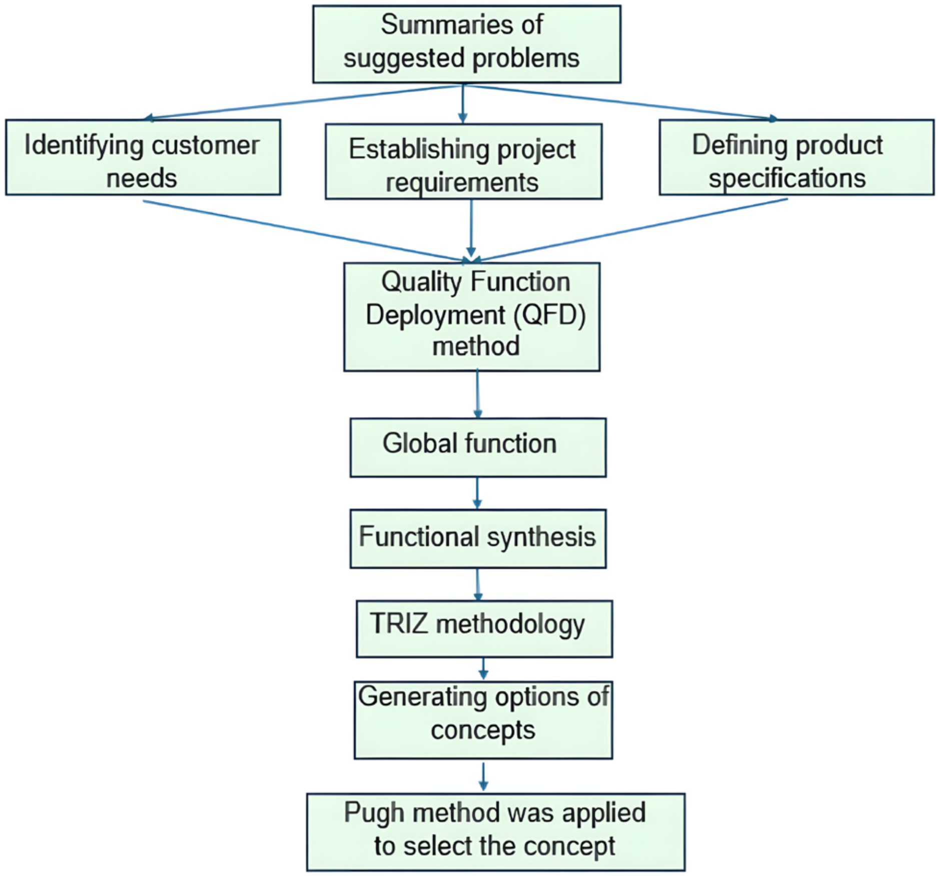
Results and Discussion

This section presents the decisions and outcomes of each step in the previously described methodology, along with the project's final product. The project began by thoroughly analyzing the problem and the market context. Government entities were identified as the primary potential customers, as they are chiefly responsible for managing and maintaining urban road infrastructure.Additional stakeholders include suppliers of raw materials and other inputs for the proposed solution. The direct users—contracted companies and their personnel—will operate the solution in the field.

Ultimately, the primary beneficiaries of the solution are road users, including drivers and passengers. The analysis of similar products and existing patents revealed numerous solutions that partially addressed the problem. Some featured a compact design or covered all required processes, while others were tailored to conditions outside the scope of this project. After identifying and translating customer needs into technical requirements, the QFD analysis was conducted. Table 1 illustrates the resulting matrix with the corresponding weights and stakeholder evaluations. The scores reflect the impact level of each requirement on fulfilling the related need without assessing the qualitative effect (positive or negative). The scale adopted was 0 for no impact, 1 for low impact, 3 for moderate impact, and 6 for high impact. Based on these values and stakeholder-assigned weights, it was possible to determine the most critical requirements for the project.

After analyzing the market, interfaces, lifecycle solutions, and stakeholders involved in the pothole maintenance scenario, a potential business model was proposed using the Business Model Canvas tool combined with functional synthesis. Based on this analysis, the route of filling potholes with precast plates was selected, as the team determined that this approach best addressed the project requirements. A morphological matrix was employed alongside the

Figure 2. The methodology applied in this work.



TRIZ methodology to support concept generation and selection.

The selected concept, illustrated in Figure 2, centers on integrating all necessary tools into a single piece of equipment capable of executing all stages of the maintenance process. The design includes a modular structure enabling automated tool replacement, storage of precast plates and bonding materials, and a dumping system. Furthermore, the equipment is designed to be self-propelled for short-distance operation and transportable over longer distances using a standard Munck truck.

Figure 4 presents the eight sequential steps defined during concept generation and solution development and the specific functions performed in each stage. The proposed machine incorporates a storage compartment for joint materials and debris, a forklift mechanism at the base for positioning precast elements, and a frontal tool alternating between an impact cutter and a vibrating compactor. It also features a vacuum for debris removal and a laser-guided marking system to delineate the cutting area. The machine is self-propelled and powered by a lithium-ion battery.

The proposed solution is considered technologically mature, integrating multiple well-established technologies in the market.

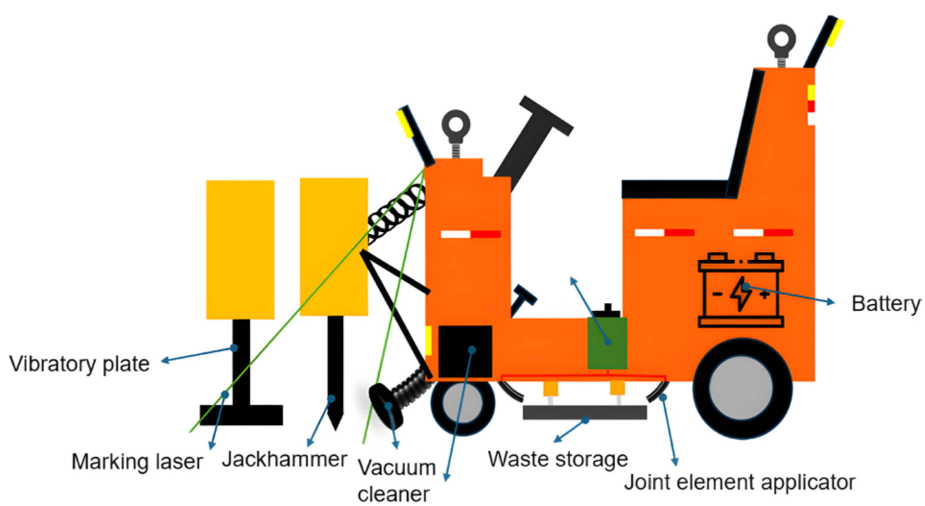
Conclusion

The methodology employed in this study proved robust and well-structured, fostering creativity among the team and enabling a comprehensive understanding of the problem addressed. The developed solution successfully met the identified functional requirements. The concept generation phase resulted in a design for equipment

Table 1. Needs and requirements of QFD.

#	Customer	Need	Customer's Weight	Customer's Rating	Intervention time	Daily productivity	Occupied area	Number of accidents	MTBF between interventions	Nº of operators	Nº of operations	Operation time	Solution volume	Solution mass	Acquisition cost	Operational cost
					min	#	m2	#	months	#	#	min	m3	kg	R$	R$
					↓	↑	↓	↓	↑	↓	↓	↓	↓	↓	↓	↓
N1	Driver	Reducing traffic congestion on roads	20%	7	6	3	6	3	0	3	3	6	6	0	1	1
N2		Avoiding risks for operators, drivers, and the population	20%	9	6	1	6	6	3	6	3	6	3	0	0	0
N3		To be long-lasting	20%	5	0	0	0	3	6	0	0	0	0	0	3	3
N4	Operator / User	Simplicity	30%	9	6	3	1	0	0	6	6	6	6	6	6	6
N5		Quick application time	30%	5	6	6	0	3	0	3	3	6	0	0	1	3
N6		Easy transportation	30%	7	3	6	1	1	0	6	0	3	6	6	3	3
N7	Public Authority	Reducing CAPEX and OPEX costs	50%	9	6	3	0	0	6	6	1	3	3	3	6	6

Figure 3. Sketch of the concept.



that promises reduced operation time, enhanced safety, minimized spatial footprint, and potentially lower costs. The proposed solution integrates multiple essential functionalities for pothole repair within a single, compact piece of equipment, demonstrating high technical feasibility and innovation.

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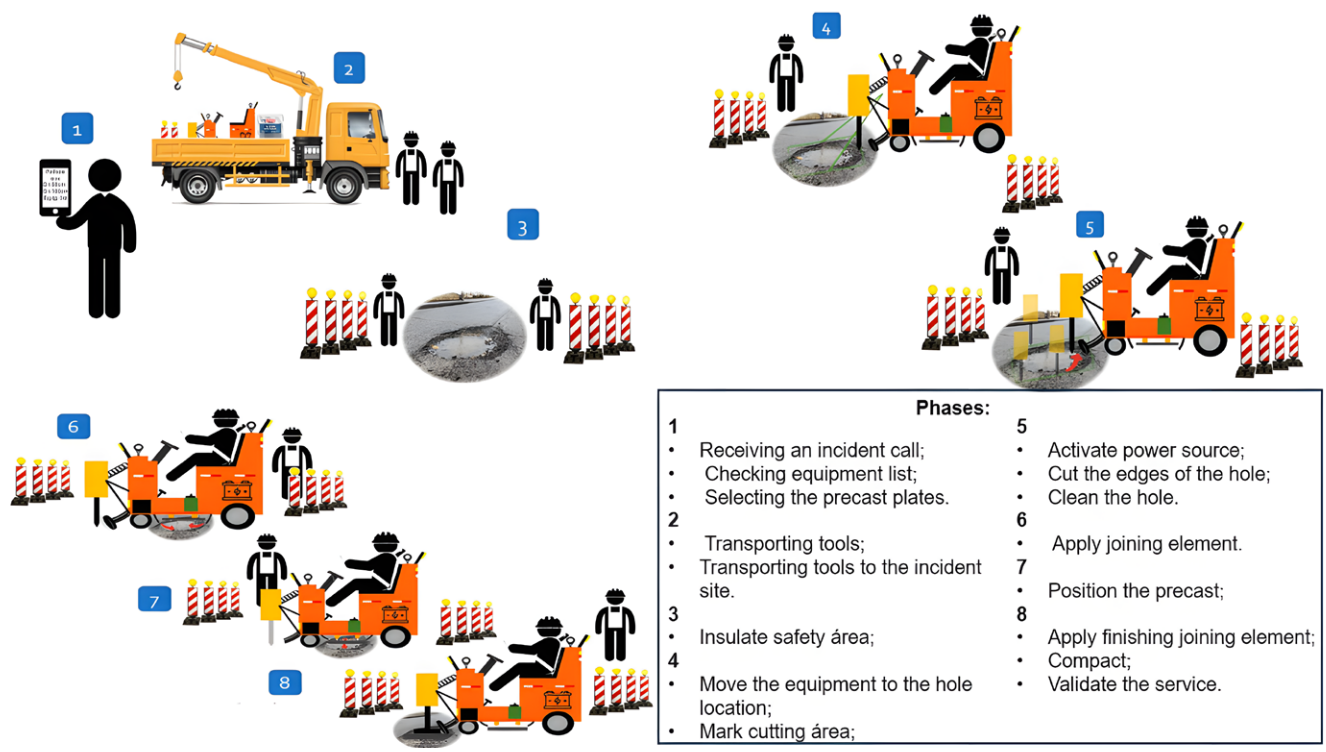
Figure 4. Concept operation phases.



approach to methodologies in product development processes.

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A Comprehensive RAM Analysis Tool Using Monte Carlo Simulations for the Oil and Gas Sector: Application and Comparison

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Ensuring the availability and reliability of complex systems, such as those in the oil and gas industry, is critical for operational efficiency and safety. Traditional analysis methods often struggle to account for the variability and uncertainty inherent in failure and repair processes, leading to suboptimal maintenance strategies. This paper introduces a Monte Carlo Simulation (MCS) tool for analyzing Reliability, Availability, and Maintainability (RAM). The tool accommodates various probability distributions and calculates key performance indicators such as availability, reliability, maintainability, and confidence intervals. Applied to a CO_2 separation plant case study, the results demonstrate the tool's enhanced capability to capture a broader range of performance metrics compared to traditional analytical methods.
Keywords: RAM Analysis. Reliability. Availability. Monte Carlo Simulation.

System reliability and availability are fundamental to maintaining operational efficiency and safety in energy, transportation, and manufacturing industries. Traditional methods—such as Fault Tree Analysis (FTA) and Reliability Block Diagrams (RBD)—offer valuable insights into component interactions and potential failure pathways. However, as systems become increasingly complex, these approaches often fail to capture the inherent variability and uncertainty of failure and repair processes. This can hinder accurate system performance prediction and lead to ineffective maintenance planning.

To overcome these limitations, this paper presents a Monte Carlo Simulation (MCS) tool developed in Python, designed to enhance RAM analysis in complex systems. The tool offers a more robust and realistic assessment than conventional analytical methods by simulating a wide range of failure and repair scenarios. The tool is applied to a CO_2 separation plant as a case study. Its results are benchmarked against traditional methods, demonstrating its ability to provide comprehensive and insightful system performance evaluations.

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Theoretical Background

Fault Tree Analysis (FTA)

Fault Tree Analysis (FTA) is a structured analytical method used to identify the root causes of failures in complex systems. The analysis starts with a top event—typically a critical system failure—and systematically traces backward through intermediate and basic events to identify underlying causes [1]. Logical gates such as "AND" and "OR" are used to model the interactions between events: "AND" gates indicate that all input failures must occur for the output failure to happen, while "OR" gates require only one input failure.

Each basic event in the fault tree is assigned a failure rate, which enables the computation of the top event's probability. Minimal cut sets—the smallest combinations of basic events that can cause the top event—are critical for highlighting system vulnerabilities. These insights inform the design of redundancy measures and risk mitigation strategies to reduce the likelihood of catastrophic failures [2].

Reliability, Availability, and Maintainability (RAM) Analysis

Reliability, Availability, and Maintainability (RAM) analysis is a comprehensive approach to evaluating the operational performance of complex systems throughout their lifecycle. Reliability refers to the probability that a system will perform its intended function under specified conditions for a given period. Availability measures the time a system is operational and accessible when needed. Maintainability evaluates the ease and speed with which a system can be restored to operational status after a failure [3].

RAM analysis integrates these three dimensions to inform effective maintenance and operational strategies. While analytical methods such as FTA provide high accuracy for systems with limited complexity, they often lack the flexibility to address systems with numerous interdependencies and stochastic behavior. In contrast, numerical methods like Monte Carlo Simulation enable uncertainty modeling in failure and repair processes, making them particularly effective for evaluating repairable systems and capturing real-world performance variability.

Table 1 summarizes the applicability of stochastic metrics and performance measures across analytical and numerical approaches.

Monte Carlo Simulation

Monte Carlo Simulation (MCS) is a statistical technique widely used to evaluate complex systems' reliability, availability, and maintainability (RAM) by modeling the inherent uncertainty and variability in system behavior. It involves performing numerous simulation iterations to produce a distribution of possible outcomes based on probabilistic models for failure and repair rates.This makes MCS especially effective in scenarios where traditional analytical methods are inadequate due to system complexity or interdependencies [4].

The approach relies on historical failure and repair data to define appropriate probability distributions—such as exponential, Weibull, and log-normal—for modeling time-to-failure and time-to-repair for individual components. The simulation process includes defining the system configuration, sampling failure and repair times, and simulating system operation over time to assess performance under realistic conditions [4].Key performance indicators (KPIs), including reliability, availability, and maintainability, are computed and aggregated across simulations to generate probabilistic outcome distributions.

Materials and Methods

This section presents the methodology implemented in the developed RAM analysis tool, which integrates Monte Carlo Simulation. The method is designed to systematically evaluate the dynamic behavior of systems under varying operational conditions.

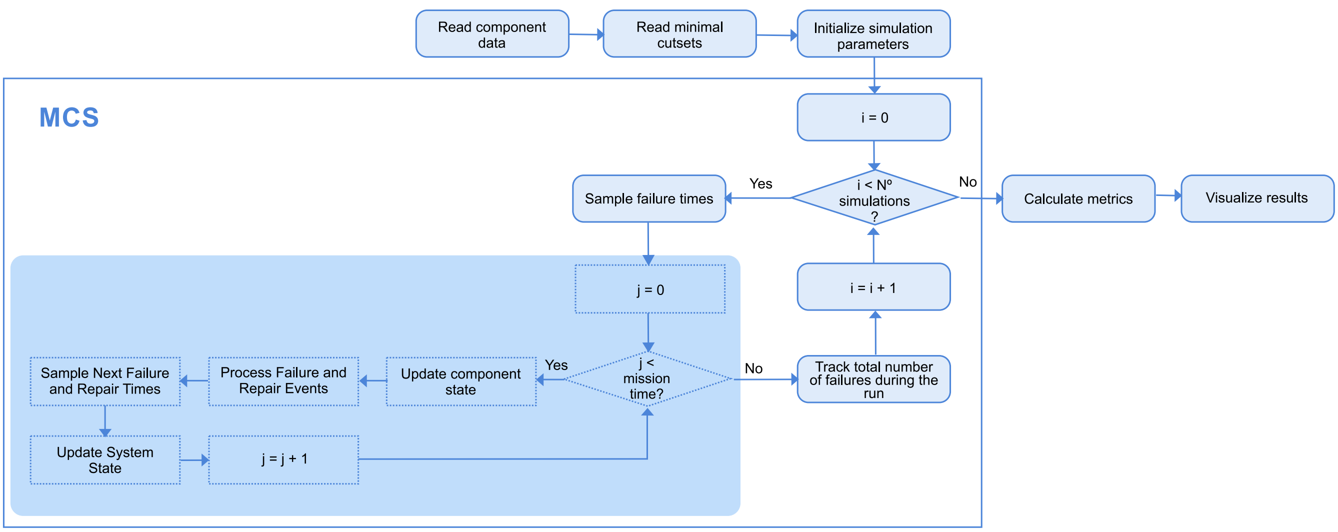
Figure 1 illustrates the methodological flowchart detailing the sequential steps during the simulation process. These include system definition, selection of statistical distributions, simulation execution, and computation of performance metrics.

The developed tool follows a structured simulation process as described below:

Table 1. Applicability of stochastic measures in discrete-time and repairable continuous-time methods.

	Reliability	Availability	MTTF	MTTR	ENF
Discrete-time	✓				
Repairable Continuous-time	✓	✓	✓	✓	✓

Figure 1. Flowchart of RAM analysis algorithm.



Read Component Data: The tool begins by importing system component data, including failure and repair rates, Mean Time Between Failures (MTBF), and Mean Time to Repair (MTTR). Users can define probability distributions for time-to-failure and time-to-repair, with optional input of additional parameters for modeling complex statistical behaviors.

Read Minimal Cut Sets: Minimal cut sets derived from Fault Tree Analysis (FTA) are loaded. These sets represent the smallest combinations of component failures that can lead to system failure. This step is essential for identifying critical failure paths and prioritizing components for maintenance or redundancy planning.

Initialize Simulation Parameters: The simulation is initialized by specifying the number of Monte Carlo iterations (N), the total mission time, and the time step increment used to advance the simulation.

Monte Carlo Simulation Process: The core of the methodology includes the following steps:

i. Simulation Loop: Executes the defined number of simulation runs.
ii. Sampling Failure Times: Generates failure and repair times for each component using the selected probability distributions.
iii. Mission Time Loop: Iteratively simulates system behavior across the mission time.
iv. Processing Failure and Repair Events: Dynamically updates component statuses based on sampled event timings.
v. Updating Component States: Continuously reflects real-time changes in the operational status of each component.
vi. Tracking Failures: Logs component and system failures throughout the simulations for performance evaluation.

Calculate Metrics: Upon completion, the tool computes key metrics, including availability, reliability, maintainability, the expected number of failures, time-to-failure and time-to-repair histograms, and confidence intervals.

Visualize Results: Output metrics are presented graphically to enhance interpretation. Visuals include probability distribution plots, performance indicator trends, and comparative charts, supporting robust decision-making.

Case Study

The proposed tool was applied to a case study involving a CO_2 separation membrane testing system to remove carbon dioxide from natural gas streams. The system includes 30 critical components, such as valves, heat exchangers, filters, and control units. Failures may occur individually or in combination, as identified by predefined minimal cut sets. To ensure confidentiality, all component input data were anonymized and slightly altered without compromising the structure, relationships, or integrity of the system model. This preserves the study's analytical value while protecting sensitive operational details.

Results and Discussion

This section compares results from the analytical and numerical approaches applied to the CO_2 separation plant. It highlights each method's strengths, limitations, and implications in terms of predictive power, accuracy, and applicability to real-world maintenance strategies.

Analytical Solution

The analytical approach evaluated system reliability over a one-year mission time (8,640 hours) using Fault Tree Analysis (FTA). Reliability was computed by assessing the failure probabilities of interconnected components at monthly intervals. However, since this method does not incorporate repair events, it tends to overestimate system degradation and does not reflect the dynamic nature of system recoverability.

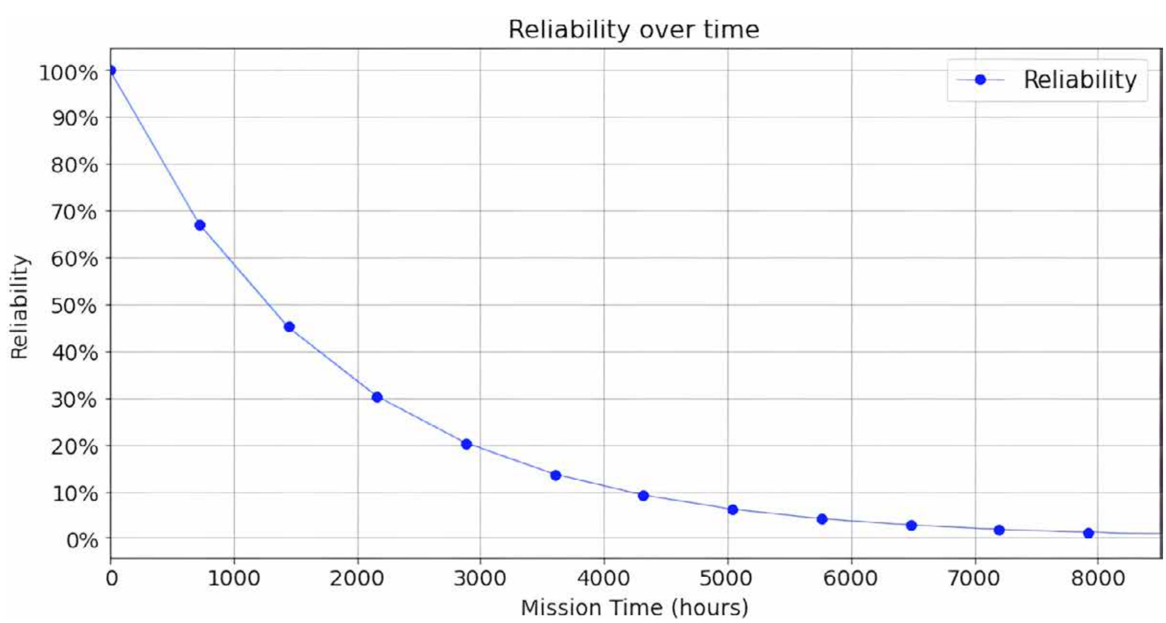
Reliability

As illustrated in Figure 2, the system's reliability follows an exponential decay over time, with noticeable declines at each monthly checkpoint. This trend reflects the cumulative effect of component aging and increased failure risk. Although the analytical method provides a valuable baseline and identifies critical weak points, its inability to model repairs limits its relevance for systems where downtime recovery is a key factor.

Numerical Solution

The numerical assessment of the CO_2 separation system's Reliability, Availability, and

Figure 2. System reliability - Analytical solution.



Maintainability (RAM) was conducted using Monte Carlo Simulations (MCS) over varying mission times. This approach captures the stochastic nature of system behavior by simulating numerous operational scenarios, thus enabling a more detailed and realistic evaluation of system performance.

Reliability

The system's reliability was analyzed over a mission time of 8,640 hours (one year) using Monte Carlo simulations with sample sizes of 1,000, 10,000, and 100,000 runs. Figures 3(a) and 3(b) illustrate the reliability curves of 1,000 and 100,000 simulations, respectively.

As observed, increasing the number of simulations leads to smoother reliability curves and narrower confidence intervals, reflecting reduced statistical uncertainty. In Figure 3(a), the reliability curve derived from 1,000 simulations shows greater variability and a wider confidence interval, indicating less precision. In contrast, Figure 3(b), based on 100,000 simulations, displays a notably smoother curve with a significantly narrower—almost imperceptible—confidence interval attributable to the Law of Large Numbers [5].

This result underscores adequate sample sizes' critical role in enhancing reliability estimates' accuracy and robustness, especially in complex systems where variability and interdependencies among components can influence overall behavior.

Maintainability

The maintainability of the CO_2 separation system was assessed using time-to-repair (TTR) data generated through Monte Carlo simulations. Figure 4(a) displays the TTR histogram from 100,000 simulations, while Figure 4(b) provides a focused view of the top 81.7% of the dataset. The Mean Time to Repair (MTTR) was calculated as 100.97 hours, establishing a baseline for expected downtime. However, MTTR alone does not adequately reflect the full distribution and variability of repair durations.

