

MODELING, SIMULATION AND DYNAMIC OPTIMIZATION APPLIED TO AN ETHANOL FED-BATCH FERMENTATION PROCESS

Paulo R. C. Vilela

University of São Paulo at São Carlos, Mechanical Engineering Department Av. Trabalhador São-carlense, 400. Zip code: 13566-590 - São Carlos, SP, Brazil vcrpaulo@gmail.com

Adriano A. G. Siqueira

University of São Paulo at São Carlos, Mechanical Engineering Department siqueira@sc.usp.br

Abstract. This paper deals with modeling, simulation and dynamic optimization applied to an ethanol fed-batch fermentation process to maximize production through obtain a robust controller to optimize the insertion of substrate in the medium. The need for replacement of oil, reducing greenhouse gas emissions and the greenhouse effect made the production and use of ethanol in Brazil the most important commercial renewable fuel program in the world today. A literature review is carried out, highlighting fermentation kinetics of alcoholic fermentation, the methodologies for estimating the kinetic parameters required to obtain a model appropriate and the optimization of fed-batch fermentation, through optimal control algorithm and robust. Modeling is presented in the state variables of the dynamic system composed of the time variation of the substrate, the product, the cell concentration and volume. The kinetic parameters are estimated by a Prediction-Error identification Method, using Matlab. The optimization of fedbatch fermentation is performed considering as objective function to maximize the productivity of ethanol, eliminating most of residual sugars at the end of the fermentation process. The optimized parameter is the input flow of substrate and applied methodology is based on a LPV (linear parameter varying) control technique. The results of identification parameters are presented as well as the LPV controller performance.

Keywords: Fed-Batch Fermentation, LPV Control, Modeling and Simulation, Parameters Estimation

1. INTRODUCTION

According to UNICA (União da Indústria de Cana-de-Açúcar) (UNICA, 2012), during the 2011/2012 harvest were ground more than 550 million tons of sugarcane, producing over 36 million tons of sugar and 23 billion liters of ethanol. Sugarcane occupies today about 7 million hectares, which corresponds to approximately 2% of all arable land in the country. These numbers make Brazil the largest producer, followed by India, Thailand and Australia.

Fermentation products, such as bread, wine and beer, are consumed since the beginning of the practice of agriculture. There are reports that show the consumption and brewing of beer before 6000 BC (VILLEN, 2009). Lavoisier, in 1789, was the first to make a quantitative study of alcoholic fermentation, identifying in addition to ethyl alcohol and carbon dioxide another compound, acetic acid. But it fell to Pasteur, in 1857, explaining the nature of the alcoholic fermentation, attributing it to the action of living organisms, yeasts, as causal agents (PACHECO, 2010).

The fermentation process does not occur by chance. Yeast uses fermentation to get energy and thus survive. The ethanol produced in the fermentation is just a byproduct of this process. Therefore becomes necessary to understand and provide the necessary and ideal conditions for yeast to produce ethanol as efficiently as possible. A way to determine which conditions are the better ones is through the study of the kinetics of alcoholic fermentation. This study has great economic and industrial potential, and that's why specialized research centers have great interest in to it.

According to ATALA et al. (2001), use of synthetic substrates (synthetic molasses) show different results than when using molasses from sugar cane. Molasses of sugarcane, despite being a good substrate, contains components that can act as inhibitors in the fermentation. Therefore, work that aims to study the kinetics of fermentation in industrial conditions should use molasses of sugarcane as substrate.

THATIPAMALA et al. (1992) applied the least squares Levenberg-Marquardt algorithm on experimental data conducted in fed-batch fermentation with different initial concentrations of product and substrate using *Saccharomyces cerevisiae* as microorganism.

LEE et al. (1995) obtained data from yield coefficients directly by experimental data. Maximum growth rates were estimated using a smooth cubic spline through cross-validation. The constant repression (k_i) and Monod $(k_g \text{ and } k_m)$ were obtained using a statistical method. The maximum concentrations of cells and ethanol were abstracted by previous data from continuous culture experiments.

