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Comparison of two Model Predictive Control for the ethanol production optimization of a two-stage bioreactor with cellular recycling

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Abstract: This paper addresses the problem of dynamic optimization of ethanol production. This process is described by a nonlinear model. A Model Predictive Control (MPC) has been implemented in order to optimize the bioprocess dynamically. Two algorithms were used together with a MPC: the Pattern Search (PS) and the Iterative Ant Colony Algorithm (IACA). They were compared with an open-loop control experimentally implemented. The MPC with the PS algorithm showed a better performance than the MPC with IACA and than the open-loop control.

Keywords: Model Predictive Control, Optimization, Pattern Search, Ant algorithm, Ethanol production.

1. INTRODUCTION

This new century presents crucial environmental challenges such as water supply, global warming and new energy sources for substitution of fossil fuels. These two last are closely dependent. Actually, the carbon dioxide CO_2 emissions with greenhouse effects are mainly connected with the use of fossil fuels for transport. Currently, ethanol is the main biofuel used in Europe. Its use reduces CO_2 emissions from 50 to 80 % compared to fossil fuels (Perréon-Delamette 2004). Ethanol production is now based on old technology with performance that requires innovative culture strategies to optimize productivity, ethanol concentration and conversion yield.

In order to overcome this challenge, an original bioprocess has been studied by several authors (Aldiguier 2006; Ben Chaabane 2006; Ben Chaabane *et al.* 2006). A two-stage continuous bioreactor with a cell recycling loop allowed a productivity of 41 g/(L.h) to be reached with an ethanol titer of 8.3°GL in the second bioreactor (Ben Chaabane *et al.* 2006). Cell viability was low, at around 42 % in the steady-state. Increasing cell viability would increase ethanol productivity up to 98 g/(L.h). The key parameter for improving ethanol production would thus be a better management of cell viability.

In this work, it is proposed a Model Predictive Control (MPC) framework. A "good" model and an optimization algorithm are necessary in order to apply a MPC. Usually, MPC problems are solved with Sequential Quadratic Programming (SQP) algorithms (Morari and Lee 1999). Unfortunately, these algorithms cannot guarantee a global convergence (Chen *et al.* 1996). Two algorithms, that can guarantee a global convergence, are compared: a pattern search algorithm and an Iterative Ant Continuous Algorithm in order to find the optimal trajectory for the MPC. The model used for the process is presented in a companion paper (Aceves-Lara *et al.* 2010).

2. THE TWO STAGE-BIOREACTOR PROCESS

The two-stage bioreactor configuration developed in the LISBP Laboratory (see figure 1) was deduced from the microbial physiology of *Saccharomyces cerevisiae* and differs from those described in the literature (Groot *et al.* 1992; Nishiwaki and Dunn 1999). Following several authors (Aldiguier 2006; Ben Chaabane 2006; Ben Chaabane *et al.* 2006), the selected configuration consists of:

- A bioreactor (R_1) dedicated to cell growth without oxygen limitation. The operating conditions with a low ethanol concentration (< 84 g/L), enabling assimilation of vitamins such as biotin (Winter 1988) give yeasts under oxido-reductive metabolism favorable to ethanol production in the second bioreactor.
- A micro-aerated bioreactor (R_2), is dedicated to ethanol production, and is coupled to an external ultrafiltration module. This configuration yields high biomass concentration to achieve high ethanol productivity.

