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REGULAR ARTICLE

Kinetic modeling and neuro-fuzzy application in ethanol production

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Autor contribution
EZG: Conceptualization. Experimental data collection. Literature review. Manuscript writing; CDZF: Conceptualization. Experimental data collection. Data storage. Data analysis. Literature review. Manuscript writing. Manuscript revision. Supervision; RMB: Conceptualization. Experimental data collection. Data storage. Data analysis. Literature review. Manuscript writing. Manuscript revision. Supervision.

Abstract

This study presents the application of kinetic modeling and Neuro-Fuzzy techniques in ethanol production. The research aims to optimize the fermentation process by employing the Adaptive Neuro-Fuzzy Inference System (ANFIS) to predict ethanol yield under different conditions. Initially, sugarcane juice was used as a raw material and subjected to fractional distillation to obtain ethanol. The experimental data were analyzed using artificial neural networks and fuzzy logic to develop a predictive model. The ANFIS hybrid model demonstrated high accuracy in forecasting ethanol production, allowing for process optimization and cost reduction. Additionally, the kinetic analysis of fermentation provided insights into substrate consumption and ethanol yield efficiency. The results indicate that the Neuro-Fuzzy approach is a powerful tool for improving bioethanol production processes, enhancing both efficiency and sustainability.

Keywords

Neuro-Fuzzy; Ethanol production; Kinetic modeling; Artificial neural networks; Fermentation optimization.

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Introduction

The use of renewable energy is one of the most important strategies for facing the challenges related to climate change and the scarcity of natural resources (SMITH et al., 2013). Renewable energy comes from natural sources that are constantly replenished and do not run out, unlike fossil fuels, which are finite and cause serious damage to the environment when burned (SAIDUR et al., 2011). Some examples of renewable energy include solar energy, wind energy, hydroelectric energy, geothermal energy and biomass (CANEPPELE; SERAPHIM, 2010). The transition to the use of renewable energy is essential to reduce greenhouse gas emissions, combat air pollution, preserve natural ecosystems and increase the share of clean sources in the energy matrix (GODINHO et al., 2023).

In this context, economic and environmental analysis stands out as a crucial point, comparing that the production of biodiesel from virgin soybean oil can not only meet energy demands, but also contribute significantly to the reduction of pollutant gas emissions. The advanced technique of this approach reinforces the continued importance of research and development of technologies that drive the transition to cleaner and renewable energy sources (FERMINO et al, 2024). To advance the adoption of renewable energy, it is crucial to support public policies that encourage research, development and installation of these technologies, as well as to raise awareness and engage society in the adoption of more sustainable practices, such as the application of models that optimize processes and reduce production costs. Modeling plays a fundamental role in the optimization of the production process in various industries and sectors, including agribusiness (CANEPPELE; SERAPHIM, 2010). It allows companies to simulate and analyze different scenarios, identifying opportunities for improvement, cost reduction, increased efficiency and improved product quality. Within optimization processes, Fuzzy Logic, also known as fuzzy logic, is highly relevant, as it operates in a branch of logic that deals with uncertainty and ambiguity, allowing systems to process vague or imprecise concepts (VASAKI et al., 2021). Fuzzy Logic relies on an Artificial Intelligence called Neuro-Fuzzy, which combines neural networks and fuzzy logic to solve complex problems involving uncertainty and imprecision (YADAV; BHASKER; UPADHYAY, 2022). In this context, the objective of this article is to develop a Fuzzy model based on results obtained in a practical class on ethanol production.

Materials and methods

Initially, the raw material used in the experiment (represented by a yellowish liquid) is applied to a thermal separation process by fractional distillation. The distillation system consists of a distillation flask, where the sample is heated, an approach to control the temperature, a condenser responsible for converting the vapors into the liquid phase and a collection flask intended for storing the distillate obtained. The process aims to selectively separate the volatile components, ensuring the production of a product with a higher degree of purity, as indicated by the colorless liquid in the Erlenmeyer flask. The experimental data are subsequently analyzed through computational modeling, using an approach based on artificial neural networks and fuzzy logic (NeuroFuzzy).

