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Modeling And Control of a Continuous Ethanol Fermentation Using a Mixture of Enzymatic Hydrolysate and Molasses from Sugarcane

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In this work, a kinetic model considering the effect of temperature was employed to assess the dynamic behavior of an ethanol fermentation process. To calibrate the model, experimental data were obtained from batch cultures using cellulosic hydrolysate from sugarcane bagasse blended with sugarcane molasses at 75% and 25% in volume, respectively, as carbon sources. The kinetic model with its parameters is applied in the simulation of a continuous fermentation process for ethanol production. The system is a typical large-scale industrial process consisting of four fermenters attached in series and operated with cell recycling. Based on dynamic simulation of the process, a suitable Infinite-Horizon Model Predictive Control (IH-MPC) was applied to deal with the fluctuation of the sugar concentration in the raw material. The control objective is to maintain the outlet sugar concentration of the fourth reactor at a desired value, by manipulating the feed flow rate. This strategy was tested for both disturbance rejection (regulatory problem) and changes in the output reference (servo problem).

1. Introduction

In the current context of biofuels production, it is evident the need to improve the process efficiency towards higher productivity and lower production costs. The control strategy also plays an important role, especially due to the changes in the raw material quality. This is even enhanced when a mixture of cellulosic hydrolysate from sugarcane bagasse and sugarcane molasses are used as raw materials in an integrated first and second-generation (1G+2G) ethanol production process.

An advantage of this integrated process is that the bagasse is already available at plant site. The 2G ethanol production may share part of the facilities where 1G ethanol production takes place (e.g. concentration, fermentation, distillation, among others) (Dias et al., 2012). However, the industrial implementation of the 1G+2G ethanol production will demand a control strategy robust enough to handle fluctuations in the composition of the medium feed to the reactor.

Recently, a few authors have studied the dynamic behavior of ethanol fermentation through modeling and simulation. Hydrolysates from sugarcane bagasse (Andrade et al., 2012, Kumar et al., 2015), woody biomass (Wang and Liu, 2014) and soybean meal (Luján-Rhenals et al., 2015) were used as raw materials. Nevertheless, suitable control strategies able to deal with disturbances related to these processes have not yet been reported.

In this context, the aim of the present work was to employ mathematical modeling to analyze the dynamic behavior of a 1G+2G ethanol fermentation process. This allowed defining the best control strategy to deal with the fluctuations of the sugar concentration in the raw material. The control was designed to maintain the outlet sugar concentration at a desired value. The performance of an advanced controller, the Infinite-Horizon Model Predictive Control (IH-MPC) (Odloak, 2004) was assessed.

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2. Process modeling

The process modeling starts with the construction of a temperature-dependent kinetic model using batch fermentation cultures. Then, the kinetic model that provided the best fit to the experimental measures was used to simulate a continuous fermentation process for ethanol production.

2.1 Batch culture

Fermentation media and microorganism

Four ethanol fermentations were performed in batch mode using a bioreactor Bioflo 115 of 1.5 L (New Brunswick, USA) at different temperatures (30, 32, 34 and 36 ºC) to calibrate the kinetic model. The microorganism used was *Saccharomyces cerevisiae* an un-named strain cultivated in the Development Bioprocess Laboratory at CTBE and originally obtained from the Faculty of Food Engineering/ State University of Campinas, originally sampled from an industrial ethanol distillery. The substrate was composed with sugarcane molasses and cellulosic hydrolysate from sugarcane bagasse. The production of cellulosic hydrolysate consisted of acid pretreatment with 1.0 % (w/v), 20 % wt of solids and 90 min (Tovar et al., 2015). The solid fraction, cellulignin, was saccharified with 8% WIS using Cellic® CTec2 (Novozymes Latin America Ltda, Brazil) and β-glucosidase from *Aspergillus niger* (Sigma-Aldrich Corporation, USA). The enzymes complex load was 15 FPU / g substrate and 33 IU/g substrate. The final concentration of substrate in term of total sugars as inverted (TSAI) was 180 g/L.

Analytical methods

The cell concentration in dry basis was determined in triplicate by gravimetry. Samplesing of 1 mL were centrifuged, washed two times with Mili-Q water and dried at 80 °C until constant weight in the analytical balance. The determination of sugars (sucrose, glucose and fructose) was carried out by high-performance liquid chromatography (HPLC) using Agilent Infinity 1260 with IR detector at 50 °C, Aminex column HPX-87P 300 mm x 7.8 mm at 60 °C and 0.5 mL/min of ultrapure Milli-Q water as eluent phase. Ethanol, acetic acid and glycerol were determined through Dionex Ultimate 3000 with IR detector Shodex RI-101, Aminex column HPX-87H 300 mm x 7.8 mm at 50 °C and 0.5 mL/min of 5 mM sulfur acid as eluent phase.

