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# Bioethanol production sustainability: Outlook for improvement using computer-aided techniques

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**Abstract**

In this work a computer-aided tool to modelling of biotechnological processes is built up with focus on developing methodologies that can be used always that a re-estimation of parameters is necessary. The ethanol fermentation process is used as a case study. The performance of a hybrid neural model and a first-principles model, both considering the effect of temperature on the kinetics, are evaluated not only by their accuracy in describing experimental data, but mainly by the difficulties involved in the adaptation of their parameters. The results show that the proposed tool is very efficient to follow changes in operating conditions and their impact on the system kinetics which is an important issue to lead the process to be operated at high level of performance.

**Keywords:** Modeling, Parameter estimation, Temperature effect, Artificial intelligence.

## 1. Introduction

There are many minor, but important, industrial problems associated with the ethanol fermentation processes to be solved nowadays, when optimal operation is a target. Among them is the lack of the processes robustness in the presence of fluctuations in operational conditions, which leads to changes in the kinetic behavior, with impact on yield, productivity and conversion. These changes are very common in ethanol plants, where they occur not only due to the variations in the quality of the raw material but also due to variations of dominant

microorganism in the process. Another issue in ethanol fermentation processes is the influence of temperature on the kinetics. It is difficult to support a constant temperature during large-scale alcoholic fermentation and variations in temperature affects productivity through changes in kinetics as well as in microorganism lifetime. Thus, a description of the influence of temperature on kinetics of the microorganism involved is essential for a reliable mathematical modeling to be used in process optimization, control and operation.
In this work an adaptive methodology for hybrid neural modeling of the effect of temperature on the kinetics of batch fermentation was proposed. The rate expressions for cell growth, substrate consumption and product formation are described by multilayer perceptron neural networks (MLPNN) and the neural network parameters are re-estimated in an adaptive scheme when there are changes in operational conditions and fluctuations in the quality of raw material. The objective of this work was to present a comparison of methodologies for the adaptive modeling of biotechnological processes. The use of first-principles and hybrid neural models **[1-3]** was evaluated considering the accuracy with which they describe experimental data and the difficulties involved in the re-estimation of the kinetics parameters.

## 2. Experiments for developing the mathematical models

*Experiments used to develop the mathematical models (first data set)*
Five batch experiments (at 28, 31, 34, 37 and 40$^{o}$C) were used to estimate the parameters of the proposed models. Details about these experiments are described elsewhere **[4]**.
*Experiments with changes in operational conditions (second data set)*
Another five batch experiments (at 30, 31.2, 34, 36.8 and 38$^{o}$C) were used to validate the methodologies for re-estimation of kinetic parameters. Sugar cane molasses was from a harvesting period different from that used in the first experiments and so, there is a change in the quality of raw material when this data set is compared to the first one.

## 3. Mathematical modeling

### *3.1. First-Principles Modeling*

First-principles models comprise the mass balance equations, with microorganism growth, substrate consumption and ethanol formation for a batch reactor described as follows:

$$\frac{\mathrm{d}X}{\mathrm{d}t} = r_{\mathrm{x}}\,;\ \frac{\mathrm{d}S}{\mathrm{d}t} = -r_{\mathrm{s}}\,;\ \frac{\mathrm{d}P}{\mathrm{d}t} = r_{\mathrm{p}} \qquad (1\text{-}3)$$

The methodology for the calculation of the kinetic parameters as a function of temperature used in this work is described below:

**(*i*)** *Determine the appropriate forms of kinetic rates.*

Eq. (4) shows the cell growth rate equation, $r_x$, which includes terms for such types of inhibitions.

$$r_x = \mu_{max} \frac{S}{K_s + S} \exp(-K_i S) \left(1 - \frac{X}{X_{max}}\right)^m \left(1 - \frac{P}{P_{max}}\right)^n X \quad (4)$$

In this study, Luedking-Piret expression was used to account for the ethanol formation rate, $r_p$.

$$r_p = Y_{px} r_x + m_p X \; ; \; r_s = (r_x / Y_x) + m_x X \quad (5\text{-}6)$$

The substrate consumption rate, $r_s$, is given by Eq. (6), describing the sugar consumption during fermentation, which leads to cell mass and ethanol formation.