In this bioprocess five concentrations appear: total biomass concentration (X_t), viable biomass concentration (X_v), glucose concentration (S), ethanol concentration (P) and the glycerol concentration (G). As it is illustrated in Figure 1 the feed flow rate (Q_{alim}) to the first reactor contains the mineral medium flow rate (Q_m), the substrate feed flow rate (Q_{S1}), the water flow rate (Q_w) and the vitamins flow rate (Q_v). For this process $Q_{alim} = Q_m + Q_{S1} + Q_w + Q_v$, $Q_{alim} = 10\,Q_m$ and $Q_v = Q_m/10$ then Q_m is expressed as $10(Q_{S1} + Q_w)/89$. First

reactor has two others flow rates; the outlet flow rate from R_1 to R_2 (Q_{12}) and the inlet flow rate from R_2 to R_1 (Q_{21}). Reactor 2 has five flow rates: a substrate feed flow rate (Q_{S2}), a purge flow rate (Q_{pg2}), a permeate flow rate (Q_p), the inlet flow rate from R_1 to R_2 (Q_{12}) and an outlet flow rate from R_2 to R_1 (Q_{21}). The concentrations of glucose that feed the two reactors are respectively S_{f1} and S_{f2}. V_1 and V_2 represent the volume of each reactor. S_{alim} is the diluted substrate concentration and is equal to $S_{f1}Q_{S1}/10\,Q_m$, what allows to write $Q_w = (89S_{f1}/100S_{alim} - 1)Q_{s1}$.

The originality of this process (Sanchez-Gonzalez 2008; Sanchez-Gonzalez *et al.* 2009) consists in the recirculation loop (Q_{12} and Q_{21}) between the second bioreactor and the first, to enhance cell viability.

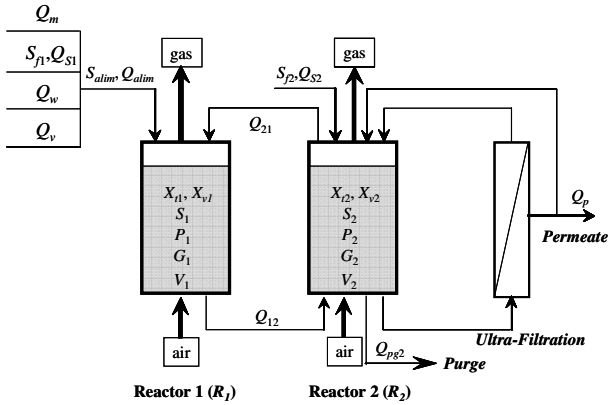

Fig. 1. Schematic diagram of a two-stage bioreactor with a cell separator for continuous ethanol production.

An initial model of this process proposed by Ben Chaabane (2006) was used in static optimization for determine the constant flow rates to apply in order to reach optimal steady-state. In this manner an industrial yield of 0.44 g of ethanol per g of glucose with a productivity of 41 g/(L.h) (Ben Chaabane et al. 2006) was obtained in our laboratory by mantained constant flow throughout the experiment. The new detailed model of this process will be presented in a companion paper (Aceves-Lara et al. 2010) submitted to another conference. The aim of this paper is to improve the ethanol production and to obtain more quickly the optimal steady-state by controlling the various flow rates during the experiment.

In the following section, the dynamic optimization procedure and the results obtained from simulations model are presented. A quantification of the profit obtained compared to the preceding results is given.

3. MODEL PREDICTIVE CONTROL FOR THE ETHANOL PRODUCTION

The Model Predictive Control has been successfully employed for solving constrained and unconstrained, linear and nonlinear problems (Cervantes *et al.* 2003; Costa *et al.* 2005; Kameswaran *et al.* 2005; Kameswaran and Biegler 2006; Van Hessem and Bosgra 2006; Kawathekar and Riggs 2007), which are often encountered in the process industries. Currently there are over two thousand online applications of MPC in the chemical process industries (Tran *et al.* 2005), mainly in the refining, petrochemical, and chemical industries as well as in pulp, paper and food processing (Qin and Badgwell 2003). In biological processes, it was mainly applied to continuous bioreactors (Zhu *et al.* 2000) and fedbatch bioreactors (Mahadevan *et al.* 2001).

