Modeling, Control and Optimization of Ethanol Fermentation Process

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Abstract: This paper presents the modelling, control and optimization of a fermentation unit of the ethanol industry. The presented model considers all the important variables that affect the ethanol production: temperature, pH and reactor feed rate. The proposed strategy is based on a two level control system. In the low level, SISO controllers are used to impose the desired closed loop dynamics of the local variables and to reject local disturbances. In the high level a MIMO optimal controller is used to maximize the ethanol production. Simulation results with a industrial scale model are presented to illustrate the advantages of the proposed strategy.

1. INTRODUCTION

Ethanol from sugar cane as a substitute for fossil fuels has proven to be concrete alternative in the fight against air pollution. In Brazil, sugarcane industries are interested in increasing their productivity from the optimization of their processes. In particular, there is a clear prospect of improved performance in the fermentation processes.

Ethanol production via fermentation by *saccharomices cerevisiae* is a process in which the formation of product is associated with cell growth. The yeast cells are subjected to stresses inherent to the process, that are caused by environmental conditions and physical-chemical factors such as high temperature, salinity, pH and high concentrations of ethanol and sugar.

In this process, the inoculum prepared in the bottom of the reactor receives the must from a flow control, until it reaches the desired level. The temperature and pH of the must are maintained around desired values using a heat exchanger and the addition of acid substances, respectively.

Several papers have been published analyzing various aspects of the fermentation control process. A methodology for obtaining the optimum process temperature for the maintenance of cell viability, reducing glycerol production and increasing efficiency is presented by Atala et al. [2001]. An analysis of how to minimize the processing time to obtain a desired production in a bioreactor is found in Cacik et al. [2001]. In Magazoni et al. [2009] an absorption chiller is used for cooling the fermenters of an alcohol and sugar producing plant, obtaining an increase of 0.8% in fermentation efficiency.

To control the reactor feeding, Modak and Lim [1987] developed an optimization scheme using a nonlinear model where the feed flow rate is a function of the state variables: concentrations of cells, substrate, product and reactor volume. Chen and Hwang [1990] suggested a different procedure for optimal feeding of substrate, using a on-off control strategy which provides less wear of the actuators. In the work of Chaudhuri and Modak [1998], a neural network model with feedback was presented to determine the optimal flow rates of substrate. Chiou and Wang [1998] developed a method for the optimization of feed-bath reactors, which avoids the fast convergence to local optimum points while increasing the probability of finding the global optimum one. Also, in Wang et al. [2001], the same method was used to estimate the kinetic parameters of the ethanol fermentation model and glycerol, using *Saccharomyces diastaticus* LORRE 316 and to determine the best feeding rate and time to maximize alcohol production.

Recently, dos Santos et al. [2006] presented an on-off control strategy based on the solution of the initial value equations, defined by phase, resulting from the application of the Principle of Pontryagin and a procedure for reducing the top indexes. The method was also used in Borges [2008] to estimate and calculate the optimal feed flow. The experiments were simulated and validated in a bench scale reactor with interesting results.

Predictive control have also been applied to bath reactor for other applications outside the ethanol industry [Rodrigues and Maciel, 1999, Ashoori et al., 2009]. However, proposed solutions do not considered all the degrees of freedom of the problem. In order to optimize the fermentation process, all the main variables (feed flow rate, temperature and pH) should be controller simultaneously if the goal is to achieve high production with minimal loss of energy and raw materials. Thus, this work presents the modeling (in industrial scale) of the ethanol fermentation process and a control structure with two layers that allows the process control and production optimization.

The rest of the paper is organized as follows. Section 2 presents the models of equipments and processes that compose the industrial ethanol fermentation system. The proposed control strategy is presented in Section 3, while Section 4 is devoted to illustrate the obtained results with some simulations. Finally the paper ends with conclusions.

