

# Model-Based Supervisory Control Structure for Plantwide Control of a Reactor-Separator-Recycle Plant

Hilda M. Moscoso-Vasquez, Gloria M. Monsalve-Bravo, and Hernan Alvarez\*

Departamento de Procesos y Energía, Facultad de Minas, Universidad Nacional de Colombia—Sede Medellín, Medellín 050041, Colombia

ABSTRACT: This work presents a methodology for designing a supervisory control structure in plantwide control (PWC). First, available PWC structures are discussed focusing on their drawbacks originating from the scarce flexibility and simplicity when implementing them in industrial environments. To overcome this, a hierarchical approach to PWC is proposed that introduces a two-layer control structure, where the regulatory layer dynamics are classified by hierarchical association and their set points are optimized on the supervisory layer to achieve collaboration among proportional-integral-derivative (PID) controllers. Here, the dynamics hierarchy is established by means of the process Hankel matrix that quantifies the effect of all input variables over each state variable of the plant. Finally, the proposed methodology is applied to a reactor-separator-recycle system for propylene glycol production, where a better process performance is reached using the hierarchical approach in comparison with a decentralized control structure.

#### ■ INTRODUCTION

The main characteristic of large-scale systems is that they consist of several interacting components. For chemical plants, mass and energy interactions represent a major obstacle when dealing with the plant control and optimization. Studies in this field have revealed that plantwide control (PWC) offers a promising solution to this problem. However, current implementation of such a control strategy is driven by economic, environmental, and safety concerns, relegating the importance of process dynamics in the plant optimization.<sup>1-3</sup>

In recent years, advances on PWC have focused on the development of control strategies for each level on the control hierarchy of a process plant: regulation, supervision, optimization, and programming. So far, PWC design methodologies have been focused on the structural decisions that must be taken on the regulatory layer<sup>1,4-6</sup> or in the design of the optimization layer,<sup>7-10</sup> solving the control problem in the regulatory or supervisory layer with MPC or optimal controllers. However, efforts in the industrial implementation of PWC strategies have failed because of the high complexity of available structures, computational requirements, and the inexistence of a simple yet formal approach to the problem.<sup>3,11</sup> Therefore, current industrial practice involves the use of local controllers with local control objectives for each unit, the integration of these objectives being hardly ever possible.<sup>12</sup> These local controllers are often proportional-integral (PI) or proportional-integral-derivative (PID) because of their simple structure and easy implementation. 13 Their reliability and practicality allow them to be easily operated without requiring expert personnel. However, because they do not consider the effect of their local control actions into the performance of the whole system, they may drive the system to undesirable control loop performance, mainly because each of the unit outputs are disturbances for other units and vice versa. 12,13

In order to overcome PID control issues, the incorporation of a coordination layer arises as the solution for integrating upper layers in the control hierarchy (optimization, plant programming)

with the control layer and thus reconcile the different models used in these layers to improve control quality. 7,11,14 The main challenge when designing these nonlinear controllers is to get a good performance, characterized by stability, time response, and accuracy, despite the presence of extreme nonlinearities in the plant.11

Considering that it is essential to find control layouts of easy implementation and tuning that at the same time use process knowledge, 3,11 this work presents a methodology for designing control structures that offer good performance with simple architectures, so they can be practical for industrial implementation. Given that an appropriate design of the lower layers can yield a good overall control performance without compromising the simplicity required for the system, 6,15 criteria based on the dynamic behavior of the process is presented in order to assess the design of PID controllers used in the regulatory layer. Additionally, the integration of a model-based supervisory layer contributes to optimization of the plant operation 14 by reflecting the rationale from the process design phase 16 and considers system performance criteria in opposition to the usual economic guided design. 7,8,17

This work is organized as follows. First, a review of the currently available control structures for PWC is done, identifying the approaches used to obtain the most common structures and discussing the main advantages and issues about each structure. In addition, a brief discussion of multivariate control strategies is made toward selecting the most appropriate one for the control policy in the supervisory layer. Then, the proposed model-based supervisory control structure is presented in detail, introducing the criteria for establishing the dynamics hierarchy and the methodology for designing both regulatory and supervisory

Received: July 1, 2014 November 15, 2014 Revised: Accepted: December 3, 2014



layers. Finally, the proposed methodology is implemented in a reactor—separation—recycle system assessing the supervisory control structure performance compared to the traditional decentralized approach.