The histogram was segmented into bins (Figure 4b) to enhance interpretability, offering a more granular understanding of system performance across various repair scenarios. The TTR data can be characterized by a Probability Density Function (PDF), whose integral over time yields the Cumulative Distribution Function (CDF), representing system maintainability.

Figure 5 presents the maintainability CDF, which enables the estimation of the probability of repair completion within a given time frame. For instance, the analysis reveals that approximately 60% of repairs are completed within 102 hours. Although a specific distribution fit (e.g., Weibull or log-normal) was not performed, the use of Monte Carlo simulations proves valuable for capturing the inherent variability in maintainability across complex, multi-component systems.

Availability

The availability of the CO2 separation system was evaluated using Monte Carlo simulations over mission times of 1, 6, and 12 months, with sample sizes of 1.000, 10.000, and 100.000 runs. Table 2 details the average availability and confidence intervals for each period.

As the number of simulations increases, the confidence intervals for mean availability narrow, consistent with the behavior observed in the reliability analysis. For example, using 1,000 simulations over one month, the 95% confidence interval for availability is relatively wide, ranging from 93.64% to 94.99%. However, with 100,000 simulations, the interval becomes significantly narrower, indicating more accurate and reliable estimates.

Figures 6(a) and 6(b) illustrate the availability curves generated from 1,000 and 100,000 simulations. Both graphs show that availability is initially high but gradually declines over time as system failures accumulate. Eventually, the curves reach a plateau, suggesting that the system enters a steady-state condition prior to the end

Figure 3. System reliability for 1,000 (a) and 100,000 simulations (b).

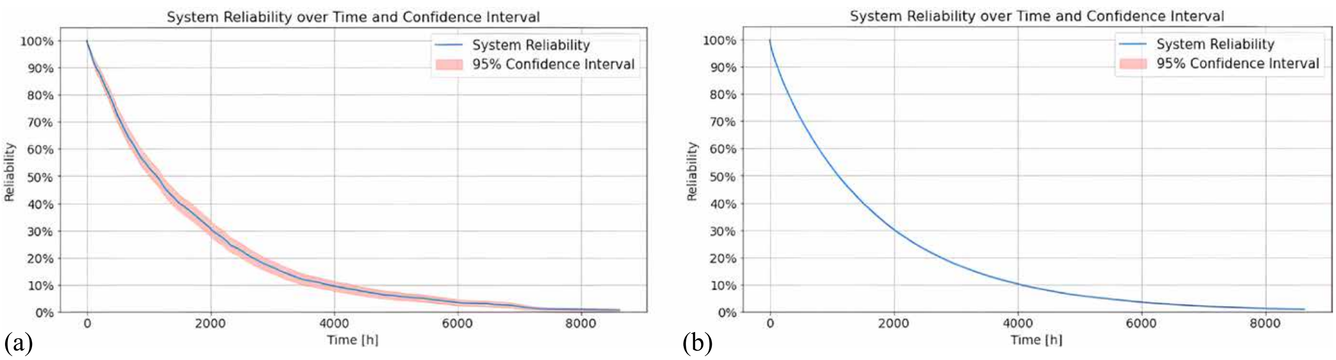


Figure 4. Histogram of all Times to Repair (a) and histogram of the 81,7 percentile of the Times to Repair (b).

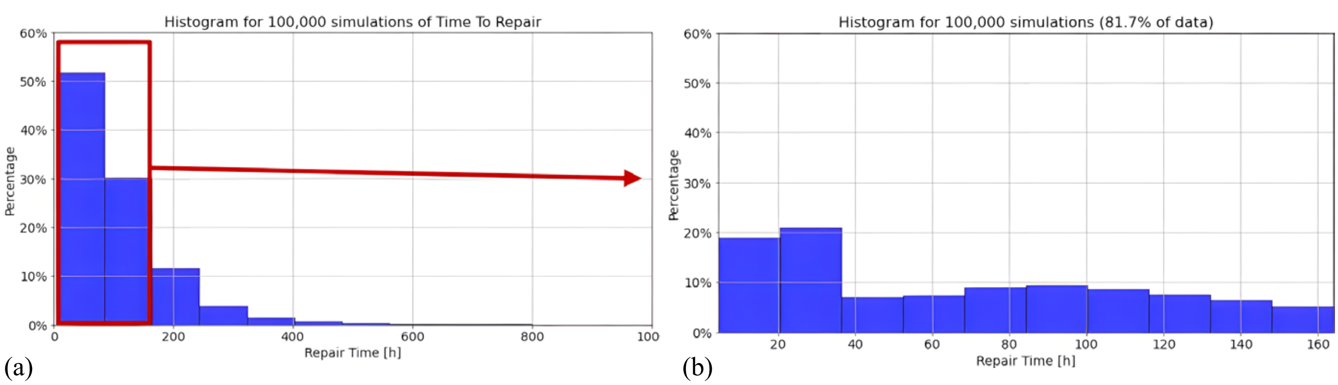


Figure 5. CDF of repair times.

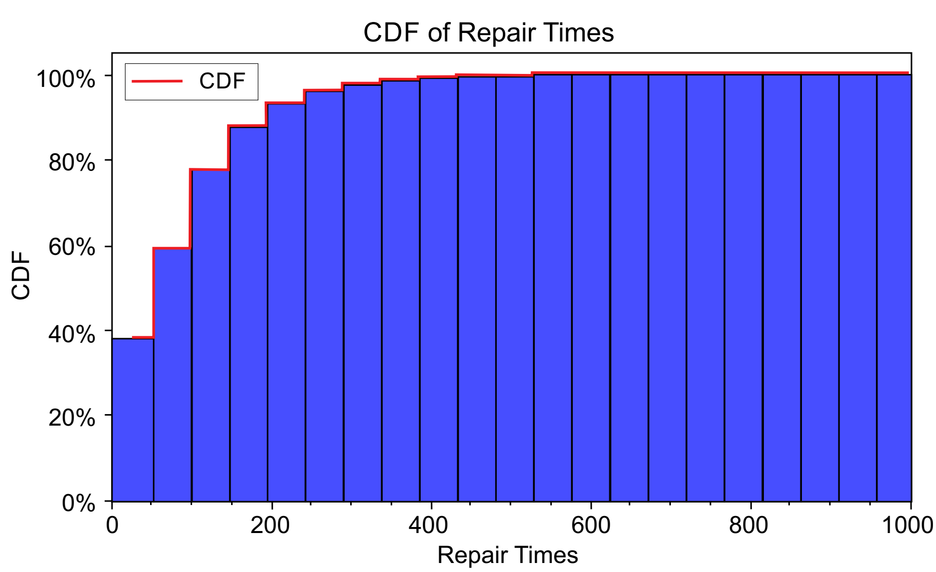
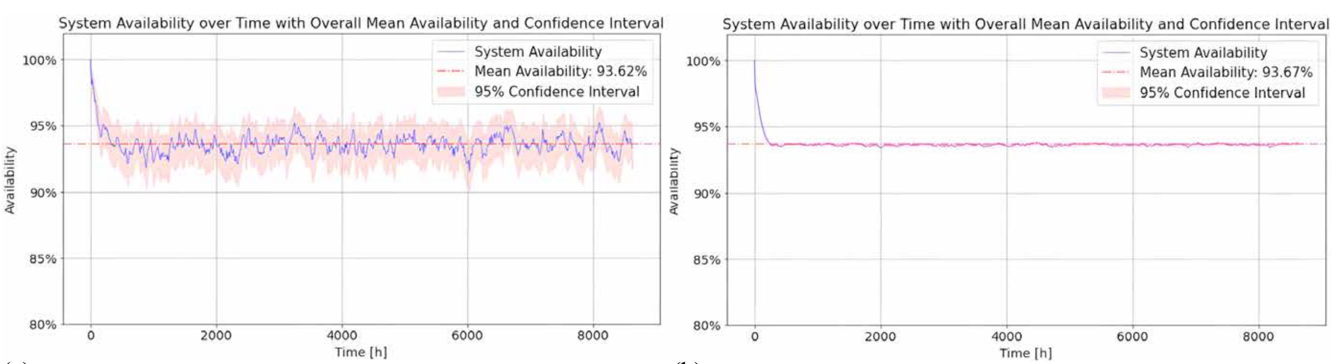


Table 2. Availability results per month.

Mission Time (months)	Number of simulations	Availability	5% percentile	95% percentile
1	1,000	94.31%	93.64%	94.99%
	10,000	94.38%	94.16%	94.59%
	100,000	94.35%	94.28%	94.42%
6	1,000	93.73%	93.43%	94.03%
	10,000	93.73%	93.62%	93.82%
	100,000	93.70%	93.67%	93.73%
12	1,000	93.75%	93.52%	93.97%
	10,000	93.67%	93.60%	93.75%
	100,000	93.67%	93.65%	93.69%

Figure 6. System availability for 1.000 simulations (a) and 100,000 simulations (b).



(a) (b)

of the mission period. This behavior reflects the balance between failure and repair processes and underscores the value of Monte Carlo simulations in capturing system dynamics over extended operational timelines.

Conclusion

The Monte Carlo Simulation (MCS) tool for Reliability, Availability, and Maintainability (RAM) analysis demonstrated significant advantages in evaluating complex systems, as evidenced by the CO_2 separation plant case study. Compared to traditional analytical methods, the MCS approach delivers more precise and comprehensive insights by incorporating the stochastic variability of failure and repair processes.

This results in narrower confidence intervals and more accurate predictions of system performance. The tool effectively simulates various operational scenarios and calculates key performance indicators—including availability, reliability, maintainability, and the expected number of failures—supporting data-driven maintenance planning and operational decision-making.

In the case study, the model estimated 6.02 individual failures and 4.5 system-level failures over 8,640 hours with 100,000 simulations, providing essential input for preventive and corrective maintenance strategies.

Overall, the findings highlight the relevance and potential of numerical simulations in enhancing the robustness, safety, and efficiency of critical infrastructure in the oil and gas industry and other high-reliability sectors.

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Mathematical Modeling and Kinetic Study of Deep Hydrodesfulfurization of Dibenzothiophenes Using $CoMoP/Al_2O_3$ Catalyst

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Deep hydrodesulfurization (HDS) is a highly effective process for removing sulfur from petroleum and its derivatives, achieving ultra-low sulfur levels, improving fuel quality, and reducing air pollution. This study estimates kinetic parameters for the HDS process using experimental data for dibenzothiophene (DBT) and 4,6-dimethyldibenzothiophene (4,6-DMDBT) on a $CoMoP/Al_2O_3$ catalyst in a fixed-bed reactor. A global power-law model provided the best fit for each dataset ($R^2 > 0.99$), while a single individual model was suitable across all data. The estimated reaction order concerning hydrogen was 0 for DBT and 1 for 4,6-DMDBT. Pre-exponential Arrhenius constants and activation energies (ranging from 90–100 kJ/mol) were also estimated and can be applied to reactor design and process optimization in HDS systems.
Keywords: Deep Hydrodesulfurization Reaction. $CoMoP/Al_2O_3$. Kinetic Modeling. Dibenzothiophene. 4,6-Dimethyldibenzothiophene.

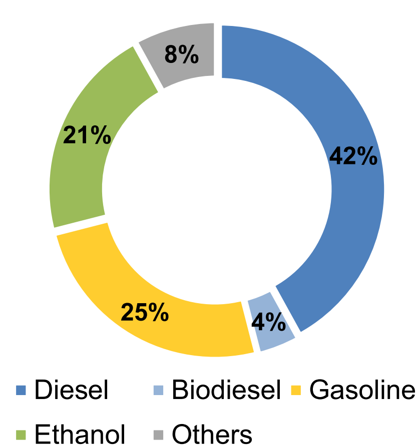
Air pollution and the environmental impact caused by high sulfur emissions from fossil fuels are pressing global concerns. When sulfur-containing fuels are combusted, sulfur dioxide (SO_2) is released into the atmosphere, forming acid rain. SO_2 is also toxic, corrosive, and detrimental to infrastructure and ecosystems. Furthermore, nitrogen oxides formed during combustion exacerbate air pollution and pose severe risks to human health [1].

In Brazil, the transport sector accounts for 33% of primary energy consumption, relying heavily on diesel due to the predominance of road transport, as shown in Figure 1. To mitigate emissions, stricter regulations have been implemented, including ultra-low sulfur diesel (ULSD) standards. ANP Resolution No. 968/2024 mandates a maximum sulfur content of 10 ppm (S-10 diesel) in urban areas, while rural regions still utilize S-500 diesel, containing up to 500 ppm of sulfur. Since 2013, the use of S-10 diesel has significantly increased, currently comprising 60% of national diesel production. A complete transition to S-10 is projected within the next decade [2]. However, achieving this goal requires improved efficiency in petroleum product hydrotreatment (HDT) units. HDT is essential for purifying feedstocks and removing contaminants through hydrogenation reactions, among which hydrodesulfurization (HDS) is specifically responsible for sulfur removal.

<u>Hydrodesulfurization (HDS)</u>

Although the HDS process is well established, achieving ultra-low sulfur levels through deep HDS remains challenging due to the complexity of

Figure 1. Fuel Consumption in Brazil.



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fuel compositions and the simultaneous removal of other contaminants. Many compounds present in the feedstock or formed during HDT reactions compete for the catalyst's active sites, thereby reducing HDS reaction rates. Nitrogen-containing compounds, in particular, inhibit the reaction by adsorbing onto the catalyst surface and delaying hydrogen activation. Additionally, coke formation, promoted by heterocyclic nitrogen compounds, significantly shortens catalyst life [3].

Modeling HDS is complex but vital for optimizing process conditions, maximizing sulfur removal efficiency, and minimizing costs. Hydrogen, a key input in this process, typically supplied in excess to increase conversion, often represents the second-highest operational cost in refineries [4]. Improving process efficiency enhances sulfur removal and reduces energy and material costs. Therefore, accurate modeling of deep HDS reactions is critical for meeting S-10 diesel production goals.

Among the primary sulfur-containing compounds in diesel, dibenzothiophene (DBT) and 4,6-dimethyldibenzothiophene (4,6-DMDBT) are recognized as the most refractory. As shown in Figure 2, both compounds transform two parallel reaction pathways. In the direct desulfurization (DDS) route, DBT and 4,6-DMDBT produce hydrogen sulfide (H_2S) and biphenyl (BPH), leading to products such as cyclohexylbenzene (CHB) or 3,3’-dimethylbiphenyl (3,3’-DMBPH). In the hydrogenation (HYD) route, DBT undergoes hydrogenation of one of its aromatic rings to form an equilibrium mixture of tetrahydrodibenzothiophene (THDBT) and hexahydrodibenzothiophene (HHDBT), which are rapidly converted to CHB. For 4,6-DMDBT, the hydrogenation pathway yields products such as methyl cyclohexyl toluene (MCHT) or dimethyl cyclohexane (DMBCH) alongside H_2S [5].

Materials and Methods

Figure 3 shows the steps taken to achieve the research objective.

Development of the Parameter Estimation Procedure

The selected mathematical models were implemented using the Environment for Modeling, Simulation, and Optimization (EMSO) software [6], employing the EML (EMSO Modeling Library), an open-source modeling language. The resulting systems of algebraic differential equations from the predefined models were solved using a multi-step integration method with the DASSLC integrator [7], applying relative and absolute tolerances of 10^{-6} and 10^{-8}, respectively.

Parameter estimation was performed using the Nelder and Mead flexible polyhedron optimization method, with relative tolerances of 10^{-6} for both the objective function and the estimated parameters [8]. The global optimum was ensured by initializing the optimization procedure from multiple starting points within the predefined lower and upper parameter bounds.

The parameter estimation results were subjected to statistical evaluation using tests integrated into EMSO, including the Student's t-test and Fisher's F-test, both conducted at a 95% confidence level. The Chi-square test was also employed to assess the goodness-of-fit of the estimated models concerning the objective function value.

Kinetic Models

For the formulation of mass conservation equations, the reactions were considered irreversible. The hydrogen was assumed to be in excess, and the catalyst bed was modeled as isothermal. The hydrogen concentration in the liquid phase and the maximum degree of vaporization of the solvents and reactants were estimated for each experimental condition. A flash calculation that employed the Soave-Redlich- Kwong equation of state to represent all components in the feed mixture were used in HYSYS do determine these parameters.

In accordance with existing literature [3], power-law models were selected to describe the

Figure 2. HDS Reaction scheme for DBT and 4,6-DMDBT.

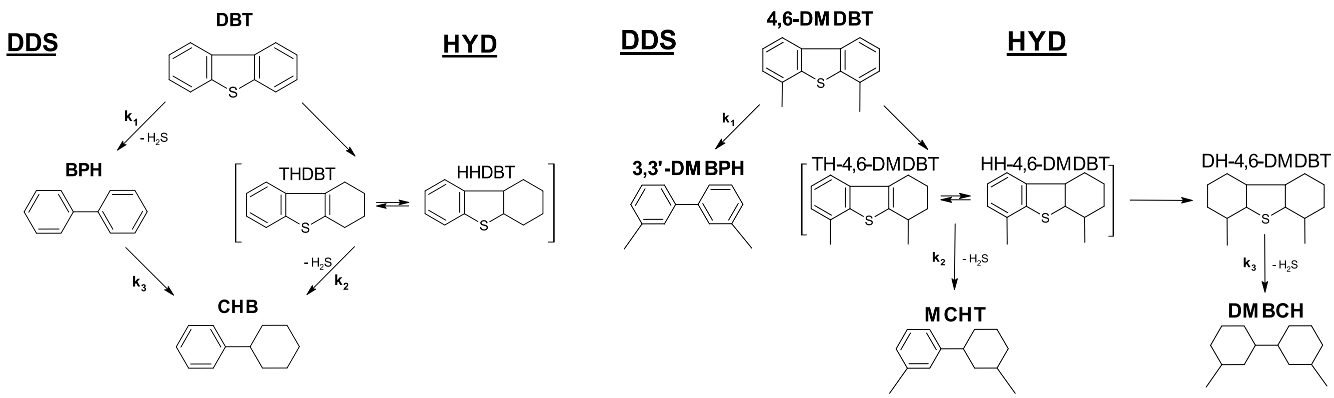
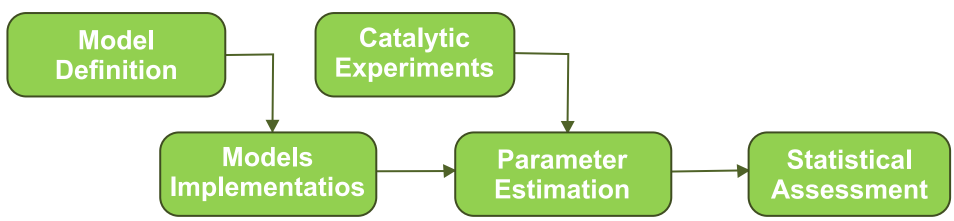


Figure 3. Method flowchart.



reaction rate, as shown in Table 1. Global models were used to evaluate the overall behavior of the HDS process and the conversion of sulfur-containing reactants. Meanwhile, individual models (Table 2) were developed to investigate the detailed reaction mechanisms and the intermediate and final product formation rates in each pathway.

To minimize parameter correlation during estimation, the kinetic parameters were reparameterized using a modified Arrhenius equation with a reference temperature (T_{ref}), as proposed by Schwaab and colleagues [9]:

$$k\ (T) = k_0 exp\left(-\frac{E_a}{RT}\right) = \ exp\ \left[-a + b\ \left(1 - \frac{T_{ref}}{T}\right)\right]$$

In this formulation, the pre-exponential factor (k_0) and activation energy E_a are replaced by the estimation parameters *a* and *b*, respectively. This transformation expresses the explicit temperature dependence of the reaction rate while reducing parametric correlation in the optimization procedure.

<u>Catalytic Experiments</u>

Initially, the procedure outlined in Section "Development of the Parameter Estimation Procedure" was validated using experimental data from previous studies conducted by the Laboratory for Development of Catalytic Processes (LDPC) [3]. These data were based on DBT, the model refractory compound, using a $CoMoP/Al_2O_3$ catalyst. Subsequently, new catalytic tests were carried out using 4,6-DMDBT, a more refractory compound, to investigate further the kinetic behavior under the technological challenge addressed in this study.

For both feedstocks, the experimental procedure followed the same protocol. The catalyst bed underwent two-step sulfidation with a 4 wt% carbon disulfide solution in *n*-hexane at a flow rate of 0.10 mL/min prior to reaction testing. All experiments were conducted in a fixed-bed reactor (PID Eng & Tech) operated in up-flow mode. Initial sulfur concentrations were 3500 mg/kg for DBT and 1000 mg/kg for 4,6-DMDBT, with *n*-hexadecane

Table 1. Global models evaluated in this work.

Name	Acronym	Models	
		DBT	4,6-DMDBT
Pseudo first Order Global Power Law	PGP	$r_{HDS} = kC_{DBT}$	$r_{HDS} = kC_{4,6-DMDBT}$
Second Order Global Power Law	SGP	-	$r_{HDS} = kC_{4,6-DMDBT}C_{H_2}$
Variable Orders Global Power Law	VGP	$r_{HDS} = kC_{DBT}^{\alpha} C_{H_2}^{\beta}$	-

Table 2. Individual models evaluated in this work.

Name	Acronym	Models	
		DBT	4,6-DMDBT
Individual Powers Law	IP	$r_{DBT} = -k_1C_{DBT} - k_2C_{DBT}C_{H_2}$ $r_{BPH} = k_1C_{DBT} - k_3C_{BPH}C_{H_2}$ $r_{CHB} = k_2C_{DBT}C_{H_2} + k_3C_{BPH}C_{H_2}$	$r_{4,6-DMDBT} = -k_1C_{4,6-DMDBT} - k_2C_{4,6-DMDBT}C_{H_2}$ $r_{3,3-DMBPH} = k_1C_{4,6-DMDBT}$ $r_{MCHT} = k_2C_{4,6-DMDBT}C_{H_2} - k_3C_{MCHT}C_{H_2}$ $r_{DMBCH} = k_3C_{MCHT}C_{H_2}$
Parallel Individual Power Law	PIP	$r_{DBT} = -k_1C_{DBT} - k_2C_{DBT}C_{H_2}$ $r_{BPH} = k_1C_{DBT}$ $r_{CHB} = k_2C_{DBT}C_{H_2}$	$r_{4,6-DMDBT} = -k_1C_{4,6-DMDBT} - k_2C_{4,6-DMDBT}C_{H_2}$ $r_{3,3-DMBPH} = k_1C_{4,6-DMDBT}$ $r_{MCHT} = k_2C_{4,6-DMDBT}C_{H_2}$

as the solvent. The gas-to-oil ratio was maintained at 400 (NL/L). Reaction progress was monitored using gas chromatography (Agilent 6890 N). The mass balance closure exceeded 95% for all experimental conditions and catalysts. The reactor achieved steady-state operation after approximately 5 hours for DBT and 7 hours for 4,6-DMDBT, with less than 2.0% conversion variations.

Experimental error was assessed through replicate measurements for each model compound. The operating conditions—temperature, pressure, and weight hourly space velocity (WHSV)—for the reference DBT dataset followed a three-level factorial design comprising 27 experiments. For 4,6-DMDBT, a partial factorial design of six experimental conditions was selected, matching the same variables. This subset was intended as a foundation for a sequential design to expand the parameter estimation dataset in the second phase. Table 3 presents the extreme values of each variable in the design.

The experimental error of the complete factorial design was calculated using the replica condition, which is the central point of all variables. The conditions for the partial planning were chosen to obtain information from the variable bounds and provide a well-distributed range of conversions. In this case, the conditions used to calculate the experimental and replication error were Temperature = 270 ºC, WHSV = 60 h^{-1}, and P = 60 bar.

Results and Discussion

Two global models were found to have acceptable adjustments ($R^2 > 0.99$) and statistical significance. Figure 4 show the model adjustment graphs for DBT and 4,6- DMDBT reagent concentration data, and Tables 4 and 5 show the results of parameter estimation.

The order for data with DBT was 0.4 ± 0.2 concerning the sulfur compound and zero concerning hydrogen. For 4,6-DMDBT, a global second-order model with an order of 1 concerning each reactant was the most appropriate. This parameter indicates whether the relevant step for

Table 3. Factorial planning conditions for experiments with each compound.

