

VOL. 65, 2018



Multivariable Model Predictive Control of a Continuous Fermentation Unit for First-Generation Ethanol Production

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This study presents the application of an advanced multivariable control strategy to a continuous fermentation process for first-generation ethanol production. The Model Predictive Control (MPC) was applied, a suitable strategy to control and optimize process systems subject to constraints. A continuous industrial fermentation process with four reactors arranged in series is considered. Based on a dynamic simulation of the process, the MPC is tested to deal with several disturbances, such as the fluctuations of the substrate concentration in the raw materials and fermentation temperature. The control objective is to maintain the substrate concentration in the last reactor and the temperature in the reactors at its desired values, by manipulating the feed flow rate and the cooling water flow rate of the external heat exchangers.

1. Introduction

A major challenge in sustainable supply of ethanol fuel is improving the existing process towards higher productivity and economic sustainability. Whit this in mind, the ethanol industry should aim to maximize profit and reduce their costs in order to gain a share of the global market. Although this endeavour seems to be a straightforward task, economic improvements must deal with the complexity of the operation of industrial ethanol plants. This can lead to several problems, such as out-of-specification products, lack of safety, higher cost, and byproducts, among others. Many of them can be handled with the implementation of a suitable control strategy to guarantee that the process variables will be kept into the desirable values (set-point) (Herrera et al., 2016). In that case, the control system must be able to deal with process complexity, nonlinearities, multiple variables, reverse responses, disturbances and precision. The optimal operation of the first-generation ethanol production process from sugarcane, especially the fermentation stage, is a challenging task. Temperature oscillations, cell stress, bacterial contamination as well as the variability of feedstock quality (molasses and sugarcane juice) are some of the major issues that difficult its control (Rivera et al., 2017). In the past, some authors have studied the dynamic behaviour and control of industrial ethanol processes through modeling and simulation (Andrietta and Maugeri, 1994, and Meleiro and Maciel, 2000). However, in the current context where the process of ethanol has been promoted as a mean to improve energy security and reduce climate change impacts, suitable control strategies able to deal with disturbances related to its production have been little reported in literature. In this context, the objective of this study was to use mathematical modeling to evaluate the dynamic behavior of a continuous fermentation unit for first-generation ethanol production. This allowed to choose a control strategy to deal with the fluctuations of both the sugar concentration in the raw material and the cooling water flow rate in each external heat exchanger. A multivariable MPC was designed to maintain the outlet sugar concentration and the operating temperature of each reactor at desired values. The proposed strategy consists in a Multiple Input - Multiple Output control system (MIMO), which has been little addressed in industrial bioprocess studies. In addition, the performance of the MPC was tested for changes in the output reference (servo problem).

2. Process Description

Figure 1 shows a schematic diagram of the continuous fermentation process for first-generation ethanol production based on studies by Andrietta and Maugeri (1994). The mathematical modeling comprising mass and energy balances was developed by Andrietta and Maugeri (1994) using data from Brazilian large-scale

Please cite this article as: Violaro F.A., Rivera E., Alvarez L.A., 2018, Multivariable model predictive control of a continuous fermentation unit for first-generation ethanol production, Chemical Engineering Transactions, 65, 67-72 DOI: 10.3303/CET1865012

industrial plants. In this study, the model is used to simulate a continuous operation to assess the dynamic behaviour of the ethanol fermentation process and to develop a robust and efficient control strategy. At this point, it is worth mentioning that the fermentation stage, despite its extensive study, still has a greater potential to increase the global efficiency of the ethanol production process (Olivéiro et al., 2010). One method to improve the current ethanol fermentation efficiency and profitability is through process intensification. Very-high-gravity (VHG) technology could be one type of improvement process aimed at obtaining high ethanol concentrations (Rivera et al., 2017).

During the simulation, sugarcane juice is converted into ethanol by fermentation in a system that contains four continuous stirred-tank reactors (CSTR) connected in series and operated with cell recycling. Each reactor has its own external heat exchanger to control its temperature (temperature affect the yeasts metabolism and reduces the ethanol concentration in the final broth). A set of centrifuges splits the outlet fermented medium from fourth reactor 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 reactor where is mixed with fresh substrate. Energy and mass balance equations are detailed in Meleiro and Maciel (2000).