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Laboratory experimentation

The work was conducted in the Chemistry Laboratory of the Sagrado Coração University Center UNISAGRADO, in the city of Bauru - SP. The sugarcane juice used in the experiment was purchased from a street vendor. After purchase, the juice was placed in 4.0 L PET bottles and stored in a simple refrigerator to be used in future work, since the objective was not to evaluate the juice, but rather to develop a model. The fermentation process was developed according to the guidelines of (GODINHO et al., 2023b). The yeast used in the laboratory work was Mauri® biological yeast 500 grams, in addition to União® crystal sugar and water.

Development of the neuro-fuzzy model

In this work, a hybrid ANFIS model was used to predict ethanol production in the laboratory. This hybrid approach is recommended for energy efficiency analyses (NARDEZ et al., 2018). Figure 1 illustrates the experimental setup used for the experimental metrology flowchart for fuzzy and kinetic modeling.

The system was modeled using the ANN (Artificial Neural Networks) method, combining logic. Fuzzy based on the Takagi-Sugeno Fuzzy inference process to define the characteristics of the ANFIS model (Figure 2) (SALEEM et al., 2021). The model was trained in 50 possible tests based on the database, developed with the results collected in the laboratory, as shown in Figure 3.

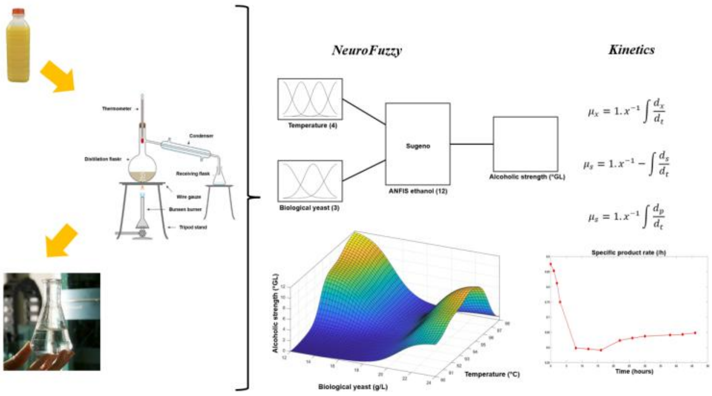

Figure 1. Experimental metrology flowchart for fuzzy and kinetic modeling.

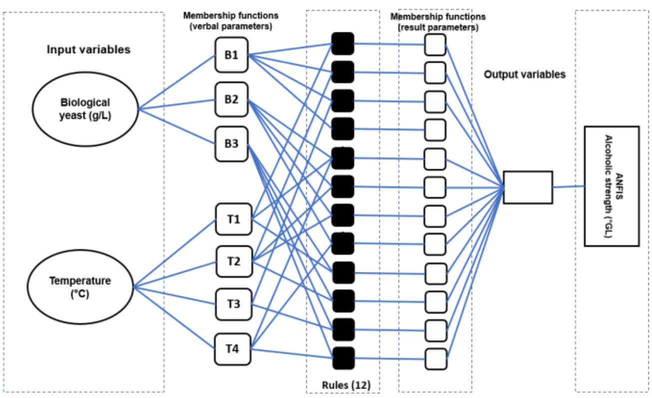

Figure 2. ANFIS model developed for ethanol production.

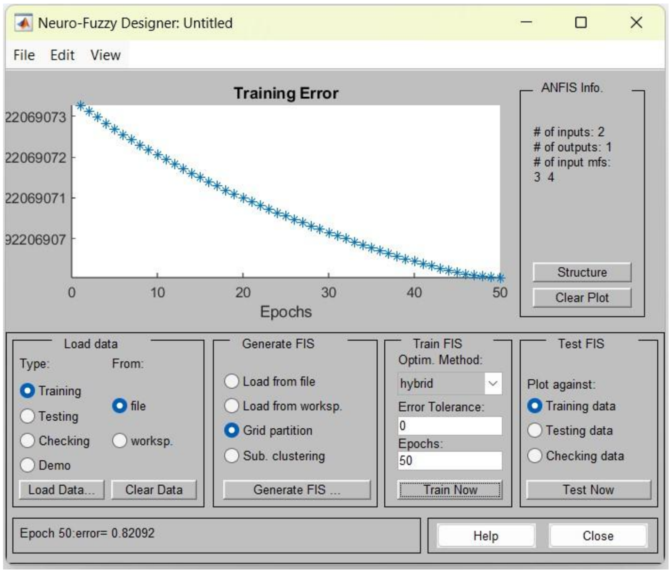

Figure 3. Training of the ANFIS model.

