Plantwide Optimizing Control for the Bio-ethanol Process

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Abstract: In this work, the Plantwide Control (PWC) problem of a continuous bio-ethanol process is investigated from a Plantwide Optimizing Control (PWOC) perspective. PWOC addresses the plantwide control problem integrating real-time optimization and control for optimal operation. Two different PWOC approaches have been considered: A Single-Layer Direct Optimizing Control approach (one-layer) and a Multi-Layer without Coordination approach (two-layer). The performance of these two PWOC approaches is compared with more traditional Decentralized architectures, demonstrating the benefits of using Plantwide Optimization-based Control strategies in bioprocesses.

Keywords: Plantwide Control, Optimizing Control, Dynamic Real Time Optimization, Ethanol.

1. INTRODUCTION

Nowadays, bioprocess industry is an important part of the worldwide economy. Specifically, the bio-ethanol industry has experienced a significant growth in the last years since ethanol, as an environmentally friendly fuel, is considered an attractive alternative energy source. Ethanol production has been continuously improved in very different ways in order to assure the economical and environmental feasibility of the process. Examples of these improvements include purification technologies for reducing energy consumption during the separation of the ethanol-water mixture (Arifeen et al., 2007), and genetic modifications of the microbial strains for building more ethanol-tolerant yeast and strains capable of carrying out simultaneously saccharification and fermentation tasks (Olofsson et al., 2008). From a process control point of view, different works have been done regarding the modelling, estimation, and control problem for the fermentation stage. However, only relatively few works (e.g. Meleiro et al., 2008, Costa et al., 2001) have addressed the control problem from the Process Systems Engineering point of view, considering the process as an integrated dynamic production system taking into account more than one single process unit (i.e. accounting for interactions between fermentation, cells recycle and flash units). In this work, the Plantwide Control (PWC) problem for the ethanol process is addressed as a large-scale real-time dynamic optimization problem due to the following facts: the nature of the process is highly nonlinear and dynamic; the process is characterized by the coupling of slow and fast dynamics; interactions between different operating units can not be neglected; and finally, economical feasibility of the process can be effectively assured if this is the main control objective of the plantwide strategy. PWC has attracted the attention of the process control community for more than 40 years, since the pioneer work by Buckley (1964). Through these years, different architectures have been used for tackling the problem of controlling a complete process. The intention of this section is to present a brief review of the several options reported for addressing PWC. A proposal of classification for different PWC architectures is shown in Fig 1, which agrees in some points with that presented by Scatollini (2009).