Experimental data obtained with yeast *Saccharomyces diastaticus*, highly tolerant to ethanol, in experiments with batch and fed batch fermentation were used to estimate the parameters of the kinetic model through Hybrid Differential Evolution (HDE) by WANG and SHEV (2000) and WANG et al. (2001). WANG et al. (2001) used the method HDE introducing a Lagrangian type method, allowing them to be used inequality constraints in the optimization problem. The

experiment was validated by comparing it with the case of constant feed and also carrying out variations in substrate concentration. The authors concluded that the optimal feeding, for the case of the model used, it is more suitable when compared to constant feed profile.

ATALA et al. (2001) and FILHO et al. (2009) considered the effects of temperature on their simulations and also that the total biomass comprises living cells (active) and dead cells (inactive) because many researchers agreed in their research that there is loss of viability during fermentation. ATALA et al. (2001) applied high rates of substrate feed, around 25 kg / (m³. H), studying the fermentation temperature of 28 °C to 40 °C, 3 °C at 3 °C. The yield reached a maximum at 31 °C, decreasing to a minimum being hit at 40 °C.

RIVERA (2006) compared the performance of the model described by ATALA et al. (2001) when the kinetic parameters are optimized using Quasi-Newton algorithm and Real Coding Genetic Algorithm (RGA)

BORGES (2008) used a strain of *Saccharomyces cerevisiae* with culture medium and diluted crystal sugar and nutritional supplements for yeast. The process of fed-batch process was used, varying the feed time of 3 to 5 hours and the concentration of sugar in the must from 217 to 285 g / L. The technique of differential evolution (DE) was used by for estimation of kinetic parameters from experiments in batch and fed batch. This method choice was used because of its high applicability in diverse areas of knowledge. A version implemented in Matlab[®] by STORN and PRICE (1996) was used for it.

LOBATO et al. (2006) and BORGES (2008) used the principle of Pontryagin with the transformation of the original problem into a problem of identification of phases with floating differential index with defined shift times. Thus the original problem is transformed into various problems defined in stages, with characteristics defined by the respective index and the sequence of events. When compared to results from the literature, the authors considered that the performance of the developed methodology was good.

PIMENTEL and COUTINHO (2012) rewrote the non-linear dynamics of the bioreactor in terms of time-varying parameters (*quasi-LPV* approach) in order to apply the linear matrix inequality framework for designing the free dynamics resulting from a partial feedback linearizing strategy.

This paper presents the first results of the development of a mathematical model for fed-batch fermentation, based in experimental data obtained using one kind of yeast at three different temperatures. The dynamic model is generated using the Matlab environment by using the Prediction-Error identification Method to estimate the kinetic parameters. The mathematical model obtained is therefore used to develop a robust controller based on LPV techniques.

The paper is organized as follows. Section 2 introduces the modeling of a fed-batch fermentation using state variables composed of the time variation of the substrate, the product, the cell concentration and volume. Section 3 presents an experiment developed to estimate and identify the parameters of fed-batch fermentation to a specific kind of yeast. Section 4 shows how the LPV control can be used to optimize the performance of fed-batch fermentation. Section 5 presents the results of the LPV control implementation in the proposed dynamic system. Section 6 summarizes the main contributions of the paper.

2. MATHEMATICAL MODELING OF FED-BATCH FERMENTATION

The objective of the fermentation kinetics is to relate productivity rates of cell growth, substrate consumption and other related parameters. Like any mathematical model, the complexity of the kinetic description invariably depends on the application made and the parameters involved (BORGES, 2008).

To properly design a control-based model is first necessary to identify the model to be used and its parameters, so some considerations must be made about this step. Model a fermentation presents as main difficulty determining the equation which manages the reaction.