The modeling was performed using the commercial software MATLAB®, licensed by the Agroenerbio Research Group of FZEA/USP, with computational assistance from the Fuzzy Logic Toolbox, the ANFIS command line function, and the Neuro-Fuzzy Designer iterative application.

The proposed hybrid ANFIS model was developed with 2 input variables, namely biological [yeast] and temperature, with 3 relevance variables for biological ($g.L^{-1}$ – 1, 2, and 3) and 4 for temperature (°C - 80, 85, 90, and 95), resulting in 24 correlations (fuzzy rules) that the fuzzy system itself develops and is described in Figure 2. In the transformation stage, the discrete values of the input variables were converted into fuzzy values (fuzzification), adopting Gaussian-type relevance functions.

In addition, an output variable was adopted, the alcohol content (°GL). Finally, the weighted average of all rule outputs was adopted, as it is the standard for Takagi-Sugeno inference systems, which is used in the MATLAB® Fuzzy system. The methodological procedures used to model the proposed ANFIS were compatible with the methods adopted by (FURLONG et al., 2019).

Kinetics of alcoholic fermentation

By analyzing the results, it was possible to obtain the instantaneous and specific velocities for certain points, based on the derivative of the equation generated by the regression of the curves.

According to Lee (2008), the formulas were extracted from the kinetics of fermentation processes, which is the analysis of the concentration values of one or more components of the cultivation system as a function of the cultivation time. Components are understood as the microorganism (or biomass), the metabolic products (metabolites) and the nutrients or substrates that make up the culture medium. This analysis is essential to optimize the production of metabolites of industrial interest and improve the efficiency of fermentation processes, as discussed by Bailey and Ollis (2012) in their studies on bioprocess engineering.

The specific speed of reproduction of microorganisms, also known as specific growth rate or specific growth rate, is an important parameter that describes how quickly a population of microorganisms multiplies under ideal growth conditions. In other words, the specific speed of reproduction indicates how many times the population doubles its size during a given time interval (SANTOS et al., 2018).

The instantaneous speed of reproduction of microorganisms, substrate consumption and product formation can be represented by the following expressions, as per (SANTOS et al., 2018) (Equations 1, 2 and 3).

$$r_x = \frac{d_s}{d_t} \qquad \text{Equation (1)}$$

$$r_s = \frac{d_s}{d_t} \qquad \text{Equation (2)}$$

$$r_p = \frac{d_s}{d_t} \qquad \text{Equation (3)}$$

where: r_x = instantaneous growth rate, in g.L^{-1}.h^{-1}, r_s = instantaneous rate of substrate consumption, in g.L^{-1}.h^{-1}, and r_p = instantaneous rate of product formation, in g.L^{-1}.h^{-1}.

The specific rate of reproduction of microorganisms, of substrate consumption and of product formation can be represented by the following expressions (Equations 4, 5 and 6).

$$\mu_x = 1.x^{-1} \int \frac{d_x}{d_t} \qquad \text{Equation (4)}$$

$$\mu_s = 1.x^{-1} \int \frac{d_s}{d_t} \qquad \text{Equation (5)}$$

$$\mu_p = 1.x^{-1} \int \frac{d_p}{d_t} \qquad \text{Equation (6)}$$

where: μ_x = specific growth rate, in h^{-1}, μ_s = specific rate of substrate consumption, in h^{-1}, and μ_p = specific rate of product formation, in h^{-1}.

The efficiency of the fermentation process refers to the capacity of a fermentation system to convert substrates (such as sugars) into desired products (such as ethanol, lactic acid, acetic acid, etc.) quickly, completely and economically, with fermentation being a biological process that occurs under anaerobic conditions, that is, in the absence of oxygen (ZANARDI; COSTA JR., 2015).