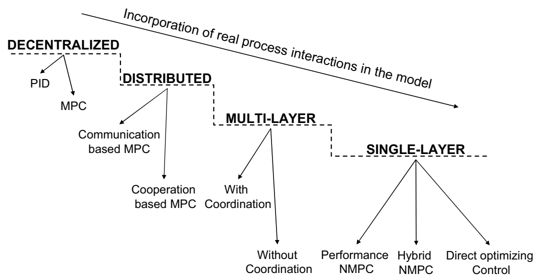

Fig 1. Plantwide Control Architectures

In the *Decentralized* scheme, many different individual regulators are used in the process without sharing any kind of information between them (i.e. each controller operates independently of the others), even though the selection of the manipulated and controlled variables might take into account the interactions in the process. The decentralized approach consists usually of SISO PID loops, although MPC controllers can also be used. As noted by Stephanopoulous and Ng (2000), most of the research activities in the topic of PWC up to year 2000, addressed the PWC problem as the selection of the best input-output pairing for the formation of SISO PID loops. Of course, as in any rule there are exceptions, and one of the most relevant examples in this case is the work by Garcia and Morari (1984), in which a multivariable control scheme based on a *Multi-layer* PWC architecture was proposed for controlling a benzene plant. Some of the many works that have addressed the PWC in a decentralized manner are Araujo et al. (2007), Larsson et al. (2003), Robinson et al. (2001), Zhen et al. (1999), Lausch et al. (1998), Luyben et al. (1997) and McAvoy and Ye (1993). Most of the works in the remaining three architectures shown in Fig 1 make use of a multivariable controller. Two main reasons motivated to move the PWC problem from the paradigm of decentralized PID towards different alternatives: the performance limitations of the decentralized architecture, and the broad industrial impact of the Model Predictive Control (MPC) framework (Venkat et al. 2007). In the *Distributed* architecture some information is exchanged between the multiple MPC controllers. Two Distributed-MPC approaches worthy of mention are the communication- and cooperation-based, which mainly differ that in the first, each controller has a local objective function, whereas in the latter the objective function in each controller is a copy of the total objective function for the complete plant (Rawlings and Stewart, 2008). Representative works addressing the PWC from the Distributed perspective are those by Sun and El-Farra (2008), Venkat et al. (2007), Mercangöz and Doyle (2007) and Venkat (2006). *Multi-layer* architecture is a hierarchical structure that follows the guidelines given by Findeisen et al. (1980), which classified the hierarchical control into multilayer and multilevel. According to Findeisen's work, in the multilayer case, the control of a system is split into algorithms (layers), whereas in the multilevel case control is divided into local goals and the action of each local control unit is coordinated by an additional supremal unit. In Fig 1 it is proposed to sub-divide the Multi-layer (or hierarchical) architecture into: *With Coordination* (denoted as Multilevel approach by Findeisen) and *Without Coordination*. Multilayer architectures should be composed by at least two different layers, in which the task of finding the control actions that should be applied to the process is split usually into: a *Real Time Optimization* (RTO) layer that computes optimal set point values for the controlled variables, and a *Control* layer which is in charge of tracking the optimal set point values (Kadam et al., 2002). In the control layer, a PID or MPC controller can be used (Kadam and Marquardt, 2004). It is important to notice that as mentioned by Biegler and Zavala (2009), the "connection" between RTO and MPC layers may suffer inconsistencies due to model mismatch (non-linear steady state vs. linear dynamic) and conflicting objectives. Therefore, in the last years a proposal for replacing the steady state RTO by a Dynamic Real Time Optimization (D-RTO) layer has emerged (Kadam et al. 2003; Kadam and Marquardt, 2004). On the other hand, regarding the *Multi-layer with coordination* architecture, the reader is referred to the work by Tosukhowong et al. (2004) in which a coordination collar is used to find for each MPC a locally feasible set point close to the global solution found by the RTO layer; and to the work by Cheng et al. (2007), in which a price-driven method is used for coordination between the RTO and the MPC layers. Additionally to the references already mentioned, the following works include examples of PWC using *Multi-layer* architecture: Ochoa et al. (2009), Kadam and Marquardt (2007), Lu (2003), Duvall and Riggs (2000) and Ying and Joseph (1999). A final mention should be done regarding the difference between the Multilayer with coordination and the Distributed architectures. As both schemes include coordination, in the Distributed case the coordination consists on exchanging some information between the local MPCs, whereas in the Multilayer with coordination, the local MPCs are not communicated between them but communicated to the RTO layer. The last PWC architecture in the classification shown in Fig 1 is the *Single-layer* scheme. Despite the very common belief that a *Single-layer* or centralized structure will be intractable for PWC (Venkat et al., 2007), in the last years some publications from both the industrial and the academic side have shown that such monolithic approach it is not only possible to implement but also gives very good results from an economic point of view (Bartusiak, 2007; Zavala et al., 2007; Franke and Doppelhamer, 2007). Works using this architecture solve online a moving horizon optimization problem, but differ in the type of objective function optimized. A first group of works denoted as *Performance NMPC* uses a performance-type objective function (in which mainly the tracking of a reference value is penalized). The second scheme includes besides the performance term, an economic penalization term in the formulation of the objective function and therefore it is denoted here as *Hybrid NMPC* (Economic+Performance). The final scheme denoted in the literature as *Direct Optimizing Control* (Engell, 2007) uses a pure economic objective function in which the usual control specifications enter as constraints and not as set points, and therefore no tracking term is penalized. References showing examples of the application of the Single-layer architecture are: Biegler and Zavala (2009), Roman et al (2009), Ochoa et al. (2009), Engell (2007), Franke and Doppelhamer (2007), Zavala et al. (2007), Bartusiak (2007), Manenti and Rovaglio (2007), Franke and Vogelbacher (2006), Toumi and Engell (2004) and Jockenhövel et al (2003). The main purpose of this paper is to present a novel approach for the PWC of the bio-ethanol process, in which the main control objective is to maximize the profitability of the whole process. The paper is organized as follows: Section 2 gives a description of the ethanol continuous process from starch, including a brief description of the relevant works that have addressed the control of the process considering it as composed of more than one process unit. Section 3 presents the Plantwide Optimizing Control (PWOC) concept proposed in this work and describes the main steps of this approach. A new method for shrinking the search region during the optimization problem that arises when applying PWOC is proposed in Section 4. The Multi-layer without coordination and the Single-layer direct optimizing architectures are used for addressing the PWC problem in the continuous bio-ethanol process. These approaches are compared in Section 5 to conventional decentralized architectures.

2. BIO-ETHANOL PRODUCTION PROCESS

The case study addressed is based on the extractive alcoholic fermentation process shown in Fig 2. A detailed description of this process is found elsewhere (Meleiro et al., 2008). The process includes saccharification, fermentation, cells recycle, flash separation, distillation and rectification. The end product considered is the ethanol obtained at the top of the rectification column, which in a further step must be sent to a dehydration unit (e.g. molecular sieves). A nonlinear dynamic model of the process has been simulated using Simulink®. The model consists of a nonlinear DAE system comprising 69 differential states and 173 algebraic equations. pH, temperature and liquid levels are regulated as usually done in industry by means of local SISO loops, which in the following will be denoted as *basic control*. After closing these basic loops, 13 input variables are left, 3 of which are identified as disturbances: starch (S_0), enzymes (Enz_1) and fresh yeast concentration (X_3) fed into the process. The remaining 10 inputs are available for improving the control strategy in the process. The process with its basic level control loops is shown in Fig. 2 (for simplicity, the pH and temperature loops are not shown). In addition to the basic loops, an internal biomass control strategy (Ochoa et al., 2009) is also shown. The combination of the traditional *basic control loops* with this biomass internal strategy is denoted in the following as *Local Control Strategy*. Two main reasons motivated implementing the biomass control. First, an optimal biomass concentration in the fermentor should be always guaranteed in order to avoid a misuse of the substrate if a higher concentration than the optimal is available. Additionally, if biomass concentration is below the optimum, a slower metabolite production rate will occur, affecting the productivity of the process. Second, yeast is only involved in a closed mass loop comprising fermentation, filter and cells recycle; i.e. no biomass is found on the streams up the fermentor nor downstream the filter. As already mentioned, the process has 10 manipulated variables available for improving the control strategy; however, 3 of them (F_3, F_7, F_{10}) are used as manipulated variables in the biomass strategy. The remaining 7 manipulated variables (F_0, F_1, F_{13}, VB_1, R_1, VB_2, R_2, which are the starch input flow, enzymes input flow, recycle flow from the flash to the fermentor and vapour and reflux rates for each column) are potential manipulated variables denoted as “Plantwide variables”.

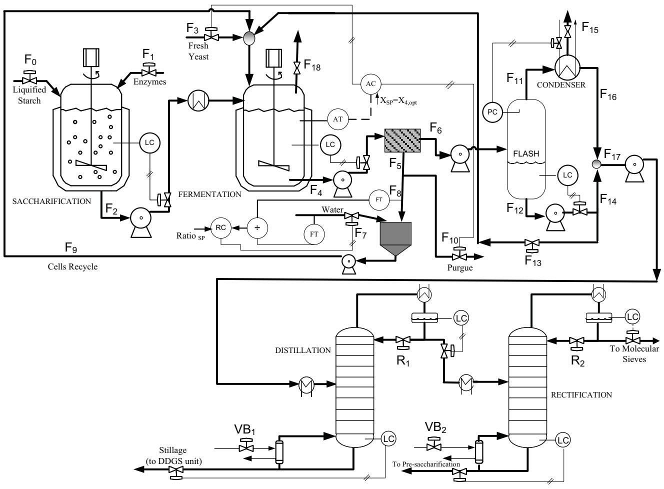

Fig 2. Bio-ethanol Process from Starch: Local Control Strategy (Basic loops + Internal Biomass Strategy).