# ■ APPROACHES TO PLANTWIDE CONTROL

Over the past 40 years, different structures have been developed and applied for PWC, namely: *centralized, distributed, hierarchical*, and *decentralized*.<sup>7,15,18</sup>

In decentralized control structures, the supervisory layer is absent. This kind of control structure involves the use of multiple PID controllers for each process variable or process unit.<sup>7</sup> Despite the fact that they are not the best way of solely controlling a highly interactive process, 12 they represent a suitable way to design the control system in the control layers of the plant hierarchy (controlled variables and input-output pairings). 1,5,6,18-21 For this purpose, multiloop control strategies<sup>22,23</sup> can be applied for the design of the regulatory layer in this approach, when the selection of controlled and manipulated variables is not straightforward. In this matter, the methodology of Alvarez and Espinosa<sup>6</sup> for selecting inputoutput pairings using the singular value decomposition (SVD) of the Hankel matrix is recommended for the design of the regulatory layer given its good performance compared with other approaches such as the SVD of the process matrix or relative gain array (RGA).

In contrast, in centralized control structures, the process control and optimization are performed by a single controller, without a supervisory or coordination layer. Traditionally, such a controller is a model predictive control (MPC) which includes a complete model of the plant with a plantwide objective function for the control input calculation. <sup>24,25</sup> Considering that MPC controllers have a large computational load attributed to robustness and reliability problems and communication bandwidth limitations, which is an issue that many times shades their good performance, the implementation of centralized architectures in many cases results being impractical and inflexible. <sup>9,18,24,26</sup>

Distributed and hierarchical structures represent good alternatives when dealing with control of chemical processes since they can incorporate the interactions in the system for its operation. These structures have several advantages regarding centralized and decentralized structures, thanks to the incorporation of predictive control and handling of time-varying constraints for the control system operation. 18 Distributed control systems involve exchange of information among local controllers to regulate the complete plant.<sup>2,12,27</sup> In these structures, the most common controllers are MPCs which, at each time step, must complete three main tasks: (i) compute the local control inputs, (ii) transmit their decisions about the local control actions, and (iii) negotiate with the other controllers which control action should be applied. 12,27 This type of control strategy deals with the same problems of centralized control, inherited from the usage of MPC controllers.<sup>3</sup>

There are two alternatives for distributed control: (i) cooperative and (ii) collaborative or coordinated. <sup>18,25,27</sup> The key difference between both alternatives is the incorporation of a supervisory layer in the coordinated structures. The coordinator in such a layer moderates the demands of individual controllers based on knowledge of the interactions among the operating units and, by an iterative procedure, correctly finds the optimal strategy for plantwide operation. <sup>2</sup> Coordination is achieved trough one of three policies: <sup>2</sup> (i) the *price-driven*, (ii)

the resource allocation approach, and (iii) the prediction-driven coordination. These are based on how the available resources are used by each individual controller. However, there is no complete interaction structure linking a subsystem with the others; rather, a subsystem interacts only with a few neighbors.<sup>28</sup> In both schemes the controllers can optimize a local objective function (as in cooperative structures) or a global one (as in coordinated structures).

Finally, the basic principle of hierarchical control is decomposition of the large-scale system into several smaller subsystems and coordination of the resulted subsystems that lead to an optimal solution.<sup>29</sup> Generally, these structures involve an optimization level which determines the optimal values of the controlled variables to the regulatory layer, comprised by MPC controllers. 9,25 These structures can also involve a coordination (supervisory) layer between the optimization and control layers, which assigns to each controller a feasible set point to achieve the control objectives set on the optimization layer. The supervisory layer then allows the integration of an optimization level when the regulatory layer is under either decentralized or distributed schemes and generally consists of an MPC or an optimal control policy. The coordinator in these structures consists of a sophisticated controller that is equipped with constraint handling and optimization capabilities. 11,16 Coordination generally involves plant economics criteria 14,30 and can be achieved under Mesarovic et al.<sup>31</sup> principles: interactions prediction and balance of interactions.

