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Setpoint temperature estimation to achieve target solvent concentrations in *S. cerevisiae* fermentations using inverse neural networks and fuzzy logic

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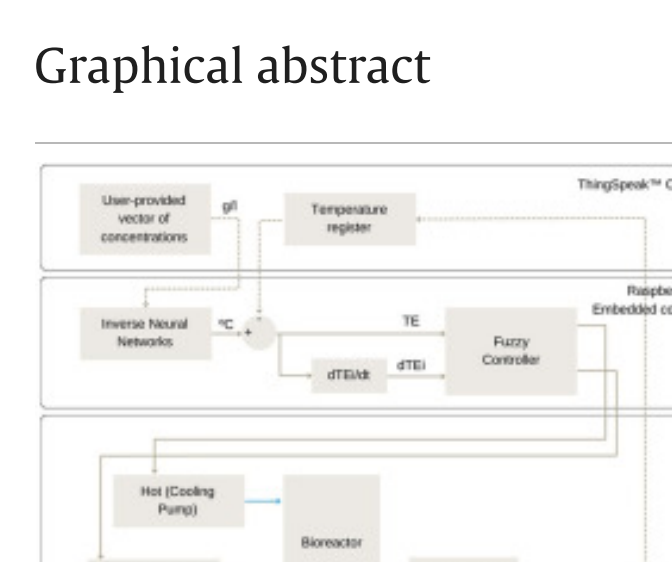
Abstract

Over the years, many technical advances have been made to improve the final quality of beers by controlling the concentrations of compounds obtained at the end of alcoholic fermentation. However, these efforts have mainly focused on increasing ethanol and reducing other compounds considered defects. This study addresses the challenge of obtaining specific concentrations of four solvent compounds (*isobutanol*, *ethyl acetate*, *amyl alcohols*, and *n-propanol*) produced by the yeast *S. cerevisiae* Safale S04, determined by an expert. A model based on four inverse neural networks (INNs) has been developed to predict the target temperature required to achieve the desired concentrations. These INNs have been trained using virtual data generated by four artificial neural networks (ANNs), as described in detail in previous work. For implementation, a fuzzy control system based on the Mamdani inference method was utilized. To experimentally validate the results, four complete fermentations were conducted. The INNs were found to be accurate tools for predicting the target temperatures based on predetermined compound concentrations, with R^2 values ranging from 0.982 to 0.986. When comparing the experimental concentration data, the most accurate prediction was achieved for *n-propanol*, with an average error of 0.18 mgL^{-1}, while *ethyl acetate* had an error of 0.25 mgL^{-1}, *isobutanol* had an error of 0.48 mgL^{-1}, and *amyl alcohols*, being the least precise prediction, had an error of 0.83 mgL^{-1}.

Graphical abstract



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Introduction

Beer is a beverage produced by alcoholic fermentation primarily from *S. cerevisiae* or *S. pastorianus* yeasts. Among the primary and secondary compounds produced during the process, some are crucial because of their significant influence on the organoleptic characteristics of the final product, such as higher alcohols and esters (Humia et al., 2019).

In the brewing industry, the concept of alcoholic fermentation does not strictly align with the biochemical process. Brewers consider that alcoholic fermentation begins when yeast is introduced into the fermentation vessel and continues until the initiation of the maturation phase (Oliver, 2013; White and Zainasheff, 2010). From a biochemical standpoint, this corresponds to a shorter period that encompasses glycolysis and culminates in the production of ethanol (Nelson et al., 2021). Nonetheless, in this study, we adhere to the definition provided by brewers.

The impact of these compounds is directly linked to their concentration in the final product. Therefore, the organoleptic characteristics could vary from pleasing to unpleasant (BJCP, 2015; BJCP, 2021a; Meilgaard et al., 1979). This is the principal reason why it is interesting to predict and control the concentration beforehand.

Research efforts have focused on the prediction, control, maximization or minimization of the most important compounds in beer, such as ethanol, diacetyl, or dimethyl sulfide (Carrillo-Ureta et al., 2001; Li et al., 2011; Zhang, R., 2018). As a consequence, fewer studies are found concerning secondary compounds, even though they contribute to the final organoleptic profile of beers, being pleasant at specific concentrations, as well as providing complexity, richness, and depth. The case of the ester "ethyl acetate" is known to exhibit a pleasant fruity aroma at low concentrations, while at high concentrations, it presents a pungent and unpleasant acetone-like odour (Smogrovicova and Domeny, 1999; Verstrepen et al., 2003).