2. SYSTEM DESCRIPTION

As pointed out, the fermentation system described in this work is a industrial scale process normally used in real sugar and ethanol plants in south and central America such as in Brazil and Guatemala. The studied process
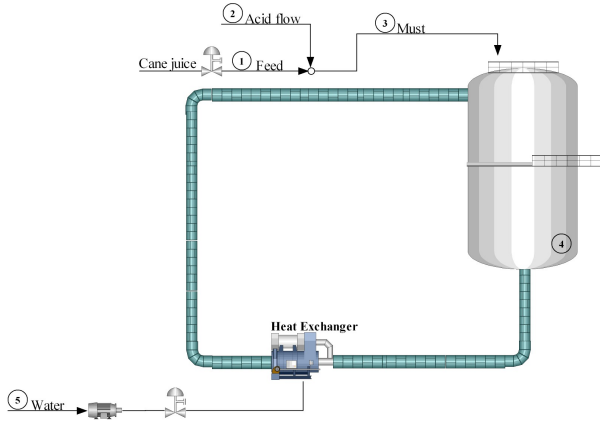

Fig. 1. Bath system

is shown in Fig. 1 where three main sub-systems are observed: (i) the reactor itself, where the fermentation occurs; (ii) the heat exchanger used to control the temperature of the process and (iii) the feed system, which considers both, the flow and pH dynamics.

The fermentation unit operation is as follows. The cane juice that is mixed with acid substance to maintain the pH in a desired value feeds the reactor until it reaches the desired level defined by the operator. The reactor is a batch unit and during each production period, a continuous recirculation of the must is performed. The must passes through a heat exchanger, which uses a coolant circulation to keep the must inside the reactor at an ideal temperature. Therefore, to obtain a complete control of this fermentation process three subsystems should be modeled: (i) the feed and pH control system, (ii) the heat exchanger, (iii) the fermentation into the reactor.
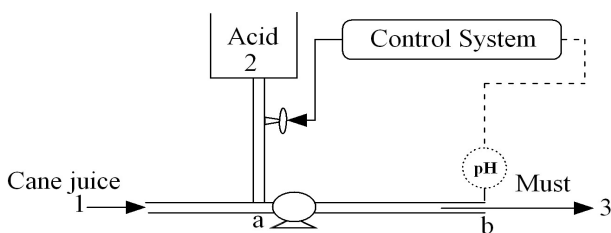
2.1 pH dynamic model

Fig. 2. pH process configuration

After extraction of the sugarcane juice, it is required that it be treated before being sent to the next steps of production. Treatment consists of chemical processes that have the finality of disinfecting and eliminating undesirable impurities in the broth. After this process the pH must be controlled. pH control is a very common process in sugar and alcohol plants. The strong nonlinearity of this process makes it one of the hardest type of SISO (single input single output) systems to be controlled. Moreover,

it is also a very important variable in the process, because large variations in pH can significantly impact the quality of the product and process efficiency.

For this work, the pH modeling was performed using the technique of invariant reaction [Gustafsson and Waller, 1983] for the system presented in da Costa Fº et al. [2010] whose configuration is illustrated in Fig. 2. The pH adjustment is done by injecting acid solution directly in the line of the duct where it passes the broth. Point a in the figure is where the mixing occurs; the pH sensor is installed in point b. Between points a and b, a pump is used to obtain the acid-broth mixture (which is considered perfect in the model). The volume $V = 474.71L$ is the total volume of all pipelines between points a and b, including the pump.

For any current i with a known pH and invariant value W_{bi}, it is possible to calculate invariant W_{ai} with:

$$W_{ai} = W_{bi} \cdot G(pH_i, K_{a1}, K_{a2}) + F(pH_i),$$

in which:

$$G(pH_i, K_{a1}, K_{a2}) = -\frac{1 + 2 \cdot 10^{(pH_i - pK_{a2})}}{1 + 10^{(pK_{a1} - pH_i)} + 10^{(pH_i - pK_{a2})}}, \quad (1)$$

$F(pH_i) = 10^{-pH_i} - 10^{(pH_i - 14)}$ and $pK_{ai} = -Log(K_{ai})$. From the system's balance for each of the invariant reaction, considering the numbers of the currents shown in Fig. 2, it is possible to express the model in state space [da Costa Fº et al., 2010]:

$$\begin{bmatrix} \dot{x_1} \\ \dot{x_2} \end{bmatrix} = \begin{bmatrix} \dfrac{F_1}{V}(W_{a1} - x_1) \\ \dfrac{F_1}{V}(W_{b1} - x_2) \end{bmatrix} + \begin{bmatrix} \dfrac{(W_{a2} - x_1)}{V} \\ \dfrac{(W_{b2} - x_2)}{V} \end{bmatrix} u \quad (2)$$

where $u = F_2$, $x_1 = W_{a3}$ e $x_2 = W_{b3}$. The output equation of the model calculates the pH implicitly. Using real pH variation data from experiments in one of the industrial plants [da Costa Fº et al., 2010], the model parameters were defined as: $pKa_1 = 6.6869$, $pKa_2 = 8.9950$, $Wb_1 = 5.8250 \cdot 10^{-4}$, $pH_1 = 4.45$ and $pH_2 = 7.00$.