Regarding the multivariate control policy for the supervisory controller, MPC controllers are the most used within distributed and hierarchical control structures, obtaining satisfactory results. However, the derivation of the control law is more complex than the classical PID controllers, and its computation must be performed in every sampling time.<sup>32</sup> Furthermore, although MPC-based structures allow the integration of dynamic interactions in the process for its control, the usage of linear models within these structures restrict their operation to a close vicinity of the operating point in which the process model was linearized. Another drawback of MPC controllers is the absence of tools for their tuning, a task that becomes even more complicated as a compromise between speed of response, decoupling of the loops, and robustness must be found.<sup>33</sup>

The possibility of achieving optimal plantwide performance through coordinated structures (hierarchical or distributed) represents a great motivation toward developing such structures. However, it must be considered that most applications involve MPC controllers which have an uneven success rate across the industry, attributed to their dependency on the multiple technical decisions that have to be made by the control engineer in the course of an implementation,<sup>34</sup> and the large investments required accompanied by the care and attention from control experts. Therefore, in order to promote the industrial application of such structures, in this work a PIDbased hierarchical control structure is proposed. Here, the coordination of PID controllers is made under the Mesarovic et al.<sup>31</sup> balance of interactions principle, extracting the dynamic interactions from the process model and using them to optimize the regulatory layer controllers set points. This would provide a better computational performance from simplifying the base-controller structure, and reduction of possible communication bottlenecks, given that no communication among controllers is required.

# DESIGN PROCEDURE FOR MODEL-BASED SUPERVISORY CONTROL STRUCTURES

As mentioned in the past section, the major drawbacks of the available PWC structures are their complex structure and communication demands, along with high computational requirements when nonlinear MPC controllers are used within these structures. The design procedure herein proposed aims to obtain a control structure with good performance but with a simple structure for its implementation on industrial environments. In order to reduce control efforts when regulating processes with strong dynamic interactions, the proposed control strategy establishes a dynamics hierarchy, allowing the classification of process variables in (i) main or critical dynamics (MaD) constituted by one dynamic behavior that relates both process dynamic characteristics and process objective, which means that MaD regulation allows the guaranteeing of product quality; and (ii) secondary or noncritical dynamics (SeDs), constituted by the other process dynamics. This classification has the advantage of (i) requiring lower control efforts since only the MaD is regulated instead of controlling every process dynamics on their nominal values and (ii) manipulating SeDs set points in an optimal way. In this way, the regulation of the MaD is achieved with less effort since the possible control actions are focused where they give better results. This approach is inspired in collaborative structures in distributed MPCs, in which controllers are optimally coordinated to achieve regulation of the whole plant. 18,29

This procedure allows the design of a two-layer hierarchical control structure, as can be seen from Figure 1: (i) regulatory

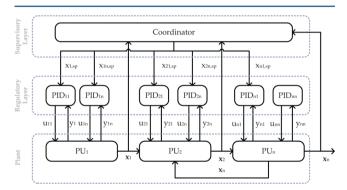


Figure 1. Proposed supervisory control structure.

layer (RL), which deals with MaD and SeDs control, and (ii) supervisory layer (SL), where SeDs set points are optimized based on the phenomenological-based model (PBM) of the process, minimizing the deviation on the MaD and reducing the control efforts on the MaD control loop. Although hierarchical control structures usually include an optimization level, its design is out of the scope of this work. Ochoa et al., Marquez et al. Marquez e

Table 1 presents the design procedure for the supervisory control structure that can be applied for either multivariate or plantwide control problems. It is based on the procedure proposed by Skogestad,<sup>4</sup> where the process analysis stage corresponds to the top-down analysis and the design of both regulatory and supervisory layers correspond to the bottom-up analysis. In the latter, a modification is made for including the design of the supervisory level. Each step is be explained in detail in the following sections.