2.2 Kinetic modeling

The kinetic model comprises the reaction rates for cell growth, r_x, substrate consumption, r_s, and ethanol production, r_p shown in Eqs. (1-3). Furthermore, the model considers the inhibition of cell growth by a high concentration of ethanol and substrate as well as by high concentration of cell.

$$r_x = \mu_{max} \frac{S}{K_s + S + \frac{S^2}{K_I}} \left(1 - \frac{P}{P_{max}}\right)^r \left(1 - \frac{X}{X_{max}}\right) X \tag{1}$$

$$r_s = \frac{r_x}{y_{x/s}} \tag{2}$$

$$r_p = \frac{r_x}{y_{x/p}} \tag{3}$$

In this study, six of the kinetic parameters, namely μ_{max}, K_s, K_I, r, P_{max} and X_{max} are modeled as function of temperature by using Eq. (4) while $Y_{x/s}$ and $Y_{x/p}$ are modeled using Eq. (5). A search procedure based on Genetic Algorithm PIKAIA (Charbonneau, 1995) is used to estimate the parameters. The least-squares criterion was used as the cost criterion to be minimized.

$$\beta(T) = Ae^{(BT)}e^{(C/T)} \tag{4}$$

$$\delta(T) = De^{(ET^3)}e^{(Fe^{(T)})} \tag{5}$$

where T is temperature and A, B, C, D, E and F are constants to be adjusted for each temperature-dependent parameter.

Table 2 shows the fitted values of the constants in Eqs. (4) and (5).

The computed profiles of the cell, substrate and ethanol at 30, 32, 34 and 36 ^oC are shown by the solid curves in Fig. 1. The experimental measures (solid symbols) used for the estimation are also shown in this figure for comparison. For all cases, R^2 ranged from 0.92 to 0.99. The Residual Standard Deviation (RSD) written as a percentage of the average of the experimental values (Rivera et al., 2007) was used as a more robust criterion to assess the goodness of fit. For all cases, RSD% ranged from 4.12 to 24.7 indicating an adequate adjustment of the model to the experimental measures.

Table 2: Optimal values of the constants in Eqs. (4) and (5)

Parameter	A	B	C	D	E	F
μ_{max}	1.2819×10^{5}	-0.184967	-210.739752	-	-	-
K_s	1.0775×10^{25}	-0.804135	-934.340651	-	-	-
K_I	5.1410×10^{14}	-0.438893	-493.199829	-	-	-
r	75.04020	-0.064570	-75.519428	-	-	-
P_{max}	9.6879×10^{4}	-0.108010	-118.501614	-	-	-
X_{max}	2.8560×10^{4}	-0.125768	-61.096556	-	-	-
$Y_{x/s}$	-	-	-	0.11039	-2.781227×10^{-5}	8.966370×10^{-17}
$Y_{x/p}$	-	-	-	0.27453	-2.971048×10^{-5}	1.061205×10^{-17}