Additionally, it should be noticed that despite the rapid increase of the bio-ethanol industry in the last 30 years and the high economic risk that this industry faces, no much effort has been done in order to improve the efficiency of the process from the optimization and control points of view. Several works have been published regarding mainly the control of the fermentation unit in the process, but to the author’s knowledge, only few works have addressed the control of the process considering more than the fermentation stage. Costa et al. (2001) used Dynamic Matrix Control (DMC) for controlling the substrate or the product concentrations in the fermentor manipulating the substrate input flow or the cells recycle rate. A second contribution by Costa et al. (2002), proposes a SISO NMPC for controlling the substrate concentration in the fermentor, manipulating the substrate input flow. Meleiro et al. (2008) presented a multivariate NMPC to control simultaneously the ethanol, substrate and biomass concentrations in the fermentor. Although the process modelled in these works considers interactions fermentor-cells recycle-flash, the control task is still focused on tracking or regulating the main state variables in the fermentor without considering the optimal economic operation of the whole process. Finally, Bartee et al.(2008), propose using MPC for controlling the process including milling, cooking, distillation etc.; however, no details regarding algorithms and implementation are given.

3. PLANTWIDE OPTIMIZING CONTROL

Online optimizing control optimizes an economic objective over a finite moving horizon during plant operation based upon a rigorous nonlinear dynamic model (Küpper and Engell, 2008). Plant limitations and product specifications are included in the optimization as constraints. This definition is used in this section as key concept for developing the basic steps of a Plantwide Optimizing Control (PWOC) approach. PWOC addresses PWC as a nonlinear dynamic online problem, in which the available manipulated variables in the process are used for achieving maximum profitability in the plant in spite of disturbances. In this way, PWOC calculates optimal values for the set of selected manipulated variables, in order to maximize a Plantwide Profitability Objective function Φ, instead of maintaining a set of controlled outputs at predefined set points. A key feature of PWOC is that input-output pairing is avoided because the output actually controlled in the process is the Plantwide Profitability and the available manipulated variables are simultaneously used for satisfying that purpose. Online optimizing control has been gaining increasing attention in the last years in different chemical process applications (Engell, 2007). However, not much work has been reported in the open literature on the on-line optimizing control of bioprocesses. In this work PWC of a bioprocess is addressed from an optimizing control perspective, considering a large-scale nonlinear Dynamic Real-Time Optimization (D-RTO) problem. The proposed PWOC approach comprises six main stages, as shown in Fig 3. In the following, a description of each stage is presented.

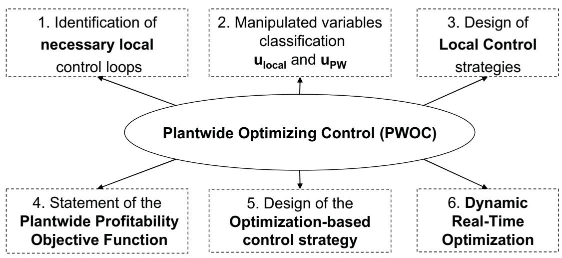

Fig 3. Plantwide Optimizing Control Stages

Stage 1: Identification of necessary control loops

Even though the goal of any chemical or biochemical process is to return a maximum profit, there are additional control objectives that should be taken into account before establishing a PWOC structure for satisfying this economic goal. These objectives are mainly related to safe operation, equipment and environmental protection and should be achieved independently of the economical performance of the plant, i.e. by using local control loops.

Stage 2: Classification of the Manipulated Variables

Manipulated variables in the process can be used in the local control loops or for the PWOC of the process. Those manipulated variables used for satisfying the local control set points are denoted as *Local manipulated* (u_{Loc}), whereas the *Plantwide manipulated* variables (u_{Pw}) are those that remain available after selecting the u_{Loc}, and that are used for maximizing the plantwide profitability objective function.

Stage 3: Design of Local Control Strategies

After identifying the necessary local control loops in the process and the local manipulated variables required for satisfying the control objectives at the local control loops, it is then necessary to address the design of those local loops (i.e. pairing manipulated-controlled variables, selection of controller type, controller tuning, etc.), as traditionally done.

Stage 4: Statement of Plantwide Profitability Function (Φ)

The next step is to establish a plantwide profitability function Φ and its constraints, in order to formulate a D-RTO problem. Statement of the objective function Φ will depend upon the specific process addressed. However, it may contain terms related to productivity of the process, raw materials and energy consumption, economic losses, etc. Constraints in the optimization problem are determined by plant and product specifications, and by limitations in the state and input variables. Since PWOC addresses the optimizing control problem for a complete plant over a finite moving horizon during plant operation, it is also important to select the prediction horizon Δt_{opt} over which the objective function and constraints will be evaluated. Δt_{opt} should not be shorter than the characteristic response time of the slowest relevant dynamic in the process (to avoid unexpected long-term performance deterioration), while at the same time it should be as short as possible to minimize computational load.

