

Evaluation of mechanical properties of starch-gelatin-sargassum polymers based on neural networks

Evaluación de las propiedades mecánicas de polímeros de almidón, gelatina y sargazo mediante redes neuronales

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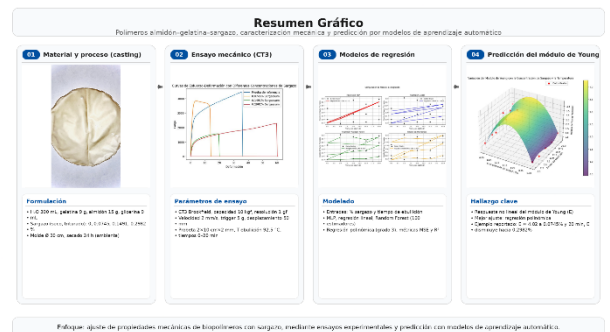
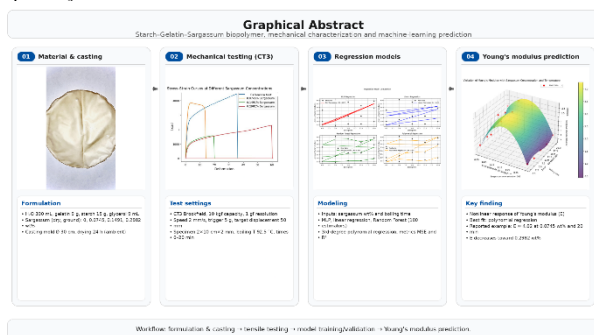


Abstract

In biodegradable polymer research, starch, gelatin, and *Sargassum* algae waste are gaining attention as a potential solution to mitigate the environmental impact of conventional plastics. This study, conducted at Universidad Tecnológica de Tula-Tepeji, evaluated the mechanical properties of a polymer composed of these components using a CT3 texture analyzer, with neural network models employed to predict such properties. Polymers were prepared with varying *Sargassum* concentrations, and their mechanical response under tensile loading was analyzed to estimate Young's modulus. The *casting* process effectively integrated *Sargassum* into the polymer, offering a potential eco-friendly alternative. Neural network predictions of the material's behavior proved accurate, demonstrating the usefulness of this approach in materials research. These findings support incorporating additional data and *Sargassum* variations in future work to further enhance predictive capability.

Resumen

En la investigación de polímeros biodegradables, los materiales basados en almidón, gelatina y sargazo atraen interés por su potencial para reducir el impacto ambiental de los plásticos convencionales. Este estudio, realizado en la Universidad Tecnológica de Tula-Tepeji, analizó las propiedades mecánicas de un polímero con estos componentes mediante un analizador de textura CT3 y modelos de redes neuronales para predecir dichas propiedades. Se prepararon polímeros con diferentes concentraciones de sargazo y se evaluó su respuesta a la tracción, estimando el módulo de Young con una red neuronal. Los resultados mostraron que el proceso de *casting* integra efectivamente el sargazo, ofreciendo una alternativa ecológica. Las predicciones de la red neuronal fueron precisas, demostrando su utilidad en la investigación de materiales. Se recomienda ampliar los datos y variaciones de sargazo en futuros estudios para mejorar la capacidad predictiva.



Biodegradable polymers, *Sargassum*, Neural networks

Polímero biodegradable, Sargazo, Redes neuronales

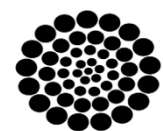
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Introduction

Due to the exponential increase in the use of plastics in the contemporary era, a growing environmental concern has been generated, driven by the transformation that these materials have caused in various sectors, such as packaging and medicine, which has evidenced their persistence in the environment and, consequently, the emerging need to seek more sustainable alternatives. [Kibria, Masuk, Safayet, Nguyen, & Mourshed, 2023]

Faced with this situation, biodegradable polymers emerge as a promising solution to the challenge posed by plastic pollution, with materials based on starch, gelatin, and *Sargassum* algae waste being identified as valuable components in the production of these polymers due to their abundance and availability. Furthermore, being renewable raw materials, they become a viable alternative for the substitution, whether partial or total, of traditional synthetic polymers. It is this combination of raw materials that promises an innovative approach by enhancing the intrinsic properties of each component to develop materials with optimized mechanical characteristics. [Tennakoon, Chandika, Yi, & Jung, 2023]