2.2 Heat exchanger modelling

The number of parameters and its nonlinear dynamics make the modelling of a heat exchanger very difficult. Starting from a nonlinear and continuous model, a state space representation of the distributed parameter system is obtained using the "Direct Lumping of the Process" technique presented in Bonivento et al. [2001]. Basically, this method subdivides the thermal exchange surface into Δx sections, that is, the state vector is defined by the temperature of the sections.

Assuming that the velocity of the fluids across the heat exchanger is constant and neglecting the effects of the metal between the sections, the mass and energy balances can be calculated applying the Energy Conservation Principle to every lump (for time t, at point $x - \Delta x$), resulting in:

$$\frac{\partial}{\partial t}(Mc_pT) = \dot{m}c_p(T_{x-\Delta x} - T_x) - UA\Delta T \quad (3)$$

where $M = a\Delta x\rho$ is the lump mass; $\dot{m} = av\rho$ is the mass flow rate; a is the section of the chamber where the fluid flows; ρ is the fluid density; c_p is the specific heat capacity; T is the fluid temperature; t is the time; v is the fluid velocity; ΔT is the temperature difference; Δx is the incremental distance; A is the surface of the space included

in the considered lump and U is the overall heat transfer coefficient.

The heat exchanger is divided into N lumps so that the space model of the system refers to a state vector T representing the temperature of each lump. This vector can be subdivided into two parts, representing the temperature of each fluid:

$$T = [T_{r1}, T_{r2}, T_{r3}, ..., T_{rN} \quad T_{f1}, T_{f2}, T_{f3}, ..., T_{fN}]^T$$

in which T_{rj} e T_{fj} are the must and water temperatures in the point jth, with $j = 0, 1, ..., N$, respectively. T_{r0} e T_{f0} are considered as part of the inputs. Therefore, the following $2N$ order system can be obtained:

$$\begin{cases} M_r c_{pr} \dfrac{dT_{r,j}(t)}{dt} = \dot{m}_r(t) c_{pr}[T_{r,j-1}(t) - T_{r,j}(t)] - UA\Delta T(t) \\[3mm] M_f c_{pf} \dfrac{dT_{f,j}(t)}{dt} = \dot{m}_f(t) c_{pf}[T_{f,j-1}(t) - T_{f,j}(t)] - UA\Delta T(t) \end{cases}$$
(4)

The parameters of the system are:

$$
\begin{array}{ll}
N = 100 & a_r = a_f = 4.6296 \cdot 10^{-2} m^2 \\
v_r = 6 m/s & \rho_r = \rho_f = 1000 kg/m^3 \\
v_f = 6 \cdot u(t) m/s & c_{pr} = c_{pf} = 4.187 kJ/(K \cdot kg) \\
U = 1 kW/(K \cdot m^2) & T_{f0} = 20^o C \\
\Delta x = 0.02 m & A = 1.53 \cdot 10^{-2} m^2
\end{array}
$$

The temperature of the water is considered constant and the length of the thermal exchanger is $L = 2m$. The must from the reactor enters in the heat exchanger with a constant mass flow rate given by $\dot{m}_r = 10^6 kg/h$ and the water mass flow rate is $\dot{m}_f = 10^6 \cdot u(t)$ (kg/h), regulated by $u(t) \in [0, 1]$, which is used as a manipulated variable to control the temperature of the must into the reactor. In a real situation, the static gain of the heat exchanger varies as a function of the input temperatures of the fluids. This important characteristic is verified in the proposed model.

2.3 Reactor modelling

The mathematical modelling of the alcoholic fermentation was performed based on mass balance equations with the correspondents kinetic rates of the cell, substrate and product as well as global balance of energy for the overall process. It will be considered a sterile feeding, that is, with a null biomass concentration. The system is illustrated in Fig. 1 and a simulator that describes its behavior was developed by da Costa F° and Normey-Rico [2010].

Thus, the volume variation during the fermentative process is described as:

$$\frac{dV}{dt} = F_3$$
(5)

in which F_3 (m^3/h) is the volumetric flow rate of must at the entrance of the reactor.