Stage 5: Design of the Optimization-Based Control Strategy

PWOC is addressed here using two different architectures: *Single-Layer Direct Optimizing Control* and *Multi-Layer without Coordination*. These frameworks will be referred in the following as the one-layer and the two-layer approaches, respectively. The structures for both approaches are shown in Fig. 4. A detailed description of the building blocks for each framework can be found elsewhere (Ochoa et al., 2009). Comparing the schemes for the two frameworks (Fig. 4), it is possible to see that both approaches have very much in common. For example, both approaches are driven by a D-RTO layer, in which the objective function to be maximized is the plantwide profitability Φ. The main difference between the two frameworks is that in the one-layer approach, the input variables applied to the real plant are given by the optimization layer (u_{Pw}=u_{opt}), whereas for the two-layer, the inputs applied to the real plant are calculated by a control layer (u_{Pw}=u_{mpc}) that uses as set points, the optimal values of the states given by the optimization layer (x_{opt}). In both cases, the decision variables of the optimization problem are the plantwide manipulated variables u_{Pw}. In the two-layer case however, a second layer (NMPC controller) is used, in which an optimization problem is also solved for minimizing a performance-type objective function Γ, which can be composed of three terms: a penalization of the deviation of the main state variables from their set points (x_{opt}), a term that prevents large changes in the manipulated variables from one sample time to the next, and a term that constraints the manipulated variables to a small envelope around the reference trajectories u_{opt}, given by the optimization layer.

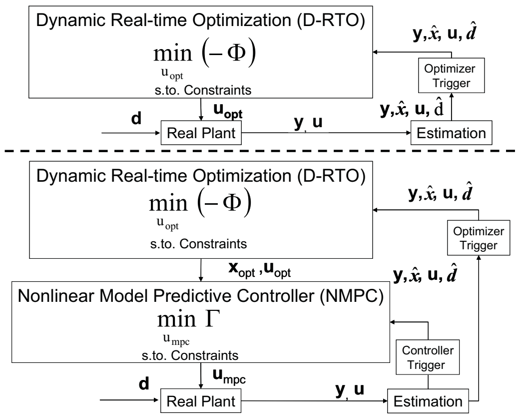

Fig. 4. Optimization-Based Control Strategies: One-layer (top) and Two-layer (bottom)

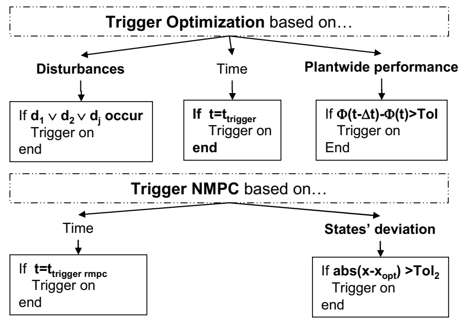

Fig. 5. Trigger for re-calling the D-RTO (top) and Controller layers (bottom)

Finally, trigger blocks in Fig. 4 deserve special mention due to their importance in the implementation of optimization-based control strategies. These trigger blocks act like switches for re-calling the optimization and control layers. An optimization-trigger for recalling the D-RTO layer can work based on a time criterion (e.g. the optimization is called periodically at a predetermined frequency), based on the disturbances dynamics (occurrence of a disturbance) or based on the performance of the plantwide profitability objective function (when Φ decreases below a certain tolerance). On the other hand, the controller-trigger can be based on a time criterion or on the state variables deviations from their optimal set points. Fig. 5 shows schematically the different criteria for activating the optimization and controller triggers.

Stage 6: Dynamic Real Time Optimization (D-RTO)

Because a nonlinear dynamic large-scale optimization problem arises in the last stage of the PWOC, an efficient feasible optimization method should be used in order to solve the problem in real time. For this purpose, different types of optimization algorithms can be used. However, the use of stochastic or evolutionary algorithms is considered here because of their reduced computational load (they do not need information about derivatives as required by gradient-based methods) and their relatively simple implementation. In this work, a stochastic method (i.e. localized random search) is used for solving the optimization problem in the PWOC. Independently of the optimization algorithm used, the method will search for the optimal solution in the space of the decision variables, which is a region bounded by the lower and upper limits of each manipulated variable (which are the decision variables of the optimization problem). This search region may be too large, resulting in long calculation times for finding an optimal solution, making difficult the solution of the PWOC problem in real time. In order to improve the efficiency of the optimization method for solving the large scale D-RTO problem, in the following section, a new stochastic-based approach for shrinking the search region of the optimization problem is introduced.

4. STOCHASTIC-BASED SHRINKING OF THE SEARCH REGION OF THE D-RTO PROBLEM

The main idea of the stochastic shrinking approach, is that for a sample time Δt (during which a disturbance took place in the process or the profitability function decreased), the changes on each plantwide manipulated variable (Δu_{PWi}) required for rejecting a disturbance, should be calculated as a function of the changes in the disturbances (Δd_j) and in the profitability objective function ($\Delta\Phi$). Mathematically, this can be written as shown in (1).

$$\Delta u_{PWi} = u_{PWi,t+\Delta t} - u_{PWi,t} = f_i(\Delta d_1, \Delta d_2, \ldots \Delta d_j, \Delta\Phi) \tag{1}$$

Where i is the number of plantwide manipulated variables and j is the number of disturbances that can be present in the process. f_i is a function that represents how much the manipulated variable i should change to reject disturbances. Specifically in this work, the use of a Gaussian distribution for describing function f_i is proposed. In this way, the changes on the manipulated variables are given in (2).

$$\Delta u_{PWi} = \xi_i\left(0\ ,\ \sigma_{u_i}\right) \tag{2}$$

Where $\xi_i(0,\sigma_{ui})$ represents a random number obtained from a Gaussian distribution with zero mean and standard deviation σ_{ui}. This standard deviation can be calculated as the maximum between different contribution terms, which represent the capability of the manipulated variable i for rejecting the different known disturbances of the process at time t, and for rejecting a decrease in Φ (that can be caused by both known and unknown disturbances), as shown in (3),

$$\sigma_{u_i} = \max(w_{i1}\Delta d_1, w_{i2}\Delta d_2, \ldots w_{ij}\Delta d_j, w_{i\Phi} z_\Phi \Delta\Phi) \tag{3}$$

where w_{ij} are gain factors that express how much a change in the manipulated variable u_{Pwi} can reject (or counteract) the occurrence of disturbance d_j, $w_{i\Phi}$ is the gain factor for the manipulated variable i rejecting the decrease in the profitability objective function Φ, and z_Φ is a dummy variable that is only activated when the objective function Φ decreases below a given tolerance Tol, that is:

$$z_\Phi = \begin{cases} 0, & \Phi(t-\Delta t) - \Phi(t) \le \mathrm{Tol} \\ 1, & \Phi(t-\Delta t) - \Phi(t) > \mathrm{Tol} \end{cases} \tag{4}$$