Figure 1: Schematic diagram of the continuous fermentation unit for first-generation ethanol production

3. Control System

Several control strategies can be used, among them; the classical feedback control is usually the first choice. However, currently control technology allows the implementation of complex control configurations and advanced control algorithms such as MPC. One of the purposes of this study is to assess the performance of a MPC strategy in a process designed to produce ethanol on actual industrial plants. The proposed strategy consists in a MIMO system where the substrate concentration in fourth reactor, S₄, and the temperature of the reactors (T₁, T₂, T₃ and T₄) must be maintained at a desired value by manipulating the feed flow rate, Fa and the cooling water flow rate in the heat exchangers (F_{i1} , F_{i2} , F_{i3} and F_{i4}), respectively.

Model Predictive Control

MPC refers to a class of control algorithms that use: (i) an explicit model of the process to predict the future response of a process along a prediction horizon and (ii) the minimization of an objective function to obtain the sequence of variation on the manipulated variable (in a control horizon) and to use the first calculation of the sequence at each time step. This control method has proven to be able to handle a wide process range, shows good performance and it is able to operate long periods without any intervention. MPC has numerous advantages when compared to other controllers, such as: easy handling for operators, intuitive and relatively easy tuning, deal with multivariable systems, easy control law to be implemented, handle with process constraints and offers a natural way to deal with feedforward control. Furthermore, convergence and stability can be theoretically assured by rigorous mathematical proofs. The improvements of this controller allow integration with a Real Time Optimization (RTO) routine preserving the stability of the closed-loop system (Alvarez, 2012).

Eq. (1) shows the general form of the transfer function model used in this study.

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$$G_{ij}(s) = \frac{K_{ij}}{\tau_{ij}s + 1} \tag{1}$$

where K_{ij} is the process gain and τ_{ij} is the time constant.

The transfer function models for the continuous fermentation process are shown in Table 1. These linear prediction models were obtained using the widely known open-loop curve reaction method and were identified around the nominal operating point with a sampling time of 0.5 h. This sampling time was applied considering the measurement time of total reducing sugars with HPLC used in an actual industrial plant. The linear models are presented in units of the process.

Output\Input	Fa (m³/h)	F _{j1} (m³/h)	F _{j2} (m³/h)	F _{j3} (m³/h)	F _{j4} (m³/h)
S₄ (kg/m³)	$\frac{0.161781}{4.360s+1}$	$\frac{-0.00225}{5.445s+1}$	$\frac{-0.00329}{4.545s+1}$	$\frac{-0.00386}{3.315s+1}$	$\frac{-0.00151}{1.315s+1}$
T ₁ (°C)	$\frac{0.015701}{2.645s + 1}$	$\frac{-0.00297}{0.715s + 1}$	$\frac{-0.00016}{5.870s + 1}$	$\frac{-0.00024}{4.320s+1}$	$\frac{-0.00019}{1.810s + 1}$
T ₂ (°C)	$\frac{0.028995}{2.540s + 1}$	$\frac{-0.00141}{2.110s + 1}$	$\frac{-0.00266}{0.905s+1}$	$\frac{-0.00012}{5.260s + 1}$	$\frac{-0.00009}{3.100s + 1}$
T₃ (°C)	$\frac{0.040870}{3.840s + 1}$	$\frac{-0.00114}{4.445s+1}$	$\frac{-0.00187}{3.220s + 1}$	$\frac{-0.00333}{1.335s+1}$	$\frac{-0.00007}{5.470s + 1}$
T4 (°C)	$\frac{0.067309}{4.885s + 1}$	$\frac{-0.00156}{6.170s + 1}$	$\frac{-0.00241}{5.090s + 1}$	$\frac{-0.00364}{3.370s + 1}$	$\frac{-0.00308}{0.625s+1}$

Table 1: Transfer function models of the system

The transfer function models were properly converted into a state-space model in discrete-time, in the incremental form as briefly described in Eqs. (2) and (3). The reader is referred to Maciejowski (2002) for details on the state-space model formulation.

$$x(k+1) = Ax(k) + B\Delta u(k)$$
 (2)
 $y(k+1) = Cx(k)$ (3)

which is assumed to be minimal. At each time step k, the MPC solves the following optimization problem:

$$\min_{\Delta uk} J_k = \sum_{j=0}^p (y(k+j/k) - y^{sp})^T Q(y(k+j/k) - y^{sp}) + \sum_{j=0}^{m-1} \Delta u(k+j/k)^T R \Delta u(k+j/k)$$
(4)

Subject to:

$$u_{min} \le u(k+j/k) \le u_{max}, \quad j = 1, 2..., m-1$$
 (5)

$$-\Delta u_{max} \le \Delta u(k+j/k) \le \Delta u_{max}, \qquad j = 1,2...,m-1$$
(6)

where u, x and y are the control, state and output vectors, respectively. A, B and C are the state, control and output matrices, respectively. y^{sp} represents the reference trajectory of the system, Q is the output reference weight and R is the control action weight.