Variable	DBT		4,6-DMDBT	
	Minimum Value	Maximum Value	Minimum Value	Maximum Value
Temperature (°C)	210	270	240	300
Pressure (bar)	30	60	30	60
WHSV (h^{-1})	4	8	8	14

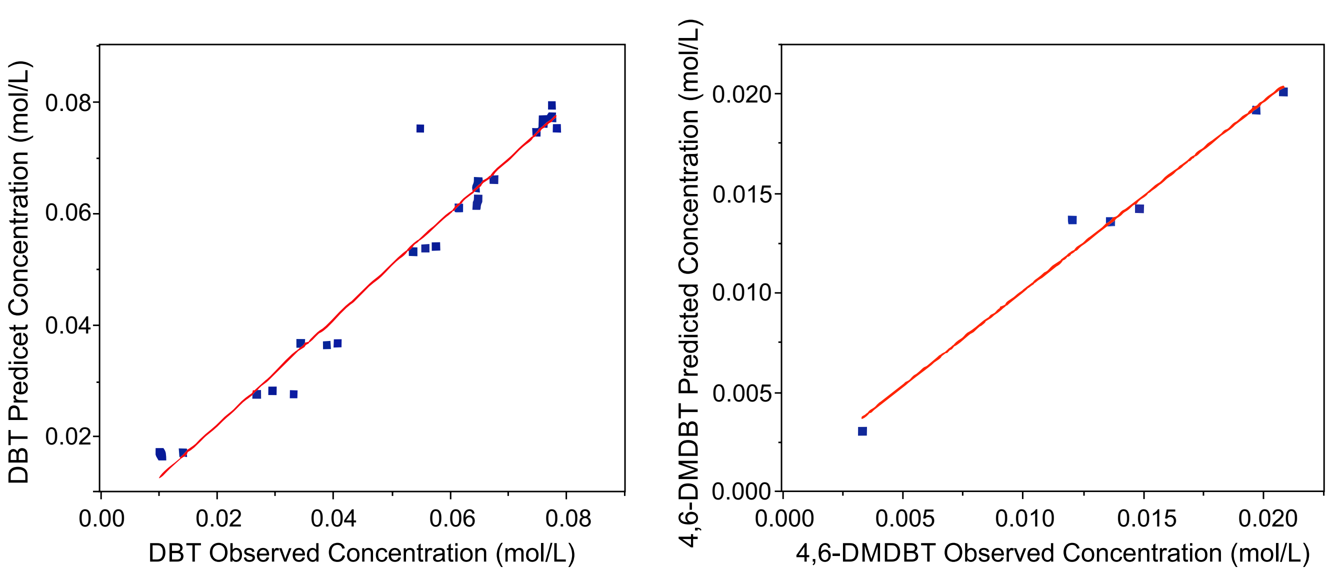
Table 4. Estimation results for global model with DBT.

Model	Parameter	Result
VGP	α	0.4 ± 0.2
	β	Not statistically significant
	a	5.0 ± 0.7
	b	24.1 ± 3.1
	E_a	86.3 ± 11.2
	$\ln k_0$	29.2 ± 3.8
	F_{obj}	24.2
	R^2	0.9902

Table 5. Estimation results for global model with 4,6-DMDBT.

Model	Parameter	Result
SGP	a	-2.7 ± 0.1
	b	19.6 ± 2.8
	E_a	88.6 ± 12.4
	$\ln k_0$	22.3 ± 2.7
	F_{obj}	15.2
	R^2	0.9948

Figure 4. Predicted *versus* observed concentrations for Global Models with DBT and 4,6- DMDBT, respectively.



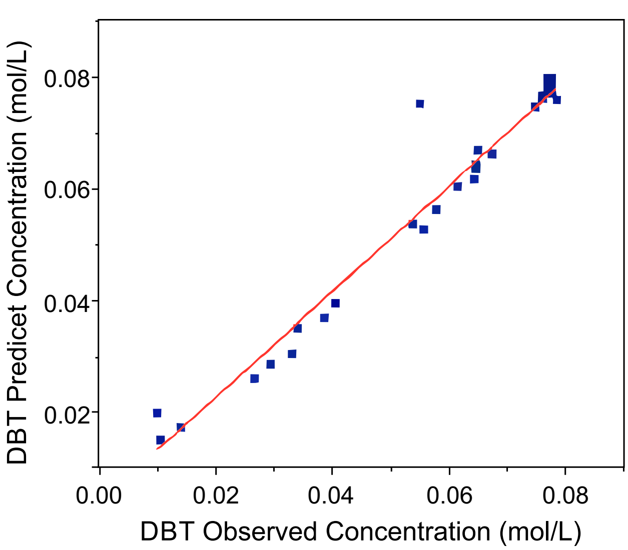
the reaction kinetics depends on hydrogen. The results indicate that DDS was the preferred route for the first compound, while for the second, it was HYD, as established in the literature [5]. In the individual models, the same model (PIP) presented acceptable fits ($R^2 > 0.98$), as shown in Figure 5 and parameters with statistical significance in Tables 6 and 7.

Figure 6 clearly shows that, despite the same models, the preferred routes for each representative compound have been inverted. The figure shows the rate of each product calculated by the models in the same temperature range (240 to 270°C). The formation rate of BPH and MCHT is higher than that of CHB and 3,3'-DMBPH, which corroborated the precedent that DDS was the dominant route for DBT, while 4,6-DMDBT predominantly followed the HYD pathway.

Conclusion

The evaluated kinetic models agreed well with the experimental data and yielded statistically significant parameters. Apparent activation

Figure 5. Predicted *versus* observed concentrations for Individual models with DBT and 4,6- DMDBT, respectively.



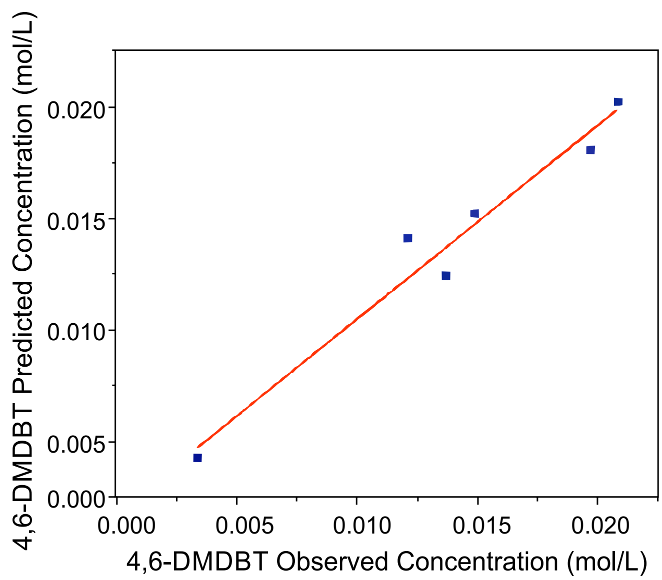


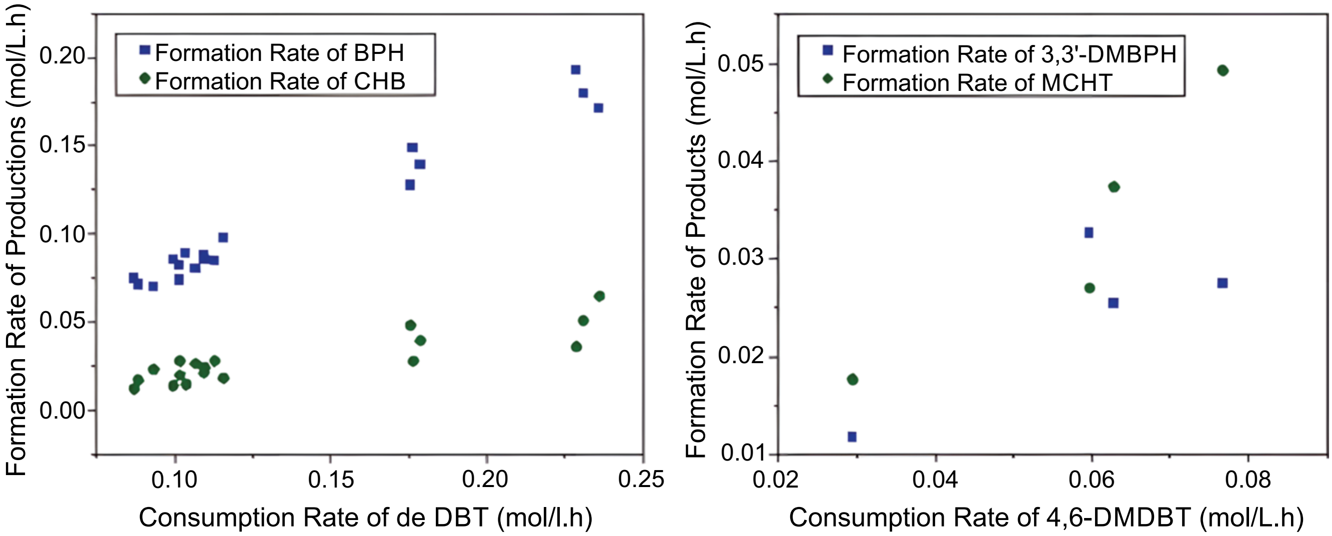
Table 6. Estimation results for best individual model with DBT.

Model	Parameter	Result
PIP	a_1	-1.5 ± 0.1
	b_1	22.7 ± 2.3
	E_{a_1}	100.5 ± 10.2
	$\ln k_{o_1}$	21.2 ± 2.4
	a_2	-1.7 ± 0.1
	b_2	22.7 ± 2.9
	E_{a_2}	101.3 ± 12.9
	$\ln k_{o_2}$	21.0 ± 3.0
	F_{obj}	89.9
	R^2	0.9884

Table 7. Estimation results for best individual model with 4,6-DMDBT.

Model	Parameter	Result
PIP	a_1	-0.6 ± 0.3
	b_1	19 ± 7
	E_{a_1}	87.6 ± 31.5
	$\ln k_{o_1}$	20.0 ± 6.7
	a_2	-2.1 ± 0.1
	b_2	19 ± 3
	E	85.5 ± 13.9
	$\ln k_{o_2}$	21.1 ± 3.0
	F_{obj}	180.2
	R^2	0.9843

Figure 6. Comparison of the product formation rate as a function of the reagent consumption rated.



energies were estimated in the 90–100 kJ/mol range, consistent with values reported in the literature. The more refractory nature of 4,6-DMDBT compared to DBT was confirmed by the need for a higher operating temperature range (240–300 °C for 4,6-DMDBT *vs.* 210–270 °C for DBT) to achieve similar conversion levels. The best-fitting global models highlighted differences in the estimated reaction order concerning hydrogen: 0 for DBT and 1 for 4,6-DMDBT. Likewise, the individual models enabled accurate predictions of product formation rates, showing the faster formation of biphenyl (BPH) for DBT and methyl cyclohexyl toluene (MCHT) for 4,6-DMDBT.

These findings reinforce the preference for different reaction pathways—DDS for DBT and HYD for the more refractory 4,6-DMDBT. These insights facilitate the adjustment of key operational parameters, such as temperature, pressure, and WHSV, for known refractory diesel feeds. They also support more accurate reactor design and process optimization to achieve ultra-low sulfur concentrations via hydrodesulfurization (HDS), ultimately enhancing fuel quality and reducing air pollution.

The next step involves conducting a sequential experimental plan to evaluate and estimate kinetic parameters for competitive reactions involving 4,6-DMDBT and nitrogen-containing compounds. This will yield a more realistic representation of refinery feed compositions while increasing laboratory efficiency through focused experimentation and more statistically robust parameter estimation.

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Predictive Maintenance Strategies for Heat Exchangers Applied in a Hybrid Project Management Framework for Oil and Gas Industries

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This study presents the development of a predictive maintenance model for heat exchangers in oil refineries, integrating agile methodologies within a structured project management framework. Conducted as a case study in an oil and gas company refinery, the research addresses challenges related to data accuracy, model reliability, and implementation. The hybrid methodology encompasses project scope definition, data collection from laboratory-scale and operational heat exchangers, and model development over 18 months. The model was validated and refined through rigorous testing, enabling the prediction of optimal cleaning schedules. Risk management strategies included applying a Risk Breakdown Structure (RBS) and SWOT analysis, resulting in optimized maintenance scheduling, cost reduction, and enhanced operational efficiency and safety. This approach provides a benchmark for improving oil and gas industry maintenance practices.
Keywords: Project Management. Predictive Maintenance. Hybrid Methods. Oil Refineries. Mathematical Models.

Project management is fundamental for successful complex ventures, particularly in the oil and gas industry, which faces significant challenges and risks. Heat exchangers are critical in this sector, ensuring facilities continuous and safe operation. These devices are essential for thermal energy exchange between fluids and are integral to oil refining and natural gas production [1,2].

The performance of heat exchangers can be severely impaired by the accumulation of deposits and fouling, which reduce heat transfer efficiency and increase operational costs [3]. Thus, strategically managing cleaning campaigns for these units requires careful planning and applying advanced predictive techniques [4].

Traditional maintenance approaches initially focused on immediate cost reduction, often neglecting long-term system reliability and availability. Maintenance practices began with Corrective Maintenance, evolving into Preventive Maintenance (PM)—a proactive approach to prevent failures. The increasing competitiveness of the oil and gas industry accelerated this transition [5]. The development of engineering concepts such as reliability, maintainability, availability, and lifecycle cost optimization emphasized the importance of minimizing equipment downtime. Consequently, preventive or scheduled maintenance became standard practice [6], eventually giving rise to modern techniques such as Condition-Based Maintenance (CBM), where maintenance decisions are driven by real-time machine condition data obtained through monitoring systems (Figure 1) [2].

In the oil and gas sector, where operations are continuous and highly complex, preventive and predictive equipment maintenance is critical [7].

Project management is vital in this context, offering significant improvements across various operational dimensions. The importance of this study can be summarized through the following contributions:

Reduction of Operational Costs: Fouling in heat exchangers increases energy consumption and necessitates frequent cleanings. An effective forecasting model can optimize maintenance schedules, yielding substantial cost savings [5].

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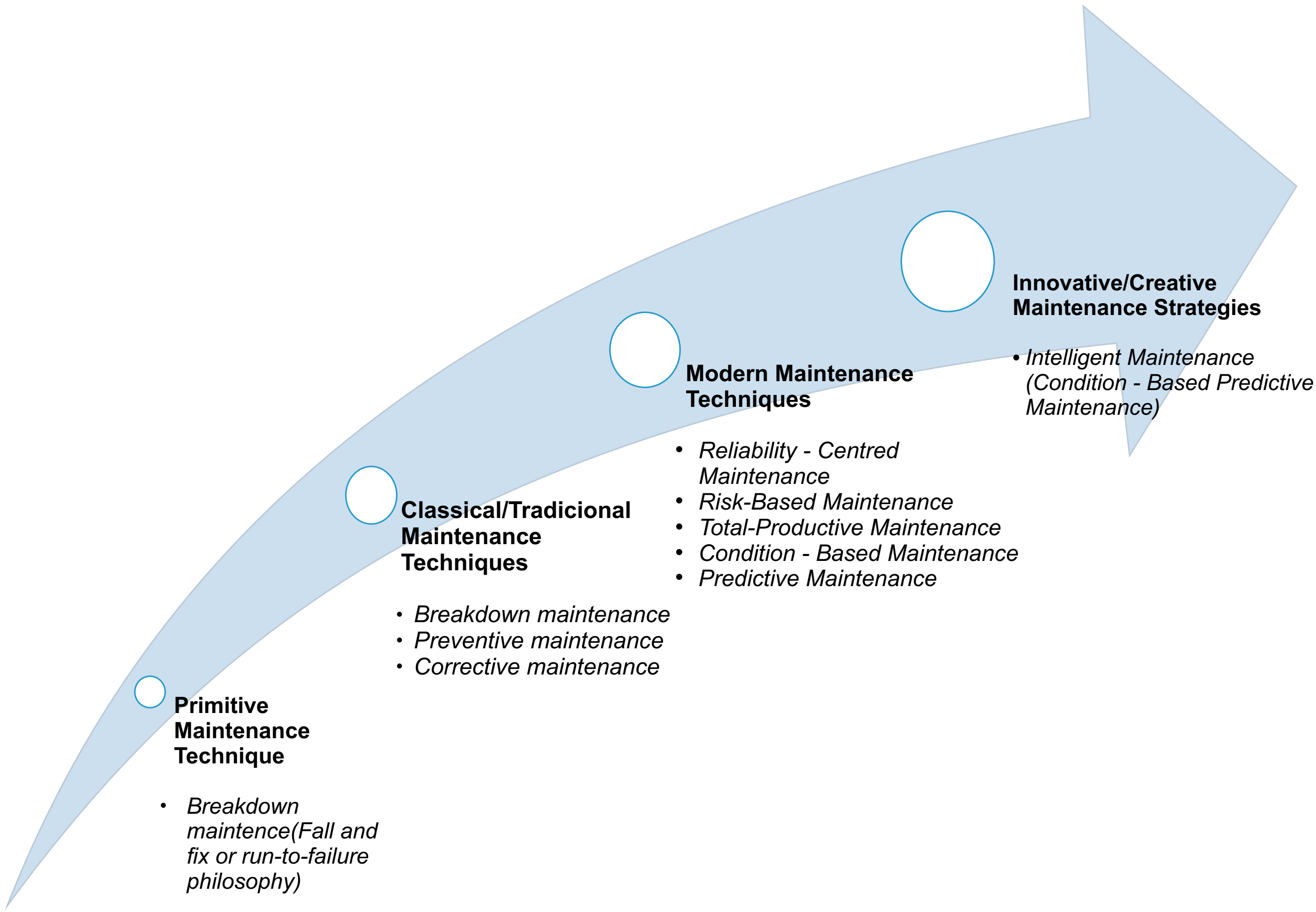
Figure 1. Evolution of industrial systems maintenance practices.



Adapted from Eyoh, & Kalawsky [2].

Extension of Equipment Lifespan: Properly managed predictive maintenance extends the operational life of heat exchangers by preventing severe degradation, thereby avoiding costly repairs or replacements [6].

Improved Operational Efficiency: Strategic project management ensures that heat exchangers operate optimally, enhancing overall process performance and contributing to the company's competitiveness [8].

Enhanced Operational Safety: Applying project management techniques to heat exchanger maintenance fosters safer industrial operations, minimizing the risk of equipment failure and associated hazards [9].

Strategic Planning Capability: Project management provides a systematic and structured approach to planning and executing cleaning campaigns, integrating technical, economic, and operational factors to achieve optimal results [3].

According to the most recent data from the Brazilian Ministry of Mines and Energy, the aggregate production of the country's oil refineries reached approximately 1.97 million barrels per day in 2020, translating to an estimated annual production of about 719 million barrels [10]. However, this output can vary significantly due to market demand, economic conditions, and refinery maintenance schedules. These fluctuations underscore the need for effective management strategies to ensure operational continuity and efficiency in Brazil's refining sector.

Therefore, the need for an effective forecasting model for heat exchanger maintenance in the oil and gas industry is evident. Such a model aims to determine the optimal timing for cleaning interventions, maximizing efficiency while minimizing maintenance costs [11]. This article explores the intersection between project management and predictive maintenance, presenting a methodological framework for developing and implementing an effective predictive model.

Materials and Methods

The method adopted in this study is grounded in applying a project proposal to a real case study conducted in 2019 at a refinery operated by an oil and gas company, as described by Souza and Marinho [12]. This practical approach was chosen to support the development of a robust mathematical model capable of predicting cleaning schedules for heat exchangers within preheat train systems.

Figure 2 illustrates the structure of the hybrid methodology, which incorporates the design of the project scope, time management, cost analysis, and risk assessment. These elements were integrated into the 18-month model development process.

Results and Discussion

A Work Breakdown Structure (WBS) is a fundamental project management tool used to define and organize a project's total scope by decomposing it into smaller, more manageable components. The WBS developed for the Cleaning Campaign Forecast Model for Heat Exchangers offers a comprehensive visual representation of the project's structure, delineating key phases such as Project Management, Acquisitions, Procurement, Development of the Mathematical Model, Testing and Certification, Project Outcome, and Closure [13].

Figure 3 presents the proposed WBS for the project. This structured approach ensures that all necessary tasks are clearly identified, appropriately assigned, and systematically executed. It facilitates effective planning, resource allocation, and monitoring of project progress.

Although the original case study adopted the Waterfall model, the current approach integrates both the Waterfall and Agile methodologies, particularly during the development and validation phases of the mathematical model for cleaning campaign prediction. This hybrid model ensures that project deliverables are aligned with the defined scope, schedule, and budget, while leveraging the flexibility of Agile practices to

Figure 2. Framework of the project.

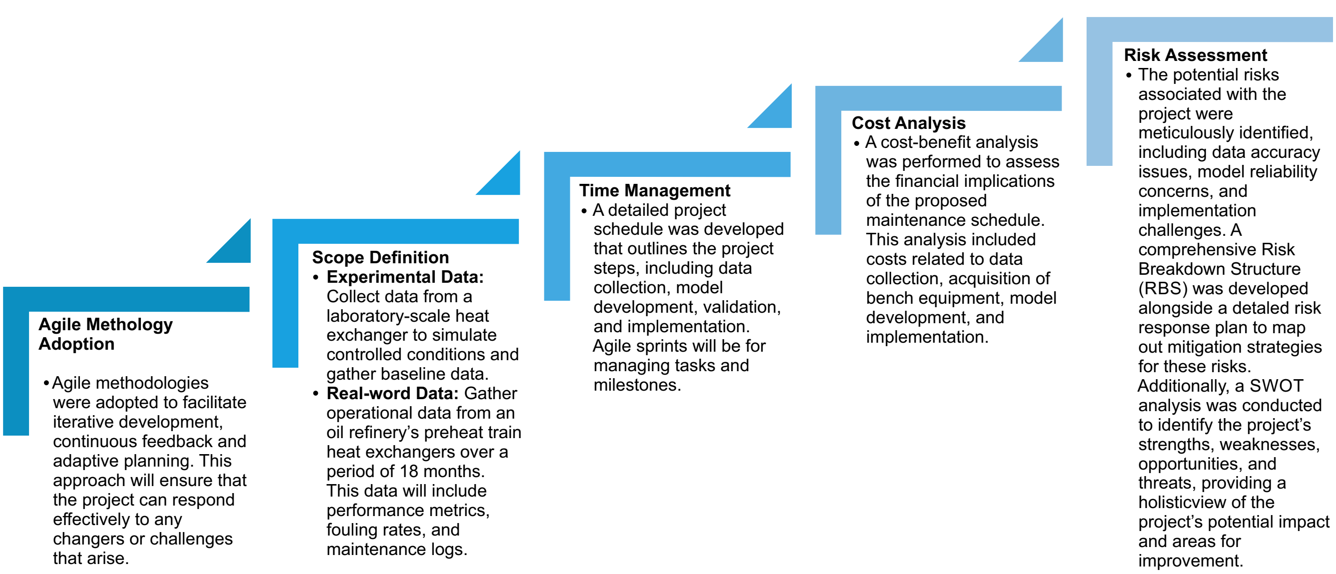
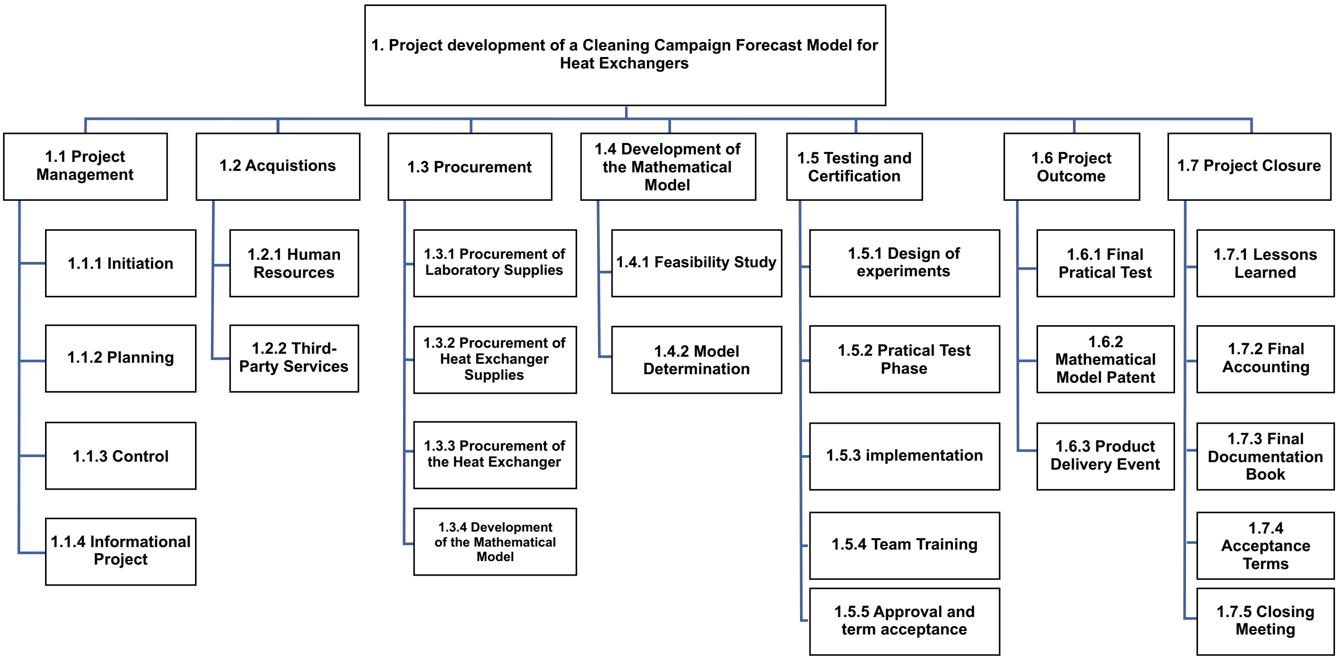


Figure 3. Project WBS.



accommodate evolving requirements and enhance the effectiveness of project execution.

In the Agile framework, the Scrum methodology organizes work into iterative cycles known as Sprints, typically lasting one month. These Sprints enable the development team to continuously refine and adapt the project as new insights and challenges emerge. The stages of the Scrum process implemented in this project include (Figure 4):

Sprint Planning: During this phase, the team defines the deliverables for the upcoming Sprint. The Product Owner prioritizes items in the Product Backlog, and the team selects tasks for the Sprint. These selected tasks are moved to the Sprint Backlog.