**Stage 1: Process Analysis.** In this stage of the procedure, the process PBM is developed, the state variables and available manipulated variables in the process are identified, and the operating point of the plant is established.

Step 1: Development of a Process PBM. As a consequence of chemical processes complexity, modeling has become a necessary and useful tool to understand and design processes. Considering that the final use of a model determines its structure, for control purposes the model must be insensitive to parameter changes.<sup>4</sup> Therefore, PBMs are suitable for this purpose. This kind of model usually is a nonlinear state—space model based on mass and energy balances that includes constitutive equations that can be either empirical or phenomenological and can be obtained following the methodology presented by Alvarez et al.<sup>36</sup>

In the proposed procedure, this type of model is used for the control structure design. Considering that the proposed control structure requires information regarding dynamic interactions in the process, the model must represent it as accurately as possible for the sake of the performance of the resulting control structure.

Although obtaining a PBM of the whole plant is a difficult and arduous task, large-scale models can be obtained by dividing the system into less complex parts (individual process units or processing stages). This can simplify the modeling task since PBMs for individual process units can be found and would only require validation of the parameters for its use in this procedure.

Step 2: Identification of Available Manipulated Variables and States of the Process. The available manipulated variables  ${\bf u}$  and the state variables  ${\bf x}$  of the process are determined from the PBM. This is made bearing in mind that all the decisions regarding controlled variables are made over the state variables, assuming that the process state is completely measured or estimated which makes  ${\bf y}={\bf x}$ . Additionally, a controllability analysis is required to evaluate whether the state behavior can be affected by process inputs.<sup>4</sup> This analysis can be performed with either graph theory, <sup>37</sup> set theory, <sup>38,39</sup> or use of the condition number or the singular value decomposition of the process matrix.<sup>4</sup> This property should be considered before the control system is designed.<sup>37</sup>

Step 3: Definition of the Process Operating Point and Span of State and Input Variables. The process operating point is a given value of the state variables vector that represents a mathematical equilibrium point of the model. This means that the derivative of a given state variable with respect to time is equal to zero at this point. On the other hand, the span of the state variables is determined with the process safety limitations. The span of the manipulated variables is determined with both safety limitations and available final control elements in the plant.

**Stage 2: Regulatory Layer Design.** On the regulatory level the individual controllers for process units are designed. Here, the control configuration is established, as well as the input—output pairings and the controller tuning.

Step 4: Establishment of Controller Configuration. In this step the following decisions are made: 4 selection of measured, controlled, and manipulated variables and the determination of the control configuration.

(a). Measured Variables. Within the total state control (TSC) paradigm embraced in this work, all state variables are either measured or estimated through a state observer.

Table 1. Proposed Plantwide Control Structure Design Procedure

	step	analysis tools and comments	model requirements					
	Stage 1: Process Analysis							
1	development of a process PBM	nent of a process PBM mass and energy balances; modeling procedure						
2	identification of available manipulated variables and states of the process	ariables and controllability analysis performed with either graph theory, set theory, or singular values						
3	definition of the process operating point and span of state and input variables	operating point and span of						
	Stage 2: Regulatory Layer							
4	establishment of controller configuration	PID (simple structure of easy implementation)						
5	selection of input-output pairings for each process unit	pairing analysis: SVD of Hankel matrix	linear discrete-time model					
6	controller tuning	single-loop PID controllers; possible ratio or cascade control	linear/nonlinear model					
	Stage 3: Supervisory Layer							
7	determination of dynamics hierarchy	SVD of the Hankel matrix; selection of main dynamics (regulatory control) and secondary dynamics (tracking control)	linear discrete-time model					
8	coordinator design	formulation of the optimization problem; determination of MaD sensitivities to SeDs	nonlinear model					
9	establishment of triggers for the optimization	selected according to the designers' desire; possible triggers: time frame, deviations on main dynamics, deviations on cost functional, $J$						