The compounds selected for the experimental phase are the solvents: *higher alcohols*, *amyl alcohols*, *isobutanol*, *n-propanol*, and ester *ethyl acetate*. However, it does not refer to the chemical characteristics of the solvents, but rather to their organoleptic characteristics, as explained by the Beer Judge Certification Program (BJCP): "solvents: acetone-like aroma" (BJCP, 2021b).

Different studies indicate that the factors that influence the production of solvents, range from yeast genetics, wort composition, to the fermentation temperature (Loviso & Libkind, 2018, 2019), the most readily monitorable and controllable physical variable in an industrial environment.

In the literature, several studies can be found that estimate or monitor the concentrations of some secondary compounds, but we have not found any that take into consideration the organoleptic profile at the end of fermentation as a mark of product quality.

Several mathematical models for predicting alcoholic fermentation variables in beers can be found. However, the majority of these models focus on the *S. pastorianus* species, with less focus on *S. cerevisiae*. At this point, we must acknowledge a challenge inherent in the beer brewing process, namely, the high variability in raw materials, recipes, brewing processes, beer styles, and the numerous combinations that can be derived from them (Kunze and Hendel, 2019), which hinders the accuracy of mathematical models. Nevertheless, neural networks have proven to be an efficient alternative for modelling non-linear complex systems in food microbiology and fermentations, whereby by understanding the data sets of certain input and output variables, we can predict the empirical relationships between these variables (Huang et al., 2007; Syu, Tsao, Austin, Celotto, & D'Amore, 1994). With these neural networks, we can generate new artificial data sets for various purposes, such as scaling from pilot plant to industrial level or for generating inverse neural networks, as will be explained later. Finally, it is important to consider that their implementation in embedded systems is relatively straightforward.

In this study, a group of four neural networks, developed in a previous work (Moya-Almeida et al., 2021), is utilized to estimate compound concentrations based on temperatures and times. By comparing simulated data generated by these neural networks with experimental data obtained from gas chromatography, R^2-values ranging from 0.939 to 0.996 have been achieved.

With these, artificial datasets were generated, which are reversed to train a new set of neural networks, where the outputs of the original ANNs are used as inputs for the new networks, and their inputs are treated as outputs; these novel networks are referred to, in this study, as inverse neural networks (INNs).

To the best of our knowledge, this technique has not been utilized for predicting solvent concentrations in beer fermentations to enhance the final product's quality, which constitutes one of the primary contributions of this study. Moreover, when this technique has been employed for other purposes, it typically involved incorporating a high number of inputs (measured variables). In contrast, this study prioritized a minimalist approach, employing only a direct input (temperature) along with time, thereby demonstrating the feasibility and high precision of this technique.

One of the limitations of the proposed method refers to the requirement for independent study and calculation of the data sets needed to train the initial ANNs, and the INNs, for each specific type of beer or microorganism. Therefore, it would be beneficial to develop a comprehensive database to store this information.

Subsequently, as a fermentation control tool, a controller based on fuzzy logic has been used due to its advantages, such as its simplicity, robustness, and easy practical implementation.

Fuzzy logic is an inconsistency-tolerant type of logic; that intends to go against the idea of only two possibilities as a solution to a given problem (on-off, high-low, 1-0). It recognizes that within the boundaries of these solutions, there exist intermediate points that represent diffusely the membership to a specific fuzzy set (Averill, 2020; Pedrycz, 2021; Zadeh, 1965).

Thus, a fuzzy rule defines the consequence that occurs from the relationships of two or more antecedents connected by fuzzy logical operators. Once the information enters these fuzzy rules, an inference method is needed to assess the outcome of the output variables of the consequent. One of the most used is the Mamdani method, these rules are of the IF x_1, x_2 – THEN y_{12} type. Subsequently, this conclusion is represented by an area resulting from the aggregation of all the areas produced by the evaluation of each fuzzy rule, for this reason, it is necessary to take it to a number which represents the solution that was found; this process is known as "defuzzification". To carry out this task there are several mathematical methods, among which the centroid method stands out. (Averill, 2020; Oussalah et al., 2001).