The mathematical model that best fits with experimental data is the model of GHOSE and THYAGI (1979) with *n* parameter different from one, Eq. (1), which takes account for both the inhibitory effects from the substrate as the product. This model is applicable to concentrations in the range 0-120 g/L (SANTOS, 2005) and conditions which only uses a single substrate (BORGES, 2008).

$$\mu = \mu_m \cdot \frac{s}{s + k_s + \frac{s^2}{k_i}} \cdot \left(1 - \frac{p}{p_m}\right)^n$$

where:

- $\mu \rightarrow$ Specific cell's growth rate
- $\mu_m \rightarrow$ Maximum cell's growth rate
- $s \rightarrow$ Substrate concentration
- $k_s \rightarrow$ Saturation constant for cell's growth
- $k_i \rightarrow$ Inhibition constant of cell's growth by the substrate

(1)

- $p \rightarrow$ Product concentration
- $p_m \rightarrow Maximum$ product concentration where microbial growth ceases
- $n \rightarrow$ Power of the term of product inhibition

Using the process of fed-batch fermentation form for ethanol production from Saccharomyces cerevisiae is indicated because it minimizes the effects of high concentrations of substrate and product, which occur at the beginning and end of the process, respectively. Equations (2) through Eq. (7) describe the dynamic behavior of the process, where x, s and p are cell concentrations, substrate and product, respectively. In the text below a description is carried out for each of the equations.

Considering that the growth rate of cells is dependent on the dilution of the cells (due to the inlet must) and the multiplication of cells (the specific growth rate of cells, Eq. (1)), has Eq. (2).

$$\dot{x} = -\frac{u}{v}x + \mu x$$
 $x(0) = x_0$ (2)

Equation (3) shows that the variation rate of substrate depends on the amount of incoming substrate being diluted in wort and the specific rate of substrate consumption, Eq. (4), by the cells.

$$\dot{s} = \frac{u}{v} \langle \langle F_F - s \rangle \sigma x \qquad \qquad s(0) = s_0 \tag{3}$$

$$\sigma = \left(\frac{1}{y_{xs}}\mu + m_s\right) \tag{4}$$

where:

- $s_F \rightarrow Must Concentration$
- $y_{xs} \rightarrow$ Cell Yield: relative to the amount of substrate diverted to cell multiplication
- $m_s \rightarrow$ Maintenance of Cellular Constant: relative to the amount of necessary substrate for cell survival

The ethanol production's rate, Eq. (5), is dependent on the dilution of ethanol in wort and the specific rate of product formation, Eq. (6), by yeast.

$$\dot{p} = -\frac{u}{v} p + \pi x \qquad p(0) = p_0 \tag{5}$$

$$\pi = \frac{y_{ps}}{y_{xs}} \mu \tag{6}$$

where:

• $y_{ps} \rightarrow$ Ethanol Yield: relative to the amount of the substrate used for ethanol's production.

The change of fermentation tank volume basically depends on the inlet must. In this case it ignores the volume change due to CO_2 production.

$$\dot{\mathbf{v}} = \mathbf{u} \qquad \qquad \mathbf{v}(0) = \mathbf{v}_0 \text{ and } \mathbf{v}(t_f) = \mathbf{v}_f \tag{7}$$

3. PROCEDURE FOR IDENTIFYING THE PARAMETERS OF THE MATHEMATICAL MODEL

The fed-batch fermentation experiments were conducted in order to approach as much as possible the methodology adopted in the industrial process. Yeast PE-2, used in the tests, was multiplied in Fermentec laboratories (FERMENTEC TECNOLOGIAS EM ACUCAR E ALCOOL LTDA.), by courtesy.

3.1 Test conditions and experimental procedures

Fermentations were carried out in bottles (fermentation tank) of a total volume of 3000 ml. The inoculum used had a total volume of 625 mL, composed of 250 g of yeast, 312 ml of water and 63 mL of wort, totalizing 25% of the total volume of wort. The must was composed of molasses and water (20% concentration), pH 4.5. The final volume of wort was near 2500 mL. There were two cycles, each one with nine fermentation tanks (Fig. 1) equally distributed on three temperatures (30 °C, 33 °C and 36 °C). Were performed 6 feeds spaced 1 hour (1 x 325 ml and 5 x 310 mL) in each fermentation tank, totaling 5 hours of feeding, as is usual in the industry (AMORIM, 2005).

Figure 1 shows the temperature control of the fermentation tanks that was performed individually using commercial temperature controller. Dichroic lamps were used to carry out the wort heating procedure until the desired temperature was reached. Temperature controllers were set so the maximum variation of these were 1 °C always reaching the maximum upper temperature controlled (30 °C, 33 °C and 36 °C).

The weight of the wort was measured using precision balances and transmitting the measurements to a computer that recorded and kept that.