A final mention should be done, regarding the calculation of the gain factors used for obtaining the standard deviation σ_{ui}. It would be desirable to calculate these gains mathematically, from the nonlinear model of the process as expressed in (5)

$$w_{ij} = \sum_{k=1}^{n} \frac{\partial u_i}{\partial x_k} \times \frac{\partial x_k}{\partial d_j} \tag{5}$$

where $\partial u_i/\partial x_k$ represents the inverse of the open loop gain between state variable x_k and input u_i; and $\partial x_k/\partial d_i$ represents the open loop disturbance gain between x_k and disturbance d_j. As the complexity of the process model increases, the complexity for calculating the w_{ij} factors analytically also increases. For this reason, these gain factors are proposed to be calculated by using Digraphs. Information regarding digraph models is found elsewhere (Maurya et al., 2003).

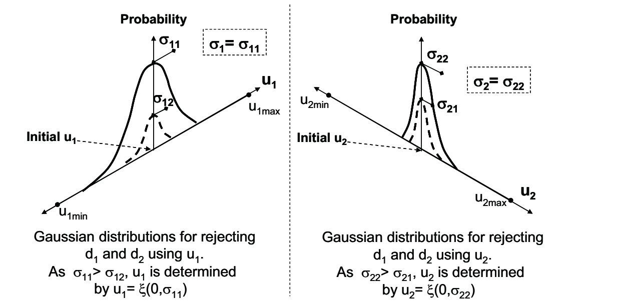

Fig. 6. Shrinking approach: Gaussian distributions for a system with two manipulated variables and two disturbances.

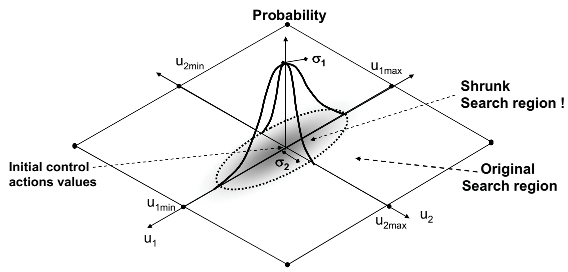

Fig. 7. Shrinking approach: Final Shrunk Search Region vs. Original Search Region.

For concluding this section, a graphical representation of the shrinking approach for a system with two manipulated variables and two disturbances that occur at the same time, is presented in Fig. 6 and 7. Fig. 6 shows the Gaussian distributions with standard deviation σ_{11} and σ_{22} for describing the manipulated variables u_1 and u_2 respectively, when disturbances occur in the process. Fig. 7 shows the Shrunk Search Region for the optimization problem, formed by the Gaussian distributions for u_1 and u_2. It is important to notice that despite the maximum standard deviation has been selected for each case, a reduction of the search space for the optimization algorithm is achieved because the original search region of the optimization problem was only bounded by the upper and lower bounds of u_1 and u_2 (see Fig. 7). The stochastic-based shrinking approach is used in section 5 for reducing the search region of the optimization problem that arises when the PWOC concept is applied to the ethanol case study. As it will be shown through this example, the PWOC problem has been solved more efficiently by applying the shrinking approach than without shrinking.

5. PWOC FOR THE ETHANOL PROCESS: RESULTS AND COMPARISON

The main purpose of this section is to show the application of PWOC to the bio-ethanol process described in Section 2 and to compare the obtained results to a typical decentralized SISO loops scheme. The decentralized architecture implemented for comparison uses seven PID control loops, in addition to the Local Control strategy introduced in Section 2. The paired PID loops (controlled-manipulated variable) are the following: E_4-G_2-F_0, G_4-F_{13}, x_{DE1}-R_1, x_{BE1}-VB_1, x_{DE2}-R_2, x_{BE2}-VB_2, where E_4, G_2, G_4, are the ethanol concentration in the fermentor and the glucose concentration in the saccharificator and in the fermentor, respectively. x_{DE1}, x_{BE1}, x_{DE2}, x_{BE2}, corresponds to the mol fractions of ethanol in the top and bottoms of the distillation and rectification columns, respectively. A special mention should be done regarding the control loop E_4-G_2-F_0, which is a cascade proposed due to the fact that the ethanol to be produced depends strongly on the glucose concentration (G_2) that comes from the saccharificator. Finally, it should be noticed that following recommendations given by Araujo (2007), and in order to do a fair comparison to the PWOC results, the controlled variables for the distillation and rectification columns in the decentralized loops are concentrations and not temperatures (or temperature differences), which are usually the real controlled variables at an industry level. On the other hand, the main objective of PWOC is to control the profitability at its maximum value, and therefore the pairing controlled-manipulated variable is avoided. In the following, the PWOC stages are applied in detail to the bio-ethanol process.

Stages 1-3: Identification and design of necessary control loops.

For the bio-ethanol process, the following control loops has been identified as *necessary local loops*: level control in all tanks, pH and temperature control in saccharificator and fermentor, and pressure control in flash, distillation and rectification. Additionally to these loops, as explained in section 2, a biomass control strategy is used. With exception of the loops involved in the biomass strategy, all local loops are SISO (e.g. PI or PID). After implementing the local loops, the process still has 7 available manipulated variables that are used as plantwide manipulated for maximizing the profitability of the process. These plantwide manipulated variables are: F_0, F_1, F_{13}, VB_1, R_1, VB_2, R_2; corresponding to starch and enzymes input flow, recycle flow from the flash to the fermentor and vapour and reflux rates for each column.

Stage 4: Statement of Plantwide Profitability Function (Φ).