(b). Control Configuration. This procedure takes advantage of PID controllers for its implementation, given that current industrial practice aims toward fewer new designs and operation of the existing facilities in new ways<sup>3</sup> and that tuning rules for PID controllers are widely available. <sup>19,42–44</sup> Here, the task of overcoming PID controller drawbacks corresponds to the model-based supervisory layer. <sup>14</sup>

(c). Controlled and Manipulated Variables. The selection of controlled variables is made through a control degrees of freedom (DoF) analysis in the system. This allows the determination of the number of variables that must be controlled in the system. Despite the TSC paradigm embraced here, this number can be lower than the total state variables. In this case, the relevance of each state variable is considered, through the  $SII_{x_k}$  calculation (see eq 5) that determines which of the state variables should be controlled.

Step 5: Selection of Input–Output Pairings. Any of the available multiloop control strategies can be used to determine the input–output pairings. Of these strategies, the SVD of the Hankel matrix has proved to have good results because it considers the dynamic behavior of the process. The Hankel matrix,  $\mathcal{H}$ , defined by (1), represents the input–output behavior of the system, since it relates a sequence of past inputs to future outputs.

$$\mathcal{H} = \begin{bmatrix} \mathbf{C}_d \\ \mathbf{C}_d \mathbf{A}_d \\ \dots \\ \mathbf{C}_d \mathbf{A}_d^{n-1} \end{bmatrix} [\mathbf{B}_d \ \mathbf{B}_d \mathbf{A}_d^{n-2} \ \dots \ \mathbf{B}_d \mathbf{A}_d^{n-1}]$$
(1)

The SVD of the Hankel matrix, presented in (2), is used to obtain a quantitative measure of the dynamic influence of each process variable and establish the input—output parings accordingly.<sup>6</sup> Such quantitative measure involves the euclidean norm of the corresponding input and output entries of the singular vectors  $(V_i \text{ and } U_i)$  with the singular values as given by (3) and (4), respectively.

$$\mathcal{H} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\mathrm{T}} \tag{2}$$

$$III_{u_k} = \sqrt{\sum_{i=1}^{p} \sigma_{ii}^2 \sum_{j=0}^{n-1} \mathbf{V}_{i,k+mj}^2}$$
(3)

$$OII_{y_k} = \sqrt{\sum_{i=1}^{p} \sigma_{ii}^2 \sum_{j=0}^{n-1} \mathbf{U}_{k+lj,i}^2}$$
(4)

where p represents the number of nonnegative singular values, i.e., the rank of the system. The matrices  $\mathbf{U}$  and  $\mathbf{V}$  are the orthonormalized eigenvectors of  $\mathcal{HH}^T$  and  $\mathcal{H}^T\mathcal{H}$ , respectively.  $\sigma_{ii}$  are the nonnegative square roots of the eigenvalues of  $\mathcal{H}^T\mathcal{H}$ , i.e.,  $\mathcal{H}$  singular values. Furthermore,  $\mathrm{OII}_{y_k}$  is the output impactability index of the kth output variable and represents the impact of process manipulated inputs  $\mathbf{u}$  as a whole over the kth output variable  $y_k$ .  $\mathrm{III}_{u_k}$  is the impact of the kth process manipulated input  $u_k$  over process outputs  $\mathbf{y}$  as a whole, called the input impactability index. It is important to highlight that the number of inputs m must be equal to the number of output variables l.

Once the  $OII_{y_k}$  and  $III_{u_k}$  of all input and output variables are computed, the input—output pairings are established by pairing the  $u_j$  with the highest  $III_{u_k}$  and the  $y_i$  with the highest  $OII_{y_k}$ . The procedure continues with the elimination of the set of variables already paired and the repetition of  $OII_{y_k}$  and  $III_{u_k}$  calculation until all of the variables are paired.

Step 6: Controller Tuning. Once pairings are established, controller tuning can be carried out using techniques for single-input/single-output (SISO) systems, because any possible interactions between control loops will be considered on the supervisory layer.