**(*ii*)** *Estimate a set of temperature dependent parameters for each temperature considered in the experiments.*

Some of the parameters in the kinetic expressions above ($\mu_{max}$, $X_{max}$, $P_{max}$, $Y_x$ and $Y_{px}$) are known to be dependent on temperature **[5]**. Let θ specify the parameters vector, which contains all the temperature-dependent parameters. The objective of the mathematical estimation of model parameters is to find out θ by minimizing the objective function, min $E(\theta)$:

$$E(\theta) = \sum_{n=1}^{np} \left[ \frac{(X_n - Xe_n)^2}{Xe_{max}^2} + \frac{(S_n - Se_n)^2}{Se_{max}^2} + \frac{(P_n - Pe_n)^2}{Pe_{max}^2} \right] \quad (7)$$

where $Xe_n$, $Se_n$ and $Pe_n$ are the measured concentrations of cell mass, substrate and ethanol at the sampling time $n$. $X_n$, $S_n$ and $P_n$ are the concentrations computed by the model at the sampling time $n$. $Xe_{max}$, $Se_{max}$ and $Pe_{max}$ are the maximum measured concentrations..

The parameters which are not temperature dependent are fixed in the values given by **Atala et al. [5]** and are: $K_s$ = 4.1 kg/m$^3$, $K_i$ = 0.004 m$^3$/kg, $m_p$ = 0.1 kg/[kg·h], $m_x$ = 0.2 kg/[kg·h], $m$ = 1.0 and $n$ = 1.5.

**(*iii*)** *Propose an equation to describe the influence of temperature and fit it to the optimized values obtained for each temperature.*

The influence of temperature on $\mu_{max}$, $X_{max}$, $P_{max}$ and $Y_{px}$, is non-linear and Eq. (8) can be used to express it:

$$\text{temperature-dependent parameter} = A \exp(B/T) + C \exp(D/T) \quad (8)$$

The influence of temperature on $Y_x$ was described by Eq. (9):

$$\text{temperature-dependent parameter} = A \exp(B/T) \quad (9)$$

In these equations, $A$, $B$, $C$ and $D$ are constants, and $T$ is the temperature in $^oC$.

### *3.2. Hybrid Neural Modeling*

In this study, the structure of the hybrid neural model is derived taking into consideration the mass balances (Eqs. 1-3) for the batch fermentation process, with neural networks describing the rate expressions for cell growth, $r_x$, substrate consumption, $r_s$, and product formation, $r_p$.
For the current study, each rate expression ($r_x$, $r_s$, and $r_p$) was modeled with a MLPNN with four inputs (concentrations of biomass, substrate and ethanol, and temperature), a single hidden layer, described mathematically by Eq. (10), and one output. Both input and output data were normalized to the range [0, 1].

$$\hat{y} = g[x,\theta] = F[\sum_{j=1}^{M} W_j f_j (\sum_{l=1}^{N} w_{jl} x_l + w_{j0}) + W_0] \quad (10)$$

In Eq. (10), θ specifies the parameter vector, which contains all the adjustable parameters of the network; i.e., the weights and biases $\{w_{j,l}\ W_j\}$.
It follows from Cybenko's theorem **[6]** that all continuous functions can be approximated to any desired accuracy with a network of one hidden layer of sigmoidal ($f(x) = 1/(1+\exp^{-x})$) hidden units (nodes) and a layer of linear output nodes. Such structure is used in this work. Nguyen–Widrow initialization algorithm is used for initialization of weights and biases and is subsequently trained with the Levenberg–Marquardt algorithm in Matlab's neural network toolbox. Training was stopped after 1000 epochs. The appropriate number of nodes to be included in the hidden layer was addressed with the cross-validation technique in order to avoid model over-fitting.

## 4. Results and Discussion

The first-principles and hybrid neural models kinetic parameters were estimated using the results of the first five experiments **[4]**. When the same models were used to describe the second data set, the prediction quality is poor. These results show that conditions such as molasses harvesting and medium composition affect the process performance (kinetics and dynamic behavior). Such changes occur frequently in industrial operations, and this reinforces the importance of adaptation of kinetic parameters.