In the production of biopolymers, the *casting* method has been demonstrated to be a simple technique, with low costs and without considerable environmental impact, that allows for obtaining homogeneous films. The versatility of this technique permits the incorporation of various biopolymers, additives, and natural reinforcements without compromising the biodegradability of the final product, which makes it ideal for the manufacturing of sustainable biopolymers with adjustable mechanical properties. [Flórez, Cazón, & Vázquez, 2023]. However, the challenge of achieving a prediction and understanding of the mechanical properties of these composite polymers persists, and it is in this landscape that advanced neural networks emerge as an as-yet-unexplored opportunity. These models, which simulate brain function in terms of data processing and pattern establishment, promise to offer precise predictions based on previously collected data, functioning not only as research instruments but also as facilitators in the design and development of new materials. [Wang, Soutis, Ando, Sutou, & Narita, 2022]

Therefore, in this study, conducted by the interdisciplinary team at the Universidad Tecnológica de Tula-Tepeji, a detailed analysis was carried out with the objective of evaluating the mechanical properties of a polymer formulated from starch, gelatin, and *Sargassum* algae waste. By means of a texture analyzer, data on the tensile strength of the polymer were collected, which, subsequently, when processed by a neural network model, revealed a precision in the prediction of its mechanical properties. [Beaumont *et al.*, 2021]

The significance of these findings is highlighted by the possibility that neural networks may transform the field of research and development of sustainable materials. With this research, it is sought not only to contribute to the scientific body of knowledge but also to pave the way for future developments focused on sustainability.

In recent decades, *Sargassum*, a specific type of marine algae, has gained notoriety, especially in Caribbean and Atlantic regions, where its excessive proliferation brings environmental and socioeconomic problems. Its rapid growth and accumulation on coastlines result in impacts such as the visual degradation of beaches, affecting tourism, and damage to marine ecosystems due to the reduction of water oxygenation and habitat alteration. This problem has led to *Sargassum* being considered a residue, but, at the same time, its abundance and properties have captured the interest of researchers and industry, who see in it a raw material with unexplored potential, transforming this challenge into a sustainable strategy that addresses both environmental aspects and the demand for new biodegradable materials. [Amador-Castro, García-Cayuela, Alper, Rodríguez-Martínez, & Carrillo-Nieves, 2021] [Robledo *et al.*, 2021]

Given the evolution and complexity of contemporary materials, advanced and precise analysis tools are demanded, and in this scenario, neural networks are positioned as an option. Inspired by the structure and function of the human brain, these networks process large volumes of data, identify patterns, and establish relationships, surpassing, in many cases, traditional analysis.

In materials science, predicting how a material will respond based on its composition and structure is crucial, and neural networks offer such prediction with high precision, in addition to allowing the exploration of new compounds, the optimization of properties, and an acceleration of the innovative process, thus establishing a new standard in the research and development of advanced materials. [Ahmed *et al.*, 2023][Taye *et al.*, 2023]

Methodology

The primary objective of the research was to evaluate the mechanical properties of polymers incorporating various concentrations of *Sargassum* and, subsequently, to predict said properties by means of neural networks. For this purpose, the methodology described below was designed.

For the preparation of polymers with variable *Sargassum* concentrations, the *casting* method was chosen, preparing samples with specific concentrations of dry *Sargassum* ground in a mortar: 0%, 0.0745%, 0.1491%, and 0.2982%. This variability allowed for the evaluation of the direct influence of *Sargassum* on the mechanical behavior of the polymer, providing results on its potential impact on the manufacturing of sustainable polymers. Starch, gelatin, and glycerin were used to obtain an edible film. The combination of these reagents in the appropriate proportions allowed for obtaining a film with suitable strength and flexibility for the mechanical tests.

In the base solution preparation process, 300 mL of distilled water was used as a solvent, to which 9 grams of Sigma-Aldrich® porcine skin gelatin were added. The mixture was homogenized through constant stirring. Before the solution reached the boiling point, 15 grams of starch were added, maintaining stirring until complete dissolution of the starch in the solution. Finally, 9 mL of glycerin were added, ensuring a homogeneous distribution of all ingredients in the reactor. At this stage, the *Sargassum* powder was also incorporated.

Once the adequate dispersion of the components was achieved, the *casting* method was used, pouring the resulting solution into 30 cm diameter silicone molds. This facilitated obtaining uniform samples with the desired dimensions, guaranteeing the consistency and quality of the final product.