Figure 1. Nine fermentation tanks equally distributed on three temperatures (30 °C, 33 °C and 36 °C) with individual temperature controllers.

The first cycle served merely to create the recycling of yeast, making the test as close as possible to reality experienced in plant. Due to this situation, no samples were taken and no acid treatment was performed in the first cycle.

The 2nd cycle was carried out with the acid treatment (pH 2.5 for 1.5 h, 1.8 g H2SO4) and samples were collected (20 mL) at the start of the process and every hour, until 9 hours of fermentation were reached. For each sample ethanol, biomass, Residual Sugar and viability analysis were performed.

3.2 Obtaining the Dynamic Model

Efficient linear parameter-varying (LPV) controllers can be designed with accurate and low complexity LPV model of the basic behavior of the system. Use of first-principle laws of physics, chemistry and biology are common to construct dynamic models. Build a complete mathematical model, consistent and compact based on expert knowledge can become a complex task due to the difficulty of distinguishing parameters whose effects are relevant to those who may be ignored (TOTH et al, 2012). The main stream LPV control-synthesis approaches are based on models defined in a state space form.

(8)

In this paper, Nonlinear Least Squares Algorithm is used to perform, through idnlgrey (Estimating Linear Grey-Box Models) function from Matlab[®] an estimation of parameters from yeast PE-2, using the dynamic model shown in Eq. (1) through Eq. (7) considering the inhibition by the product and the substrate.

The solution of differential equations to obtain parameters was performed using three different methods (FORSYTHE, 1977):

- Forward Euler's Method: method of first order, has a lot of instability and the global error is proportional to the step size.
- Runge-Kutta 23: Uses a simple second and third order pair of formulas for medium accuracy.
- Runge-Kutta 45: Uses a fourth and fifth order pair for higher accuracy. Since this one uses higher order formulas, it usually takes fewer integration steps and gives a solution more rapidly.

The method with the best performance, as well as the response time as the final error was the Runge-Kutta 45 method.

3.3 H∞-Control for linear parameter varying (LPV) systems

An LPV system has dynamic matrices of state-space representation dependent on a vector of parameters $\rho(t)$ which vary with time (SIQUEIRA et al., 2011).

Let consider an LPV system given by Eq. (8).

$$\dot{\mathbf{x}} = \mathbf{A}(\rho(t))\mathbf{x} + \mathbf{B}_{1}(\rho(t))\mathbf{w} + \mathbf{B}_{2}(\rho(t))\mathbf{u}$$
$$\mathbf{z} = \mathbf{C}_{1}(\rho(t))\mathbf{x} + \mathbf{D}_{11}(\rho(t))\mathbf{w} + \mathbf{D}_{12}(\rho(t))\mathbf{u}$$
$$\mathbf{y} = \mathbf{C}_{2}(\rho(t))\mathbf{x} + \mathbf{D}_{21}(\rho(t))\mathbf{w}$$

where:

- **x**: Vector of State Variables
- w: Vector of External Perturbations
- u: Vector of Control Inputs
- z: Vector of Controlled Outputs
- y: Vector of Measured Outputs.

The input/output signals dimensions and the state dimension can be defined by the matrices $\mathbf{A} \in \mathbb{R}^{nxn}$, $\mathbf{D}_{12} \in \mathbb{R}^{p1xm2}$ and $\mathbf{D}_{21} \in \mathbb{R}^{p2xm1}$. The time varying parameters $\rho(t) = [\rho_1 \dots \rho_L]^T$ are assumed limited by its minimum and maximum value and the rate of variation of these parameters are assumed well defined in the entire time interval, satisfying $|\dot{\rho}(t)| \leq \mu_i$.