In the present study, the formulation of the closed loop optimization problem is expressed as a MPC using the dynamic model previously described in (Aceves-Lara *et al.* 2010) and rewritten as:

$$\frac{d\xi}{dt} = f(t, \xi, u) \tag{1}$$

where ξ are the system states variables, (*i.e.* X_{t1}, X_{v1}, S_1, P_1, G_1, X_{t2}, X_{v2}, S_2, P_2 and G_2) and u is the vector of the control variables, (i.e. Q_{S1}, Q_{S2}, Q_{12}, Q_{21}, Q_p, Q_{pg2}, S_{f1} and S_{f2}). This nonlinear model is used in a MPC framework to choose the control action. The MPC controller chooses the future control value *i.e.*, the four flow rates and the two feed concentrations that minimizes the following objective function:

$$J = \min_{\substack{\{Q_{S1},\,Q_{21},\,Q_p,\,Q_{S2}\} \\ S_{f1},\,S_{f2}}} \left(\sum_{l=t}^{t+H_p} W_x(\eta_l - \eta_l^*) + \sum_{l=t}^{t+H_c} W_u \Delta u_l^{\,2} \right) \qquad s.t. \begin{cases} h(z) = 0 \\ g(z) \le 0 \end{cases} \tag{2}$$

where z = [S_1 P_1 X_{t2} S_2 Q_{S1} Q_{12} Q_p Q_{pg2} Q_{S2} Q_m Q_w Q_v].

Furthermore we define $(\eta_l - \eta_l^*) = \begin{cases} P_2 - \eta_l^* & If\ P_2 \le 64 \\ Y_{P/S}^{ind} - \eta_l^* & If\ P_2 > 64 \end{cases}$,

$$Y_{P/S}^{ind} = \frac{P_2 Qp}{Q_{S1}S_{f1} + Q_{S2}S_{f2} - S_2\left(1 - \frac{X_{t2}}{\rho}\right)Q_{pg2} - S_2 Q_p},$$

$W_x = \begin{cases} 0.1 & If\ P_2 \le 64 \\ 100000 & If\ P_2 > 64 \end{cases}$ and $W_u = [1 \quad 10 \quad 1 \quad 1 \quad 0.1] I_5$. H_p is the prediction horizon, H_c is the control horizon and I_5 is the identity matrix. The r_l^* variable represents a reference trajectory which enable to reach the set point $s*$. This variable is defined as the output of a first order system:

$$\eta_{i+1}^* = \kappa \cdot \eta_i^* + (1 - \kappa) s* \tag{3}$$

with $\kappa = (1-\beta)^{T_s/t_c}$ and $s* = \begin{cases} P_2 = 64 & If\ P_2 \le 64 \\ Y_{P/S}^{ind} = 0.5 & If\ P_2 > 64 \end{cases}$

The parameters value are: $\beta = 0.98$ (the term β signified that the system have reached a β percent of set point $s*$), $t_c = 10\,h$ (the term t_c represent the converge time to reach the value $\beta\, s*$) and T_s is a sampling time.

The optimization is subject to the following equalities constraints for vector $h(z)$:

$$\begin{aligned} Q_{12} + Q_{S2} - (Q_{21} + Q_p + Q_{pg2}) &= 0 \\ Q_m + Q_{S1} + Q_w + Q_v + Q_{S2} - (Q_p + Q_{pg2}) &= 0 \end{aligned} \tag{4}$$

to respect mass balance.

And four inequalities constraints for vector $g(z)$:

$$S_1 \le 120$$
$$S_2 \le 120 \quad (5)$$
$$X_{t2} \le 200 \quad (6)$$
$$P_1 \le 84 \quad (7)$$

according to previous works reported by Winter (1988).

When the optimum future value of input flow rate is determined, it is applied. In the following control cycle, the next optimum control value of input flow rate is determined again. To apply a MPC requires solving simultaneously an optimization problem and the system model equations. A sampling time of $T_s = 0.5\,h$ was chosen, with a prediction horizon H_p of 10 hours and a control horizon H_c of 1 hour. The optimization algorithms used will be explained in a next section. MPC optimization needs to use an algorithm which assures global convergence in a shortly time. Pattern search is one possibility, another is Ant Colony Algorithms.