The following profitability objective function is proposed to be maximized for the ethanol process addressed in this work:

$$\begin{aligned}\Phi = {} & w_1 \int_{t_0}^{t_0+\Delta t_{opt}} x_{ED_2} D_2\,dt - w_2 \int_{t_0}^{t_0+\Delta t_{opt}} F_0 S_0\,dt + w_3 \int_{t_0}^{t_0+\Delta t_{opt}} x_{ED_2}\,dt \\ & - w_4 \int_{t_0}^{t_0+\Delta t_{opt}} F_4\,dt - w_5 \int_{t_0}^{t_0+\Delta t_{opt}} VB_1\,dt - w_6 \int_{t_0}^{t_0+\Delta t_{opt}} VB_2\,dt \\ & - w_7 \int_{t_0}^{t_0+\Delta t_{opt}} x_{WD_2} D_2\,dt - w_8 \int_{t_0}^{t_0+\Delta t_{opt}} x_{EB_1} B_1\,dt - w_9 \int_{t_0}^{t_0+\Delta t_{opt}} x_{EB_2} B_2\,dt\end{aligned} \tag{6}$$

where w_i are weighting factors. The first term in (6) is related to the productivity of the process (expressed as the product between the ethanol concentration and the distillate flow rate in the top of the rectification column); the second term penalizes raw material consumption; the third term is a quality soft constraint; the following three terms in the second line of the equation (accompanied by w_4, w_5 and w_6) are used for penalizing the energy consumption in the process (pumping power and steam consumption). Last part of the equation contains a term that penalizes the presence of water at the top of the rectification column (related to post-processing costs in the dehydration unit) and two terms associated to economic losses due to the presence of ethanol in the bottom of the columns. t_0 is the initial time for the optimization routine and Δt_{opt} is the prediction horizon over which the objective function and constraints are evaluated. Δt_{opt}=15 hours has been selected taking into account the slow dynamic response of the process to changes in its inputs.

Stage 5: Design of the Optimization-Based Control Strategy

In order to compare the one- and two-layer approaches, PWOC for the ethanol case study is addressed using these two approaches shown in Fig. 8. It must be noticed that the biomass control is run in cascade with the D-RTO layer (in both frameworks), from which it receives the optimal set point value that should be locally tracked. In both cases, the objective function to be maximized in the D-RTO layer is given by (6). The complete formulation of the optimization problem addressed in the D-RTO layers is given in (7). As can be seen, the decision variables of the optimization problem are the values for the u_{Pw}. The last inequality constraint is used inside the optimization loop for assuring that the solution of the optimization problem will guarantee a long-term ethanol concentration at the top of the rectification column (x_{ED2}) equal or higher than the concentration obtained if the plantwide manipulated variables were kept constant at u_{Pw}^* (values of the manipulated variables at the time t_0). The performance-type objective function Γ in the NMPC layer of the two-layer approach (bottom of Fig. 8) penalizes deviations of the ethanol concentration in the fermentor (E_4) and in the top of the rectification column (x_{ED2}), respectively, from their optimal set points values given by the D-RTO layer during a prediction horizon Δt_{mpc}=2 hours, as stated in (8). The terms Q and R are weighting matrices, which can be seen as tuning parameters for the NMPC. Schwartz et al. (2006) present a method for determining MPC tuning parameters that lead to optimal results from either an operational or financial standpoint. Finally, the trigger conditions used in the simulation study for addressing the PWOC problem of the ethanol process are shown in Fig. 9.

$$
\begin{aligned}
&\min_{u_{PW}} (-\Phi(\dot{x}, u, t_0, \Delta t)) \\
&\text{s.t. } f(\dot{x}, x, u, d, t) = 0 \\
&\quad x_i(t_0) = x_{0i}, u_{min} \le u \le u_{max} \\
&\quad x_{ED_2}\left(t_0 + \Delta t_{opt}, u_{PW}\right) \ge x_{ED_2}\left(t_0 + \Delta t_{opt}, u_{PW}^{*}\right)
\end{aligned}
\qquad (7)
$$

$$
\Gamma = \int_{t_{0,mpc}}^{t_{0,mpc}+\Delta t_{mpc}} Q(x_{ED2} - x_{ED2,opt})^2 dt + \int_{t_{0,mpc}}^{t_{0,mpc}+\Delta t_{mpc}} R(E_4 - E_{4,opt})^2 dt \qquad (8)
$$

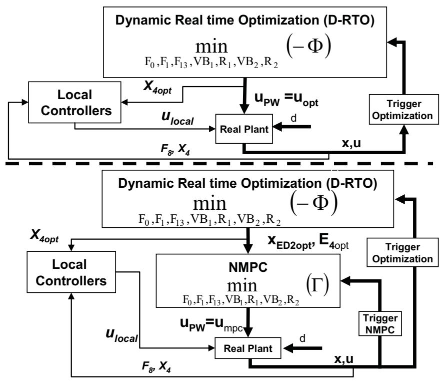

Fig. 8. Optimization-Based Control Strategies for the ethanol process: One-layer (top) and Two-layer (bottom)

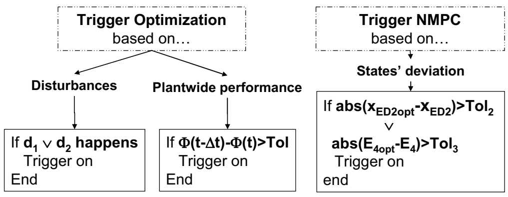

Fig 9. Trigger conditions for the ethanol PWOC: Optimization (left) and NMPC (right) layers.