The cell growth rate is defined as follows

$$\frac{dX}{dt} = \mu X - \frac{F_3}{V} X - K_d X$$
(6)

where μ (h^{-1}) is the specific growth rate and K_d (h^{-1}) is the global coefficient of cell death. The factor F_3/V (h^{-1}) is the dilution rate as the feed is added during the fermentation process.

The substrate consumption S is modelled by the following equation:

$$\frac{dS}{dt} = \frac{F_3}{V}(S_i - S) - \mu \frac{X}{Y_{X/S}} - m_X X$$
(7)

in which $S_i = 200 kg/m^3$ is the feed substrate concentration, $Y_{X/S}$ (kg/kg) is the yield factor of the biomass based on the substrate consumption and $m_X = 0.2 kg/(kg \cdot h)$ is the cell maintenance coefficient.

The ethanol formation P is written as:

$$\frac{dP}{dt} = Y_{P/X}\mu X + m_P X - \frac{F_3}{V} P$$
(8)

where $Y_{P/X}$ (kg/kg) represents the yield factor of the ethanol based on cell growth and $m_P = 0.1 kg/(kg \cdot h)$ is the ethanol production associated with cell growth.

The dead biomass concentration into the reactor X_d is calculated as:

$$\frac{X_d}{dt} = K_d X - \frac{F_3}{V} X_d$$
(9)

where $K_d = K_{dT} \exp{(K_{dP}P)}$ (see Tab. **??**).

Through the energy balance of the system, the variation in the fermentation temperature T_{r0} during the process is described by:

$$\frac{dT_{r0}}{dt} = \frac{F_3}{V}(T_i - T_{r0}) + \frac{\dot{m}_r(t)}{\rho_1 V}(T_{rN} - T_{r0}) + \frac{\mu X}{Y_{X/S}} \frac{\Delta H_S}{\rho_1 c_{p1}} + \frac{m_X X \Delta H_S}{\rho_1 c_{p1}}$$
(10)

where ΔH_S is the heat released during the fermentation process whose value is $151 kcal$ per kilogram of substrate consumed and $T_i = 28^o C$ is the feed temperature.

In the model shown, the specific growth rate μ is expressed as a function of the limiting substrate concentration, of the inhibitory effects of the substrate, ethanol and cell concentrations, and as function of the reduction constant from pH of the reactor $\Lambda(pH)$. Thus, it has the following equation:

$$\mu = \frac{\mu_{max}}{\Lambda(pH)} \frac{S}{K_s + S} e^{-K_i S} \left(1 - \frac{P}{P_{max}}\right)^n \left(1 - \frac{X + X_d}{X_{max}}\right)^m$$
(11)

where $m = 1$ and $n = 1.5$ are constant values, μ_{max} (h^{-1}) is the maximum specific growth rate, $K_s = 4.1 kg/m^3$ is the substrate saturation constant, K_i (m^3/kg) is the substrate inhibition coefficient, P_{max} (kg/m^3) and X_{max} (kg/m^3) are, respectively, the ethanol concentration and the biomass concentration when cell growth ceases.

Although the dependency between the cellular activity and pH can not be explained by a mathematical expression, it is found in the literature an adequate adjustment for many microorganisms [Nielsen and Villadsen, 1994]. In this work, $\Lambda(pH)$ is calculated for $pH < 4.5$ and $pH > 5.3$ decrease the cells growth, according to the following function:

$$\Lambda(pH) = k_3 \cdot \left(1 + \frac{k_1}{10^{-pH}} + \frac{10^{-pH}}{k_2}\right)$$
(12)

in which $k_1 = 10^{-5.3}$, $k_2 = 10^{-4.5}$ e $k_3 = 0.4633$. The parameters used in equations showed above were described as function of temperature by Atala et al. [2001]whose expressions were determined, using the industrial yeast *Saccharomyces cerevisiae* and cane molasses as the substrate.