According to Stanbury, Whitaker and Hall (2016), the efficiency of a fermentation process can be assessed through several critical parameters, such as substrate conversion, process yield, fermentation speed, contamination level, efficiency in product recovery and optimized use of available resources.

The formula for calculating the efficiency of the fermentation process is as follows, according to (FERRO, 2023) (Equation 7).

$$EE = \frac{P}{S_c} x100 \qquad \text{Equation (7)}$$

where: EE = energy efficiency, in %, P = product obtained in fermentation and S_c = substrate consumed.

Results and discussion

Neuro-Fuzzy model results

When applying Neuro-Fuzzy modeling, it is crucial to perform rigorous tests to validate the developed model, ensuring that it generalizes well to new data and maintains the robustness required for practical applications, as shown in Figure 4. These tests usually include cross-validation and prediction error analysis, which allow the model to be adjusted and improved based on its actual performance. Using tests in this context ensures that the modeled system is efficient and reliable in real-world operations, such as in industrial control processes or optimization of complex systems. The proposed ANFIS hybrid model presented adequate behavior and was compatible with the training and validation data. For graphical representation, different Fuzzy surface models were obtained, and minimum and maximum energy points were verified for different dosages, depending on the concrete components (Figure 5).

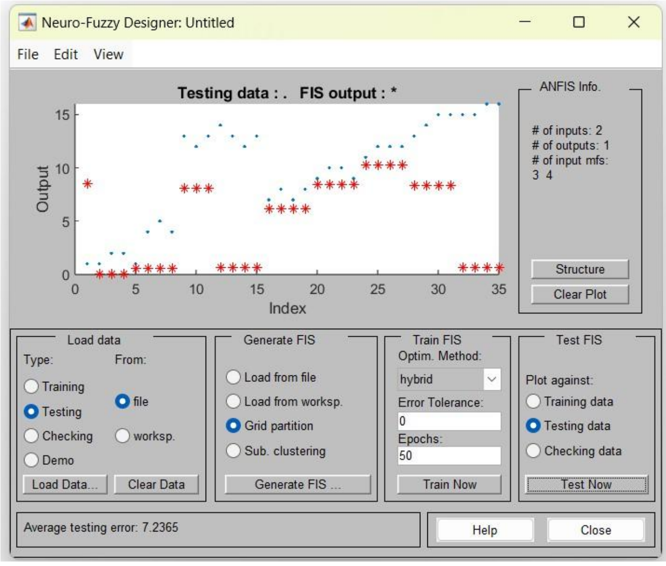

Figure 4. Testing the ANFIS model.

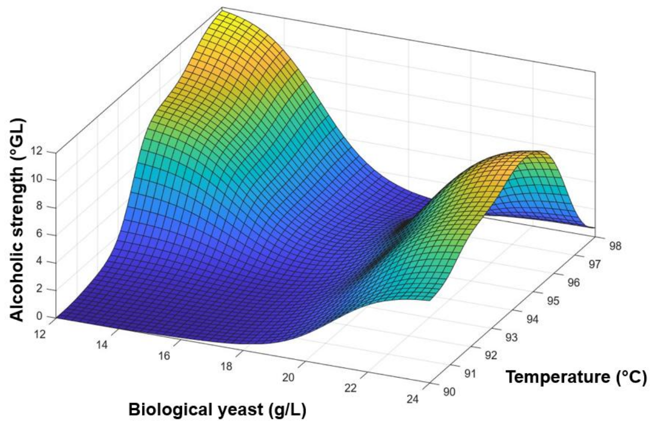

Figure 5. 3D graph for bioethanol production using different temperatures and yeast doses.

Resulting kinetic velocity models

The graph of the specific velocity of the product, evaluated during fermentation, is shown in Figure 6. The use of Neuro-Fuzzy modeling has emerged as an effective approach to deal with complex systems, especially in those where uncertainty and nonlinearity are predominant. This technique combines Fuzzy logic, which is useful for modeling uncertainty and imprecision, with artificial neural networks, which have the ability to learn from data and identify patterns (CANEPPELE; SERAPHIM, 2010).