Daily Scrum: A short meeting is held to assess progress, discuss obstacles, and plan the day's work. This routine promotes transparency and synchrony within the team. Sprint Review: At the end of each Sprint, the team presents completed tasks to stakeholders. This stage offers an opportunity for feedback, validation, and adjustments based on practical insights.

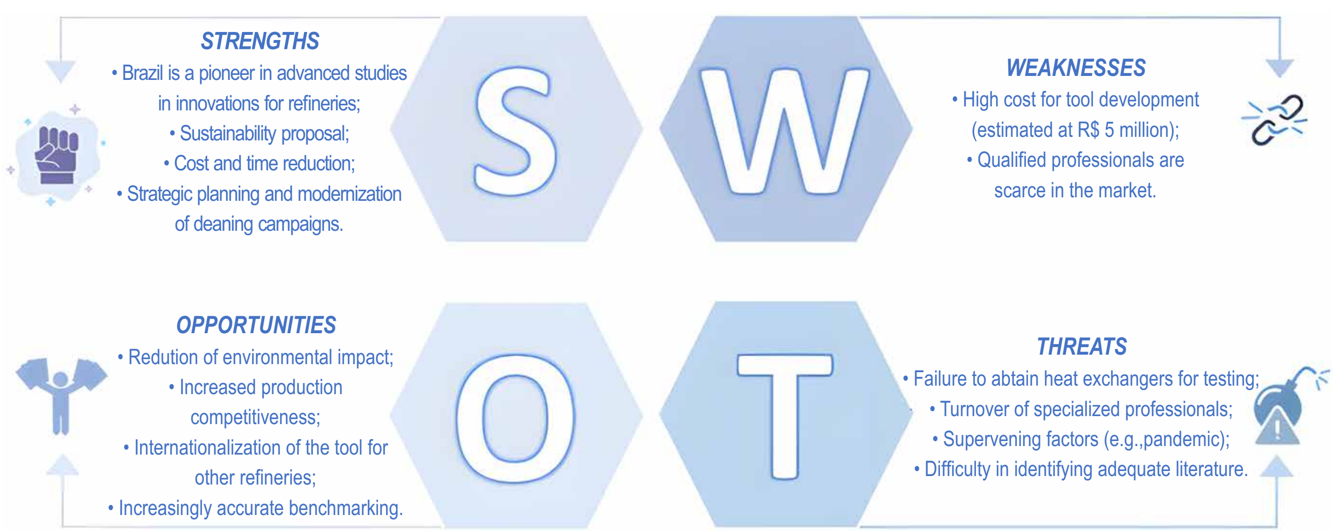
Sprint Retrospective: Following the Sprint Review, the team reflects on the Sprint process, identifying lessons learned and areas for improvement to enhance future performance.

Integrating these Scrum elements fosters a structured yet adaptable environment that supports continuous delivery of high-quality outcomes. This approach also ensures responsiveness to stakeholder feedback and evolving project dynamics. A SWOT analysis (Figure 5) and a Risk Response Plan (Table 1) were developed to complement the implementation of Agile methodology. The SWOT analysis comprehensively evaluates internal strengths and weaknesses and external opportunities and threats, providing strategic insights for decision-making. The Risk Response Plan, in turn, outlines critical risks and corresponding mitigation strategies, contributing to proactive project governance and resilience against potential disruptions.

The quality requirements for this project encompass several critical elements necessary for developing a reliable and applicable mathematical model. Central to this effort is data from both a

Figure 4. Scrum process.

Figure 5. SWOT analysis.



bench-scale shell-and-tube heat exchanger and a full-scale operational heat exchanger installed in a refinery plant. This dual-source data collection provides a robust dataset for validating and fine-tuning the model to ensure real-world applicability.

Using Microsoft Excel® VBA and MINITAB® as analytical tools is crucial in modeling. These tools offer powerful capabilities for data analysis and statistical validation. These tools support the generation of accurate, replicable outcomes, reinforcing the reliability of the predictive model. Complementing these technical components, integrating Agile methodologies—particularly Scrum—with traditional project management frameworks provided a flexible and effective structure, well-suited to the dynamic and highly regulated oil and gas sector. This hybrid management approach enabled efficient execution across all project phases, including planning, resource allocation, model development, and implementation. The iterative nature of Scrum, with recurring Sprints, supported ongoing improvements and responsiveness to emerging challenges, such as compliance requirements, environmental constraints, and rapid technological changes.

Table 1. Critical points of the risk response plan for technical execution failure.

Risk	Probability	Severity	Exposure	Response	Action Description	Responsible
Failure in the Mathematical Model Definition	Medium	Medium	Medium	Mitigate	Identify possible failures, evaluate model variables, and adjust parameters.	Technical Team
Failurein Heat Exchanger Testing	Low	Low	Low	Mitigate	Require performance and certification test reports after equipment manufacturing; If a defect is identified in the equipment, report the problem to the supplier for repair.	Supplier and Technical Team
Failure in Adapting the Obtained Data	Medium	Low	Medium	Mitigate	Identify possible failures, evaluate model variables, and adjust parameters; • Provide data through the Plant's Heat Exchanger Battery Sponsor.	Technical Team, Technical Leader, and Sponsor

Agile tools like Daily Scrums and Sprint Retrospectives promoted transparency, accountability, and continuous process optimization. Together, these elements ensured that the project maintained alignment with its technical goals while remaining adaptable to the realities of industrial environments.

As described by Pessoa and colleagues [11], the mathematical model developed for this study introduces an innovative yet simplified method for predicting fouling rates in crude oil heat exchangers within preheat systems at refineries. Fouling—a common issue in thermal systems—is affected by fluid velocity, temperature, fluid composition, and equipment configuration. This model streamlines predictions by focusing on mean fluid velocity and effective temperature, resulting in a low error margin validated against operational data from a Brazilian refinery. Its adaptability to varying operational conditions makes it a practical tool for optimizing maintenance strategies and mitigating the economic losses associated with fouling.

This technical rigor and methodological flexibility integration highlights the project's commitment to precision, efficiency, and industrial applicability in solving complex maintenance challenges.

Conclusion

As demonstrated in this study, implementing predictive maintenance strategies in preheat train heat exchangers shows substantial promise in improving operational efficiency in the oil and gas industry. The project has effectively addressed the challenges posed by fouling in heat exchangers by developing a precise and validated mathematical model using data from laboratory and operational environments and adopting a hybrid project management approach. Integrating advanced tools such as Microsoft Excel® VBA and MINITAB® enabled rigorous data handling and statistical analysis, supporting accurate modeling and decision-making. This method contributes to optimized maintenance schedules, reduced equipment downtime, and significantly minimized omic losses, affirming the strategic importance of predictive maintenance for the reliability and sustainability of refinery operations.

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The authors gratefully acknowledge SENAI CIMATEC and the project management team for their invaluable support and the opportunity to contribute to knowledge advancement in the oil and gas sector.

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Production Automation in Brazilian Pharmaceutical Industry: A Foresight Study Based on Scenario Analysis, Technology Roadmap, and System Dynamics

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This study proposes a technological foresight for automating a pharmaceutical industry production line in Brazil. To achieve this, a future scenario analysis and a technology roadmap were developed based on industrial needs identified through a literature review conducted over the past decade, along with a system dynamics mapping. The results discuss the potential impacts of automation and offer insights to guide decision-makers. This investigation could benefit pharmaceutical industries in developing countries by enabling more agile manufacturing processes and a diversified product supply to treat diseases and respond to public health emergencies.

Keywords: Production Automation. Scenario Analysis. Technology Roadmap. System Dynamics.

Technological disruptions in the Digital Age have presented significant challenges to organizational work processes, particularly manufacturing. The concept of Industry 4.0 has gained global relevance, driven by three primary factors: digitalization, integration of the horizontal and vertical value chain, and digitization of product and service supply chains through innovative business models and customer engagement [1].

A 2024 report by the Dubai Future Foundation identified "living with autonomous robots and automation" as one of the key megatrends. Initially dominant in the automotive sector, robots and process automation are increasingly penetrating other manufacturing environments, fostering efficiency and innovation while raising ethical and societal concerns [2]. Globally, task automation reached 34% in 2024 and is projected to rise to 42% by 2027 [2]. In parallel, the World Economic Forum's 2023 report on the future of work indicated that artificial intelligence is expected to increase by 75% by 2027 [3]. Although the growth rate of industrial robotics has slowed due to post-pandemic economic challenges, long-term projections suggest that service robots—especially in manufacturing, healthcare, and logistics—will expand by approximately 21.5%, particularly in the Middle East [2].

Brazil and other developing nations must invest in technological foresight to automate production lines and achieve similar advancements. Technological foresight is a strategic process for anticipating future scientific and technological developments that may influence industry, the economy, and society. It focuses on altering technological trajectories and strengthening institutional competitiveness and survival [4–6].

From an industrial standpoint, foresight helps identify trends in technology, demographics, regulations, and consumer lifestyles [7], all of which are deeply connected to innovation, research and development (R&D) management, and entrepreneurial opportunities. Foresight is particularly valuable when rapid response is needed for crises or public health emergencies, aligning with the concept of "future preparedness" [8].

Methodologically, foresight involves mapping the innovation process and examining how multiple factors and stakeholders interact to

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anticipate the outcomes and risks of technological change [4,9]. There are two primary foresight approaches: patent analysis and scenario-based methodologies. Both approaches face constraints related to time and resources [10]. While patent analysis can help industries build proprietary production platforms using emerging technologies, it often entails high costs. Sole reliance on imports of pharmaceutical products is also not viable. A more feasible strategy for countries like Brazil is to conduct technological foresight analyses that evaluate existing technologies' future configurations, identify uncertainties, and mitigate risks. This approach supports the prioritization of R&D initiatives [11]. Adequate foresight requires integrating both quantitative and qualitative methods. This study selected scenario analysis, technology roadmapping, and system dynamics to provide comprehensive conceptual, strategic, and operational insights [12].

This work is significant because it applies a combined foresight methodology to identify safe, innovative, and sustainable opportunities for technological advancement in pharmaceutical manufacturing. Therefore, this study aims to propose a technological foresight for automating a pharmaceutical industry production line in Brazil.

Materials and Methods

A literature search was conducted in the Web of Science, Scopus, and ScienceDirect databases using the query: "technology roadmap" AND "scenario" AND "industry". The goal was to identify industrial foresight applications employing a combination of these methods over the past decade (2014–2024). The search returned 388 results. Eight studies were selected after applying filters related to method relevance, smart manufacturing, and eligible publication types (articles, reviews, and conference papers). These represented generalized insights applicable to various industrial sectors, as no pharmaceutical-specific studies were found for the selected period.

Scenario Analysis

The literature review revealed key themes for identifying uncertainties in future industrial manufacturing. Six variables were selected, each representing one dimension of the STEEP framework (Social, Technological, Environmental, Economic, and Political). These variables included:

- Availability of digitally competent professionals;
- Adoption of science-based technologies (e.g., big data, cloud computing, AI);
- Sustainable practices in manufacturing;
- Agile logistics and supply chain operations;
- Openness to international markets;
- Laws and regulations for good manufacturing practices.

These served as the basis for constructing a morphological matrix, combining variable components to produce four distinct scenarios, with one column summarizing the most probable scenario configuration.

Technology Roadmap

The technology roadmap presented a sequential visualization of alternatives for automating a pharmaceutical production line. The roadmap detailed the responsibilities of actors and their interactions with the intended technologies, organized by short-term, medium-term, and long-term implementation goals [13,14].

System Dynamics

System dynamics modeling provides a simulation-based understanding of a context's structural and functional performance. It supports technology foresight by addressing disruptions and complex scenarios, informing policy and strategic decisions [15]. This method helps understand individual variable behavior and their interrelations, guiding decision-making and encouraging beneficial behavioral shifts [16,17].

A structural map of these variables and their interconnections was developed using Vensim® PLE software (Windows version 8.1.0 Double Precision x64, 2019).

Results and Discussion

A multidisciplinary team was assembled to develop the scenarios. The analysis showed that full automation of a pharmaceutical production line requires a multifactorial approach. Scenario 1, characterized by regressive conditions, appeared unlikely given the industry's current state. Most probable outcomes were aligned with intermediate scenarios (Scenarios 2 and 3), particularly due to advancements in digital skills and increasing adoption of digital technologies.

While digital tools improve productivity and reduce human error and accidents, the complete substitution of human labor remains uncertain. Emerging trends suggest a redefinition of job functions rather than eliminating human roles. Automation fosters product quality standardization but has not yet resolved all environmental sustainability challenges.

Logistical decisions rely partially on human input until organizations fully trust digital systems. In Scenario 4—the most transformative scenario—legal and political structures become decisive factors. While national market expansion seems feasible, boosted by experiences during the COVID-19 pandemic, international market entry may still face obstacles due to strong foreign competition. The configuration of these scenarios is illustrated in Table 1, which uses a morphological matrix with variables combined two-by-two to derive the most probable outcomes.

After constructing the scenarios, we developed a technological roadmap (Figure 1) to guide the full implementation of automation in the production process of a pharmaceutical industry. This roadmap considers the configurations and uncertainties identified in the previous step. It organizes them across different time horizons: short term (up to 2 years), medium term (2 to 5 years), and long term (5 to 10 years) on the horizontal axis, with the stakeholders responsible for each stage represented vertically. Beyond this timeline, the technological foresight process should be reviewed and updated periodically, in response to ongoing global developments.

To enable the implementation of automation technologies in the pharmaceutical manufacturing process, we identified several variables that influence behavior and contribute to the effectiveness of the roadmap stages. Figure 2 presents these interactions, mapped through a system dynamics analysis using the Vensim® computational tool.

Critical factors influencing the technological infrastructure in the health sector include auxiliary variables such as equipment costs, maintenance time, digital literacy, data analysis expertise, and green manufacturing aligned with ESG (Environmental, Social, and Governance) principles. Additional factors include delivery times for the domestic market, international sales potential, and the variety of products offered for future therapies. These variables play a strategic role in supporting the Brazilian Unified Health System (SUS). Their relevance stems from the growing pressure of rising healthcare costs, an aging population, the incorporation of new technologies and products, and other factors that impact the service and industrial sectors, further aggravating the country's dependence on imported health-related goods [18].

To reduce dependence and mitigate the negative impacts of legacy technological advances, this prospecting process can support Brazilian pharmaceutical industries in making informed decisions to enhance resilience. Adopting this forward-looking mindset will contribute to national progress and improve competitiveness in industrial health production with developed countries. Furthermore, it can inform government initiatives prioritizing knowledge, education, and—most importantly—innovation, thereby strengthening the Health Economic and Industrial Complex [18,19].

Table 1. Morphological matrix with scenario analysis.

STEEP contributors		Scenario 1	Scenario 2	Scenario 3	Scenario 4	Most probable scenario
Social	Analogic x Digital competences	Old generation people working with many papers and using hard physical strength in processes	Half/half old generation and younger people working with less paper and partially using physical strength in processes	Most of professionals are younger working with no paper, less physical effort and more digitally capable	Processes totally digitally automated with no human working on production lines	Most of professionals are younger working with no paper, less physical effort and more digitally capable
Technological	Mechanical based x Digital and wireless based	Fully human-operated equipments	Part of equipments is operated by human and other part are digitally driven - Al and big data	Fewer equipments are operated by human and most part are digitally driven - Al, big data, sensors, robots	All equipments are operated by robots or remotely	Fewer equipments are operated by human and most part are digitally driven - Al, big data, sensors, robots
Environmental	Environment polluting x ESG practices	High emissions of carbon and high production trash	Low emissions of carbon and high production trash	No emissions of carbon and few production trash	Totally green manufacturing	Low emissions of carbon and high production trash
Economic-1	Dependant x Autonomous logistics	Internal logistics dependent of human action between production phases	Internal logistics few dependent of human action between production phases	Internal logistics half/half dependent of human action and robots between production phases	Internal logistics performed by robots	Internal logistics few dependent of human action between production phases
Economic-2	Strictly National x International vending	National actuation with poor visibility and fidelity by local customers	National actuation with high visibility and fidelity by local customers	National and international actuation with poor visibility and fidelity by foreign customers only	International actuation with high visibility and fidelity by customers in whole world	National and international actuation with poor visibility and fidelity by foreign customers only
Politics/Legal	Poor x Full adoption of fabrication good practices	Almost no quality warranty and standardizing of products developed	Around of 50% quality warranty and standardizing of products developed	Over than 70% quality warranty and standardizing of products developed	Totally quality warranty and standardizing of products developed	Totally quality warranty and standardizing of products developed

Figure 1. Technological roadmap for automating the manufacturing process.

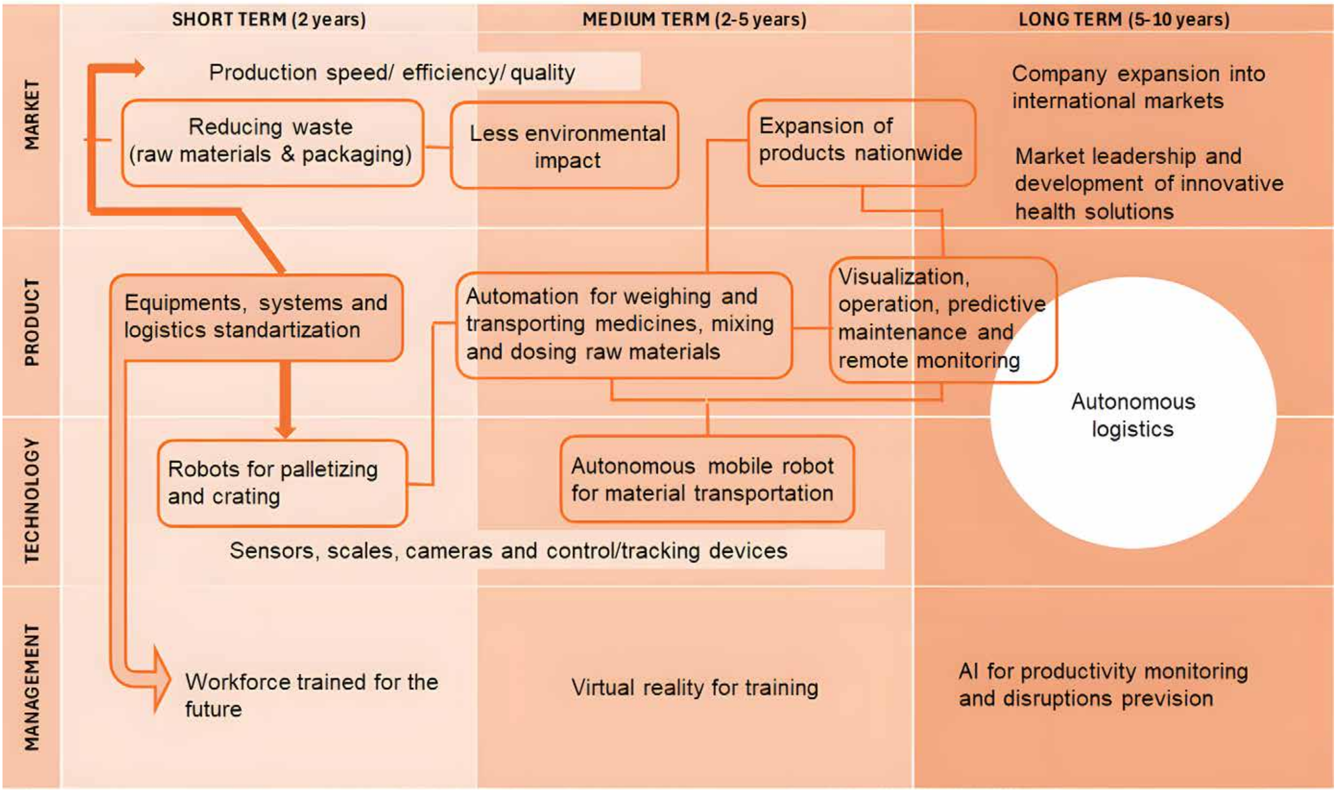
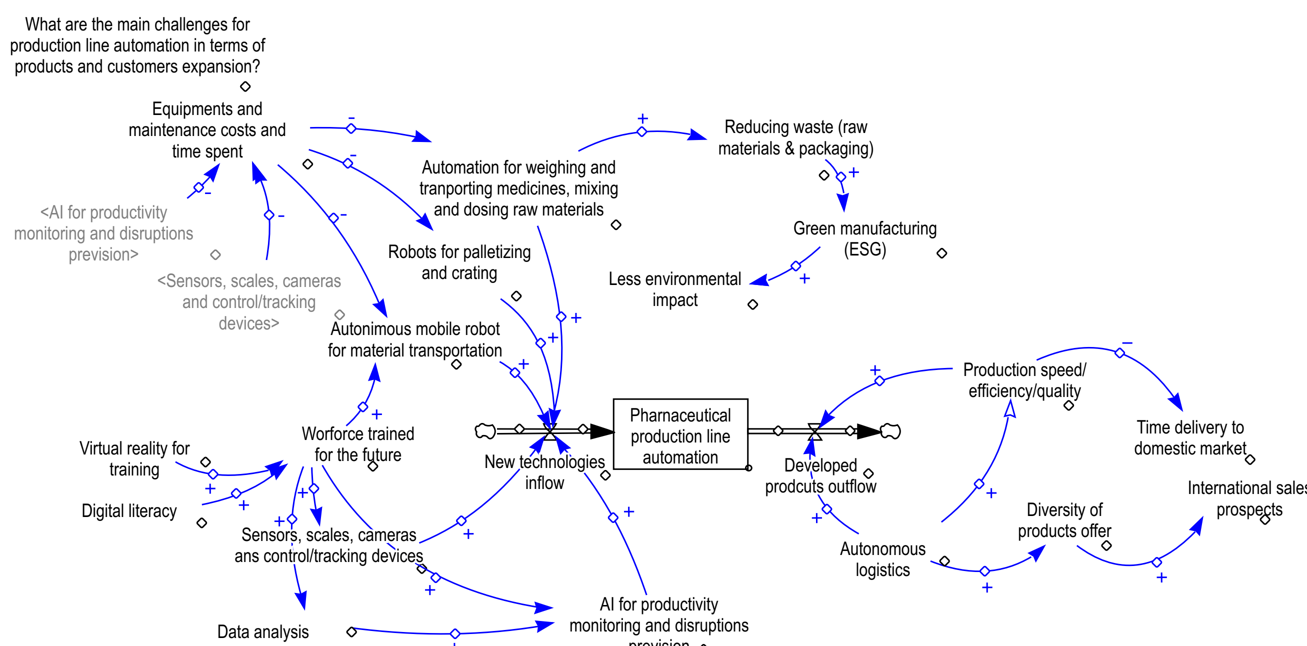


Figure 2. Dynamic analysis of the system.



To achieve this, the public and private sectors must align and articulate strategic actions, guided by insights from this technological foresight study.

These strategies should foster a high level of innovation, dynamism, and autonomy. The result will be time savings in development processes and the provision of rapid health solutions for Brazil's population and other under-resourced countries that urgently need to combat infectious diseases.

Conclusion

The foresight process represents a viable and cost-effective strategy for technological prospecting in industrial automation. It significantly reduces the financial and operational risks associated with developing new technologies.

This approach is particularly advantageous for individuals or organizations with limited technological expertise, constrained development resources, or insufficient time to engage in a complete technological development cycle, from conception through implementation.

Foresight processes prove especially valuable in contexts like the pharmaceutical industry, where multiple equipment modules must be integrated to form complex platforms or production lines. Despite requiring only a limited number of experts in future studies and situational analysis, these investigations can be highly comprehensive and effective when they incorporate complementary methods. Such a systematic approach allows for mid-course corrections and well-informed decision-making.

Moreover, a thorough and structured foresight evaluation reduces foreign dependency on healthcare technologies, streamlines production and distribution processes, and enhances national technological sovereignty. This is particularly critical for investments in bioproducts targeting diseases of primary future concern, including metabolic, chronic, and infectious diseases. It also becomes essential in scenarios demanding rapid response, such as health crises, natural disasters, or public health emergencies.

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Factors Limiting the Management of Technological Platforms ("Core Facility") to Support Scientific Health Research

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This study aimed to identify the main limiting factors in managing technological platforms—health research support units equipped with multi-user equipment and specialized staff. A review of the scientific literature was conducted, covering three thematic blocks: multi-user units, core facilities, and technological platforms, searched in the PubMed database. To correlate the limitations identified with management practices adopted in various organizations, analysis categories related to management and outcomes were developed. Based on the literature, key limitations were identified in the operation of these specialized research support units, allowing for the definition of essential analytical points for establishing a management model.
Keywords: Multi-User Units. Core Facilities. Technological Platforms.

The sustained and rapid development in recent decades of core technologies that underpin life sciences research has transformed biological science into an increasingly multidisciplinary field. This transformation has made it technically and economically unfeasible for individual health research laboratories to master all these technologies independently. Many institutions have adopted multi-user infrastructures to address this challenge and support competitive science. These platforms are especially well-suited to keeping pace with the sector's rapid technological advancements [1–3].