For the pH modelling, it is considered the carbon system $(H_2CO_3 + HNO_3)$ to represent the neutralization phenomena of feeding. Considering the illustration in Fig. 1, the model equations are:

$$\frac{dW_{a4}}{dt} = \frac{F_3}{V} \cdot (W_{a3} - W_{a4}) \qquad (13a)$$

$$\frac{dW_{b4}}{dt} = \frac{F_3}{V} \cdot (W_{b3} - W_{b4}) \qquad (13b)$$

3. CONTROL STRATEGY

The proposed control strategy is illustrated in Fig. 3. This structure, whose objective is to operate the plant to obtain the maximum of ethanol, is divided in two parts:

- Global Control System: in this top layer, the optimizer computes the optimum pH, temperature (T) and level (H) in the reactor to maximize the ethanol production. It works as master controller and defines the set-point for the slave loops.
- Local Control System: this layer is composed by three slave loops which work in cascade with the optimizer. The objective of these local controllers is to keep the fermentation process in the operating point (pH, T, H) defined by the upper layer.
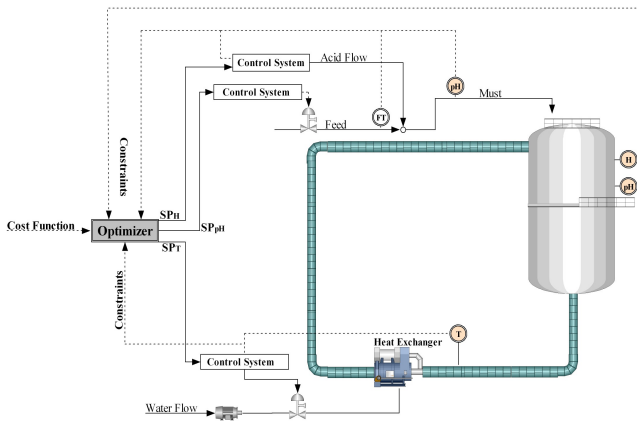

Fig. 3. Automation and control system

The complete model composed by the three sub-systems described in section 2 will be used to simulate the process behavior in section 4 and to compute the predictions in the optimal controller. As in industrial practice, simple low order models are used to tune the local controllers, and these models are obtained from the behavior of the complete model near an operation point.

3.1 Local Control System

In the proposed approach PID (*Proportional-Integrative-Derivative*) controllers are used in the pH temperature and level control loops because they are the typical structures used in industry.

The PID algorithm used here is [da Costa Fº et al., 2009]:

$$C(s) = \frac{K_c(1 + \frac{1}{T_i s} + T_d s)}{\alpha T_d s + 1}, \alpha \in [0, 1] \qquad (14)$$

where Kc is the proportional gain, T_i is the integrative time (in hours), T_d is the derivative time (in hours) and α defines the low pass filter of the derivative action (in the PI case, $T_d = \alpha = 0$). Also, a set-point filter ($F(s) = \frac{1+\beta s}{1+\gamma s}$) can be used, when necessary, to obtain smoother set-point responses. Moreover, the PID algorithm includes a anti-windup strategy.

To tune the temperature PID controller, a simple first order plus delay model is used to represent the relationship between the temperature and the cooling flow in the heat exchanger. The following values were obtained for a fast response with a small overshoot:

$$K_c = -4000, \quad T_i = 0.05, \quad T_d = 0.03, \quad \alpha = 0.1.$$

A simple PI with a reference filter was enough to control the level in the reactor, that is an integrator system ($K_c = 250$, $T_i = 1$, $\gamma = 0.5$, $\beta = 1$). This tuning is done in order to obtain responses without overshoot, as no control action can decrease the level.

Because of the high gain variability of the pH model (see the curve in Fig. 4), the PI controller for this loop was implemented with a scaled gain:

$$K_c = \frac{1}{|K_2(u_2)|} \qquad T_i = 0.003$$

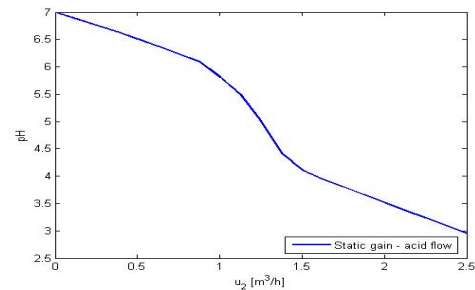The proposed PI allows to obtain a closed-loop system

Fig. 4. Static curve pH - acid flow

with smooth response and rise time similar to the open loop one.

As pointed out the set-points for the Local Control System are given by the optimization process described in the following.

3.2 Global Control System

The Global Control System is based on a NMPC (Nonlinear Model Predictive Control) technique, which is implemented to determine the control signal that minimizes a given cost function at each sampling time, using a prediction horizon and a nonlinear model of the process. The sampling period, that is called here the processing time ΔQ, is defined by the operator.