An aspect that needs to be taken into consideration is the reliance on advanced techniques for measuring this type of compounds, such as Gas Chromatography (Martins et al., 2020; Villacreces et al., 2022), which involves sampling and sending samples to laboratories, incurring additional costs. This further emphasizes the importance of developing models for economically predicting compound concentrations, which could potentially be implemented online.

Finally, we believe that this type of system has potential applications for craft brewers, characterized by their limited purchasing power, which leads them to not implement advanced controllers but rather on-off controllers with hysteresis. For this reason, we have consistently considered that the proposed methods can be implemented on low-cost and readily accessible devices.

This study aims to showcase that the utilization of an INN in conjunction with a fuzzy logic temperature control system can effectively predict and sustain the optimal fermentation setpoint temperature to obtain the target concentrations of four solvents: *isobutanol*, *propanol*, *amyl alcohol* and *ethyl acetate*, by employing solely the temperature and its rate of change as input variables for the controller. Therefore, the goal is to develop an efficient control system with a low cost and relatively simple implementation.

The main contributions are summarized below:

- We propose a method to calculate average setpoint temperatures for obtaining expert-determined concentrations of four solvent compounds in *S. cerevisiae* fermentations.
- We have demonstrated the feasibility of calculating these setpoint temperatures through the implementation of INNs, which were trained with artificial datasets generated by ANNs trained with experimentally obtained datasets, despite the complex variability of compounds resulting from alcoholic fermentation with *S. cerevisiae*.
- The experimental results demonstrate that, at least on a pilot plant scale, temperature and its error derivative are sufficient as controlled variables, and when combined with the use of Fuzzy Control, highly accurate outcomes are achieved.
- To the best of the authors' knowledge, this is the first work that estimates parameters for bioreactor control with the ultimate goal of predicting concentrations of secondary compounds, taking into account final organoleptic quality considerations in alcoholic fermentations, based on expert knowledge.

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Section snippets

Related works

In this section, a review is conducted on applications of neural networks in fermentations and fuzzy control in bioreactors. …

Hardware and software

Matlab® R2021b U2 (MathWorks, Natick, MA, USA) was used for data analysis, ANNs training, fuzzy controller, and a hardware-embedded standalone application.

A Raspberry Pi 3B+ (Raspberry Pi Fdn, Cambridge, UK) was used for the implementation of the hardware-embedded standalone application. Also, it was used as a communication channel between the temperature sensor and a ThingSpeak™ channel (MathWorks, MA, USA), where the collected data was stored.

All fermentations were carried out in a 23 L …

Fuzzy control

As a first step, the development of the Fuzzy Controller (FC) was carried out.

The universe of discourse for the linguistic variable TE is [−4, 4] °C, which encompasses the range of values above and below the sensor measurement that the controller takes into account for implementing control functions. For *dTE*, the universe of discourse is $[-6\text{x}10^{-3}, 6\times10^{-3}]$ °C ·s^{-1}; which represents a maximum limit of 1.8 °C of increase or decrease in temperature every 300s (equation (3)). As a consequence, …

Conclusions

To the best of the authors' knowledge, this is the first study that predicts the optimal temperature necessary to achieve expert-designated concentrations of a set of solvent compounds (*isobutanol*, *n-propanol*, *amyl alcohol*, *ethyl acetate*) produced by the yeast *S. cerevisiae* Safale S04 during the alcoholic fermentation process.

The study has demonstrated the remarkable accuracy of inverse neural networks in predicting the temperatures required to achieve user-specified final concentrations, using …

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CRediT authorship contribution statement

Vinicio Moya-Almeida: Conceptualization, methodology, software, validation, formal analysis, investigation, data curation, resources, visualization, writing—original draft preparation, funding acquisition, language review, writing—review and editing, experimentation Belén Diezma-Iglesias: resources, visualization, writing—original draft preparation, writing—review and editing, supervision Eva Correa-Hernando: resources, visualization, writing—original draft preparation, writing—review and …

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work the authors used GPT-3.5 with the exclusive objective of enhancing the language. After using this tool, the authors reviewed and edited the content as needed and takes full responsibility for the content of the publication. …

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Vinicio Moya Almeida reports financial support was provided by Secretaría de Educación Superior, Ciencia, Tecnología e Innovación de la República de Ecuador. …

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