Search and find a dynamic controller K (ρ), given by Eq. (9), is the solution to the problem involving LPV sytems which has output feedback control with H ∞ , providing internal stability and bounded L₂ gain between perturbation signal **w** and output signal **z**.

$$\dot{\mathbf{x}}_{\mathbf{K}} = \mathbf{A}_{\mathbf{K}}(\rho(t), \dot{\rho}(t))\mathbf{x}_{\mathbf{K}} + \mathbf{B}_{\mathbf{K}}(\rho(t), \dot{\rho}(t))\mathbf{y}$$

$$\mathbf{u} = \mathbf{C}_{\mathbf{K}}(\rho(t), \dot{\rho}(t))\mathbf{x}_{\mathbf{K}} + \mathbf{D}_{\mathbf{K}}(\rho(t), \dot{\rho}(t))\mathbf{y}$$
(9)

Closing the loop between systems given by Eq. (8) and Eq. (9), for all $t \ge 0$ and every possible trajectory ($\rho(t)$, $\dot{\rho}(t)$), taking into account null initial conditions, Eq. (10) is valid.

$$\int_{0}^{T} \mathbf{z} \mathbf{d}\tau \leq \gamma^{2} \int_{0}^{T} \mathbf{w}^{\mathrm{T}} \mathbf{w} \mathrm{d}\tau$$
(10)

It is important to observe that the controller matrices explicitly depend on the time-varying parameter $\rho(t)$ and its derivative $\dot{\rho}(t)$.

Solving the set of Linear Matrix Inequalities (LMIs) given by Eq. (11), Eq. (12) and Eq. (13), , minimizing γ , the controller is obtained.

$$\begin{bmatrix} \mathbf{N}_{\mathbf{X}} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} \dot{\mathbf{X}} + \mathbf{X}\mathbf{A} + \mathbf{A}^{\mathrm{T}}\mathbf{X} & \mathbf{X}\mathbf{B}_{1} & \mathbf{C}_{1}^{\mathrm{T}} \\ \mathbf{B}_{1}^{\mathrm{T}}\mathbf{X} & -\gamma\mathbf{I} & \mathbf{D}_{11}^{\mathrm{T}} \\ \mathbf{C}_{1} & \mathbf{D}_{11} & -\gamma\mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{N}_{\mathbf{X}} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} < \mathbf{0}$$
(11)

$$\begin{bmatrix} \mathbf{N}_{\mathbf{Y}} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} -\dot{\mathbf{Y}} + \mathbf{A}^{\mathrm{T}}\mathbf{Y} + \mathbf{A}\mathbf{Y} & \mathbf{Y}\mathbf{C}_{1}^{\mathrm{T}} & \mathbf{B}_{1} \\ \mathbf{C}_{1}\mathbf{Y} & -\gamma\mathbf{I} & \mathbf{D}_{11} \\ \mathbf{B}_{1}^{\mathrm{T}} & \mathbf{D}_{11}^{\mathrm{T}} & -\gamma\mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{N}_{\mathbf{Y}} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} < \mathbf{0}$$
(12)

$$\begin{bmatrix} X & I \\ I & Y \end{bmatrix} > 0$$
(13)

where:

- $N_X \rightarrow Any$ base of a null space of $[C_2 D_{21}]$
- $N_{Y} \rightarrow Any$ base of a null space of $[B_{2}^{T} D_{12}^{T}]$

After solving the LMIs mentioned above (Eq. (11), Eq. (12) and Eq. (13)) in terms of X and Y, Eq. (14) is used to obtain the LPV controller.

$$A_{K} = N^{-1} \left(\dot{\mathbf{X}} \dot{\mathbf{Y}} + \dot{\mathbf{A}}_{K} - \mathbf{X} \left(\mathbf{A} - \mathbf{B}_{2} \mathbf{D}_{K} \mathbf{C}_{2} \right) \mathbf{Y} - \dot{\mathbf{B}}_{K} \mathbf{C}_{2} \mathbf{Y} - \mathbf{X} \mathbf{B}_{2} \dot{\mathbf{C}}_{K} \mathbf{M}^{-T},$$

$$B_{K} = N^{-1} \left(\mathbf{B}_{K} - \mathbf{X} \mathbf{B}_{2} \mathbf{D}_{K} \mathbf{y} \right)$$

$$C_{K} = \left(\mathbf{C}_{K} - \mathbf{D}_{K} \mathbf{C}_{2} \mathbf{Y} \mathbf{M}^{-T}, \mathbf{D}_{K} = \mathbf{D} \right)$$
(14)

where N and M satisfy $I - XY = NM^{T}$ and $D_{cl} = D_{11} + D_{12}D_{K}D_{21}$.