The D-RTO problem was solved by the direct Sequential approach using a Monte Carlo localized random search optimization method, which is simple to implement, have broad applicability and do not require the computation of gradients (Spall, 2003). Basically, the algorithm consists of three main steps. First, an initial guess θ_0 of the optimal point is randomly picked and the number of iterations *k*, is set to zero. Second, an independent random vector d_k is generated, and added to the current optimal value θ_k. Third, it is checked if $-\Phi(\theta_k+d_k) < -\Phi(\theta_k)$; if this condition is satisfied, the new optimal value is set as $\theta_{k+1}=\theta_k+d_k$, otherwise, the second step is repeated (random generation of d_k). The algorithm stops when either, the maximum number of iterations has been reached or a convergence criterion has been fulfilled. For testing the PWOC approach, simulation studies were carried out using the nonlinear model of the process as the real plant. Results presented in this Section correspond to the simulation of the system starting at an optimal steady state. After 6 hours of operation at this steady state, a disturbance on the starch feed concentration enters the process (20% reduction of the starch concentration). At this moment, the optimization trigger is switched on and the D-RTO layer is called in order to calculate the new values for the plantwide manipulated variables that drive the process to optimal operation (maximal profitability). The localized random search method was used as previously explained for maximizing the profitability objective function, subject to the constraints given in (7). The optimization algorithm was selected to be run each time during 50 iterations after making a balance between performance and computational time for real-time implementation. The shrinking approach described in Section 4 was used for reducing the search space of the optimization problem. Specifically, the gain factors w_{ij} and $w_{i\Phi}$ in (3) were calculated using Digraphs. After calculating the gain factors, the standard deviation σ_{ui} of the Gaussian distribution that describes the probability of change of each manipulated variable for rejecting the disturbances was calculated as the maximum between different contribution terms. Then, precisely this Gaussian distribution for each manipulated variable was used for generating the vector d_k, in order to allow the optimization algorithm to make moves only in the region described by these distributions. Fig. 10 and 11 show the simulation results obtained of applying the PWOC to the ethanol case study, in presence of a disturbance on the feed concentration. PWOC was run using the two optimization-based control frameworks shown in Fig. 8. The first of these frameworks is the PWOC-one-layer (solid line) and the second is the PWOC-two-layer (dashed line). These two approaches are compared to the behaviour of the process when two different decentralized PID schemes are used, which in the following are denoted as: Decentralized 1 (described at the beginning of this section) and Decentralized 2. The only difference between both decentralized schemes is that in Decentralized 2, the E_4-G_2-F_0 loop is replaced by a D_2-F_0 loop, in order to keep constant the flow of product that goes to the dehydration unit. At this point it is important to remark that all the control approaches compared in this section use the Local Control Strategy mentioned in the Stages 1-3 of this Section, as part of the local control loops in the regulatory level. In the following Figures, the term *Two-layer SP* is used for denoting the set point values of the state variables E_4, x_{ED2} in the NMPC layer and for X_4 in the local control loop. These set point values are given by the D-RTO layer: $E_{4sp}=E_{4,opt}$, $x_{ED2,sp}= x_{ED2,opt}$ and $X_{4sp}=X_{4,opt}$. Also, the set point values for the state variables controlled in the decentralized schemes (including biomass concentration in the fermentor) correspond to the starting steady state values. Results shown in Fig. 10 are related to the fermentation section. It can be seen that using PWOC (both the one- and two-layer) results in a lower ethanol concentration in the fermentor than when using Decentralized schemes. Decentralized 1 achieves the highest ethanol concentration (E_4), which is not surprising because one of its control objectives is precisely to keep E_4 at its set point (original steady state value); and it is doing so by feeding a lower substrate flow rate (F_0), as shown in Fig 10-top-right. Fig 10-bottom-left shows the dynamic behaviour of the biomass concentration. It can be seen that both PWOC approaches keep a lower biomass concentration, due to the fact that they are actually tracking the optimal set point value, given by the D-RTO layer, and not just maintaining a fixed set point value (as done in the Decentralized schemes). At this point, analyzing the process as conventionally done as if it were conformed just of a fermentation unit, wrong conclusions could arise, in which decentralized strategies will be claimed suitable enough or even, much better than the optimization-based approaches. However, it must be noticed that independently of the control scheme, the product of a bio-ethanol plant (after dehydration) is ethanol at purity higher or equal than 99.6% wt. Since the profitability of the plant is closely related to the net flow of this final product, and the latter is proportional to the net flow of ethanol in the fermentor output, which is given by $E_4 \times F_4$ (ethanol concentration × total output flow in the fermentor), then it can be concluded that the one- and two-layer approaches would lead the process to higher cumulative profitability values than the decentralized, because their total net flow of ethanol at the fermentor output is higher (See Fig. 10-bottom-right) in spite of their lower ethanol concentration. These results are confirmed in Fig 11, where the benefits of the PWOC approaches and the drawbacks of the decentralized schemes become evident when the profitability objective function (Fig 11-top) is compared for the different control approaches. Analyzing Fig 11, it is possible to conclude that PWOC results in a much more effective response to the disturbance than the Decentralized schemes, from an economical point of view. Specifically, the PWOC-one-layer reaches the highest cumulative profitability for the process, having at the same time the highest cumulative production rate and a higher ethanol concentration than the decentralized architectures. The PWOC-two-layer allows at the beginning a small decrease of its objective function (when compared to the initial value), despite the fact that this approach drives the process towards the highest product concentration (Fig 11-bottom-left). However, for the first 20 hours after the disturbance appearance, the two-layer approach kept the profitability on average at the same value than the starting steady state, and after this, it was able to improve its objective function value, reaching even at the end the same optimal value than the one-layer. Furthermore, it can be seen that the Decentralized schemes result not only in lower profitability, but also in lower product concentration and in the case of Decentralized 1, in the lowest cumulative flow of product. Of course, it can be argued that the product concentration resulting in the decentralized schemes is lower because precisely these controllers are doing their jobs regulating the controlled variables at their set point values. However, it must be noticed that regulation of the controlled variables at fixed set points might deteriorate the profitability of the process, because when a disturbance enters the process, the optimal operating point may also move. How much this point moves can not be generalized because it depends on the process and the nature of the disturbances, and in many cases disturbances can not be predicted. If well it is completely true that over the years process industry has been operating under fixed set point policies relying on PID SISO loops, without reporting enormous economical losses, it is also true as stated by Prett and García (1988), that the apparent savings in doing so (i.e. minimization of both design effort and maintenance) are in majority of cases nonexistent and in the long run result in more costs than the use of multivariate techniques. Following the analysis in Fig 11, comparing only the decentralized approaches, it is clear that Decentralized 2 is more convenient from an economic view, because at the end of the period, at least it reaches a profitability value close to the starting point, despite of resulting in less ethanol concentration in the fermentor (Fig 10-top-left).