Regarding sample collection, time intervals were established for obtaining samples from each batch: 0, 5, 10, 15, and 20 minutes after heating had begun. This collection scheme allowed for obtaining a complete view of the material's evolution as time progressed and temperature increased. This process was carried out in a batch reactor, Atlas Syrris® brand, designed for small-scale chemical reactions with temperatures up to 200°C.

To determine the mechanical properties of the polymers, a CT3 Brookfield® texture analyzer was used, capable of applying up to 10 kgf with a resolution of 1 gf. Through this equipment, the stress-strain behavior of the samples was recorded, providing data on the behavior of the materials elaborated with *Sargassum* residue at a boiling temperature of 92.5 °C. The tests were performed using specimens of 2 cm x 10 cm x 2 mm. The Brookfield® machine was programmed with a trigger of 5 g, a target deformation of 50 mm, and a speed of 2 mm/s for the tensile test.

With the obtained data, a neural network model was designed to predict the stress in the Young's modulus of the polymers. Thanks to this tool, which simulates the human brain's capacity to establish patterns, it was possible to predict with notable precision the mechanical properties of the polymer, evidencing the advantages of neural networks over traditional methods.

A series of predictive models were included in the study to obtain the relationship between *Sargassum* concentration, boiling time, and Young's modulus. The use of a Multilayer Perceptron Neural Network provided by the Python sklearn library was explored in conjunction with other algorithms, including Linear Regression, third-degree Polynomial Regression, and Random Forest Regression with 100 estimators.

The dataset encompassed different *Sargassum* percentages and boiling times. An average of Young's moduli was obtained from three measurements, and after processing, the training of the models proceeded. Subsequently, metrics such as the Mean Squared Error and the coefficient of determination R^2 were calculated to evaluate the effectiveness of each model in the prediction.

Furthermore, the predictive capacity of each model was visualized through graphs, which facilitated the qualitative comparison among them. As part of a practical application, the Polynomial Regression model was used to predict Young's modulus as a function of *Sargassum* concentration and boiling time.

Additional research is suggested to optimize the architecture of the Multilayer Perceptron Neural Network, including the number of neurons and hidden layers, in order to improve predictions and obtain a better understanding of the analyzed relationships.

It is important to highlight that the neural network model not only has applications in this research but also presents revolutionary potential in the field of materials science. The prediction, with a high level of precision, of the properties of composite materials can facilitate and accelerate the design of more sustainable and efficient solutions. Therefore, this approach represents a significant advance and a tool to face environmental challenges such as plastic pollution. The graphical representation of the polymer after drying is shown in Figure 1.

Results

Once the process with *Sargassum* at its different concentrations was completed, Figure 1 shows the polymer after being dried at room temperature for a period of 24 hours. This image will be essential for understanding the properties and transformations of the material under study.

Box 1



Figure 1

Graphical representation of the polymer with Sargassum after its drying process at room temperature, evidencing a characteristic brownish hue, possibly attributed to the interaction of intrinsic compounds of the Sargassum with the polymeric matrix.

After detailed observation of Figure 1, it is evident that the polymer, upon the incorporation of *Sargassum*, acquires a brownish hue, which could be due to the presence of certain pigments or compounds inherent to *Sargassum*. These, when interacting with the polymeric matrix, trigger this peculiar coloration, which could have not only aesthetic but also functional implications, directly influencing its applicability in certain industrial sectors.

The stress-strain graph, shown in Figure 2, constitutes a fundamental tool in materials engineering, used to evaluate mechanical properties with a particular focus on strength. In this study, the mechanical properties of a polymer were analyzed as a function of its *Sargassum* concentration, a natural resource widely distributed in coastal areas. Three different *Sargassum* concentrations were considered [0.0745%, 0.1491%, and 0.2982%], which were compared with a *Sargassum*-free reference sample.

The stress-strain curves of the polymers with *Sargassum* concentrations of 0.0745% and 0.1491% show a similar trend, with a gradual increase in load as deformation increases. These curves exhibit linear elastic behavior in the initial stages, suggesting an initially elastic response of the materials.

On the other hand, the curves corresponding to the *Sargassum* concentration of 0.2982% present a slightly different behavior. Greater initial stiffness is observed, which could indicate superior resistance to deformation compared to lower *Sargassum* concentrations. However, these curves also show elastic behavior in the initial stages, followed by a transition towards plastic behavior as deformation increases.

It is relevant to note that, at the highest *Sargassum* concentrations [0.2982%], the stress-strain curves tend to reach a maximum load before experiencing a gradual decrease. This could be related to the interaction between the *Sargassum* particles and the polymer matrix, which would lead to flow behavior or structural weakening under these conditions.