3.4 Reduction of the problem to a finite number of dimensions

The solution of LMIs given by Eq. (11), Eq. (12) and Eq. (13) represents a convex problem with infinite dimensions and limited if its dependence on $\rho(t)$ in another parameter is taken into account. To represent this system in a finite number of dimensions, it is necessary to discretize these points.

The matrices $X(\rho)$ and $Y(\rho)$, unknown, are solution of LMI if they satisfy the inequalities in all discretized points. Thus, to set the X and Y matrices as a function of ρ defining a criterion for variation of it, it is necessary to set these matrices using basic functions that have dependency on ρ , whose shape is shown in Equation (15)

$$\mathbf{Z}(\rho) = \sum_{i=1}^{M} \mathbf{f}_i(\rho) Z_i$$
(15)

where $f_i(\rho)$, i = 1, ..., M, is continuously differentiable. The basic functions of the matrices are chosen have a similar behavior of the system to be controlled.

The above concepts (Section 3.3 and Section 3.4) have been implemented in Matlab[®], with the differential equations which represent the kinetic behavior of the yeast PE-2 to achieve a robust controller for the system.

4. RESULTS AND DISCUSSIONS

In this section, the results of each part of the paper development are presented.

The experiment was conducted as described in section 3.1. Figure 2 shows the variations of biomass (g/l), product (g/l) and substrate (g/l) concentrations and the volume of the tank (l). In all three studied cases, the feed ended after 5 hours of fermentation, as seen in Fig. 2. The data obtained are close to those BORGES (2008) obtained in their experiments, with slight difference in the concentration of cells (biomass), at which cell's growth was less pronounced in the experiment carried out for this work.

The conversion rate of substrate into biomass $(y_{xs} [g/g])$ and the conversion rate of substrate to product $(y_{ps} [g/g])$ were obtained according to Eq. (16) and Eq. (17), respectively. The productivity $(Q_p [g/(l.h)])$ was calculated according to Eq. (18).

$$y_{ps} = \frac{p \underbrace{v} \underbrace{c} p_0 v_0}{\underbrace{b} \underbrace{c} v_0 \underbrace{s}_F + v_0 s_0 - v \underbrace{c} \underbrace{s} \underbrace{c}$$
(16)

$$y_{xs} = \frac{x \underbrace{y} \underbrace{r}_{v_0} x_0 v_0}{\underbrace{r}_{F} + v_0 s_0 - v \underbrace{s}_{F}}$$
(17)

$$Q_p = \frac{p_F - p_0}{t_F} \tag{18}$$

A comparison between the conversion rates and productivity at each temperature examined was executed and is shown at Fig. 3. Higher temperatures (above 35 °C) favor bacterial growth (AMORIM, 2005), thus impairing the substrate to product (ethanol) conversion rate and consequently decreasing productivity. Table 1 shows the experimental initial conditions and final results of the experiment at each temperature.



Figure 2. Volume, Biomass, Substrate and Product concentration at three different temperatures (30 °C, 33 °C and 36 °C).



Figure 3. Comparison between Substrate-Biomass Conversion Rate (y_{xs} [g/g]), Substrate-Product Conversion Rate (y_{ps} [g/g]) and Productivity (Qp [g/(l.h)]) at three different temperatures (30 °C, 33 °C and 36 °C)

	T = 30 °C	T = 33 °C	T = 36 °C			
S ₀ [g/l]	0	0	0			
X ₀ [g/l]	234,0	251,4	190,1			
P ₀ [g/l]	34,47	34,47	34,47			
V ₀ [I]	0,984	0,984	0,990			
V _F [I]	2,534	2,511	2,518			
F [l/h]	0,25	0,25	0,25			
t _F [h]	9	9	9			
S _r [g/l]	1,56	1,48	1,52			
y _{ps} [g/g]	0,588	0,578	0,568			
y _{xs} [g/g]	0,092	0,061	0,184			
Q _p [g/(l.h)]	7,77	7,74	7,63			

Table 1. Experimental results of fed-batch fermentation.