4. PATTERN SEARCH ALGORITHMS

Pattern search (PS) methods are direct methods characterized by a series of exploratory moves that consider the behavior of the objective function at a pattern of points, all of which lie on a rational lattice. These algorithms were used by Fermi (Lewis *et al.* 2000) in parameters estimation. Recently, it was used for building energy optimization (Wetter and Wright 2003). Basically, pattern search methods can be explained as follows: There is an iterate $x_k \in \Re^n$ at an iteration point k and a step-length parameter $\Delta k > 0$. Then, the optimum is successively searched at the points $x_+ = x_k \pm \Delta_k e_i \;\; i \in \{1,\ldots,n\}$, until a x_+ is found for which $f(x_+) < f(x_k)$. If $f(x_+) > f(x_k)$, then Δ_k is reduced by half; otherwise, the step-length parameter is left alone, setting $\Delta_{k+1} = \Delta k$ and $x_{k+1} = x_+$. In the latter case, the step-length parameter can also increase, by a 3 factor. The iteration is done again until Δk is deemed sufficiently small. One important feature of pattern search that plays a significant role in the global convergence analysis is that it does not need to have an estimate of the derivative of f at x_k.

Optimization was made with a generalized pattern search (GPS) algorithm of the Matlab function "*patternsearch*" (Genetic Algorithm and Direct Search Toolbox, Mathworks) and differential model equations were solved with ode113. The parameters used for the optimization were: a mesh contraction of 0.0001 and a mesh expansion of 3.

5. ANT COLONY ALGORITHMS

The optimization based on natural systems, like ants algorithms, dates from the beginning of the 90's. Ant Colony Optimization (ACO) is a paradigm for designing metaheuristic algorithms for combinatorial optimization problems. The first Ant Algorithm was presented in 1991 (Colorni *et al.* 1991; Dorigo *et al.* 1991) and, since then, many variants of the basic principle were reported in the literature. ACO algorithms are based on the behavior of ant's colony (Dorigo *et al.* 1996) in order to find an optimal solution. This method is based on the deposit and evaporation of pheromones. This algorithm can be explained in a simplified way: Ants start moving randomly. Then, when they find their food, they come back towards their colony, marking their way with pheromones. The role of pheromone is to guide other ants towards the food. If other ants find the same way, they stop their random displacements and follow the same one reinforcing pheromone concentration on their return. This process is a positive feedback, because a way with more pheromone becomes more and more attractive. At the same time, the pheromone evaporates and the least reinforced ways end up disappearing, which leads all the ants to follow the shortest way.

At the beginning, ant colony algorithms were mainly used to produce quasi-optimal solutions for the travelling sales problem (TSP). After, these algorithms have been modified in order to solve dynamic problems. One of these algorithms is known as CACA (Continuous Ant Colony Algorithm) that takes up some ideas from genetic algorithms (GA) (Jayaraman *et al.* 2000; Rajesh *et al.* 2001). Nevertheless searching optimum in continuous regions using either GA or CACA is troublesome (Zhang *et al.* 2005). Another interesting ant algorithm is IACA (Interactive Ant Colony Algorithm) (Zhang *et al.* 2005). IACA is based on the idea to discretize the time and the control variables, but without discretizing the state variables. IACA evaluated the complete trajectories traversed by the ants and after that updated the pheromone concentration of each node. The great advantage of this algorithm is that it does not require discretizing states variable and it is easy to implement and is more efficient than GA and CACA since searching optimum among finite candidates is easier and simpler than in continuous region (Zhang *et al.* 2005). Unfortunately, IACA algorithms were used in order to find only one trajectory for simple problems without nonlinear constraints.

In this work, a Model Predictive Control is proposed with an IACA variation algorithm for nonlinear constraints.