The stress-strain graph provides a detailed view of how *Sargassum* concentration influences the mechanical properties of the polymers.

These results have significant implications in the field of materials engineering and may be of great interest in applications where improving the strength and toughness of polymeric materials through the incorporation of *Sargassum* is sought.

Box 2

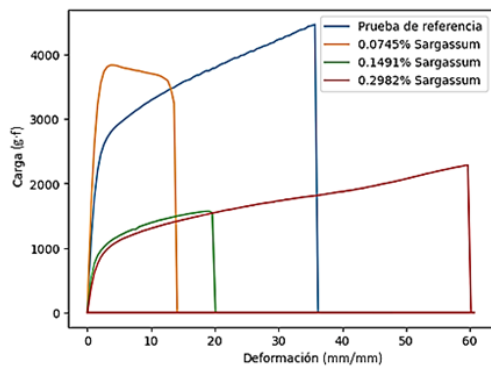


Figure 2

Stress-strain graph illustrates the impact of *Sargassum* concentration on the mechanical properties of the polymers, with load expressed in grams-force [g.f], samples treated after 20 minutes of boiling in the reactor.

In the analysis of regression models, the relationship between *Sargassum* concentration and boiling time in the determination of Young's modulus was studied, employing various approaches: Multilayer Perceptron Regression, Linear Regression, Random Forest Regression, and Polynomial Regression.

To ensure the coherence of the analysis, one row with 0.1491% *Sargassum* was omitted, thereby avoiding potential anomalies. Subsequently, the average of the three Young's modulus values present in the dataset was calculated, generating a column denominated "Average Young's Modulus," which was later used in the training of the models.

The metrics used to evaluate the efficacy of each model were the Mean Squared Error and the Coefficient of Determination R^2 , which provided information on the model's precision and its capacity to explain the variability of the data.

The generated graphs, shown in Figure 3, show that the data, represented by black markers, present considerable fluctuation. In Figure 3a, the red line represents the Multilayer Perceptron regression; according to the behavior of said line, it is demonstrated that this model fails to fit the data satisfactorily.

The same occurs with the Linear Regression model, shown with the blue line in Figure 3b, thereby demonstrating that the correlation is not strictly linear.

Box 3

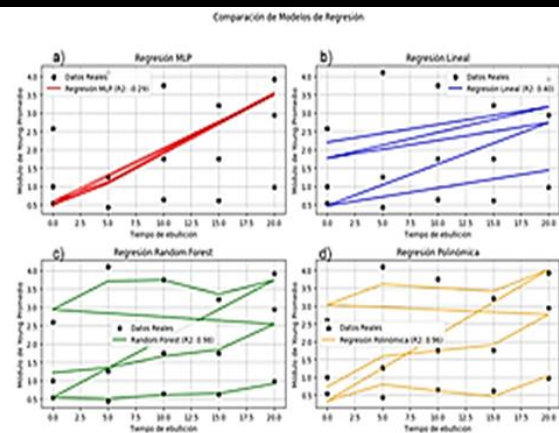


Figure 3

Graphical comparison of the regression models analyzed. The black markers represent the original Young's modulus data, evidencing their variability. The red trace corresponds to the predictions of the MLP Regression model; the blue line illustrates the behavior of the Linear Regression model; the green hue denotes the estimations of the Random Forest Regression; and the orange curve reflects the adaptability of the Polynomial Regression to non-linearities in the dataset. This representation aims to offer a clear and concise visualization of the performance and adaptability of each model in relation to the dataset studied.

Furthermore, the Random Forest model, shown with a green line in Figure 3c, proved to be more versatile in capturing certain variations in the data, as evidenced by its R^2 value. Polynomial regression, shown in Figure 3d with an orange line, with a curvature adjusted to the data, managed to model the present non-linearities more effectively, which translates into greater prediction accuracy.

A prediction was made using the Polynomial Regression model to estimate Young's modulus at a *Sargassum* concentration of 0.0745% and a boiling time of 20 minutes, obtaining an approximate value of 4.02. This result provides key information on the material's behavior under these specific conditions.

The importance of this predictive approach lies in its capacity to anticipate trends based on experimental data, which facilitates process optimization and informed decision-making.

In academic and industrial settings, having accurate predictive models is crucial for guaranteeing reliable results and understanding complex outcomes.