Using the data obtained from the experiments described above (Tab. 1) and applying the method described in section 3.2, was obtained the mathematical model for yeast PE-2 in the temperature range $30-36^{\circ}$ C. Table 2 shows the initial conditions (parameters to star the method) and the parameters estimated using the method of Runge-Kutta 45. Stopping criteria adopted were 100 iterations or variation of less than 10^{-8} between two consecutive iterations. Table 3 shows a comparison between the two different methods applied to get the model. The method chosen to continue the paper was Runge-Kutta 45 because it had a better approximation at all temperatures examined between the experimental data and the model obtained. Experimental data and results of estimated parameters model are shown at Fig. 4, Fig. 5 and Fig. 6.

Among the estimated parameters, the one who showed no significant change with temperature was Maintenance of Cellular Metabolism constant (ms), as shown in Tab. 2.

	T = 30 °C		T = 33 °C		T = 36 °C	
	Initial	Estimated	Initial	Estimated	Initial	Estimated
mi_max	0,1323	0,1277	0,1323	0,1018	0,1323	0,3128
p_max	98,3583	110,6718	98,3583	100,5807	98,3583	100,1301
n	0,9018	0,9445	0,9018	0,9251	0,9018	0,5206
ks	1,2403	0,6084	1,2403	1,7155	1,2403	22,4115
ki	84,0121	307,4217	84,0121	89,1689	84,0121	109,7352
ms	0,0051	0,0118	0,0051	0,0122	0,0051	0,0122
m	0,1	0,1927	0,1	0,0877	0,1	0,0639
x_max	105	101,9126	100	105,2812	105	100,1607

Table 2. Initial parameters and parameters estimated using method Runge-Kutta 45.

Table 3. Comparison between the methods Runge-Kutta 23 and Runge-Kutta 45 in parameter estimation.



Figure 4. Results of parameter estimation for temperature 30 ° C, comparing the experimental data and the parameter estimation. (a) Biomass (g/l) (b) Substrate (g/l) (c) Product (g/l) (d) Tank Volume (l)



Figure 5. Results of parameter estimation for temperature 33 ° C, comparing the experimental data and the parameter estimation. (a) Biomass (g/l) (b) Substrate (g/l) (c) Product (g/l) (d) Tank Volume (l)



Figure 6. Results of parameter estimation for temperature 36 ° C, comparing the experimental data and the parameter estimation. (a) Biomass (g/l). (b) Substrate (g/l). (c) Product (g/l). (d) Tank Volume (l)

Elaboration of LPV controller for the process was performed for each of the parameters estimated and temperatures analyzed (shown on Tab. 2). Figure 7 shows the variation obtained in product concentration (g / l) and Tank Volume (l) for temperature 33° C.



Figure 7. Results of applying the LPV control at a temperature of 33 ° C. (a) Increase of product concentration (g/l). (b) Changing of the feed function

As shown in Fig. 7, changing the way of feeding the substrate (Fig. 7b) resulted in an increase in the final concentration of product (Fig. 7a)

5. CONCLUSIONS

Taking into account the errors of the experimental results (analysis and methodology) can be stated that the model expressed satisfactorily the behavior of yeast. It is still possible to conclude that, due to changes in parameter values for each of the temperatures measured, the temperature is an important factor in the modeling of fermentation processes.

Using a LPV controller based on the model gives an improved robustness to the system, thus being less susceptible to variations inherent to the process.

Other variables can be inserted in the model in order to adapt it for use with various types of substrate (water and molasses; molasses, sugar cane juice and water) in order to make the model closest to the industrial reality.

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7. REFERENCES

AMORIM, H. V, 2005. Fermentação Acoólica: Ciência e Tecnologia. Piracicaba. São Paulo. Fermentec, 448 p.