It is assumed that this layer is already available from the control system installed in the real process plant. However, most of industrial PID controllers are poorly tuned or operating in manual mode. Therefore, the criteria provided in this section can be used as performance assessment tools to verify if the existent structure is adequate for the process under analysis. Also, it must be noted that no decomposition of the plant is required to implement this procedure and all plant dynamics are considered for the design of the control structure.

Stage 3: Supervisory Layer Design. For designing the supervisory layer, the dynamics hierarchy is established first and then the optimization problem regarding the coordination policy is formulated. Here, the main tools are the process PBM developed in stage 1 and an adequate objective function.<sup>14</sup>

Step 7: Determination of the Dynamics Hierarchy. Considering that the control objective on a process is mostly a product quality related variable, the other process variables can be maintained around nominal values admitting tolerances. Therefore, control efforts can be reduced if only this qualityrelated variable is controlled on its desired set point. The determination of such a variable is a key step when designing control loops, and until now it has been highly conditioned to the designer's expertise. To tackle this, a dynamics hierarchy of the process can established taking into account that the SVD of the process matrix provides a measurement of the significance of a variable inside the system. 22 Moreover, the SVD of the process Hankel matrix provides the same information but includes the dynamic behavior of the process. Recalling that in this work all state variables are measured, the state impactability index defined in (4) can be expressed for the kth state variable, SII<sub>x</sub>. defined by eq 5. This index is thus used to determine the most important state variable within the process and define the control objective.

$$SII_{x_k} = \sqrt{\sum_{i=1}^{p} \sigma_{ii}^2 \sum_{j=0}^{n-1} \mathbf{U}_{k+nj,i}^2}$$
 (5)

here U and  $\sigma$  are found by the SVD of the Hankel matrix (see (2)), p is the number of singular values ( $\sigma$ ), U matrices are the orthonormalized eigenvectors of  $\mathbf{HH}^{\mathrm{T}}$ , and n is the number of state variables. Since the  $SII_{x_k}$  represents the effect of all the input variables over each state variable, the most important state variable in the process, i.e., MaD, will be selected as the state variable  $x_k$  with the highest  $SII_{x_k}$ .

The establishment of the dynamics hierarchy of the process facilitates the selection of the critical variable of a process in a way that the dynamic behavior of the process is completely considered. In this sense, there are no process information losses in contrast with decentralized or distributed control schemes, and without requiring any heuristic decisions, which constitutes one of the main contributions of this work.

Step 8: Coordinator Design. In this step, the objective function to be minimized with the SeD set points as degrees of freedom is formulated.

As mentioned before, the available strategies for coordination in distributed or hierarchical control structures are based on optimal or MPC control policies, which lead to high computational costs. To overcome this, and to maintain the simplicity of the control structure, the optimization is based on the interactions of MaD with SeDs under a collaborative control approach, considering that SeDs set points are selected in an optimal way so MaD is easily regulated. Here, the effect of every SeD over the MaD is exploited and explicitly extracted from the process nonlinear model with some mathematical transformations. A sensitivity-driven coordination criteria is proposed without requiring the solution of an optimal control problem. Here, sensitivity refers to a certain function,  $S_i(\mathbf{x}(t),\mathbf{u}(t)): \mathcal{R}^n \times \mathcal{R}^m \to \mathcal{R}$ , that relates the influence of each SeDs over the MaD. Such a function is obtained directly from the process model by differentiating the MaD over each SeDs from its corresponding equation on the steady-state

model of the process, considering the other SeDs constant. Therefore, the sensitivity function of the MaD regarding changes in the *i*th SeD  $x_i$ ,  $S_i$ , is given by (6).

$$S_{i}(\mathbf{x}(t),\mathbf{u}(t)) = \frac{\partial x^{*}}{\partial x_{i}} \bigg|_{x_{j\neq i}}$$
(6)

where  $x^*$  represents the MaD and  $x_i$  represents the jth SeDs, with  $i \neq j = 1, ..., n - 2$ . SeDs set points are the result of solving the optimization problem described by (7).