4. Simulation Results

Simulation codes were implemented in Matlab to test the performance and capability of the MPC to deal with disturbances on: substrate concentration in the feed stream, S_0 (to simulate changes in the raw material quality), recycle rate RR, temperature in the feed stream, T_0 (to simulate warmer days) and cell concentration of the recycle stream, Xo (to simulate cell death). In addition, a set-point change (servo problem) in substrate concentration in the fourth reactor, S_4 was also considered. The initial conditions of the simulation are: Fa = 104.48 m³/h, F_{j1} = 616.20 °C, F_{j2} = 392.66 °C, F_{j3} = 208.44 °C and F_{j4} = 87.23 °C. The control parameters are Q = [10 40 30 85 30] and R = [20 0.1 0.05 0.08 0.01] for S_4, T_1 , T_2 , T_3 and T_4 , respectively. The control horizon is m = 25 and the sampling time of the controller is Ts = 0.5 h. Table 2 shows the values of concentration of substrate (S), concentration of ethanol (P), concentration of cells (X), temperature in the reactor (T),

temperature of the reagent fluid at the exit of the heat exchanger T_c and temperature of the cooling fluid at the exit of the heat exchanger (T_i) at t = 0.

The process constraints considered are: 50 < Fa < 150 with a maximum variation of 15 at each step, $200 < F_{j1} < 1000$, $150 < F_{j2} < 700$, $50 < F_{j3} < 350$ and $20 < F_{j4} < 350$ with a maximum variation of 50, 50, 30 and 30 at each time step, respectively.

Reactor	S (kg/m ³)	P (kg/m ³)	X (kg/m ³)	T (°C)	T _c (°C)	T _j (°C)
S ₁	54.43	41.74	29.37	33.88	31.42	30.33
S ₂	21.76	56.28	30.44	33.68	31.39	30.18
S ₃	5.310	63.60	30.99	33.63	31.42	30.10
S ₄	0.979	65.53	31.13	33.64	31.95	29.60

Table 2: Steady-state of the system

Figure 2 shows the manipulated and controlled variables during the simulation. The first disturbance is applied to the process from the steady-state. This disturbance is a sudden increase of S_0 (180 to 190 kg/m³), which has a large effect on the controlled variables. The substrate concentration S_4 suddenly increased to a value of 1.42 kg/m³, while temperatures T_1 , T_2 , T_3 and T_4 decreased to 33.4, 33.37, 33.41 and 33.49 °C, respectively. The control system is able to bring the outputs S_4 , T_1 , T_2 , T_3 and T_4 to the reference values by decreasing largely Fa, F_{j1} , F_{j2} , F_{j3} and F_{j4} to values of 72.8, 369.87, 392.66, 83.0, 25.67 m³/h, respectively.



Figure 2: Controlled (S₄, T_1 , T_2 , T_3 and T_4) and manipulated variables (Fa, F_{j1} , F_{j2} , F_{j3} , F_{j4}) of the simulation for the fermentation process in closed-loop. Set-point (dashed line)

The second disturbance is an increase of the recycle rate RR (0.3 to 0.32). It was applied after the system reached a new steady state. In this case, S₄ decreased to 0.842 kg/m³, while the temperatures in the reactors show a slight increase, $T_1 = 33.53$ °C, $T_2 = 33.53$ °C, $T_3 = 33.51$ °C and $T_4 = 33.53$ °C. The control system manipulated Fa, F_{j1}, F_{j2}, F_{j3} and F_{j4} to values of 82.827; 460.63, 238.79, 115.35 and 38.17 m³/h, respectively, in order to balance RR in the system and adjust the fermentation temperatures.