6. IACA APPLIED TO MPC

The algorithms proposed in order to apply IACA for MPC can be described by the nine following steps. At the beginning it is necessary to initialize the two vectors $u_{\max}$ and $u_{\min}$ as follows:

$$u_{\max} = [Q_{S1_{\max}} \quad Q_{21_{\max}} \quad Q_{P_{\max}} \quad Q_{S2_{\max}} \quad S_{f1_{\max}} \quad S_{f2_{\max}}]$$
$$u_{\min} = [Q_{S1_{\min}} \quad Q_{21_{\min}} \quad Q_{P_{\min}} \quad Q_{S2_{\min}} \quad S_{f1_{\min}} \quad S_{f2_{\min}}]$$

1. Divide the time $[t \quad t + H_p]$ into *N* segments.

2. Choose an area of initial order, $w(i)_j^{(k)}$ (*i*=1,…,6 quantity of control variables; j=1,…,*N* the prediction horizon $H_p = NT_s$; *k*, iteration of optimization procedure). For each variable the search range is given by:

$$w(i)_j^{(k)} = u_{\max}(i)_j^{(k)} - u_{\min}(i)_j^{(k)} \quad (8)$$

3. Divide the control variables $u(i)$ into *p* segments. Figure 2 shows an example of the area formed by the time discretization and the control variables.

4. Place m ants ($m = N$ x p) in each node. The algorithm proposed here follows the method of Zhang *et al.* (2005) which placed the ants in each node at the difference of Asgari and Pishvaie (2008) which placed them in the nodes of the first column of time.

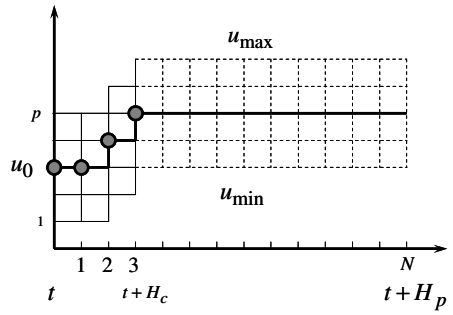

Fig. 2. Area formed by the discretization of time in N interval and the control variable in p segment.

Repeat:

5. Move randomly the ants from the left to the right. A turn is finished when an ant arrives at time $t + H_p$.

$$u(i)_j = u_{\min}(i)_j^{(k)} + \frac{(route_j - 1)w(i)_j^{(k)}}{p-1} \tag{9}$$

where $route_j$ is obtain by concatenation of the previous nodes until the node at instant j.

6. When the m turns are completed, it is necessary to update the objective adjustment of cost function:

$$fit(l) = \begin{cases} 0 \quad if \quad \dfrac{J_{\max} - J(l)}{J_{\max} - J_{\min}} < 1 \\ 1 \quad if \quad \dfrac{J_{\max} - J(l)}{J_{\max} - J_{\min}} = 1 \end{cases}, \; 1 \le l \le m \tag{10}$$

where $J_{\max} = \max(J(l))$ and $J_{\min} = \min(J(l))$. The value of the pheromone is thus:

$$\tau(i)_j = \varpi\, \tau(i)_{j-1} + q \sum_l fit(l), \; 0 \le \varpi \le 1, \; 0 \le q \le 1 \tag{11}$$

7. The ants turns that did not respect the nonlinear constraints will disappear.

It is necessary to update the pheromone density until the pheromone density will be equal to one or which cycles exceeds the limit used. Pheromone density is updated as:

$$P(i)_{jl} = \frac{\tau(i)_j}{\sum_{l=1}^{p} \tau(i)_j}; \quad l = 1,2,...,p \tag{12}$$