The NMPC is designed to maximize the ethanol concentration by solving, at each ΔQ, the following problem in the decision variables SP_H, SP_L and SP_{pH} [Logsdon and Biegler, 1989]:

$$min \; J(SP_H, SP_H, SP_{pH}) = - \int_t^{t+N} P(t)dt$$

Subject to:

$$\dot{P}(t) = Y_{P/X}\mu X(t) + m_P X(t) - \frac{F_3}{V}P(t)$$
$$H(t) \leq SP_H(t) \leq 14.4$$
$$20 \leq SP_T(t) \leq 40 \qquad (15)$$
$$4 \leq SP_{pH}(t) \leq 6$$

where t is the current time, N is the prediction horizon (in hours), P is the ethanol concentration obtained using the

non-linear model presented in previous sections [1] , SP_H is the level set-point, SP_T is the temperature set-point and SP_{pH} is the pH set-point.

The constraints in the decision variables are defined using the following ideas: (i) the minimum level should be, at each step, the current level, because in this batch system there is no way to decrease it; (ii) the maximum level is defined by the reactor capacity; (iii) for T and pH, the limits are given by the secure operation ranges normally defined in industrial practice.

The tuning parameters of this control strategy are N and ΔQ ($\Delta Q \leq N$). As the process has a fixed end time (in this application 8 hours) the maximum value of N is 8 hours. Due to the fermentation process has a slow dynamics it is expected to obtain better results using bigger values of N. The effect of ΔQ can be analyzed as follows. A small value of ΔQ imposes constraints to the practical implementation of the control system because of the time needed for the optimization procedure and also because of the dynamics of the local loops. On the other hand, big values of ΔQ gives less degree of freedom to the optimization and a poor performance is expected. Next section presents some simulations to illustrate these points and to evaluate the tuning and performance of the proposed control system.

4. SIMULATION AND RESULTS

The process model was developed in Matlab® Mathworks and the function *fmincon* is used for the NMPC optimizer. To illustrate the advantages of the proposed control system, some comparative results will be presented. In these simulations the proposed controller is compared to the one currently used in conventional ethanol plants, where the feeding, pH and temperature evolution are pre-defined by the process operator.

Some criteria were considered in the simulations following real data from the industrial process: the maximum time of fermentation process is set to $8h$ and the maximum level in the reactor is $14.4m$ ($900m^3$). The initial conditions were: $V_0 = 300m^3$ ($H_0 = 4.8m$), $X_0 = 31kg/m^3$, $S_0 = 0kg/m^3$, $P_0 = 33kg/m^3$, $X_{d0} = 0kg/m^3$, $T_{r0_0} = 30^oC$ e $pH_r = 5.01$. The ethanol concentration obtained without the optimizer is approximately $73.8066g/L$, considering a volume of $900m^3$. That is, the fermentation production is calculated using $G_P = (V_F(L) - V_0(L)) \cdot C_e(g/L)$. In this case, $G_P = 44283960g \approx 44284kg$ of ethanol per vat.

To analyze the controller tuning several tests were made with different values of N and ΔQ. In the Table 1 is showed some of the obtained results, that confirms the previous analysis. Note that, as expected, the effect of N is much important that the effect of ΔQ.

One of these cases ($N = 7$ and $\Delta Q = 2$) was selected to present detailed simulation results (see Figs. 5, 6 and 7). The obtained final concentration of ethanol is $C_e = 78.8547g/L$ and the production in the vat is $G_P \approx 47313kg$, which should generate an increase in the production of 6.84% of ethanol per reactor if compared with the process without the NMPC controller. It is rel-

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[1] This equation considers, implicitly, the relationship between P and the level, temperature and pH.

N	ΔQ	$C_e(g/L)$	N	ΔQ	$C_e(g/L)$
1	0.5	75.3532	4	2	78.4193
1	1	74.4925	4	4	77.7028
2	0.5	76.9376	7	1	78.8394
2	1	76.7099	7	2	78.8547
2	2	76.2838	7	4	78.8528
4	1	78.4707	7	7	78.7567