Then, a new disturbance was applied; the feed stream temperature T_0 was increased from 28 to 30 °C. From this disturbance, S_4 achieved 0.8964 kg/m³ while temperatures achieved values of T_1 = 33.87 °C, T_2 = 33.57°C, T_3 = 33.52°C and T_4 = 33.52°C. In this case, the control system increased largely the value of F_{j1} to 863.93 m³/h. This control action was enough to maintain a suitable fermentation temperature in the first

reactor, avoiding changes in the temperature of the subsequent reactors. On the other hand, there were no significant changes in Fa, F_{i2} , F_{i3} and F_{i4} .

The fourth disturbance is a decrease of Xo by 5 kg/m³. Under this change, S₄ was increased to a value of 1.07 kg/m³ while T₁, T₂, T₃ and T₄ decreased to values of 33.44, 33.48, 33.49 and 33.48 °C, respectively. In this case, the control action was also effective and brings the outputs to the set-point. The manipulated variables stabilized the system at the following values: Fa = 76.19, F_{j1} = 668.14, F_{j2} = 214.91, F_{j3} = 105.16 and F_{j4} = 49.15 m³/h.

Another control system test is a change in the S₄ set-point (servo problem). The set-point was decreased from 0.9795 to 0.7675 kg/m³. As observed in Fig. 2, the control system is able to follow the new reference. The Fa, F_{j1} , F_{j2} , F_{j3} and F_{j4} are adjusted to the values of 74.06, 610.49, 192.49, 89.26 and 22.88 m³/h, respectively.



Figure 3: Yield and Productivity (kg/m³ h) responses of the simulation for the fermentation process in closed-loop (continuous line) and open-loop (dashed line)



Figure 4: Effects of changes in S₄ (servo control) on yield and productivity (kg/ m^3 h)

Additionally, the ethanol productivity and fermentation yield were evaluated in the closed-loop process simulation and compared to an open-loop scenario. Figure 3 shows the behavior of ethanol productivity and fermentation yield during the simulation of the process. The results show that when S_4 , T_1 , T_2 , T_3 and T_4 are controlled simultaneously, fermentation yield is kept near to it nominal value. On the other hand, the ethanol productivity is adversely affected with respect to its initial value (t = 0) for the different disturbances simulated.

In order to observe the effect of the operating point on yield and productivity, another servo control test was performed. Two steps changes of 0.1 kg/m^3 were applied to the set-point of the substrate concentration in the fourth reactor, S₄. From Fig. 4, it can be seen that for an increase in the S₄ set-point, the yield suffered a slight drop (-0.07% and -0.14%), while the productivity increased. In the case of a decrease of the S₄ set-point, the yield increased 0.07% and 0.14%, and productivity decreased -1.85% and -3.89%. The servo problem has shown that changes in S₄ has opposite effects on productivity and yield, which means that the values that increase productivity decrease yield and vice-versa. Further studies could be made to explore the process values and control strategies that allow the process to reach an optimal operation in terms of yield and productivity. From Fig. 4 it can also be seen that the controller was able to keep the controlled variable in the set-point values. In addition, it can be observed that changes in S₄ have more influence in productivity than on yield for the closed-loop system. Studies on the ethanol fermentation process behavior and its use in the development of a suitable control strategy such as MPC could allow the development of optimal structures and efficient systems for biomass conversion.

5. Conclusion

The control system was able to regulate the operating conditions to accommodate the disturbances with the lowest changes in the fermentation process outputs. The results indicate that Fa, F_{j1} , F_{j2} , F_{j3} and F_{j4} were successfully chosen as manipulated variables capable to regulate the substrate concentration in fourth reactor, S₄, and the temperatures of the reactors (T₁, T₂, T₃ and T₄) at desired values and to avoid large variations in yield and productivity. The implementation of highly dimensional MIMO control systems has been little addressed in industrial bioprocess studies. This strategy is suitable to deal with the interaction and multivariable nature of the process. An analysis of the effect of the disturbances on yield and productivity when the operating point is fixed indicates that a simple control strategy is not adequate to optimize the process operating variables. In this direction, a major challenge is the enhancement of the control structure with the implementation of a Real Time Optimization (RTO) routine. This routine would determine the operating values of outputs and inputs that produce the maximum economic profit or the lowest operating costs in the fermentation process. Moreover, further studies are required to implement more complex control configurations with several controllers to regulate the substrate concentration and the temperature for each reactor with different sample times.

Acknowledgements

The authors acknowledge the support provided by FAPESP (grant numbers 16/22075-0 and 15/20630-4).

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