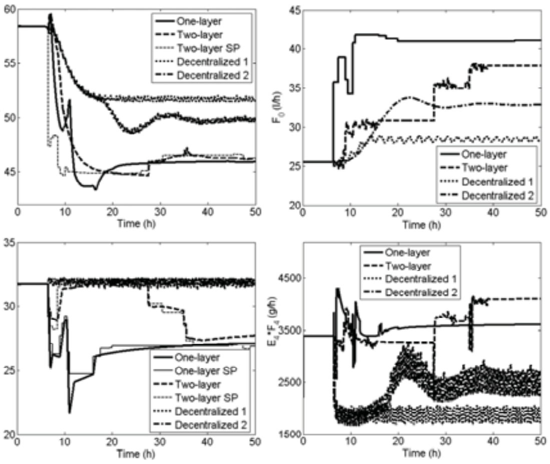

Fig. 10. PWOC results vs. decentralized control for the fermentation section: Ethanol Concentration (top-left), Starch Input Flow (top-right), Biomass Concentration (bottom-left) and Ethanol Net Flow (bottom-right).

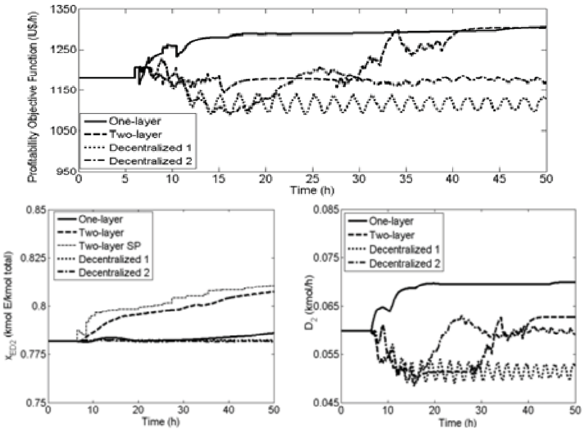

Fig. 11. PWOC results vs. Decentralized Control: Plantwide Profitability (top), Ethanol concentration in the distillate (left) and Distillate flow rate (right) at rectification section.

A final remark about the PWOC schemes should be done. If well both approaches reach the same profitability value at the end of the period (50 hours), and the two-layer has an optimal behaviour from a performance point of view (which is its "final" objective function), it might not be satisfactory at all from an economic view. Finally, it is important to highlight that independently of the optimization-based control framework selected (one or two-layer), the PWOC improves the profitability of the process when compared to the decentralized control strategies, and thus, it is a promising alternative for addressing the plantwide control problem of chemical or biochemical processes in which the profitability of the process is at risk when disturbances appear. On the other hand, in order to evaluate the performance of the shrinking approach, several simulation studies applying the PWOC with shrinking and without shrinking the search region of the optimization problem were carried out. Fig. 12 shows the advantages of the shrinking approach. By running the optimization algorithm using the same number of iterations in the two cases, the shrinking approach has not only achieved a higher profitability, but also applied smoother control actions, which is an important fact for the stability of the process and is in general desirable.

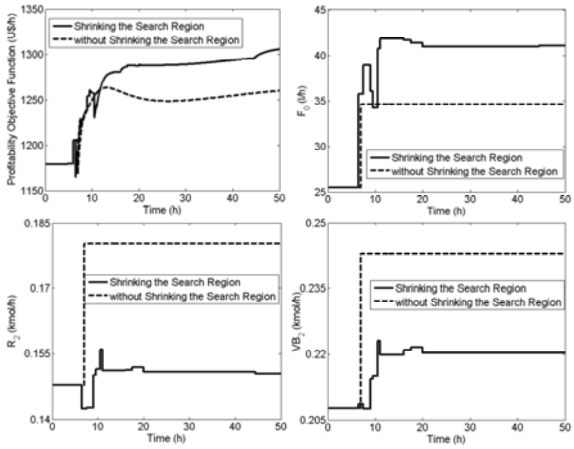

Fig. 12. One- layer PWOC: Shrinking vs. without Shrinking the Search Region. Profitability (top-left), Starch Input Flow (top-right), Reflux rate in the rectification (bottom-left) and Vapour flow rate to the rectification (bottom-right).

Analyzing the profiles for F_0, R_2 and VB_2 (Fig 12), it can be seen that when no shrinking is used (dashed lines) each manipulated variable change in a step-type policy with higher amplitude and longer period than when using shrinking (solid lines). Finally, it must be noticed that the main advantage of using the shrinking approach is that the probability of change for each manipulated variable is a function of the capability that each of them has for rejecting each disturbance (or the number of disturbances that occur at the same time, including those unknown), that means that the optimization algorithm does not waste time testing large changes in the manipulated variables that just reject in a weak way (or are not able to reject) the disturbances. When no shrinking is used, each manipulated variable is allowed to change from its lower to its upper bound, without any restriction, whereas the shrinking approach bounds the search region according to the standard deviation calculated for each manipulated variable, and it is precisely this standard deviation that contains the information about the cause-effect relationship between each manipulated variable and each disturbance.

6. CONCLUSIONS

A Plantwide Optimizing Control (PWOC) approach for bioprocesses has been presented based on the Optimizing Control concept. The main stages for PWOC and a stochastic-based shrinking approach for reducing the search space of the optimization problem have been introduced. PWOC has been applied to the bio-ethanol process, showing much better results from an economical point of view than when the process is only controlled by conventional control loops. It has been shown that PWOC is a very promising alternative for controlling chemical or biochemical processes in which the economical feasibility is at risk when disturbances appear. Finally, the shrinking approach was successfully tested resulting in an improvement of the optimization routine for real-time applications (i.e. higher productivities were obtained for the same number of iterations during optimization). Future work will be directed towards extending the shrinking approach for being applied with deterministic optimization methods.

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