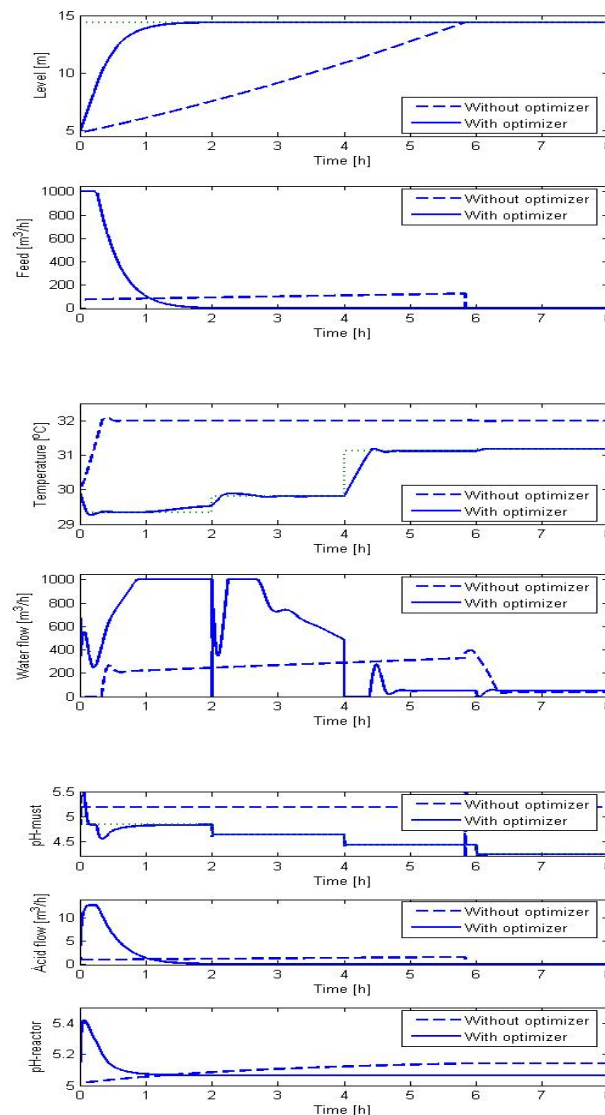Table 1. Ethanol concentrations for some values of N and ΔQ

Fig. 5. Controlled variables of the system

evant to remember that these values are on an industrial scale, in which an apparently small gain produces significant results. For comparison purposes, suffice it to say that in a plant that has six vats, this corresponds to an increase in the production of $11450t$ ethanol per crop.

5. CONCLUSIONS

This paper presented the development of a complete model and a optimization based controller of ethanol fermentation process. The proposed strategy is based on a cascade control structure. Three slave SISO controllers deal with
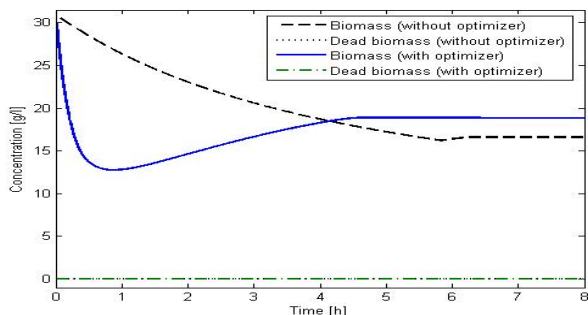
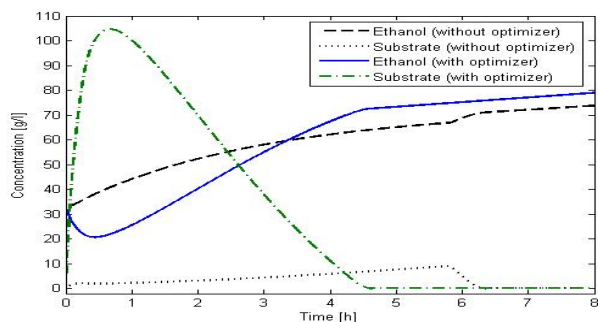Fig. 6. Performances of the system with and without optimizer

Fig. 7. Performances of the system with and without optimizer

the principal process variables and disturbances and receive the optimal set-points from a MIMO master predictive controller which maximizes the ethanol production.

Since the model was developed in industrial scale, the results obtained in the simulations can satisfactorily represent a real operation unit. From the comparative results presented in the simulations it is concluded that the proposed strategy can be used in practice to improve the performance of current plant operation strategies. As the low level layer uses simple PID controllers normally installed in industry, the implementation of the proposed strategy can be easily tested in practice executing the NMPC in a industrial PC connected with the PIDs.

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