In light of a global economic slowdown, declining research and development (R&D) funding, and rising equipment costs, research institutions have been compelled to plan their budgets more strategically, especially regarding the management of technological platforms. This context has driven the shift toward centralized research support infrastructures that facilitate the sharing of resources. These centralized platforms offer access to multi-user equipment, technologies, and services more robustly and sophisticatedly than traditional independent laboratory structures [4,5].

Initial funding for a technological platform typically covers the acquisition and installation of equipment. However, long-term operational expenses are rarely accounted for, making sustainability a complex challenge. These ongoing costs include equipment maintenance, service upgrades, technology development, and specialized personnel recruitment and training [1,6].

Given the scarcity of resources, efficient management of technological platforms has become essential. The starting point for this efficiency is identifying the operational challenges these units face. Therefore, this paper aims to review relevant literature and outline the primary limiting factors in the management of technological platforms.

Materials and Methods

This study is based on a review of the scientific literature, focusing on three thematic search blocks: multi-user units, core facilities, and technological platforms. As the study focuses on health research institutions, the PubMed database—home to over

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36 million articles and publications in the health sciences—was selected for the literature search.

The search was performed in April 2024, with no restrictions on publication date. Exclusion criteria included articles written in languages other than English, duplicates, and those unrelated to the research topic. After the selection process, the full texts of the included articles were reviewed to identify the limiting factors and to develop analysis categories relevant to the management of technological platforms.

Results and Discussion

By analyzing a range of conceptual perspectives in the literature, ten categories of analysis relevant to the management of technological platforms were identified. These were further consolidated into seven broader management areas, grouped under two overarching dimensions: management practices and results. This framework enabled the correlation of these categories with the operational limitations observed.

Analysis Categories

Understanding the relationships between specific management practices, their outcomes, and their correlation with known limitations is essential for improving the functionality and sustainability of technological platforms.

Table 1 presents the analysis categories identified, highlighting both commonalities and differences among the authors. For instance, financial management and technical research staff are recurring categories across all reviewed studies, while infrastructure, noted by Lejeune and colleagues [7], is mentioned by only one author.

In this study, the ten categories of analysis were reduced to seven and classified into management processes and results, as shown in Table 2. Thus, a new standardization and closer approximation to current business management practices were proposed [8].

Management Limitations

The literature review on the management of technological platforms identified limitations in managing these specialized support units for scientific research. Table 3 shows the limitations mentioned by the authors, correlating them with the categories of analysis proposed in this study. The authors also referred to the limitations in the texts analyzed as challenges, problems, or barriers.

A.1. Resources (Capital and Intellectual)

Regarding partnerships with other public research institutions or the private sector, the following limitations were identified: weak relationships between universities and companies [4]; conflicts of interest between public research institutions and the private sector [9,10]; and the short lifecycle of new technologies, coupled with diverse methodologies and the burden of specialized knowledge, which can overwhelm institutional capacity. This challenge reinforces the need to share R&D infrastructure among public research institutions [11,12].

Challenges related to equipment maintenance and availability include limited financial resources for equipment maintenance and updates [13,14], and the variability in service quality and response time from equipment maintenance providers, which often depends on the region [15,16]. Another important infrastructure-related challenge is adequate data storage and management systems [17,18].

Furthermore, fully leveraging the potential of available equipment depends on the expertise of the personnel operating it, which requires ongoing training [12]. A recurring issue is the presence of unqualified personnel, which has been identified as a key factor in the lack of rigorous research procedures [14,19].

A.2. General Administration

Within the general administration category, several structural limitations were identified,

Table 1. Analysis categories identified in the literature review.

N	Turpen et al (2016)	Hockberger et al (2018)	Lejeune et al (2020).
1	General administration	General management	-
2	Research and technical staff	Research and technical staff	Highly qualified personnel
3	Financial management	Financial management	Finacial Performance
4	Resource management	-	Resources
5	-	-	Infrastructure
6	Communication	Communication of services	-
7	Strategic planning	Self-assessment	-
8	Customer base and satisfaction	Customer base and satisfaction	Technological platforms performance
9	Institutional impact	Customer publications and grants	Collaboration
10	-	Educational and outreach activities	Public visibility

Table 2. Proposed analysis categories.

Item	Analysis Categories	Dimension
A.1	Resources (Capital/Intellectual)	Management
A.2	General administration	Management
A.3	Financial management	Management
A.4	Communication	Management
A.5	Strategic Planning	Management
B.1	Customer base	Results
B.2	Institutional impact	Results

such as the absence of formalized procedures for proposing, establishing, evaluating, and renewing technological platforms [20,21] and the lack of a standardized set of policies to ensure their efficient and sustainable operation [15,20]. Additionally, the need to develop a business model focused on the long-term sustainability of technology platforms was highlighted [1,20,22], along with the importance of advisory committees capable of setting targets and guiding institutional research investments [20,23]. A particular challenge is the lack of standardized processes for assessing the lifecycle of each technology, which is problematic given the short lifespan of many new technologies. This hinders both strategic and operational management of these high-investment assets [1,11]. Staff turnover also poses a significant limitation, leading to a loss of institutional knowledge and exposing the organization's inability to retain highly qualified personnel [5,12,13,17,24].This challenge is often linked to dissatisfaction among technical staff regarding their status and career recognition

Table 3. Limitations of technology platform management.

Analysis Categories	Limitations / Challenges / Barriers / Problems	Authors
A1. Resources (Capital/Intellectual)	Limited relations between universities and companies.	[4]
	Existence of a conflict of interest in partnerships between research centers and the private sector.	[9,10]
	No sharing of infrastructure between platforms.	[11, 12]
	No resources for maintenance and replacement of equipment.	[13, 14]
	No quality assurance in the provision of equipment maintenance services.	[15, 16]
	Lack of data storage/management infrastructure.	[17, 18]
	No training for the technical team to make full use of the equipment's potential / No development of specialized personnel.	[12, 14,19]
A.2. General administration	No business model for the research area.	[1, 20, 22, 25, 34]
	Lack of formalized rules for using the technological platform structure.	[20, 15]
	A lack of systematization of the presence and use of advisory committees and other organizational structures.	[20, 23]
	No formal process for evaluating and renewing platforms.	[14, 21]
	No formal process for acquiring a new platform.	[20, 21]
	No monitoring of the life cycle of new technologies.	[1, 11]
	High staff turnover.	[5, 12, 13, 17, 24]
	No recognition for the careers of technical staff.	[7, 11, 25, 26, 27]
	Lack of management knowledge among the team.	[18, 23, 27, 28, 29, 30]
A.3. Financial management	No costing and pricing models.	[11,13, 18, 20]
	No good funding systems in place for platforms.	[11]
	No system for financing and managing the budget.	[1, 6, 7, 31]
	No system for attracting external funding.	[22, 32]
A.4. Communication	No access to reliable information on technological platforms	[4, 20, 26, 33]
	Difficulty in communication between the platform team and the user	[3]
A.5. Strategic Plannin	No definition of the presence and role of technology platforms in strategic research planning.	[20, 33]
B.1.Customer base	Insufficient qualification of users to use equipment / No training of users.	[13, 16, 19]
B.2. Institutional impact	No tools for institutional evaluation of technological platforms. No performance indicators.	[1, 7, 23, 25, 30, 32]

within the institution [7,25], reinforcing the need for a work environment that offers competitive salaries, career stability, a respectful culture, and formal recognition for staff contributions [11,26,27]. Other personnel-related issues include a shortage of human resources, excessive workload, and difficulties hiring skilled labor [24].

Technology platforms function simultaneously as research laboratories and small business entities. Therefore, effective management is essential; however, most scientific health research institutions lack the necessary managerial competencies to perform these duties adequately [18,23,27–30].

A.3. Financial Management

One of the primary challenges in financial management is developing sustainable pricing models that make technological platforms attractive to both academic and private-sector users [11,18,20]. Institutions must define mechanisms that support comprehensive cost-recovery models over time [16]. Additional issues include covering operational costs, securing and managing diverse funding sources, poor budget management, and inadequate financial support [6,7,13,20,31].

An underexplored area in current planning is the strategic pursuit of donations with fewer restrictions, given the inherently high risk associated with research activities [22]. Another barrier to attracting investment is the limited development of automated methodologies capable of demonstrating the real impact of technological platforms within research environments [32].

A.4. Communication

Information about technological platforms and their available resources is often either inaccessible or incomplete, indicating a need for improved communication strategies to enhance visibility [20,26,33]. A particular barrier to industry engagement is the lack of clear information on the availability and application of these resources within research institutions [4]. Communication is also critical in facilitating interactions between platforms and their users. Many platforms consider communication a sensitive issue, and engaging with users remains a persistent challenge [3].

A.5. Strategic Planning

One notable limitation is the exclusion of technological platforms from the strategic planning processes of their host institutions [20]. Additionally, many platforms lack strategic plans [33], hindering their ability to align operations with institutional goals.

B.1. Customer Base

A critical challenge for technological platforms is ensuring that potential users are adequately trained to conduct experiments independently [16]. One of the most frequently reported problems is the misuse of equipment by unqualified users, which reflects insufficient training and undermines the quality and reproducibility of research [13,19].

B.2. Institutional Impact

Evaluation tools that can assess the necessity and effectiveness of technological platforms within institutions are urgently needed. These tools are essential for informed strategic decision-making and investment planning [23,30]. The absence of performance indicators significantly impedes the strategic and operational management of these platforms [1].

One of the most pervasive management challenges is assessing the institutional impact of technological platforms [24]. This is hampered by the lack of specific performance indicators and the inherent difficulty in measuring both quantitative and qualitative outcomes [7,32].

Conclusion

Technological platforms have become essential to health research development across multiple countries, driven by continuous advancements and the increasing sophistication of scientific equipment. The fast pace of technological progress requires substantial initial investments and careful planning to ensure the sustainability and excellence of services offered by these units.

This study on the management limitations of technological platforms confirms a direct relationship between the proposed analysis categories and the challenges identified.These findings allow for the identification of key areas for managerial intervention to improve service quality and efficiency.

This article's potential contributions lie in supporting the identification of connections between existing management limitations and the practical strategies that can be adopted to create a tailored management model for these complex research infrastructures.

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Governance of Reesearch and Innovation Networks in the National Institutes of Science and Technology (INC)

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This study aimed to investigate and characterize current knowledge regarding research and innovation networks primarily formed by researchers and the governance mechanisms present in the National Institutes of Science and Technology (INCT). To this end, an exploratory study was conducted to understand the environmental context, operational dynamics, and composition of actors within these institutes. The findings revealed a strong predisposition toward establishing research network environments comprising individual and institutional actors. Most INCTs operate through institutional mechanisms in governance, primarily structured around coordination bodies and management committees.
Keywords: Network Governance. Research and Innovation Networks. Institutes of Science and Technology.

The advent of the information and knowledge era has significantly transformed organizations, making them more adaptable. Within this new context, it has become necessary to revise core organizational strategies, including: (i) the flexibilization of infrastructure, making it more horizontal; (ii) the organizational culture, associated with the profiles of its actors; and (iii) a predisposition toward the intensive use of information and communication technology tools [1–3].

This transformation in organizational and societal environments has amplified the use of network structures as spaces for collaborative production. Simultaneously, governance and management structures have emerged as essential mechanisms for guiding decisions and operationalizing actions within these networks. In this regard, it is critical to consider the factors involved in forming and structuring networks to inform the adoption of more suitable governance models. The literature highlights several key aspects: trust among actors, the quality of relationships, network structure and coordination, mobilization, knowledge sharing, consensus on norms, objectives, and results, and network sustainability [4–9].

Research on network governance addresses elements related to the configuration of decision-making environments, such as rules, sanctions, formal agreements, and control mechanisms. These also encompass coordination and leadership, typically discussed in the context of relationships among network members [10]. Governance mechanisms that foster and enhance the participation of network actors via platforms are characterized by knowledge sharing, capacity and resource assessment, metric development and communication, and the adaptation of resources and routines [11].

The INCT Program was established through an initiative of the Ministry of Science, Technology, and Innovation (MCTI) and implemented by the National Council for Scientific and Technological Development (CNPq). Its goal is to expand funding opportunities for broad and impactful scientific research and technological development projects.

The program is grounded in several core pillars: (i) the formation of research networks, (ii) the consolidation of institutional partnerships, (iii) a multidisciplinary approach to strategically important national themes, (iv) the training and

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qualification of highly skilled human resources, and (v) long-term investment. The INCT Program replaced the Millennium Institutes Program through MCT Ordinance No. 429, dated July 17, 2008, and was reissued in 2014 via MCTI Ordinance No. 577, dated June 4, 2014. Its mission is to mobilize and cohesively integrate excellence groups in frontier and strategic scientific areas essential for the country's sustainable development [12].

Given this context, and to expand the understanding of governance structures within research and innovation networks, this study seeks to characterize the current knowledge regarding researcher network formation and governance mechanisms in science and technology institutes. The research focuses on the INCT Program, which addresses themes across major knowledge areas: Agricultural Sciences, Energy, Engineering and Information Technology, Exact and Natural Sciences, Humanities and Social Sciences, Ecology and Environment, Nanotechnology, and Health.

Materials and Methods

This study employed an exploratory and descriptive research design. Data collection techniques included extracting secondary data from scientific databases and public documents available on institutional and government websites to support the analysis of governance-related information within the INCT.

A detailed review of each INCT was performed to identify data indicating the presence of network formation and/or governance mechanisms. However, the investigation encountered limitations due to some INCT websites being non-functional or duplicated, often linked to the institutional websites of federal higher education institutions (IES).

An extensive analysis was also conducted to understand the interaction dynamics and network formation among the INCTs. Data on research themes and inter-institute connections were collected between September and October 2023. Through an exploratory approach, directed links on the web pages were mapped, and the data were organized into a spreadsheet for database construction. This structure enabled the application of Social Network Analysis (SNA), providing deeper insights into the relationships identified.

Results and Discussion

A comprehensive analysis was conducted on 159 institutional websites identified between August and October 2023. Of these, 112 were functional, allowing for the investigation of network formation initiatives and associated governance mechanisms. However, 47 websites had non-functional links, limiting data collection from those sources.

Table 1 presents a summary of INCT websites distributed by the central area of knowledge. Based on the information collected, the INCT Program currently includes 104 active institutes and engages 2,300 institutions, 12,000 researchers, and 485 partnerships with public and/or non-governmental organizations. In human resource development, 79 graduate programs have been created, encompassing 566 courses and the training of 12,700 researchers. Seven hundred eighty-seven agreements have been signed regarding international cooperation, involving 1,318 international researchers, 154 companies, and 592 associated laboratories. Regarding scientific, technological, and innovative outputs, the program has generated 79,000 academic publications, filed 1,410 patent applications, and has 12 patents in the market [13].

In a recent initiative to expand and strengthen the Program, CNPq launched the INCT Call – CNPq No. 58/2022. This call included funding from the National Fund for Scientific and Technological Development (FNDCT) and was carried out in partnership with the coordination for the Improvement of Higher Education Personnel (CAPES) and the State Research Support Foundations (FAPs). As a result, more than 100

Table 1. Overview of the operational status of the hotsites investigated.

SITES ORGANIZED BY MAJOR KNOWLEDGE AREAS
Agrarian- 19 sites - 11 operational
Energy - 6 sites - 4 operational
Engineering and Information Technology - 22 sites - 18 operational - 1 duplicated
Health - 46 sites - 32 operational
Nanotechnology - 5 sites - 5 operational
Humanities and Social Sciences - 13 sites - 12 operational
Exact and Natural Sciences - 10 sites - 10 operational
Ecology and Environment - 38 sites - 20 operational - 2 duplicated

new INCTs were selected, bringing the total number of institutes in operation across Brazil to 204. This expansion marks another significant milestone in advancing Brazilian science, as it supports research projects of strategic relevance for scientific, technological, and innovation development [12].

The analysis of the INCT institutional websites provided valuable insights into their organizational structures, particularly about their respective areas of expertise. Most institutes operate with institutional governance mechanisms, typically structured around a coordinating body and a managing committee. In some cases, although a formal structure was not explicitly outlined, mechanisms for coordinating the participation and activities of members were still implemented [8].

Several INCTs emphasized the development of virtual environments as alternatives for creating, sharing, and disseminating knowledge. These digital spaces promote communication, enhance interactions and relationships, and foster collaborative learning and knowledge co-creation. In line with the findings of Perks and colleagues (2017), such virtual communities leverage the potential of digital communication to support knowledge exchange and interaction among participants more effectively.

Another notable feature was the formation of research network environments comprising research institutions, universities, individual researchers, and national and international research groups [7]. These networks are typically established either through institutional initiatives focused on advancing specific emerging themes or through organic collaboration among members seeking to share experiences and knowledge and engage in joint production [10].

Figure 1 illustrates the potential of the research networks formed by the institutes and presents the institutional network established within the INCT context. It offers an analysis of eight thematic working groups and their institutional interconnections. These networks encompass major knowledge areas such as Health, Humanities and Social Sciences, Exact and Natural Sciences, Nanotechnology, Ecology and Environment, Engineering and Information Technology, Agrarian Sciences, and Energy. Most of these connections are established through Higher Education Institutions (IES), except for the Energy sector.

The graph presented in Figure 2 enabled the identification of patterns and visualizations of the relationships among network elements, contributing to a more in-depth understanding of the research network's dynamics. INCTs operate through a collaborative research model involving both national and international researchers and institutions. The goal is to

Figure 1 - Network of institutions developed in the context of the INCT.

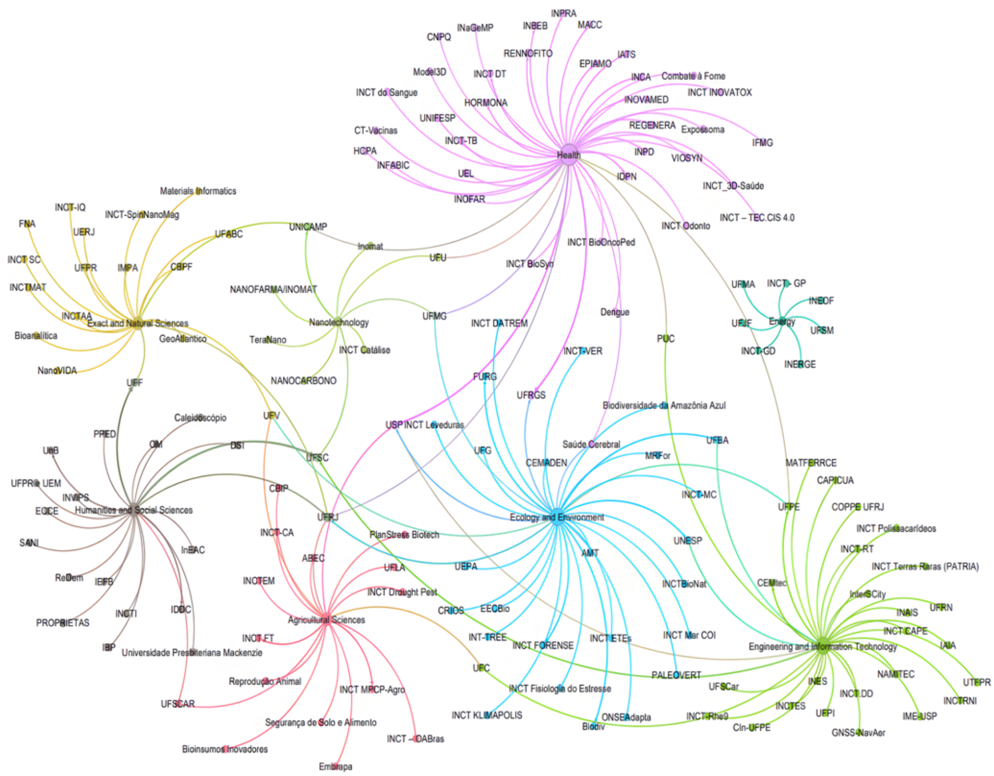
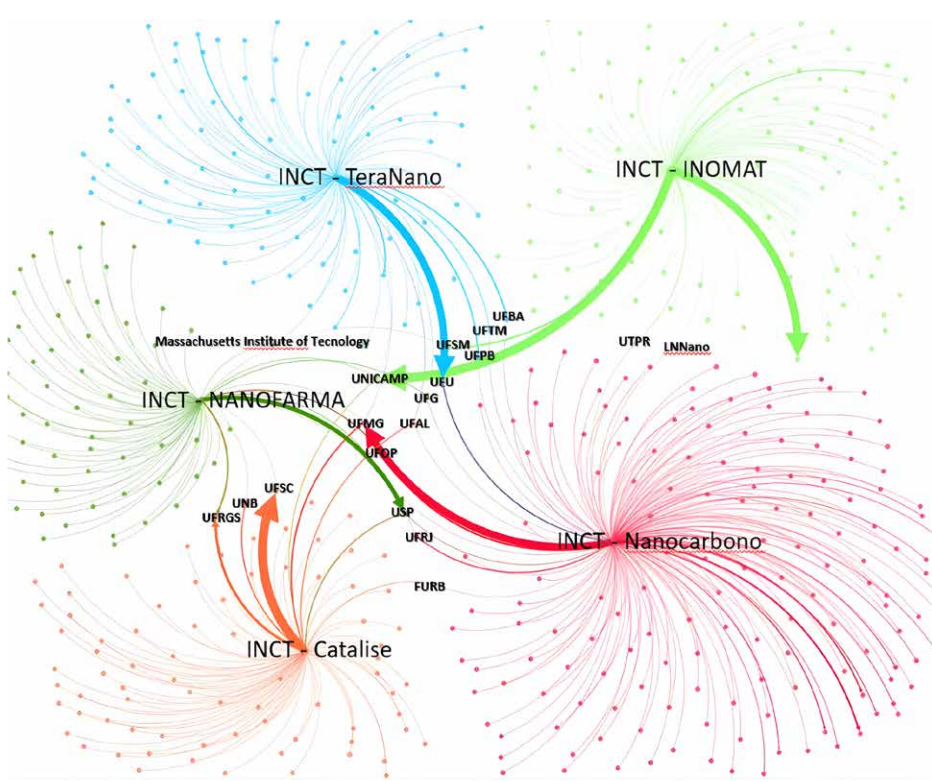


Figure 2 - Network developed under the INCTs for the nanotechnology area.



generate and disseminate knowledge to support the technological development of products and services. These efforts span all significant areas of activity within the institutes, with a central focus on societal benefits and strengthening public policies.

To illustrate this network analysis further, a specific focus was placed on the INCTs operating in Nanotechnology, demonstrating the potential for collaboration among national and international researchers and partner institutions. Notably, INCTs in this field tend to form interconnection hubs primarily through universities. Figure 2 presents the network configuration formed by these institutes, where the nodes represent individual researchers and partner institutions, and the edges indicate the number of established connections. The network comprises 400 researchers and 91 partner institutions, revealing a robust and highly interconnected structure.

The authors Vieira and colleagues (2016), Oliveira, Sanz, and Chaves (2022), Da Costa Filho-Edes and Barbosa (2022), Maia and colleagues (2015), and Ferreira and colleagues (2015) have examined the characteristics of mapping and forming research networks based on scientific collaborations among researchers within the INCTs [14–18]. In this context, it is evident that the research networks established within these institutes, aimed at collaborative and integrated research, serve as a robust coordination mechanism for scientific activity.

Conclusion

The results of this study indicate the existence of institutional governance mechanisms within the INCTs, predominantly structured around coordination bodies and management committees. These research networks comprise universities, research institutions, individual researchers, and research groups—both nationally and internationally. The findings demonstrate the significant potential of these networks in generating, sharing, and transferring knowledge. These environments function as coordination mechanisms that enhance communication, foster relationships and interactions, support collaborative learning, and co-create new knowledge. In this context, developing and implementing effective governance mechanisms within these networks becomes essential to further reinforce coordination and institutional cooperation among researchers and research groups. Such mechanisms are critical for fostering joint project development, maximizing the potential of the research networks, and contributing meaningfully to advancing knowledge to address societal challenges and inform public policy.

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Environmental Disasters and the Interface with One Health in Rio Grande do Sul: Challenges and Perspectives

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Using the One Health approach, this study aimed to examine the effects of climate disasters on the human-animal health interface in the context of Rio Grande do Sul. The research analyzed the impact of extreme weather events, such as floods and droughts, on public health, emphasizing the interdependence between humans, animals, and the environment. A systematic review assessed the literature on disasters within the One Health framework. As a result, interdisciplinary collaboration across various sectors has been emphasized as essential to addressing the challenges posed by environmental disasters. Such collaboration enables the formulation of more robust and practical strategies to mitigate the impacts of climate change.

Keywords: One Health. Climate Disasters. Animal-Human Health. Rio Grande do Sul.

Weather and climate significantly influence the water and energy systems and are essential to maintaining planetary balance and supporting human activity. However, extreme weather and climate events are major drivers of natural disasters.

Brazil is particularly vulnerable to climate change [1], and the state of Rio Grande do Sul (RS) has been severely impacted by floods since April 2024 [2]. These events, attributed to climate change, have led to environmental imbalances directly affecting human health. According to Martins Filho [2], a combination of a heatwave, a humidity corridor from the Amazon, and intense winds resulted in unprecedented precipitation, submerging large areas under water.

Natural disasters arise when extreme environmental events disrupt social systems, causing damage that surpasses local capacity to manage the crisis [3]. These events have profound implications for public health, animal health, and the environment—highlighting the relevance of the One Health approach. Initiatives such as "One World, One Health," led by the World Health Organization (WHO), the World Organisation for Animal Health (OIE), and the Food and Agriculture Organization (FAO), emphasize the interconnectedness of human, animal, and environmental health [4].