8. The best profile found $u(i)_j^*$ will be taken as a new base line for the next iteration.

$$u_0(i)_j^{(k)} = u(i)_j^* \quad j = 1,2,...,N; \quad k = 1,2,3,... \tag{13}$$

9. The new search area $w(i)_j^{(k+1)}$ will be reduced with the constant coefficient ϖ:

$$w(i)_j^{(k+1)} = \varpi\, w(i)_j^{(k)} \tag{14}$$

and the new bounds $u_{\max}(i)_j^{(k+1)}$ and $u_{\min}(i)_j^{(k+1)}$ can be updated as:

$$u_{\max}(i)_j^{(k+1)} = \frac{2u_0^*(i)_j^{(k)} + w(i)_j^{(k+1)}}{2} \tag{15}$$

$$u_{\min}(i)_j^{(k+1)} = \frac{2u_0^*(i)_j^{(k)} - w(i)_j^{(k+1)}}{2} \tag{16}$$

The algorithm finishes when the difference between the two best iterations will be lower than a bound ε. On the opposite case, the procedure will be started again.

7. RESULTS AND DISCUSSION

Simulations for continuous mode have been made using the operating conditions reported by Ben Chaabane (2006). The optimization objective is twice: until $P_2 \le 64 g/L$ the objective is to maximized P_2, when $P_2 > 64 g/L$ the objective is to maximized the industrial yield. MPC framework has started after fifteen minutes of simulation and has been applied with a white noise of 5%. The simulation results of the two optimization algorithms were compared with experimental results (Ben Chaabane 2006) obtain with an open-loop control.

Figure 3 shows the state variables in the bioreactor R_1 (total X_{t1} and viable X_{v1} biomass, substrate S_1 and ethanol P_1 concentrations). It can be noticed that MPC with a PS gives the best results: higher biomass and ethanol concentrations with a null residual substrate. It can also observe that MPC with IACA have a good result in the first 17 hours, but after 17 hours the trajectory for the state variables was not advisable. It can be due to a convergence problem with the second optimization objective $Y_{P/S}^{ind} = 0.5$.

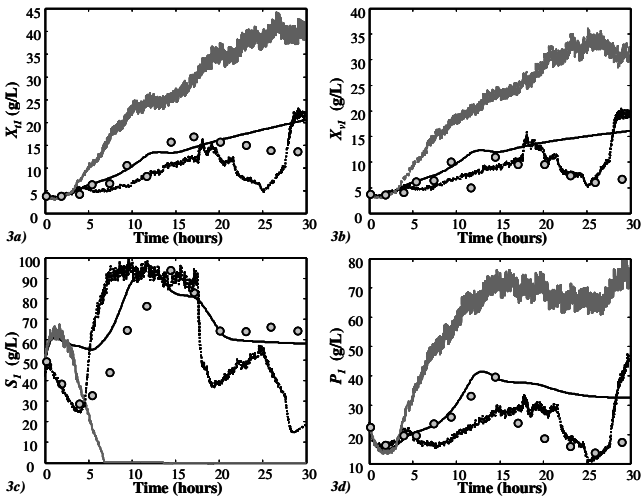

Fig. 3. State variables in bioreactor R_1: total biomass (X_{t1}), viable biomass (X_{v1}), substrate concentration (S_1), ethanol concentration (P_1); experimental data (O), model simulation (–), MPC with pattern search algorithm – – and MPC with IACA algorithm ▪▪▪

Figure 4 shows the concentrations of total X_{t2} and viable X_{v2} biomass, substrate S_2 and ethanol P_2 concentrations in the second bioreactor R_2. The MPC with PS algorithm gives here also better results than an open-loop control. An optimal ethanol concentrations was obtained in a smaller time than the others methods. Furthermore, IACA could not found a

good trajectory and is less robust than MPC with PS algorithm. In this figure it is shows clearly that MPC with IACA could converged to the first optimization objective $P_2 = 64 g/L$, but unfortunately the search of the second optimization objective $Y_{P/S}^{ind} = 0.5$ failed and was not stable.