Figure 4 shows the predictions of the models, highlighting the trend of Young's modulus as *Sargassum* concentration increases. It is observed that, from a certain point [0.2982% *Sargassum*], the modulus begins to decrease, suggesting that an optimal concentration exists for improving the mechanical properties of the polymer without compromising its resistance. This information is fundamental for the design of materials with adjustable properties depending on the *Sargassum* concentration used.

Box 4

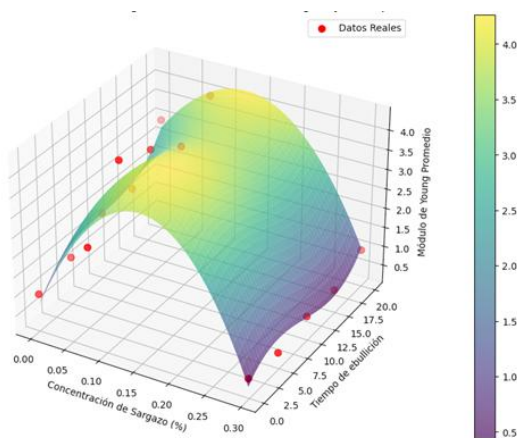


Figure 4

Representation exhibiting the model predictions in relation to Young's Modulus and *Sargassum* concentration, marking an increase in the Young's Modulus value that undergoes a decrease with the increment in *Sargassum* concentration, reaching a lower point near 0.2982%.

The *casting* method has been demonstrated to be an effective way to incorporate *Sargassum* into polymer films, offering considerable potential for the development of environmentally friendly materials.

Furthermore, the neural network used in this study has exhibited a notable capacity to predict the mechanical properties of the material, which highlights its importance as a valuable tool in materials science. To further improve its predictive capabilities, it is recommended to expand the dataset, including a greater variation in the *Sargassum* percentage. This expansion could provide deeper insights and enhance accuracy in future research on materials.

Conclusions

It has been found that, after the room-temperature drying process, the polymer mixed with *Sargassum* acquires a brownish-reddish hue. This chromatic variation could be closely linked to pigments inherent to *Sargassum*. Beyond representing an aesthetic change, this application could confer new functionalities to the material, thus expanding its spectrum of applications in different industrial sectors.

The collected data, reflected in the stress-strain graph, suggest a direct correlation between the proportion of incorporated *Sargassum* and the mechanical characteristics of the polymer. It is observed that low concentrations, specifically 0.0745% and 0.1491%, are associated with linear elastic behavior in their initial stages. In contrast, a higher concentration of 0.2985% tends to increase stiffness and promote structural weakening of the material.

Regarding the importance of using regression models for predicting material behavior, this work has demonstrated the efficacy of various regression models in determining Young's modulus as a function of *Sargassum* concentration and boiling time.

It is important to highlight that Random Forest regression has shown remarkable versatility and adaptability to data series compared to conventional linear models. On the other hand, polynomial regression has proven to be particularly efficient in detecting and handling data with high non-linearity.

The capacity to foresee behaviors and trends from experimental data is key for decision-making focused on process optimization and risk reduction, especially if the model is fed with sufficiently robust amounts of data for effective training. According to what is shown in Figure No. 3, where a comparative view of different regression models is provided, it is demonstrated that the selection of the appropriate model is crucial for obtaining accurate interpretations and predictions, always in accordance with the nature of the analyzed data.

Regarding the relevance of Young's modulus, during this investigation a special focus has been given to this fundamental property that reflects the capacity of a material to resist variations in its length when subjected to an external force.

The obtained data suggest that both *Sargassum* concentration and boiling time have a significant influence on this property.

Declarations

Conflict of interest

The authors declare that they have no conflict of interest. They have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Author contribution

Hernández-Hernández, Celia Massiel: conceptualization, editing, and writing.

Hernández-González, Sonia: results analysis and advisory.

Melo-Máximo, Lizbeth: project advisory, data acquisition, and drafting.

Nolasco-Arizmendi, Víctor Alfredo: experimentation, characterization, results analysis, conceptualization, writing, and review.

Availability of data and materials

The data generated and analyzed during the present study are available upon reasonable request from the corresponding author. The experimental materials and protocols used are described in the manuscript and, where applicable, can be provided upon request.

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Abbreviations

ANN	Artificial Neural Network
CT3	Brookfield texture analyzer model used
MLP	Multilayer Perceptron
MSE	Mean Squared Error
R ²	Coefficient of determination

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Support

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