### *4.1. Results for First-Principles Modeling*

For the re-estimation of the parameters, Eqs. (1-3) were solved using a FORTRAN program with integration by an algorithm based on the fourth-order Runge-Kutta method. The temperature dependent parameters ($\mu_{max}$, $X_{max}$, $P_{max}$, $Y_x$ and $Y_{px}$ in Eqs. 4-6) were determined by minimizing Eq. (7) using a quasi-newton algorithm. The FORTRAN IMSL routine DBCONF was used for this purpose. This procedure was repeated for each temperature considered (30, 31.2, 34, 36.8 and 38°C). The parameters that are not temperature-dependent

were not altered. In order to describe the correlation between temperature and the parameters, the data was smoothed and interpolated and the expressions given by Eqs. (8) and (9) were fitted. Figure 1 shows the behavior predicted by Eqs. (8) and (9) with temperature and the optimized parameters estimated from the experimental data in the range of 30-38°C. The performance of the model with re-estimated parameters in describing the experimental data at 31.2°C is shown in Figure 2. It can be seen that the model with re-estimation of the temperature dependent kinetic parameters described accurately the experimental data.

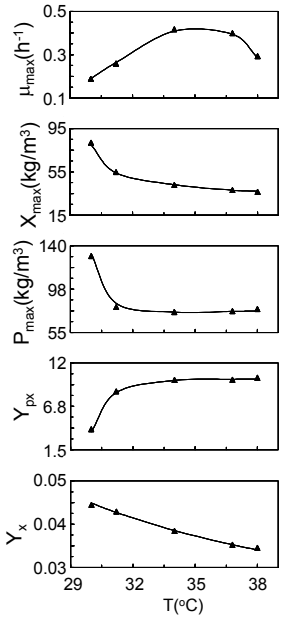


Figure 1. Parameter behavior with temperature at 30, 31.2, 34, 36.8 and 38°C

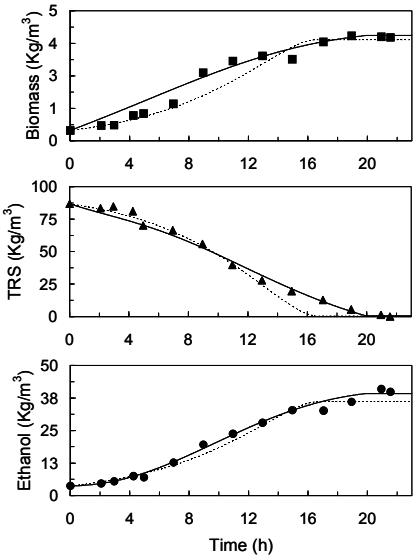


Figure 2. Experimental (cell mass, X(■); substrate, S(▲) and ethanol, P(●)) and modeling (Hybrid neural model—; First-principles model---) results with parameters reestimation at 31.2°C

## *4.2. Results for Hybrid Neural Model*

The neural network parameters were reestimated for the new experiments using the methodology detailed as follows. Initially, the appropriate neural network architecture, including the initial parameter set, is determined. After this step, if there are changes in operational conditions and/or fluctuations in the quality of raw material, the model can be directly adapted by minimizing Eq. (7). In this case, θ specify the parameter vector, which contains all the neural network parameters. The variables $X_n$, $S_n$ and $P_n$ are the concentrations computed by the hybrid neural model at the sampling time $n$. If a minimum is reached, the re-

estimation is terminated. If not, the neural network parameters are adapted and a new iteration begins with the hybrid neural model simulation. The result at 31.2°C is shown in Figure 2. It can be noticed that the adapted hybrid neural model effectively tracks the desired trajectory of experimental observations for concentrations of biomass, substrate and product.

## 5. Concluding remarks

Comparing the adaptation procedures, the re-estimation of the network weights was simpler than the re-estimation of the kinetic parameters of the first-principles model. Even considering that the rate equations and the functions that describe the parameters dependence with temperature are known in the first-principles model, the estimation problem is complex and time consuming. This suggests that using a first-principles model in a situation where frequent re-estimation is necessary could be a limitation. The updating of the hybrid neural model, however, is straightforward. The structure of the neural network (number of layers and of neurons in each layer) was fixed and the weights were reestimated. The use of this computer-aided tool enables the implementation of an on-line re-estimation procedure. Although this could not be a very significant advantage for a process well studied and known as the alcoholic fermentation, it can make a great difference for less known biotechnological processes, as it enables a rapid determination of a mathematical description that can be used for on-line optimization, soft sensor and control.

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