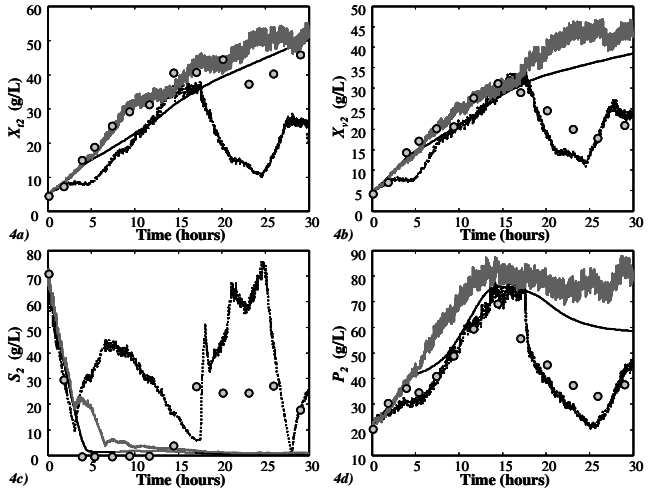

Fig. 4. State variables in bioreactor R_2: total biomass (X_{t2}), viable biomass (X_{v2}), substrate concentration (S_2), ethanol concentration (P_2); experimental data (o), model simulation (–), MPC with pattern search algorithm — — and MPC with IACA algorithm ▪▪▪

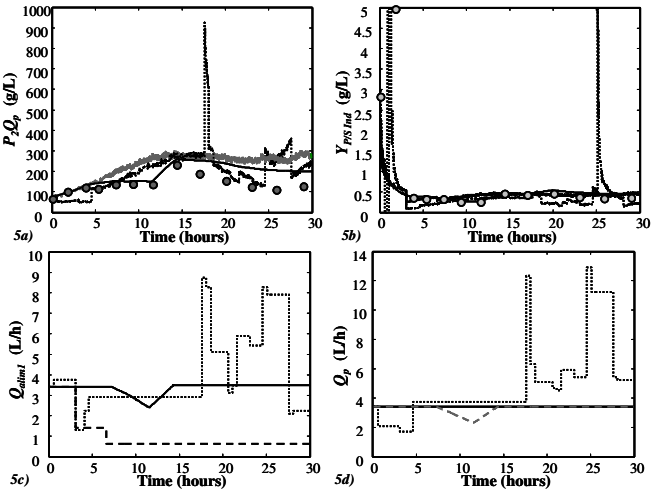

Fig. 5. Performance variables: ethanol flow rate (P_2Q_p), Industrial yield ($Y_{P/S}^{ind}$) and control variables: substrate feed flow rate (Q_{S1}), permeate flow rate (Q_p); experimental data (o), model simulation (–), MPC with pattern search algorithm — — and MPC with IACA algorithm ▪▪▪

Figure 5 shows the ethanol production P_2Q_p, the industrial yield $Y_{P/S}^{ind}$, the substrate feed flow rate Q_{S1} and the permeate flow rate Q_p obtained with an open-loop control and MPC with a PS algorithm and IACA. MPC with PS algorithm gives a better trajectory with a gain of 10 hours. This method applied only two control actions for Q_{S1} and a constant value for the permeate flow rate Q_p. Concerning the industrial yield $Y_{P/S}^{ind}$, the open-loop control and MPC with PS algorithm are near to optimal. Therefore, MPC with PS algorithm shows that it is a robust controller. On contrary, IACA algorithm was not stable, for the second optimization objective $Y_{P/S}^{ind} = 0.5$. This could be due by the number of cycles (20) that was used in order to reduce the estimation time or to the values of the matrix W_u, since it was constant for the two optimization objectives. It can be observed that after 17 h the control variables values for the substrate feed flow rate Q_{S1} and the permeate flow rate Q_p have high variations.