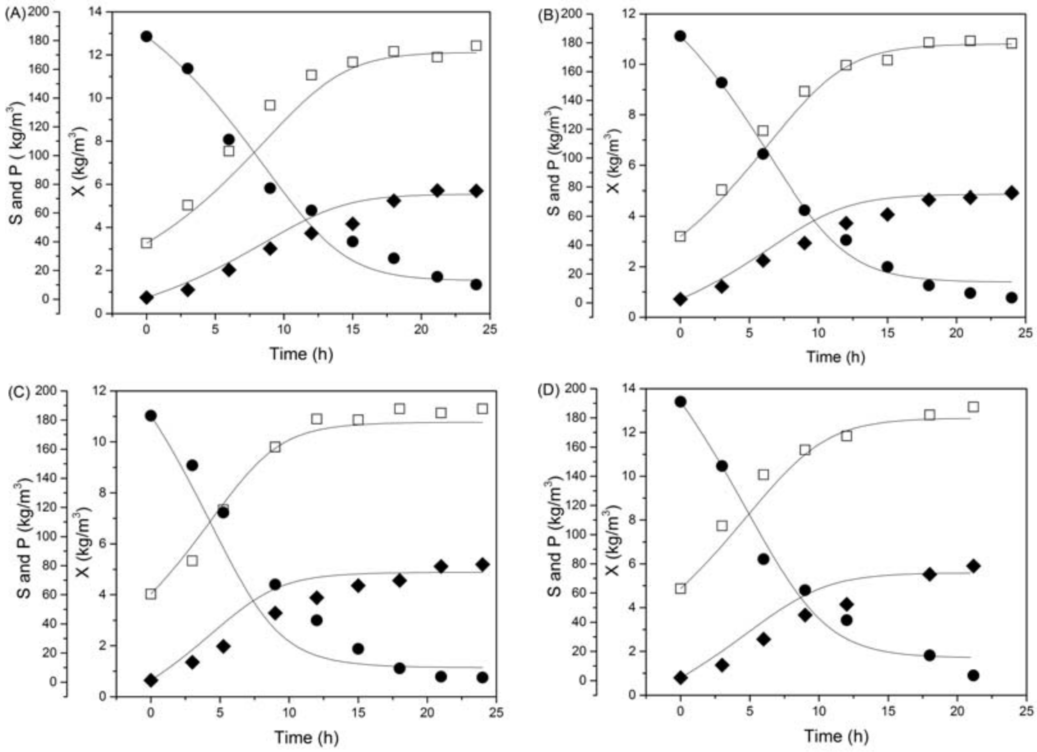

Figure 1: Experimental measures (substrate (●), cell (□) and ethanol (♦)) compared with the performance of the model (—) at: (A) 30 °C; (B) 32 °C; (C) 34 °C and (D) 36 °C.

2.3 Scale-up possibility for a continuous industrial process for ethanol production

After the kinetic model has been fitted, it is used to simulate a continuous operation to assess the dynamic behavior of the ethanol fermentation process and to develop a suitable control strategy. The general scheme of the continuous fermentation process based on that proposed by Andrietta and Maugeri (1994) is illustrated in Fig. 2. The system is a typical large-scale industrial process composed of four fermenters arranged in series and operated with cell recycling.

In this simulation study, a mixture of cellulosic hydrolysate from sugarcane bagasse and sugarcane molasses is converted into ethanol by a fermentation process carried out using the yeast *Saccharomyces cerevisae*. A set of centrifuges splits the outlet fermented medium into two phases. The light phase is sent to a distillation unit in which the ethanol is obtained. The heavy phase is submitted to an acid treatment and diluted with water before being recycled to the first fermenter. The reader is referred to Andrietta and Maugeri (1994) and Meleiro and Maciel (2000) for details on the mass and energy balance equations.

During the dynamic simulation, the concentration of cell, substrate and ethanol in the fourth fermenter reached values of 31.95 kg/ m^3, 0.46 kg/ m^3 and 63.42 kg/ m^3, respectively obtaining yield of 84%, with a productivity of 7.7 kg/ m^3h. For the simulation, optimized operating conditions were considered: feed flow rate = 100 m^3/h, inlet substrate concentration = 180 kg/ m^3, fermenter temperature = 33.5 °C, recycle rate = 0.3, and volume of the fermenters, V_1 = 210.374 m^3, V_2 = 268.037 m^3, V_3 = 316.663 m^3, V_4 = 208.208 m^3. The magnitude of these values shows that the process is designed to produce ethanol on typical industrial distilleries in Brazil (Andrietta and Maugeri, 1994).