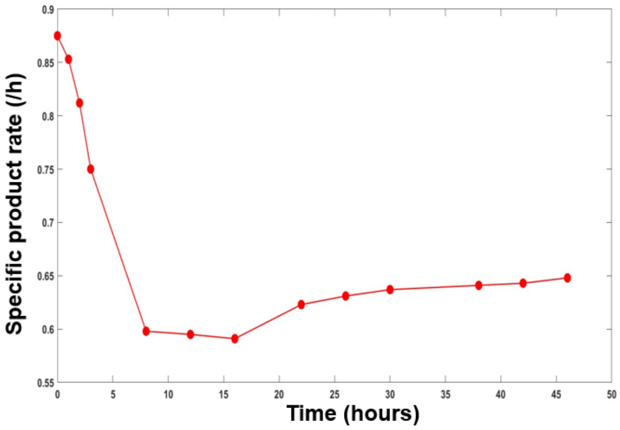

Figure 6. Curve of the specific speed of the product in h^{-1}.

The specific rate of ethanol production over time is a fundamental parameter in the optimization of fermentation processes, directly influencing the industrial efficiency of biofuel production. In recent studies, the kinetic analysis of alcoholic fermentation revealed that the specific rate of ethanol production tends to increase during the initial phases of fermentation, reaching a peak that corresponds to the maximum metabolic activity of yeasts. For example, Govindaswamy & Vane (2007) observed that, in fermentations conducted with Saccharomyces cerevisiae, the specific rate of ethanol production reached its maximum value in the first 12 hours of the process, coinciding with the logarithmic phase of cell growth.

As discussed by Fan et al. (2014), after reaching the peak, the specific rate of ethanol production generally decreases due to substrate depletion and the accumulation of inhibitory products in the medium, such as ethanol itself. These authors reported that, in a batch system, the specific rate of ethanol production began to decline significantly after 24 hours of fermentation, resulting in a total production rate of ethanol production lower than expected for continuous processes. Understanding these patterns is crucial for implementing control strategies, such as the gradual addition of substrate or the use of bioreactors with cell recycling, which can maintain fermentation activity at optimal levels for longer periods.

In addition, the same authors emphasize the importance of correlating the specific rate of ethanol production with environmental variables, such as temperature and pH of the medium, which can significantly influence fermentation performance. In their experiments, they demonstrated that maintaining optimal pH conditions (between 4.5 and 5.0) resulted in greater stability of the specific rate of ethanol production over time, preventing the abrupt drop observed in suboptimal conditions. This knowledge is essential for the optimization of industrial processes, where maximizing productivity and minimizing operating costs are primary objectives.

Conclusions

Neuro-Fuzzy modeling has proven to be an effective approach for predicting and improving complex systems, ensuring robustness and reliability in the analysis of industrial processes. The proposed ANFIS hybrid model showed adequate behavior, compatible with the training and validation data, demonstrating its applicability in the optimization of integration systems. In addition, a kinetic analysis revealed that a specific ethanol production rate reaches an initial peak, followed by a drop due to substrate depletion and accumulation of inhibitors, highlighting the importance of precise control of variables such as temperature and pH to maximize process efficiency.

This study concludes that significant variations in total energy demand can occur for different dosages and that this information can be used to predict dosages with lower energy input, with mechanical resistance to compression of characteristics similar to those with higher input. It was also found that this change can generate savings in the energy cost of dosages of around 24.77% for a conventional reinforced concrete construction.

Finally, it is inferred that the ANFIS hybrid model can be the necessary apparatus for prediction and energy savings, making the concrete production process more sustainable. This research confirmed the need for studies on the energy balance in the production process of environmentally sustainable concrete, with investigations almost always focused on the insertion of non-conventional materials in the concrete. This is only the study of the growth kinetics and substrate consumption. It is important to emphasize that in order to choose yeast, in addition to the kinetics study, it is also important to analyze the sensory characteristics of aroma and flavor developed by the yeast in the final product.

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