The Ministry of Health has adopted the One Health approach in Brazil, encouraging multidisciplinary cooperation to develop integrated solutions [5]. This approach recognizes the intrinsic link between environmental equilibrium and health outcomes [6]. The COVID-19 pandemic reinforced the urgency of addressing biodiversity and health in an integrated manner [7], underscoring the need to update national strategies to combat climate change, preserve biodiversity, and ensure food security and clean water access.

The recent environmental disaster in Rio Grande do Sul exemplifies the extreme weather events expected to become increasingly frequent. Therefore, developing new national disaster preparedness and management strategies is imperative. In recent years, the intensification of natural disasters in the region has been linked to global warming. Changes in sea surface temperature (SST) also play a significant role in climate variability [8], contributing to the severe flooding observed.

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Managing environmental risks such as floods remains a global challenge [9]. Solutions like dam construction—as illustrated by the Wivenhoe Dam in Australia—can be effective when accompanied by planned urban development [10]. However, inadequate land-use planning and improper waste disposal practices increase the risk of flooding and the spread of waterborne diseases. Land-use changes, such as deforestation and converting natural landscapes into urban areas, reduce vegetation cover and increase soil impermeability, worsening flood risks in areas with poor drainage infrastructure [11]. Therefore, effective land and waste management practices and structural measures like dams are essential. In addition, nature-based solutions—such as preserving riparian forests—are fundamental to flood mitigation [12].

Materials and Meethods

Method

This study employed a systematic review of the existing literature on climate disasters in the region and their impacts on health. The review followed the PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) guidelines to ensure methodological rigor and transparency.

Data Collection

The literature search encompassed VHL, SciELO, Medline-PubMed, Google Scholar, Web of Science, and the Integrated Research Database of PUC-Rio. Search terms included "climate change AND Rio Grande do Sul" and "floods AND Southern Brazil." The review period spanned from 2019 to 2024. Exclusion criteria included duplicate records and articles that did not directly address the relationship between climate change and flooding in southern Brazil or lacked relevant empirical data.

After screening and selection, data from the remaining studies were organized into an Excel® spreadsheet and categorized by themes such as disasters, one health, and public policies. As illustrated in Figure 1, 27 articles were included in the final analysis.

Results and Discussion

This study's main findings and discussion are presented in two subsections, beginning with the results of the systematic literature review.

Results from the Article Search Method

The search strategy initially identified 1,487 publications. After applying the date filter (2019–2024), 450 articles remained. Following abstract screening, duplicates, studies conducted outside Brazil, and those considered irrelevant were excluded. Three researchers independently reviewed the remaining articles.

Following the final selection process, 3 peer-reviewed articles and 24 additional documents from the Integrated Research Database of PUC-Rio were included, resulting in a total of 27 articles analyzed. The predominant methodological approaches across the selected studies were qualitative, including case studies, document analysis, and interviews. Between 2018 and 2020, publications increased, followed by a decline in 2021–2022. As illustrated in Figure 2, a renewed increase occurred in 2023.

Figure 3 shows the main keywords identified in the articles. " Climate change" appears more frequently in the articles, corresponding to 25%, which corroborates the hypothesis that climate disasters have a direct link with climate change. Next, we have One health, master plan, public health, and Rio Grande do Sul, with a 7% incidence in the articles analyzed.

Environmental Disasters and One Health: Implications and Spread of Diseases in the Context of Rio Grande do Sul

Climate events are increasingly frequent, including floods, landslides, droughts, and

Figure 1. PRISMA 2020 flowchart.

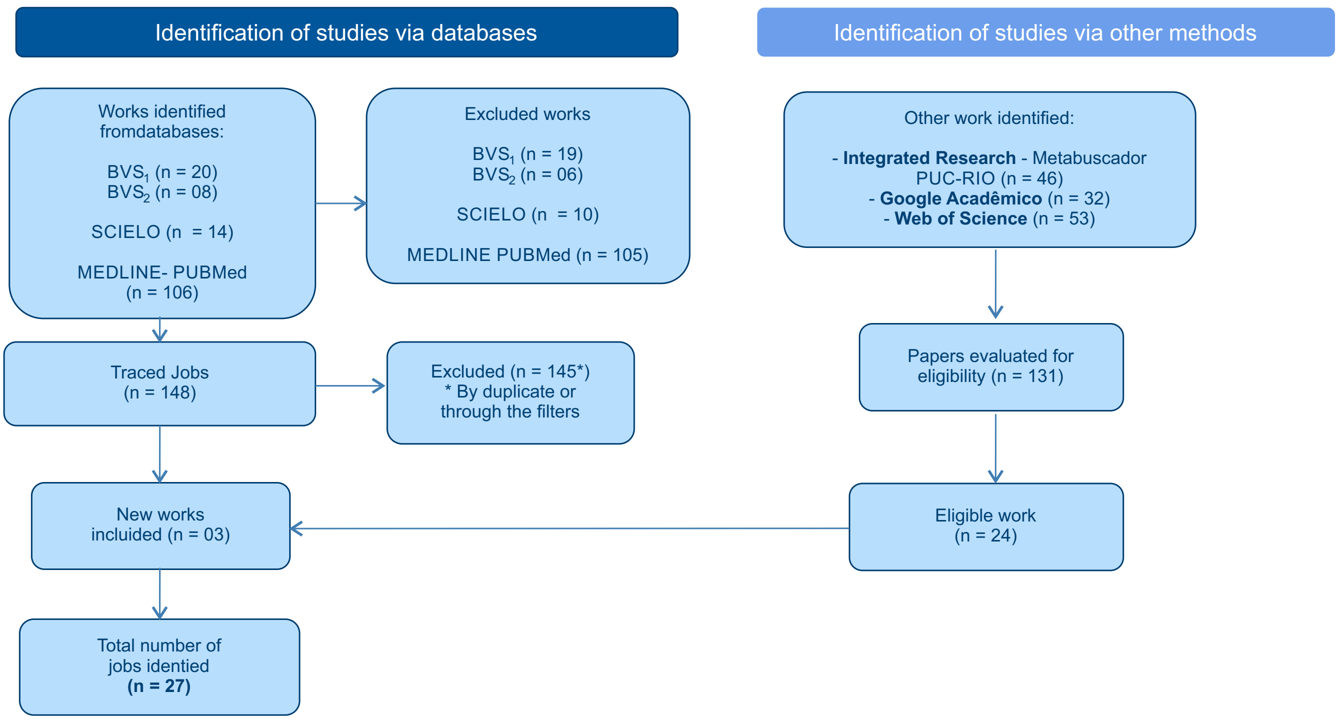


Figure 2. Number of articles per year of publication.

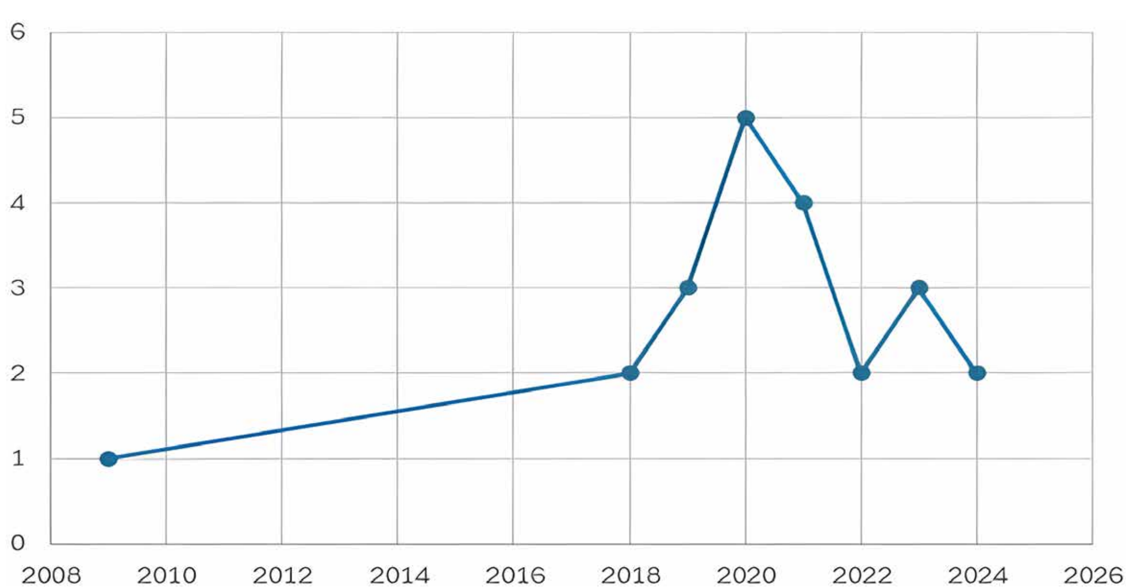
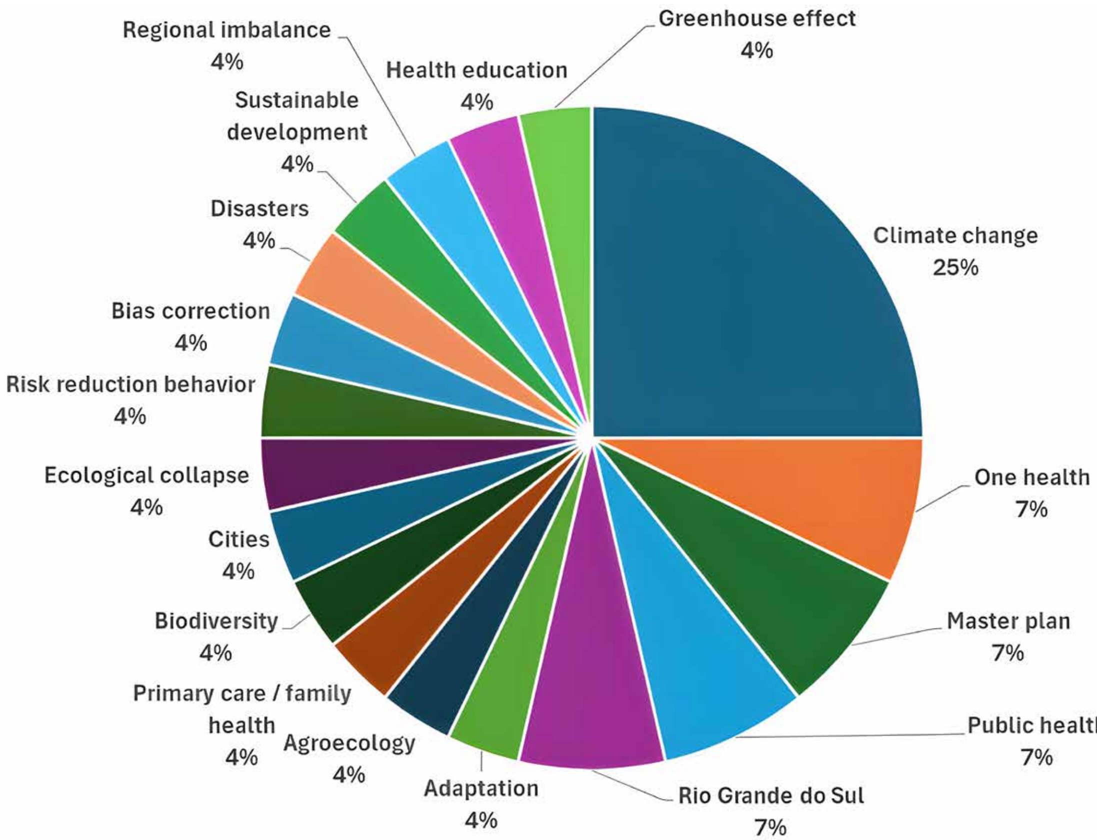


Figure 3. Most frequent keywords.



hurricanes, causing human and animal casualties, the spread of disease, and socioeconomic losses. These natural disasters are influenced by regional characteristics such as geology, soil, topography, and vegetation [13]. They may result from both internal dynamics of the Earth, such as earthquakes and volcanism, and external dynamics, such as storms and floods [14]. According to Castro (2023) [15], natural disasters can be classified into four levels of intensity, ranging from minor to severe, each with corresponding degrees of damage and loss.

Such events mobilize governments and society in search of rapid responses to minimize the loss of life and mitigate socioeconomic impacts—although some damages are irreversible. Rio Grande do Sul has experienced significant disasters, leading to human life and biodiversity losses. Floods and dam failures have disrupted biological cycles and essential environmental services, directly affecting community health and quality of life [16]. Consequences include polluted water bodies, the loss of flora and fauna, food insecurity, increased communicable diseases, and psychological and physical stress among affected populations [17]. Addressing these challenges requires an integrated approach rooted in the One Health paradigm, which links governmental decision-making and public policies to collaborative knowledge from diverse institutions [18]. Effective policies must consider local territorial characteristics, balancing identity preservation with operational efficiency [19].

The government of Rio Grande do Sul reported an increase in climate-related disasters between 2003 and 2021, with higher incidence rates from 2015 onward [8]. In 2023, Fiocruz's Climate and Health Observatory reported emergency and calamity decrees impacting 1,170 health facilities—including 548 clinics—resulting in a rise in medical emergencies and exacerbating chronic illnesses [20]. Between 2017 and 2021, droughts, floods, and heavy rains affected 482 municipalities, impacting approximately 4.44 million people. In 2023, floods and flash floods affected 51 municipalities and 47,904 individuals. By 2024, new flooding events impacted 478 cities, affecting over 2.39 million people [21,20]. These extreme weather events elevate the risk of infectious disease outbreaks, necessitating swift public health responses [2]. Post-flood scenarios often see spikes in diarrheal illnesses and vector-borne infections, highlighting the urgent need for targeted health interventions [2].

A recent study reported nearly a 300% increase in hepatitis A cases following the Rio Grande do Sul floods, emphasizing the importance of preventive actions in post-disaster settings [22].

Climate change and environmental degradation contribute to a rise in emerging infectious diseases in humans and animals, with cross-species pathogen transmission posing a significant global health risk [23]. The analysis confirmed increased frequency and intensity of rainfall, extreme weather events, floods, droughts, tropical cyclones, and El Niño effects. The Intergovernmental Panel on Climate Change (IPCC) [24] has demonstrated how urbanization intensifies these phenomena by altering wind patterns, precipitation levels, and water runoff in urban areas.

Large-scale environmental disasters—such as the recent floods—underscore the urgent need to protect vulnerable populations, despite existing deficiencies in safety infrastructure. The Health Sector Disaster Preparedness and Response Guide [25] emphasizes that health outcomes depend heavily on the quality of emergency response, recovery, and reconstruction efforts. The interconnection between human and animal health during floods underlines the necessity of integrated public policies and coordinated governance. Embedding public health principles within disaster response strategies is imperative, especially in climate change. Interdisciplinary networks—such as those documented by Hoff (2023) [26] and Schramm (2024) [27]—have significantly influenced policy development. These networks, in partnership with governmental bodies, civil society, social movements, the armed forces, and academic institutions, have played a critical role in crafting policies to mitigate these crises' impacts.

Conclusion

With the progression of climate change, natural disasters are expected to become increasingly frequent, especially in large urban areas, where environmental, social, and economic repercussions will be more severe. Effective responses will require interdisciplinary cooperation and partnerships between national and international institutions to formulate and implement robust disaster preparedness and response strategies.

Integrating the human-animal-environment triad into public policy is essential. Actions such as comprehensive urban planning, efficient drainage systems, and strengthening infrastructure are critical for mitigating risks, increasing resilience, and ensuring that public health challenges are addressed in an integrated and sustainable manner.

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Life Cycle Assessment in Agave Cultivation and Processing: A Review

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Agaves thrive in arid and semi-arid environments and can be transformed into various products through processing and refinement. The Life Cycle Assessment (LCA) methodology is employed to assess the environmental impacts of these processes. This study analyzes LCA studies related to the cultivation and processing of agave, identifying the main topics explored, relevant environmental impacts, and existing gaps. Information such as the functional unit, life cycle impact assessment methods, databases, software, objectives, and conclusions of the primary studies was evaluated. Various applications of agave and their potential environmental impacts were observed, with cultivation and processing showing comparatively lower impacts than other plants, mainly due to reduced water consumption and lower greenhouse gas (GHG) emissions.
Keywords: Agave. Biomass. Carbon Footprint. Water Footprint. Life Cycle Assessment.

Agaves comprise a group of more than 200 species of succulent plants that flourish in arid and semi-arid environments, having adapted to adverse conditions and low water availability [1,2]. These plants are native to semi-desert regions of the Western Hemisphere, including the southwestern United States, Mexico, Central America, northern South America, and the Antilles [1].

Agave's applications vary depending on the species. These plants can produce tequila, carpets, tapestries, doormats, stretchers, bags, and biomass for biofuel and bioproduct generation [3].

Brazil is among the leading producers and exporters of natural fibers from Agave sisalana Pierre, particularly in Bahia, which spearheads production alongside other northeastern states such as Paraíba, Ceará, and Pernambuco. This region concentrates the production of agave fiber, a crucial subsistence resource in the semi-arid areas of Bahia due to its drought resistance and phytochemical composition [1,4,5]. In Mexico, the cultivation of Agave tequilana Weber var. 'Blue' holds significant economic and social relevance, generating employment in agriculture and industrial processing, and substantially contributing to tequila exports [1,6].

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Given the diverse products derived from agave, it is essential to assess the environmental performance of its production processes to evaluate their sustainability. One of the industry's principal tools for this purpose is Life Cycle Assessment (LCA) [7]. This approach entails compiling input and output data related to material and energy flows across the entire life cycle of a product system, estimating the environmental impacts generated at each stage. ISO 14040/2009 (Principles and Framework) and ISO 14044/2009 (Requirements and Guidelines) offer a structured framework for conducting high-quality assessments [7,8].

This study aims to analyze the trends and findings of research on the application of Life Cycle Assessment (LCA) to the cultivation and processing of agave. The goal is to identify and compare the environmental impacts associated with agave across different life cycle stages and highlight current research gaps.

Materials and Methods

The article selection process was conducted through the ScienceDirect and Scopus databases, which provide comprehensive access to global research and analytical tools. Predefined keyword sets were combined using the Boolean operators "AND" and "OR," as shown in Table 1. The selected terms were associated with Life Cycle

Table 1. Quantities of articles.

Repositories	Agave AND (Cultivation OR Farming OR Growth) AND "Life cycle assessment"	Agave AND Processing AND "Life cycle assessment"	Duplicates
Science Direct	48	65	56
Scopus	4	4	
Selected	6	1	

Assessment and the cultivation and processing of agave. Searches were conducted in English within the "ARTICLE TITLE, ABSTRACT, KEYWORDS" fields, and the "Research articles" filter was applied. The review was performed in May 2024. Review articles were excluded, as this study aimed to analyze trends in primary research, particularly those involving experimental or observational data.

Articles were then filtered to remove duplicates and to exclude those whose titles or abstracts did not align with the research topic or were not fully available. This selection involved reading each article to confirm whether the search terms were the focus of the research rather than mentioned in passing. Specifically, the selected studies had to involve agave biomass (although other biomasses could also be included) and must have conducted LCA analyses focusing on cultivation or processing to identify the primary environmental impacts related to agave.

Table 1 presents the number of publications retrieved from the repositories using the selected search terms. A total of 65 articles were initially identified, of which only 7 met the inclusion criteria.

Results and Discussion

Table 2 presents the selected studies in descending chronological order based on their year of publication. It outlines each study's central objective, functional unit, database used, LCA software, life cycle impact assessment (LCIA) method, impact categories considered, and main conclusions.

The impact categories identified across the analyzed studies include:

- Global Warming Potential (GWP)
- Stratospheric Ozone Depletion (SOD)
- Terrestrial Acidification (TA)
- Freshwater Eutrophication (FE)
- Freshwater Ecotoxicity (FET)
- Terrestrial Ecotoxicity (TET)
- Human Carcinogenic Toxicity (HCT)
- Fossil Resource Scarcity (FRS)
- Ionizing Radiation (IR)
- Ozone Depletion Potential (ODP)
- Photochemical Oxidation Formation Potential – Human health (HOFP)
- Photochemical Oxidation Formation Potential – Ecosystems (EOFP)
- Terrestrial Acidification Potential (TAP)
- Freshwater Eutrophication Potential (FEP)
- Human Toxicity Potential – Cancer (HTPc)
- Human Toxicity Potential – Non-cancer (HTPnc)
- Fossil Fuel Potential (FFP)
- Water Consumption Potential (WCP)
- Acidification Potential (AP)
- Photochemical Oxidation Potential (PCOP)
- Eutrophication Potential (EP)
- Renewable Energy Use (REU)
- Non-renewable Energy Use (NREU)
- Greenhouse Gas Emissions (GHG)
- Fine Particulate Matter Formation (PMFP)
- Cumulative Energy Demand (CED)
- Water Consumption (WC)

- Global Warming (GW)
- Ozone Formation – Human Health (OFHH)
- Fine Particulate Matter Formation (FPMF)
- Ozone Formation – Terrestrial Ecosystems (OFTE)
- Human Non-carcinogenic Toxicity (HnCT)
- Land Use (LU)
- Mineral Resource Scarcity (MRS)

These diverse impact categories highlight the comprehensive nature of environmental performance assessments within LCA agave cultivation and processing studies. Despite methodological variations across studies, global warming potential, water consumption, and cumulative energy demand were among the most consistently analyzed and reported categories. Such consistency reflects these indicators' critical importance in evaluating the sustainability of agave-based production systems.

The literature reveals a wide range of proposals using the LCA methodology for agave, resulting in variations in the software, impact categories, and functional units selected. Among the studies, midpoint impact categories were more frequently evaluated than endpoint categories, with Ecoinvent being the most commonly used database. The Global Warming Potential (GWP) was the most frequently used impact category in the reviewed analyses. This category assesses the contribution of various greenhouse gases (GHGs) to global warming, expressed in carbon dioxide equivalents (CO_2 eq). Evaluating this impact helps identify which stages of the agave life cycle emit the most GHGs and how those emissions can be reduced. For instance, Yan and colleagues (2020) reported that the global warming impact of agave was 62% lower than corn's and 30% lower than sugarcane's, highlighting its significantly lower carbon footprint [13].

Table 2. Selected studies with the agave plant that conducted Life Cycle Assessment (LCA)

Ref.	Objective	Functional Unit/ Database	Software/ Method of LCIA	Impact Categories	Main Conclusions
[9]	Evaluate the environmental impacts of current agave bagasse management practices and compare them with alternative valorization processes, where the bagasse is anaerobically digested or processed and used as reinforcement in a polylactic acid (PLA) bioplastic composite.	1.1 tons of agave bagasse / N.F	SimaPro 9.5.0 / ReCiPe 2016 v1.1	GWP, SOD, TA, FE, FET, TET, HCT, FRS	PLA production chains need further development and standardization to reduce their environmental footprint. The low methane yield in anaerobic digestion does not offset its impacts.
[10]	Evaluate the environmental impacts of mezcal production from Agave cupreata in Michoacán, Mexico. The central issue is the influence of management options for vinasse, bagasse, and biomass energy. The study was conducted using life cycle assessment (LCA).	A 0.75-liter bottled mezcal produced/ Ecoinvent	N.F / ReCiPe midpoint	GWP, PMFP, FEP, CED	Regulations should focus on forest management to make sustainable use of wood (FSC systems), improving road conditions to reduce fuel consumption, and encouraging practices such as avoiding the use of agrochemicals during the growth of the agave, promoting the application of agroforestry systems, and organic pest control that can benefit the maintenance of agave cultivation in the long term. The results of this research can assist producers in prioritizing the reduction of material intensity and environmentally damaging emissions and monitoring progress.

Ref.	Objective	Functional Unit/ Database	Software/ Method of LCIA	Impact Categories	Main Conclusions
[11]	Compare the environmental performance associated with electricity generation from combustion and gasification processes of sugarcane and agave bagasse.	1 MJ of electricity produced/ Ecoinvent	SimaPro 8 / ReCiPe 2016	GWP, ODP, HOFP, EOFP, TAP, FEP, HTPc, HTPnc, FFP, WCP	In the cultivation stage, the main factors causing environmental damage are fertilizer use, diesel consumption, and emissions to air and water, with sugarcane cultivation having an impact 2 to 6 times greater than that of agave (except for FEP and HTPc). Combustion of sugarcane bagasse is the scenario with the highest environmental impact, followed by combustion of agave bagasse and gasification processes.
[12]	Agave juice and sugarcane molasses were compared as potential feedstocks for producing bioethanol in Mexico in terms of their environmental impact and economic factors.	1 MJ of energy / Ecoinvent	SimaPro 8 / ReCiPe 2016	GWP, ODP, HOFP, EOFP, TAP, FEP, HTPc, HTPnc, FFP, WCP	Production of bioethanol from agave juice had a lower environmental impact compared to sugarcane juice, attributed to lower pesticide, coal, and water consumption. Bioethanol production was the most impactful stage (>60%) due to low ethanol yields from fermentation. Economically, neither feedstock is viable with the current Mexican energy grid, but with 26.5% renewable energy, bioethanol production from agave juice becomes feasible.
[13]	The objective of this article was to conduct the first comprehensive LCA and economic analysis of 1st and 2nd generation (2G) ethanol produced from Australian grown agave, using data collected from a 5-year field experiment in Queensland.	1 GJ of fuel ethanol produced / Ecoinvent	SimaPro 8.4 (2018) / N.F	GW, SOD, IR, OFHH, FPMF, OFTE, TA, FE, TET, FET, ME, HCT, HnCT, LU, MRS, FRS, WC	Agave outperforms first-generation biofuel crops like corn and sugarcane in water-related environmental impacts and offers competitive ethanol yields. Despite its high land-use impact, agave can be cultivated on land unsuitable for food. It is a promising feedstock for biofuels in arid regions, with a yield of 7414 L/ha/year after 5 years, but it is economically unviable without government subsidies.
[14]	To investigate the economic and environmental feasibility of bioethanol production from Mexican lignocellulosic biomass, including wood species, grasses, bagasse, and crop residues. Comprehensive process modeling, economics, and life cycle assessment (LCA) were employed to understand the effects of these feedstock compositions on bioethanol yield, economic performance, and environmental impact within an integrated biorefinery environment that coproduces heat and power.	1 kg of biomass/ Ecoinvent 3	N.F / CML V3.03	GWP, AP, PCOP, EP	Overall, wood and agricultural wastes are competitive economically and environmentally, while lawns have had poor performance and the bagasse mixed results. The correlations based on biomass compositions suggest a proportional limit for a balanced process and GWP savings, facilitating rapid biomass screening and the identification of ideal raw material compositions.