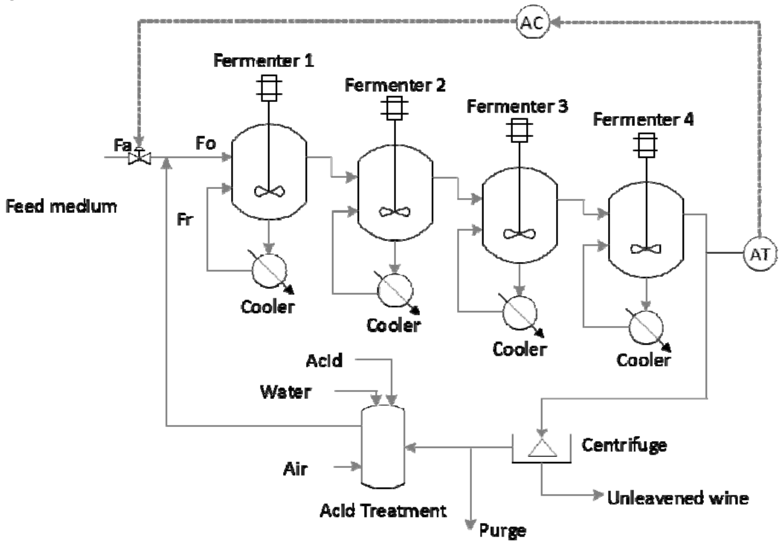

Figure 2: General scheme of the continuous fermentation process

3. Process Control

One of the purposes of this work is to assess, through simulation, a control strategy. The proposed strategy consists in a Single Input - Single Output control system (SISO) where the sugar concentration in fourth fermenter, S_4, must be maintained at a desired value by manipulating the feed flow rate, Fa. At this point, the following control notation must be introduced: y: controlled variable (S_4), u: manipulated variable (Fa). The control configuration is shown in Fig. 2. An important consideration is that the levels and the temperatures in all four fermenters are perfectly controlled.

The challenge of controlling a continuous industrial process for ethanol production is addressed by the use of a control algorithm called Infinite-Horizon Model Predictive Control (IH-MPC). Model Predictive Control refers to a class of control algorithm that utilize an explicit process model to predict the future response of a plant (Camacho and Bordons, 2004). MPC attempts to optimize the process behaviour by computing a sequence of future control actions. The main advantages of IH-MPC formulation are the following: the possibility to include process constraints in the control problem; properties such as feasibility, convergence and stability are assured (mathematical proofs). In practice, all those properties are revealed in a reliable closed-loop system, with a smooth operation. Furthermore, IH-MPC is a modern, practice and flexible control algorithm with a low computational load. Recent versions of this controller allow the integration with a Real Time Optimization (RTO) routine preserving the stability of the closed-loop system (Alvarez, 2012).

The MPC formulation considered is based in the work of Odloak (2004). It presents an MPC that guarantees stability by setting the prediction horizon as infinite and including a terminal state constraint. The feasibility is assured by the incorporation of slack variables in the optimization problem of the MPC, softening the terminal state constraint.

The prediction model was obtained using the System Identification Toolbox of Matlab®. At first, a continuous transfer function model was identified around the selected operating point:

$$y(s) = \frac{5.27 \cdot 10^{-3}}{(1.475s+1)(1.483s+1)} u(s) \tag{6}$$

The linear model in Eq. (6) is presented in process units. It was obtained from data sampled at each 0.5 h. Moreover, the transfer function model was properly converted into a state-space model in discrete-time, in the incremental form as suggested in Odloak (2004). The state-space form is the suitable structure of the process model for the control algorithm implementation.

The continuous industrial process for ethanol production was simulated in Matlab®. In order to test the performance and the capability of the control system to deal with disturbances, the sugar concentration in the feed stream S_0 is introduced as a disturbance twice during the simulation. The servo problem is also considered. After the system is recovered from the disturbances, it is introduced a set-point change in S_4. For this simulation, the set-point for S_4 was defined as 0.5 kg/m^3. As mentioned above, this controller considers a single linear model for prediction. The initial conditions of the simulation are: S_0 = 180 kg/m^3, Fa = 100 m^3/h. The process variables were scaled for the controller calculations so as to avoid numerical problems. The controller parameters are the output reference weight Q = 100, the control action weight R = 1, the control horizon m = 3. The sampling time of the controller is Ts = 0.5 h. The process constraints considered are Δu_{max}=0.5, Fa_{max} = 250 m^3/h, Fa_{min} = 50 m^3/h, S_4^{SP}= 0.5.

First, at t=0 the process has to reach the steady-state, the value of S_4 is initially 1.04 kg/m^3. The controller deals with a servo problem. It brings the process output S_4 to the set-point of 0.5 kg/m^3 and it reaches the steady-state in 20h, approximately. Fig. 3 shows the manipulated variable Fa and controlled variable S_4 along the simulation. The first disturbance occurs at time t=50 h with a sudden decrease of 20 kg/m^3 in the substrate concentration of the feed S_0. Hence, the new S_0 is 160 kg/m^3. This disturbance has a large effect on the controlled variable S_4, as well as both on yield and productivity, as depicted in Figs. 3 and 4. The control system is able to bring the output S_4 to the reference value by increasing largely the feed flow rate Fa to 148 m^3/h.