- ATALA, D. I. P.; COSTA, A. C.; MACIEL, R.; MAUGERI, F, 2001. Kinetics of ethanol fermentation with high biomass concentration considering the effect of temperature. Applied Biochem. Applied Biochemistry and Biotechnology, Vol. 91-93, p.353 - 365.
- BORGES, P. C. S, 2008. Otimização dinâmica da fermentação alcoólica no processo em batelada alimentada. Thesis (Masters Degree in Chemical Engineering) Universidade Federal de Uberlândia, 141 p.
- FILHO, M. V. A. C.; MONTEIRO, J. B.; MAGAZONI, F. C.; COLLE, S., 2009. *Modeling, Simulation And Analysis Of Ethanol Fermentation Process With Control Structure In Industrial Scale*. 22nd International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, p. 10, Foz do Iguaçu, Paraná, Brazil.
- FORSYTHE, G. E.; MALCOLM, M. A.; MOLER, C. B, 1977. Computer Methods for Mathematical Computations. Prentice-Hall.
- GHOSE, T. K.; THYAGI, R. D, 1979. Rapid Ethanol Fermentation of Cellulose Hydrolysate: Product and Substrate Inhibitionand Optimization of Fermentor Design. Biotechnology and Bioengineering, 21, 1401-1420.
- LEE, Y.; LEE, W. G.; CHANG, Y. K.; CHANG, H. N, 1995. Modelling of Ethanol Prodiction by Saccharomyces cerevisiae from a Glicose and Maltose Mixture. Biotechnology Letters, 17, n°8, 791-796.
- LOBATO, F. S.; OLIVEIRA-LOPES, L. C.; MURATA, V. V, 2006. *Optimal Feed Policy For Fed-Batch Fermentation With Events Identification Based On Switching Structures*. XXII IACChE (CIIQ) 2006/ V CAIQ AAIQ Associación Argentina de Ingenieros Químicos IACCHE Interamerican Confederation of Chemical Engineering.

- PACHECO, T. F, 2010. Fermentação Alcoólica com Leveduras de Características floculantes em reator tipo torre com escoamento ascendente. Thesis (Masters Degree in Chemical Engineering) - Universidade Federal de Uberlândia, 107 p.
- PIMENTEL, G.; COUTINHO, D, 2012. Controle Robusto Por Realimentação Linearizante Parcial De Bioreatores Em Modo De Operação Descontínua Com Alimentação. Revista Controle & Automação. Vol.23 nº.2. p. 138-152. APR. 2012.
- RIVERA, E. A. C, 2006. Otimização De Bioprocessos: Avaliação De Desempenho Das Abordagens Determinística E Por Algoritmos Genéticos. Thesis (PhD in Chemical Engineering) – Universidade de Campinas, 194 p.
- SANTOS, K. G.; LOBATO, F. S.; MURATA, V. V, 2005. Controle on-off de um fermentador batelada alimentada para altas concentrações de substrato. VI Congresso Brasileiro de Engenharia Química em Iniciação Científica, Campinas - São Paulo, 6 p.
- SIQUEIRA, A. A. G., TERRA, M. H., BERGERMAN, M., 2011 Robust Control of Robots: Fault Tolerant Approaches. London : Springer, v.1. p.228.
- THATIPAMALA, R.; ROHANI, S.; HILL, G. A., 1992 Effects of High Product and Subtrate Inhibitions on the Kinectics and Biomass and Product Yields During Ethanol Batch Fermentation. Biotechnology and Bioengineering, 40, p. 289-297.
- TOTH, R., HEUBERGER, P.S.C. & HOF, P.M.J. Van den, 2012 Prediction-error identification of LPV systems present and beyond. In J. Mohammadpour & C. W. Scherer (Eds.), Control of linear parameter varying systems with applications (pp. 27-60). Heidelberg Springer.
- UNICA, 2012. "1^a ESTIMATIVA DA SAFRA 2012/2013 12/04/2012". União da Indústria de Cana de Açúcar. 12 Apr. 2012 < http://www.unica.com.br>
- VILLEN, R. A., 2009. Biotecnologia Histórico e Tendências. Escola de Engenharia de Mauá.
- WANG, F. S.; SHEV, J., 2000 Multiobjective parameter estimation problems of fermentation processes using a high ethanol tolerance yeast. CHEMICAL ENGINEERING SCIENCE, 55, 3685-3695.
- WANG, F. S.; SU, T.; JANG, H., 2001. Hybrid Differential Evolution for Problems of Kinetic Parameter Estimation and Dynamic Optimization of an Ethanol Fermentation Process. Ind. Eng. Chem. Res., 40, 2876-2885.

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