Ref.	Objective	Functional Unit/ Database	Software/ Method of LCIA	Impact Categories	Main Conclusions
[15]	Conduct Life Cycle Assessment (LCA) of sisal fiber production in Tanzania and Brazil based on primary data, covering approximately 45% of global production. The specific objectives are to evaluate the effects of local differences in agricultural and fiber processing practices, and to assess the influence of methane emissions from waste disposal on the overall environmental performance of sisal fiber production, using modeling and scenario analysis.	One metric ton of sisal fiber/ Ecoinvent v2.2	N.F / ReCiPe Midpoint v1.12	REU, NREU, GHG	This study shows that sisal fiber produced in Tanzania or Brazil has low emissions of non-renewable energy (NREU) and greenhouse gases (GHGs) from cradle to port. Environmental performance of sisal fiber may vary significantly based on local practices, location and assumptions. Disposal of waste in open ponds can increase GHG emissions, but these can be mitigated by short disposal periods, bare ponds or use of waste to generate biogas. In all scenarios, NREU and GHG emissions from sisal fibres are 75% to 95% lower than those of glass fibres.

Other commonly assessed categories included terrestrial acidification potential and human toxicity (both carcinogenic and non-carcinogenic).Terrestrial acidification is primarily caused by pollutants like NH_3, NO_x, and SO_2, which form acids upon contact with water vapor and adversely affect soil, aquatic systems, and biodiversity [11].Human toxicity assessments help identify harmful substances in the life cycle and support measures to mitigate human exposure to such substances. Studies comparing agave to other biomasses—notably sugarcane—consistently indicated that agave has a lower environmental impact [11,12]. Parascanu and colleagues (2021) state that these differences stem primarily from cultivation practices. Sugarcane requires higher inputs of chemical compounds and fertilizers, leading to greater emissions into water and air.

A notable difference in Water Consumption Potential (WCP) was also observed, as sugarcane cultivation depends heavily on irrigation, unlike agave [11]. This reinforces agave's advantage in terms of a lower water footprint.

Conclusion

The comprehensive literature review underscores the need for expanded Life Cycle Assessment (LCA) studies focused on the cultivation and processing of agave. The selected articles—most of which are recent—enabled a detailed analysis of the diverse methodological approaches used in this field.

This study highlighted a growing concern about the environmental impacts of agave throughout its life cycle. Agave has demonstrated consistently lower environmental impacts compared to other biomass sources, particularly regarding water use and carbon emissions. Nevertheless, areas for improvement remain. The results indicate the need for policy support to promote strategies that reduce environmental impacts and incentives to enhance the economic viability of agave-based bioproducts.

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Bibliometric Analysis of Publications Related to Solid Oxide Fuel Cell (SOFC)

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The growing interest in renewable energies amid global energy challenges highlights the promising technology of solid oxide fuel cells (SOFCs) due to their efficiency, low pollutant emissions, and flexibility in using renewable sources. This study conducts a bibliometric analysis, identifying over 18,000 documents distributed across 1,800 journals worldwide. Between 2014 and 2024, there has been a significant increase in academic output on the topic, recently surpassing 141 publications annually. However, Brazil still shows a relatively modest presence in this research area. The study underscores the increasing potential of SOFCs and points to research and development opportunities that remain to be explored.
Keywords: Renewable Energies. Solid Oxide Fuel Cell (SOFC). Energy Efficiency. Pollutant Emissions. Technological Development.

This study conducts a bibliometric analysis of publications related to solid oxide fuel cells (SOFCs). Bibliometric analysis is a valuable tool for quantitatively and statistically assessing the landscape of a research field, identifying publication patterns, and exploring interconnections between study areas [1].

Researchers widely use this approach to evaluate the development of a scientific domain or to map its multidimensional characteristics [1].

The Scopus database, recognized as the largest repository of abstracts and citations from peer-reviewed literature, is commonly employed in bibliometric analyses. It includes scientific journals, books, and conference proceedings and serves as a fundamental source for this study [2].

Fuel cells—devices that convert chemical energy into electrical energy—have attracted attention due to their high efficiency (60–80%) and low environmental impact compared to combustion engines [3]. These systems operate continuously using fuel and an oxidant, typically hydrogen and oxygen from the air, with nearly zero pollutant emissions, positioning them as a sustainable energy solution [4,5].

SOFCs, in particular, have gained interest due to their high efficiency, rapid reaction kinetics at elevated temperatures, and fuel flexibility. They allow the use of natural gas, biomethane, and ethanol—fuels that are widely available in Brazil. This makes the development of SOFCs strategically important for the country, both economically and environmentally [6].

Considering the relevance of this technology, the present study analyzes global and national (Brazilian) publications on SOFCs indexed in the Scopus database. It identifies key research outputs, highlights potential areas for future investigation, and outlines the main themes consolidated in recent years. The data were compiled and analyzed using the Bibliometrix R package, a statistical tool for bibliometric research (Table 1 and 2).

Results and Discussion

Annual Scientific Production

The study analyzed 18,150 documents published between 2014 and 2024, with Brazil contributing only 228 of these documents. Figure 1a illustrates the annual distribution of articles globally during this period, while Figure 1b highlights the Brazilian contribution. There is a clear global growth trend

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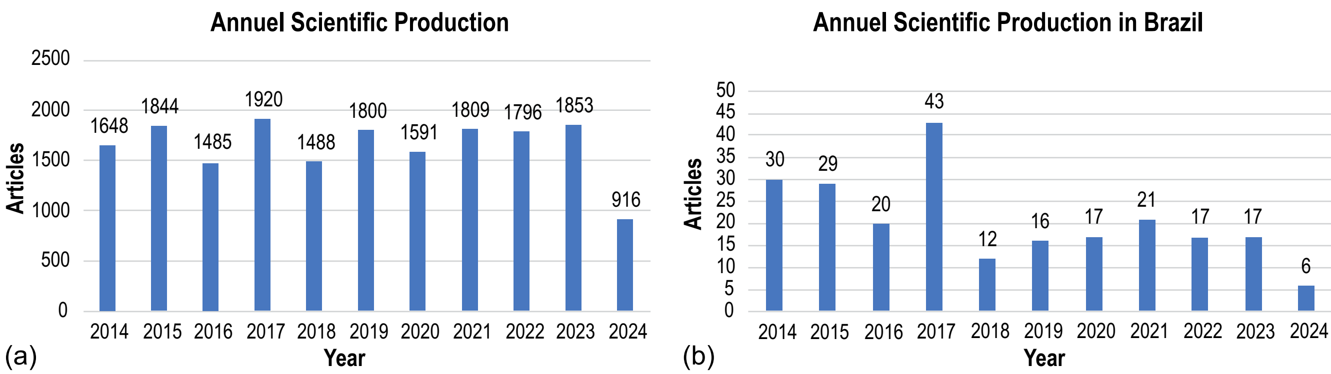
Table 1. Main information about the data generated by Bibliometrix.

Description	Results
MAIN INFORMATION ABOUT DATA	
Timespan	2014:2024
Sources (Journals, Books, etc)	1811
Documents	18150
Document Average Age	5,15
Average citations per doc	17,5
DOCUMENT CONTENTS	
Article	14057
Conference paper	3204
Review	705
Authors	22435
Documents by author	1,24
Authors per document	0,81
Co-Authors per Doc	5,23
International co-authorships %	26,15

Table 2. Main information about the data generated by Bibliometrix linked to Brazilian institutions or researchers.

Description	Results
MAIN INFORMATION ABOUT DATA	
Timespan	2014:2024
Sources (Journals, Books, etc)	89
Documents	228
Document Average Age	5.95
Average citations per doc	12.67
DOCUMENT CONTENTS	
Article	155
Conference paper	61
Review	10
Authors	230
Documents by author	1,01
Authors per document	0,99
Co-Authors per Doc	5,5
International co-authorships %	50,88

Figure 1. Number of articles per year between 2014 and 2024 worldwide (a) and in Brazil (b).



in research and publication in this area, indicating its contemporary relevance as a driving force for the field's development.

In the Brazilian context, the scarcity of studies dedicated to solid oxide fuel cells (SOFC) is notable, suggesting a nascent research area with vast potential for exploration.

Countries of Corresponding Authors

The data reveal an intriguing distribution of the countries of origin of the corresponding authors of the analyzed documents. Figure 2 provides a comprehensive view of this distribution, highlighting the twenty most prominent countries contributing to the examined research. Notably, China leads unequivocally, followed by South Korea and the United States. Brazil, on the other hand, ranks 21st, with 106 documents.

Most Relevant Sources

Figure 3 highlights the 20 most relevant sources when analyzing the documents. Notably, the International Journal of Hydrogen Energy leads with 1,784 published documents, followed closely by ECS Transactions, with 1,356 articles in the field. In the Brazilian context, as shown in Figure 4, ECS Transactions and the International Journal of Hydrogen Energy lead with 22 publications each, followed by Ceramics International with 19 publications. These data indicate a trend of journals addressing the SOFC topic more frequently, providing valuable insights for selecting journals for future investigations.

Observing the growth of the primary publication sources on Solid Oxide Fuel Cells (SOFC) from 2014 to 2024, both globally and in Brazil, clear trends stand out. Globally, the International Journal of Hydrogen Energy and ECS Transactions lead with consistent growth, followed by the Journal of Power Sources, Ceramics International, and the Journal of the Electrochemical Society. In Brazil, ECS Transactions and the International Journal of Hydrogen Energy remain significant, with notable growth in Ceramics International. Additionally, Materials Science Forum and Revista Materia show gradual increases, reflecting the country's growing interest and expansion of SOFC research.

Most Relevant Affiliations

The leading global institutions involved in SOFC research and publication are highlighted in Figures 5 and 6. In Figure 6, Kyushu University leads globally with 570 articles, followed by Huazhong University of Science and Technology with 474. In the Brazilian context, shown in Figure 7, the Materials Science and Engineering Postgraduate Program stands out with 21 articles, followed by the Federal University of Rio de Janeiro and the University of São Paulo with 12 articles. These figures demonstrate the strong engagement of universities and research centers in the study and development of this topic.

Figure 2. Distribution of the corresponding authors' countries of origin.

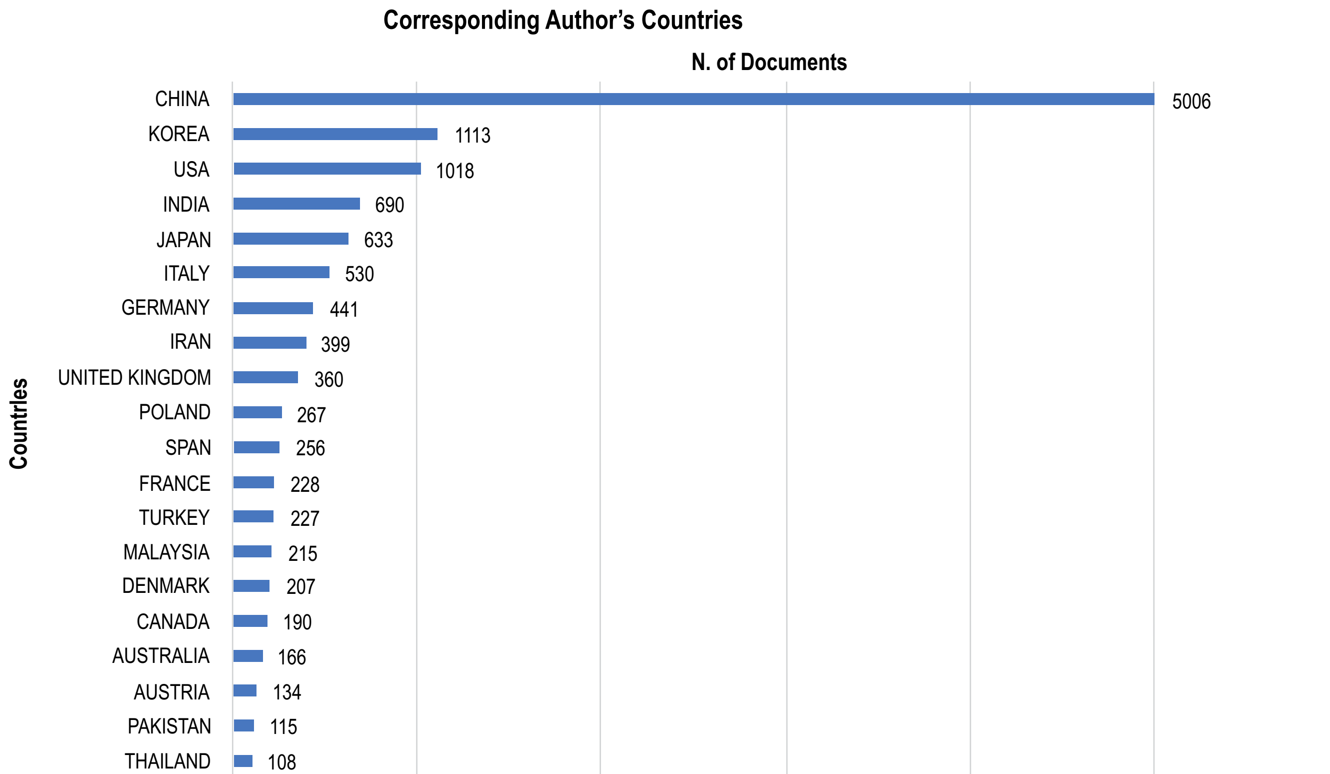


Figure 3. Most relevant sources with their respective number of publications in the SOFC field.

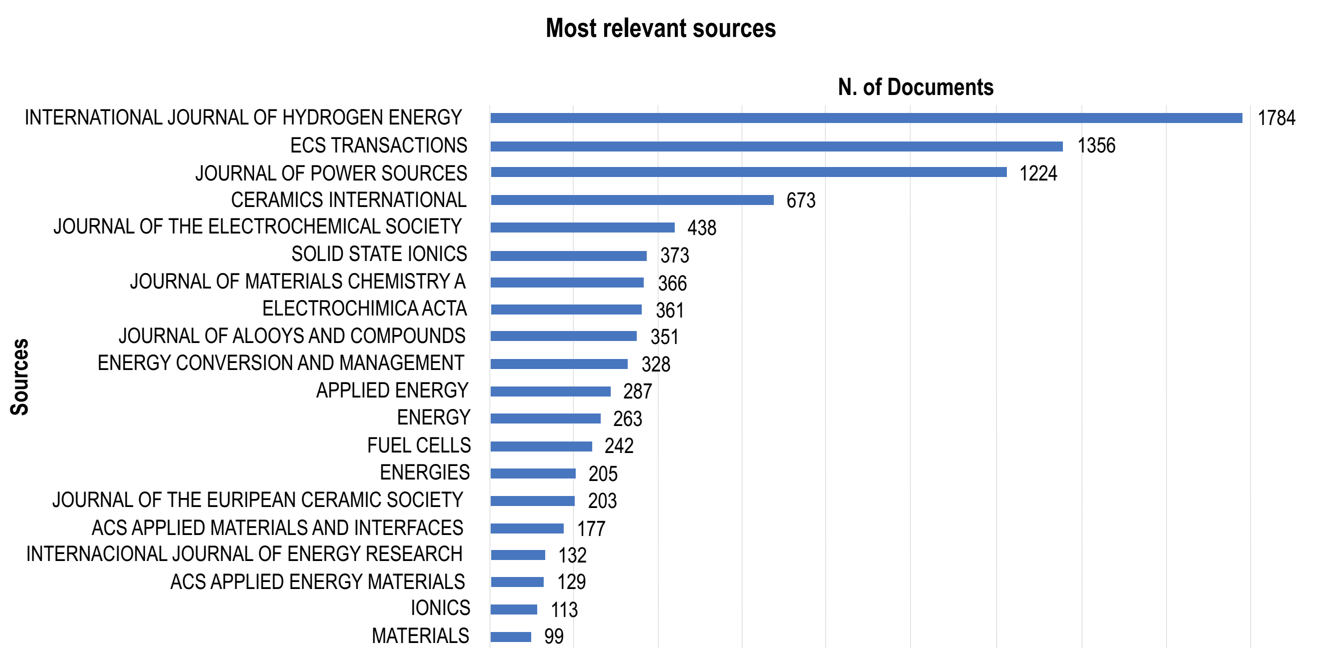


Figure 4. Most relevant sources with their respective number of Brazilian publications in the SOFC field.

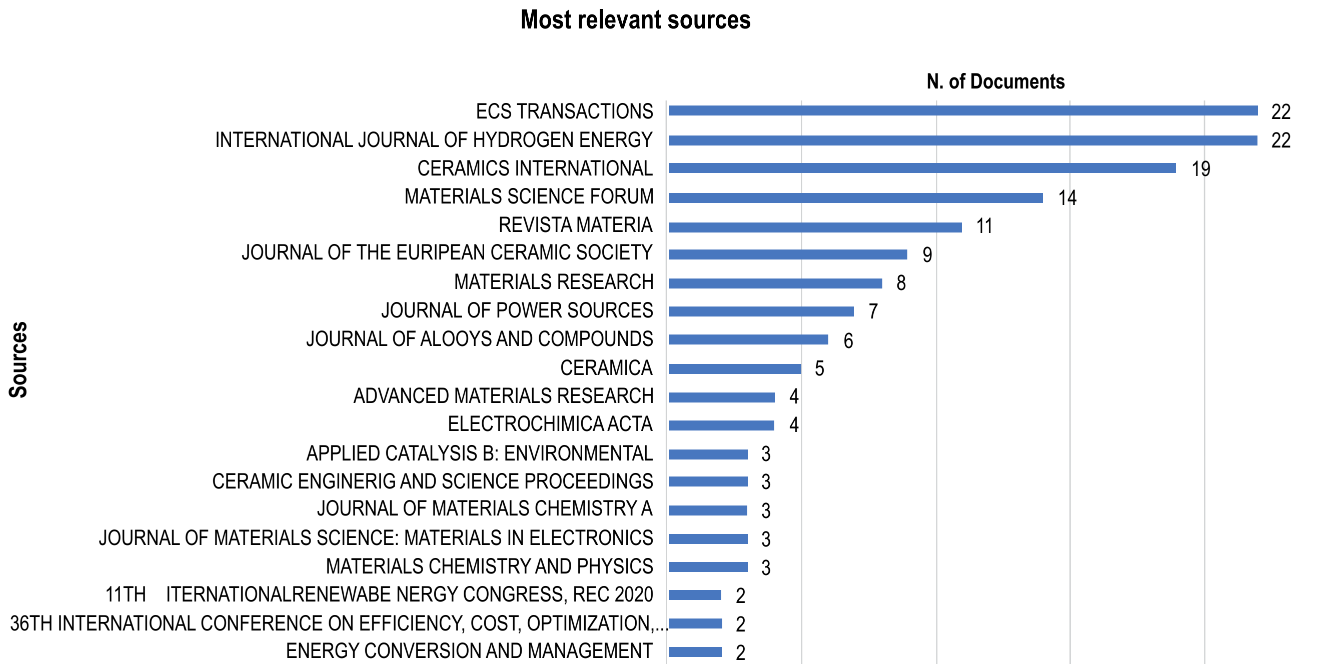


Figure 5. Most relevant institutions and their respective number of produced articles.

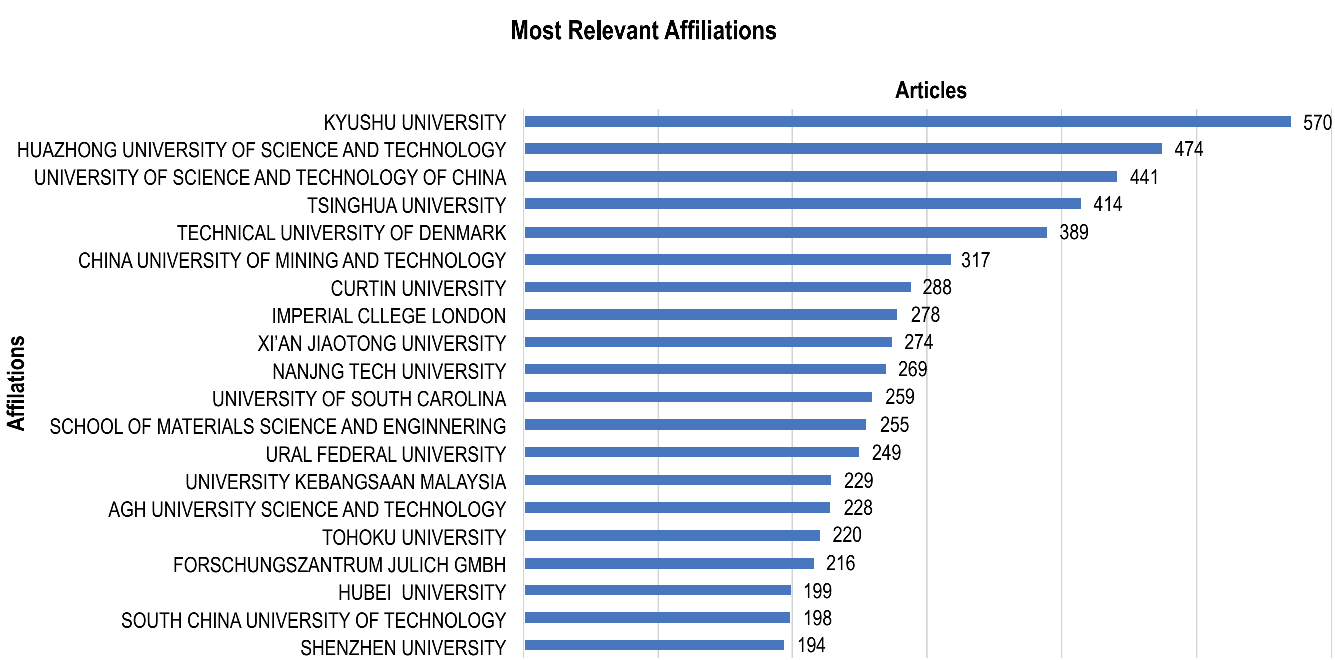
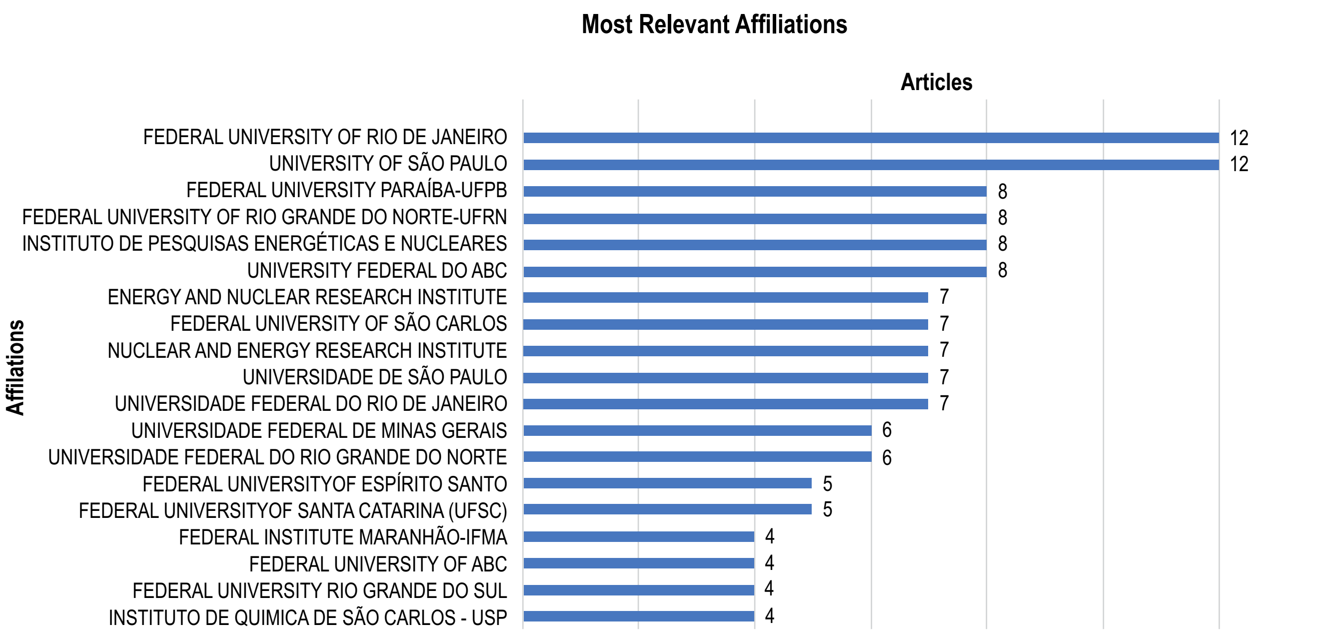


Figure 6. Most relevant Brazilian institutions and their respective number of produced articles.