Figure 6 shows others operating conditions which were applied experimentally or estimated by the MPC controllers. The worst results were obtained for the MPC with IACA algorithm. PS algorithm was very constant for the recirculation flow rate Q_{21}, the purge flow rate Q_{pg2} and the diluted substrate concentration S_{alim}. On contrary, these two flow rates have a high variation for the MPC with IACA, may be due to values used in matrices W_u and W_x. In figure 6c it can be noticed that open-loop control used a high substrate concentration in order to obtain a good ethanol concentration whereas with the MPC with a PS algorithm, since it is not necessary to vary the concentration all time when the correctly operational conditions are changed. Figure 6d shows substrate feed flow rate Q_{S2} for the second bioreactor. In Figure 6d can be seen the same two changes in the operational conditions found by the PS algorithm that reach the best trajectory. Furthermore, PS algorithm was more stable that IACA algorithm. In general IACA was not very stable for all control variables after it was estimated the second optimization objective. It should be noted that during the first 17 hours the optimization algorithm maximizes the first objective (the ethanol concentration) and that during the last 13 hours it maximizes the second objective (the industrial yield).

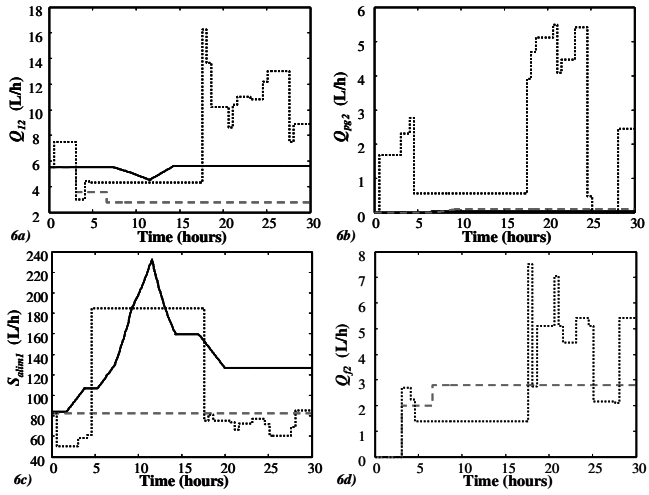

Fig. 6. Control variables: recirculation flow rate Q_{21}, purge flow rate Q_{pg2}, diluted substrate concentration S_{alim}, substrate feed flow rate Q_{S2}; model simulation (–), MPC with pattern search algorithm — — and MPC with IACA algorithm ▪▪▪

Finally, the results are summarized in Table 1. In this table, it can be noticed clearly the advantage of to use a MPC with a gain of 16 % in the ethanol flow and 14 % in the ethanol concentration.

Table 1. Comparison between experimental data obtain in open loop case (Ben Chaabane 2006) and closed loop simulation results from MPC controller with PS algorithm

Maximum	X_{t2}	X_{v2}	S_2	P_2	$Y^{ind}_{P2/S2}$	P_2Q_p
Experimental	46.1	31.4	4.2	69.5	0.45	236
MPC with PS	51	44	1	80	0.45	275

8. CONCLUSIONS

This paper presented an approach of dynamic optimization of ethanol production by using an optimal closed loop control. Two algorithms were proposed for applied a model predictive control (MPC); a Pattern Search algorithm (PS) and an Interactive Ant Colony Algorithm (IACA). The design and performance of the proposed method were applied in a two-stage bioreactor with cellular recycling process during 30 hours. MPC with PS algorithm compared to open loop (*i.e.*, uncontrolled) situations, led to gain 10 hours of time to arrive to the best ethanol concentration. Ethanol flow and ethanol concentration obtained with the PS algorithm were stables by applying only two changes within operational conditions. PS algorithm was most robust than IACA; convergence time need for PS was two hundred times faster than IACA.

The final objective of this work is to validate online the method proposed in an experimental laboratory pilot. The lack of sensors of this kind of bioprocess imposes to develop a nonlinear observer (software sensor) in order to reconstruct the non measured state variables.

9. ACKNOWLEDGEMENTS

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