After 100 hours of simulation, when the process has reached the steady-state, a second disturbance was introduced in the process. There was an abrupt increase from 160 kg/m^3 to 190 kg/m^3 in S_0. In this case, the control system acts manipulating Fa to balance the sugar increase in the feed. The new value of Fa is lower than the last steady-state, Fa = 80.2 kg/m^3. In this disturbance, the control action was effective and brings S_4 to the set-point. Another control system test was a change in the S_4 set-point, i.e., the servo problem. The set-point was increased from 0.5 kg/m^3 to 0.8 kg/m^3. Notice that the control system is able to follow this new reference. The feed flow rate is adjusted to the value 91.6 m^3/h at steady-state.

To finish the discussion, it is important to observe the behavior of the yield and the productivity along the simulation in Fig. 4. The final value of the process yield was around 0.84. The steady-state values of the yield remained almost constant during the simulation, exhibiting different values only during transient stages. This result indicates that controlling S_4, in the scenarios considered in this work, the yield is maintained controlled indirectly.

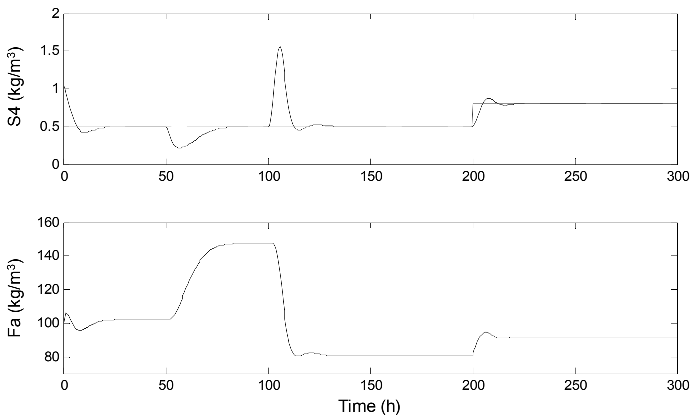

Figure 3: Input and output of the simulation for the fermentation process in closed-loop. Set-point (- - -)

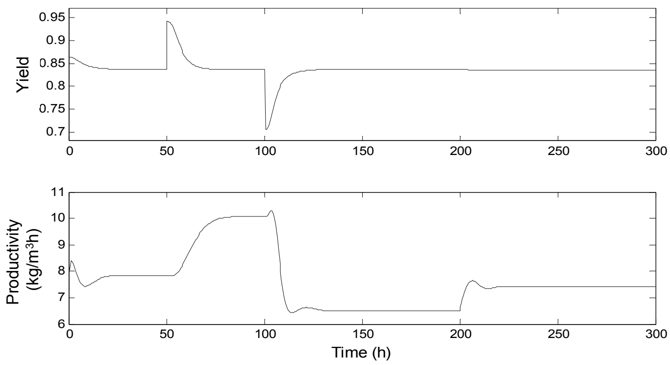

Figure 4: Yield and Productivity (kg/m^{3}h) responses of the simulation for the fermentation process in closed-loop.

On the other hand, the productivity is highly affected for the different events simulated. At the first steady-state it is equal to 7.85 kg/m^{3}h, then after the first disturbance it reaches a higher value, 10.1 kg/m^{3}h. This result is due to an increase in both S_0 and Fa. The second disturbance also affects the productivity, reduced to 6.5 kg/m^{3}h. In this case, the change in the set-point (for the servo problem) increases productivity, reaching 7.4 kg/m^{3}h. Here, the new value of Fa had a more pronounced effect on productivity than the yield.

4. Concluding Remarks

The temperature-dependent kinetic model was suitable to describe the ethanol fermentation from a mixture of cellulosic hydrolysate from sugarcane bagasse and sugarcane molasses. With the use of a continuous model that considered the developed kinetic, it was possible to assess the dynamic behavior of the fermentation process for the production of ethanol. This analysis was necessary to design a suitable control strategy able to address disturbances related to the process as well as set-point changes. Disturbances in the inlet substrate concentration can affect significantly the ethanol productivity. On the other hand, the proposed control strategy was able to maintain the yield through the regulation of sugar concentration in the fourth fermenter. The development of suitable controllers in industrial-scale ethanol fermentation that uses cellulosic hydrolysate as raw material is required. It can be a valuable tool to make the integrated first and second-generation ethanol industry commercially viable. Further works should include the viable cell dynamics in the process model. Moreover, assessment of several control strategies to optimize the process operation is recommended.

Acknowledgments

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