Most Cited Articles in Word

Table 3 presents the 20 most cited articles globally between 2014 and 2024, including the total number of citations. Table 4 lists Brazil's 20 most-cited articles during the same period. The authors and their affiliations were attributed based on the first author of each article.

Conclusion

This study analyzed 18,150 documents from 1,811 international scientific journals and 228 publications authored by Brazilian researchers across 89 journals between 2014 and 2024, using data from the Scopus database and the Bibliometrix R package. The findings demonstrate that research on renewable energy sources—particularly hydrogen and solid oxide fuel cells (SOFCs)—has shown steady growth, with a clear trajectory for future expansion.

The main objective was to conduct a bibliometric analysis of publications focused on SOFCs. Despite the relatively limited volume of literature in certain regions, the analysis identified specific areas needing further investigation and with strong potential for technological development, thus signaling a promising field for future research.

The bibliometric mapping also revealed a notable scarcity of studies on SOFCs within the Brazilian context, underscoring the country's untapped potential for further exploration. The study identified global and national publication trends, major research institutions, and key contributing authors, offering a broad and informative overview of SOFC-related research in Brazil and internationally.

These insights guide future research efforts, providing researchers with a clearer understanding of the principal journals publishing in this field. Moreover, the results highlight underexplored research themes, which could foster the development of innovative solutions for climate change mitigation and environmental sustainability through hydrogen production from renewable sources.

Additionally, the analysis identified the International Journal of Hydrogen Energy and ECS Transactions as the leading journals in terms of publication volume. There has also been a recent increase in the number of Brazilian authors contributing to this field. Brazil's primary research center is the Postgraduate Program in Materials Science and Engineering, followed by the Federal University of Rio de Janeiro (UFRJ) and the University of São Paulo (USP), indicating a growing—albeit still comparatively modest—presence in the global research landscape.

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Table 3. The most cited articles worldwide related to SOFC.

Authors	Affiliations	DOI	Total Citations
HOU Q et al.	Harbin Institute of Technology	10.1115/ES2020-1650	2020
MILCAREK RJ et al.	Arizona State University	10.1115/ES2020-1634	2020
LAVERNIA A et al.		NA	2020
RODRÍGUEZ JC et al.	National Energy Technology Laboratory	10.1115/POWER2020-16620	2019
GEMMEN RS et al.	National Energy Technology Laboratory	10.1149/09601.0025ecst	2019
JOHNSON RW et al.	Stanford University	10.1016/j.mattod.2014.04.026	1358
BUTTLER A et al.	TU München	10.1016/j.rser.2017.09.003	1303
SCHMIDT O et al.	Imperial College London	10.1016/j.ijhydene.2017.10.045	1229
MAHATO N et al.	Indian Institute of Technology Kanpur	10.1016/j.pmatsci.2015.01.001	1188
DUAN C et al.	Colorado School of Mines	10.1126/science.aab3987	1005
GAO Z et al.	Northwestern University	10.1039/c5ee03858h	728
DING D et al.	Georgia Institute of Technology	10.1039/c3ee42926a	711
LI M et al.	University of Sheffield	10.1038/nmat3782	708
SENGODAN S et al.	Ulsan National Institute of Science and Technology	10.1038/nmat4166	612
MEFFORD JT et al.	The University of Texas at Austin	10.1038/nmat4000	591
DUAN C et al.	Colorado School of Mines	10.1038/s41586-018-0082-6	515
GU W et al.	Southeast University	10.1016/j.ijepes.2013.06.028	515
GIDDEY S et al.	CSIRO Energy	10.1021/acssuschemeng.7b02219	492
DUAN C et al.	Colorado School of Mines	10.1038/s41560-019-0333-2	433
GRAVES C et al.	Technical University of Denmark	10.1038/nmat4165	419

Table 4. The most cited articles in Brazil related to SOFC.

Authors	Affiliations	DOI	Total Citations
DA SILVA FS et al.	São Paulo State University (Unesp)	10.1016/j.ijhydene.2017.08.105	297
GÓMEZ SY et al.	Federal University of Santa Catarina (UFSC)	10.1016/j.rser.2016.03.005	283
FERNANDES MD et al.	Federal University of Minas Gerais (UFMG)	10.1016/j.ijhydene.2018.07.004	96
DA SILVA AAA et al.	Military Institute of Engineering	10.1016/j.apcatb.2017.01.069	81
LO FARO M et al.	Institute for Advanced Energy Technologies "Nicola Giordano" (ITAE) of the Italian National Research Council (CNR)	10.1016/j.apcatb.2017.08.010	65
DA SILVA MJ et al.	Nuclear and Energy Research Institute (IPEN)	10.1016/j.jeurceramsoc.2015.10.005	65
STEIL MC et al.	Université Grenoble Alpes	10.1016/j.apenergy.2017.04.086	63
GUAITOLINI SVM et al.	Federal University of Espírito Santo (UFES)	10.1109/IREC.2018.8362573	55
RODRÍGUEZ-LÓPEZ S et al.	Ceramics and Glass Institute (CSIC)	10.1016/j.jeurceramsoc.2017.03.054	54
LIMA CGM et al.	Universidade Federal da Paraíba (UFPB)	10.1016/j.ceramint.2014.12.093	53
LOUREIRO FJA et al.	Universidade Federal do Rio Grande do Norte (UFRN)	10.1016/j.jeurceramsoc.2019.01.013	50
DA SILVA CA et al.	Federal University of Rio de Janeiro (UFRJ)	10.1016/j.ijhydene.2015.06.019	48
ALIOTTA C et al.	Università degli Studi di Palermo	10.1016/j.apcatb.2016.02.044	43
SARRUF BJM et al.	Federal University of Rio de Janeiro (UFRJ)	10.1016/j.ijhydene.2019.04.075	42
NOBRESA SD et al.	Nuclear and Energy Research Institute (IPEN)	10.1149/2.107403jes	36
SARRUF BJM et al.	Federal University of Rio de Janeiro (UFRJ)	10.1016/j.ijhydene.2018.01.192	34
AUGUSTO BL et al.	Federal Fluminense University (UFF)	10.1016/j.ijhydene.2014.05.088	34
LO FARO M et al.	Institute of Advanced Energy Technologies	10.1007/s10800-015-0849-5	33
TARRAGÓ DP et al.	Federal University of Rio Grande do Sul (UFRGS)	10.1016/j.powtec.2014.09.037	30
SANTOS JRD et al.	Universidade Federal da Paraíba (UFPB)	10.1016/j.electacta.2018.08.018	29

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Quality of Scientific Production Validation of Research Traceability Standars

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Without a specific standard for evaluating the quality of research output, funding agencies and academic journals have placed a growing emphasis on implementing study monitoring procedures. Within this context, this study validated research traceability standards that can contribute to improving the quality of scientific production. A qualitative study was conducted with a community of researchers to identify and validate traceability standards to ensure scientific research quality. Ten standards related to scientific traceability and reproducibility were identified, with particular emphasis on the description of methodology and data sharing, which emerged as the most relevant.

Keywords: Scientific Research. Quality. Traceability.

Scientific research is essential for societal advancement, providing a foundation for in-depth exploration of phenomena based on their inherent characteristics and modes of operation [1]. The scientific community broadly acknowledges that rigorous methods and reliable results are indispensable for research integrity and scientific knowledge advancement. Notably, nearly 30% of article retractions are attributed to scientific error or the inability to verify results, which may only represent a fraction of the broader issue [2]. This scenario poses particular risks in an environment increasingly reliant on external funding, while suffering from a shortage of human resources and stable research infrastructure. As such, the reliability of scientific data is paramount—not only for the progression of science, but also for maintaining the trust of the public and collaborators within research teams. Individual scientists and institutions are responsible for the quality and integrity of the research they produce and disseminate [3].

In recent years, quality management within the Research and Development (R&D) sector has become increasingly critical, driven by the growing demand for researchers to demonstrate adherence to the highest methodological standards. Implementing quality management criteria, particularly those related to scientific traceability, facilitates impartial monitoring and verification across all domains of research and development. Although no universal standards for research quality currently exist, relevant quality criteria from established standards and manuals should be adapted and applied wherever feasible to ensure data compliance [4]. In this context, the application of quality principles—such as data traceability—proves to be highly beneficial, reinforcing the positive intersection between Quality Management and scientific research.

This study aimed to identify and validate scientific traceability standards, thereby contributing valuable insights to the scientific literature. The objective was to enhance the transparency and reproducibility of the research process by establishing clear standards that other investigators can adopt and replicate.

Materials and Methods

This qualitative study was conducted in two stages. Figure 1 illustrates the process for validating the identified criteria.

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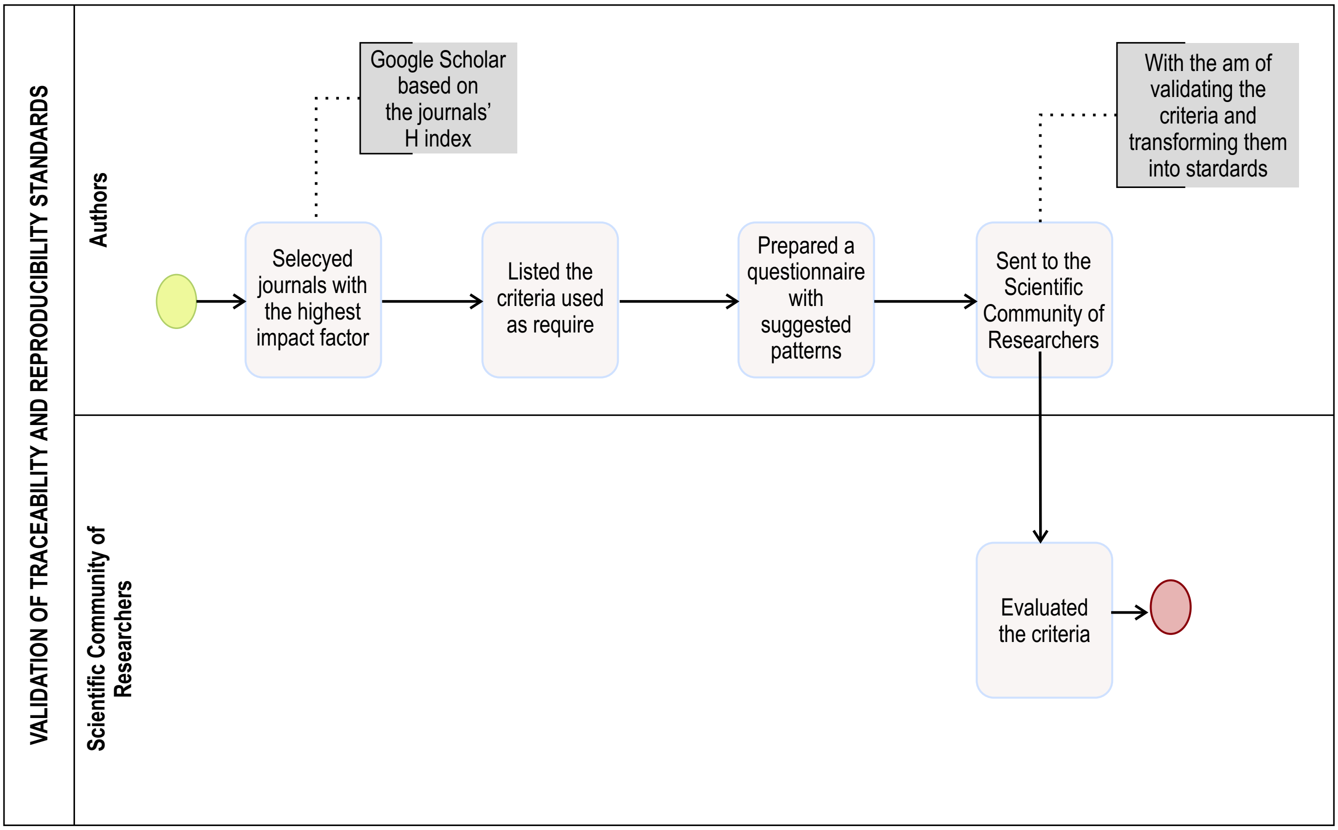
Figure 1. Diagram of the standards validation steps.



In the first phase, the journals with the highest impact factor in January 2023 were selected, they were: Nature, The New England Journal of Medicine, Science, IEEE/CVF Conference on Computer Vision and Pattern Recognition and The Lancet with H5 indexes of 444, 432, 401, 389 and 354, respectively [5]. The criteria for publication in these journals related to traceability and reproducibility were evaluated and described in Table 1—the criteria for publication in these journals related to traceability and reproducibility

In the second phase, the selected criteria were sent to a scientific community of researchers, in person or remotely, and answered by 31 researchers from the Oswaldo Cruz Foundation, a health research institution of the Brazilian Government with relevant scientific production. The researchers were randomly assigned and responded to the questionnaire using the criteria listed in Table 1.

The researchers who participated in the study assigned percentage values to each traceability criterion, reflecting the relative importance of each standard compared to the others. The total of all assigned percentages equaled 100%, ensuring a balanced assessment. The data were organized and analyzed according to the value attributed to each standard by the participants, based on perceived importance. The study complied with ethical standards, having been approved by the Federal Institute of Bahia Research Ethics Committee under opinion number 079685/2022.

Results and Discussion

Traceability refers to the ability to map and follow the entire pathway of a process, from its initial stages to its conclusion. In the research context, this implies monitoring the investigative process from conception to final output. With the

Table 1. Criteria related to traceability and reproducibility evaluated by the scientific community.

Criteria related to the traceability and reproducibility evaluated by the scientific community		
1	**Method**	Description of the methodology used
2	**Material (Equipment and Reagents)**	
3	**Artifacts (Collection instruments)**	
4	**Dataset (What data was used)**	Sharing and making data and/or codes available
5	**Where data is stored/can be found**	
6	**Peer review**	Other criteria
7	**Presence of bibliographic references**	
8	**Technical terms used in scientific research**	
9	**Indication of software, equipment or tools used**	
10	**Availability of results**	

rapid advancement of technological innovation, growing competitiveness, and increasing pressure for productivity, quality assurance tends to be overlooked in scientific research and publication [6].

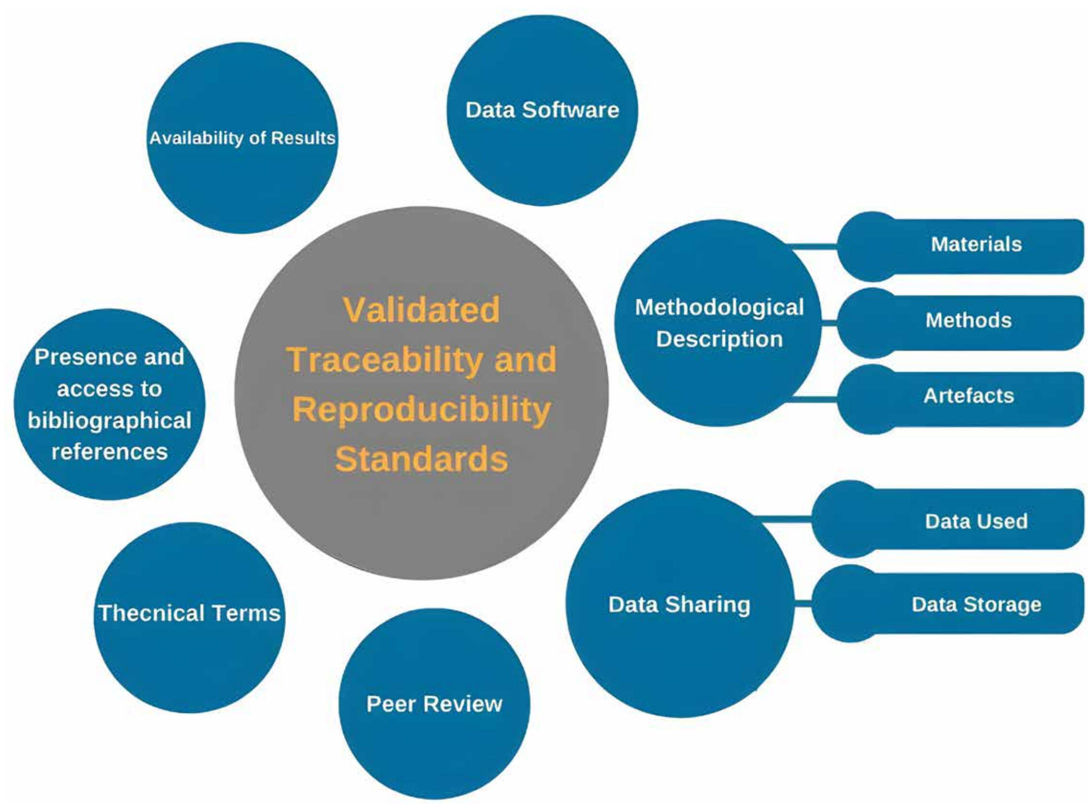
Recognizing the importance of traceability necessitates a broader reflection on the foundations of science. Science must be grounded in the capacity to critically evaluate conclusions drawn by researchers, particularly those that have exerted or may exert significant influence. In this regard, ensuring traceability is indispensable for confirming or revising findings. Achieving this requires transparency in data and full disclosure of the methods employed in generating it. Clear, intelligible, and traceable documentation—including detailed accounts of data acquisition processes and any subsequent modifications—is essential both during the research and after publication [7].

Moreover, research findings that lack traceability tend to be less reliable and less valuable. Methodological approaches that systematically pursue predictive statistical models through trial-and-error steps often fail to report unsuccessful attempts, which may also hold scientific value. The omission of such results, simply because they did not meet the researcher's expectations, undermines the study's reproducibility and replicability. This practice contributes to a body of irreproducible findings that ultimately threaten scientific disciplines' credibility, utility, and foundational principles [8].

At the conclusion of the second phase of this study, the scientific community engaged in the research validated a set of traceability and reproducibility standards. These validated criteria are presented as formal traceability standards, as shown in Figure 2.

For the scientific community surveyed, the standards presented in Figure 2 were deemed critical for ensuring research quality.The standard most strongly associated with methodology encompasses the parameters, procedures, rules, and/or techniques, including computational approaches, used to construct and explain

Figure 2. Validated traceability and reproducibility standards.



knowledge generation [9]This standard was further subdivided into:

i) Materials – the resources employed in the research, including equipment, instruments, and biological or chemical products;

ii) Method – the approach used to conduct the study or experiment, including the procedures adopted to obtain results;

iii) Collection artifacts or instruments – objects created explicitly for the study, such as design products, prototypes, or software.

The second key standard, data sharing, is fundamental to timely disseminating studies, knowledge, and new lines of inquiry, thereby accelerating scientific discovery. It also enables the reuse and validation of previously generated data for future research efforts [10]. This standard was subdivided into:

iv) What data was used – a description of the datasets included in the research;

v) Where the data can be found – information on how to access the data, including files, systems, or repositories used in the study.

vi) The sixth standard, results availability, ensures that quality-assured data associated with the study's findings are accessible [11].

vii) Bibliographic references – this standard supports the validation of the research and situates the study within the broader context of existing literature. This facilitates a deeper understanding of the subject matter and allows readers to expand their knowledge of the topic [11].

viii)Technical terms or vocabulary help to identify key concepts and ideas presented in the study, improving clarity and efficiency in reading. This standard establishes a shared language to precisely convey concepts related to the research theme [11].

ix) Software or tools refers to digital programs used throughout the research and publication process, including those for document creation, image editing, data analysis, and more.

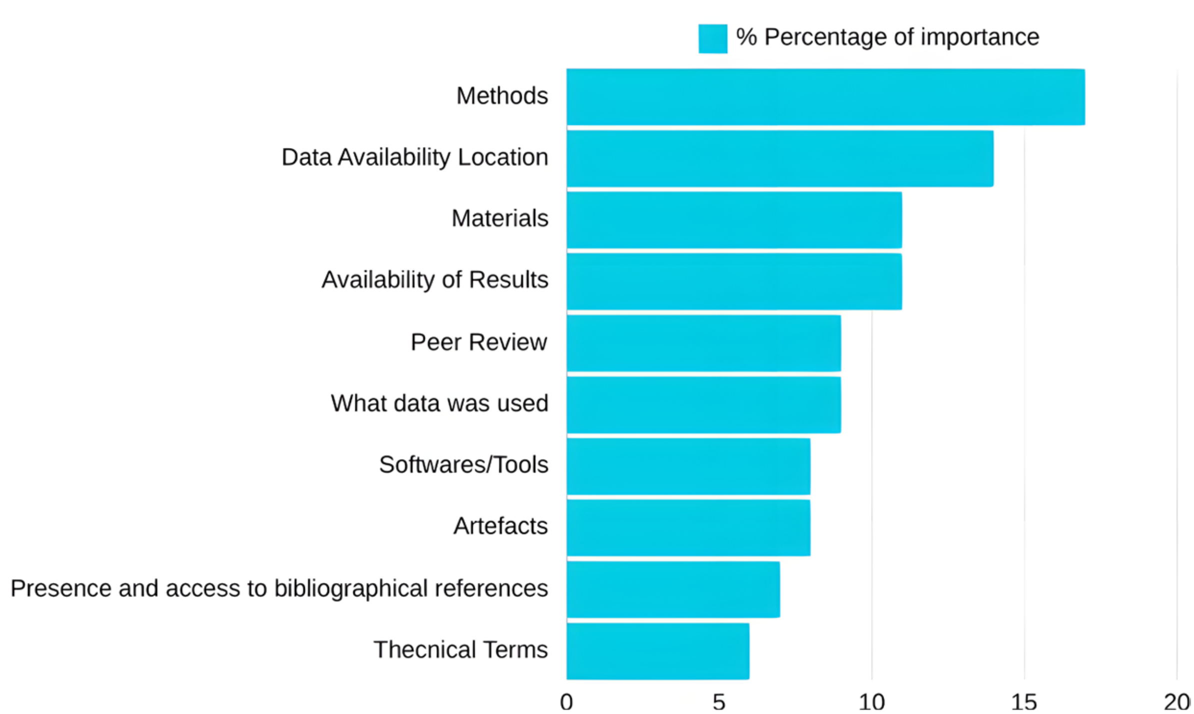
x) The standard peer review is widely recognized as a collaborative and essential component of scientific publishing. It involves submitting research for evaluation by domain experts to verify scientific validity and uphold rigorous quality standards, ultimately ensuring that only robust and credible research is published [12].

Together, these results enabled the identification of a comprehensive set of criteria—previously uncodified as a unified framework—proposed as a potential scientific standard for traceability and reproducibility. Furthermore, the consultation with researchers allowed the assignment of relative importance to each criterion, as illustrated in Figure 3.

The standards related to methods—materials, method, and artifacts—were assigned relative importance scores of 11%, 17%, and 8%, respectively, totaling 36% for the methodology standard. Among these, the method component stood out with 17%, underscoring the significance of establishing efficient and well-structured research methods. The criteria associated with data used and data accessibility received scores of 9% and 14%, respectively, up to 23% for the data sharing standard, which was identified as the second most critical domain.

The remaining standards—peer review, references, technical vocabulary, software/tools, and results availability—were rated at 9%, 7%, 6%, 8%, and 11%, respectively. These results demonstrate that, from the respondents' perspective, the methodology and data sharing standards are the most significant for ensuring the quality of scientific research. Scientific research must continually aim to generate meaningful and valuable knowledge for society, offering explanations of facts and phenomena aligned with the public and social interest. The dynamic nature of knowledge construction necessitates regularly updating

Figure 3. Criterion x Importance.



scientific understanding [13,14]. Within this context, researchers, scientists, research institutions, and universities play a vital role in producing scientific outputs. Applying traceability standards effectively communicates the critical rigor required for scientific credibility and reliability to the broader society.

Conclusion

Concerns regarding scientific research quality, integrity, and usefulness are becoming increasingly visible. They must be addressed not only by individual researchers but also by institutional managers and all stakeholders involved in producing and disseminating scientific knowledge. Scientific outputs must ensure the generation of credible, verifiable information to support sound decision-making, thereby offering tangible value to society through high-quality research.

The absence of traceability and reproducibility presents potential risks, particularly when viewed through good research practices. Conversely, re-evaluating data in light of enhanced transparency can significantly contribute to scientific rigor and quality improvement.

This study identified and validated ten traceability and reproducibility standards that authors and journals can adopt to improve the clarity, accountability, and repeatability. While all ten standards were acknowledged, the methodology and data sharing standards emerged as the most relevant according to the researchers surveyed. These findings suggest the need for further investigation into the specific reasons for the perceived prominence of these standards and the identification of minimum essential parameters necessary to ensure their effective implementation in scientific research workflows.

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