$$\min_{x_{1,\text{sp}},\dots,x_{n-1,\text{sp}}} J = \alpha(x_{\text{ss}}^* - x_{\text{sp}}^*) + \sum_{i=1}^{n-1} \beta_i \frac{1}{S_i}$$
(7)

 $x_{i,\text{spmin}} \leq x_i \leq x_{i,\text{spmax}}$ 

$$\Delta x_{i,\text{spmin}} \leq \Delta x_{i,\text{sp}} \leq \Delta x_{i,\text{spmax}}$$

This aims to minimize the error on the MaD and the control efforts by finding the new values of the SeDs to which the MaD is more sensitive, and therefore, will have an improved response to small changes on the SeDs.

Here the parameters of eq 7 are discussed:

- (a) x<sub>sp</sub>\* is the set point of the MaD.
  (b) x<sub>ss</sub>\* corresponds to the x\* value that would be achieved should the system reach steady state with the  $x_{i,sp}$  values determined during the optimization, extracted from the nonlinear steady-state model of the process. It is a way of predicting the future state of the process, but considering only a time step forward, in contrast to MPC that covers a larger horizon.
- (c)  $S_i$  corresponds to the sensitivity of MaD to changes on the ith SeD at the current values of the process state, which intends to drive the optimization problem toward the SeDs values that help in achieving the fastest return of the MaD to its required value.
- (d)  $x_{i,\text{spmin}}$  and  $x_{i,\text{spmax}}$  are the limiting values for SeDs set points that allow stable operation and achievement of the desired value of the MaD. These are extracted from the reachable set  $\mathcal{R}_{x}$ . The reachable set contains all of the points in the state-space to which the system can be taken from its operating point through the available control inputs. 46 In this way, this constraint allows ensuring that the control system will be able to drive the process toward new admissible set points in which the system can be stabilized. Therefore, the supervisory layer considers the controllability and stability of the process.
- (e)  $\Delta x_{i,\text{spmin}}$  and  $\Delta x_{i,\text{spmax}}$  are the maximum and minimum changes possible in the SeDs set points, limited by the actual admissible change of the manipulated variables  $\Delta u$  by the installed final control element.
- (f)  $\alpha$  corresponds to the weight of MaD error.  $\beta_i$  are scaling constants such as all  $S_i$  are on the same order of magnitude, considering that the variables are in process units, i.e., not normalized. Although there appear to be multiple parameters to be tuned, the determination of each  $\beta_i$  is made by fixing one of them constant and adjusting the others just as adjusting the proportional constant in a PID controller. The selection of the constant  $\beta_i$  is recommended to be  $\beta_i = 1$  for the  $S_i$  with the lowest magnitude order. Also,  $\alpha$  and  $\beta_i$  are selected considering the relative importance of the error on the MaD compared to the control efforts.

The objective function (7) has some relevant characteristics: (a) The effect of the disturbances over the process is known since it uses current state measurements and control actions of

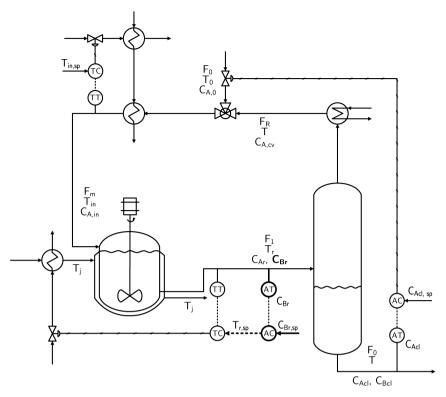


Figure 2. P&ID for the RSR system. The MaD closed loop is indicated in thicker lines than those of the SeDs closed loops.

the process to compute the sensitivities  $S_i$  instead of disregarding it as made in MPC and optimal control policies.

- (b) Steady-state sensitivities are computed with current measurements, so they are updated to account for the dynamic evolution of the system and optimize the next step for the process. The proposed optimization considers only the following time step with an algebraic expression, while MPC has a larger set of control inputs to be determined (control horizon) over a larger time horizon (prediction horizon) by solving the differential equations that compose the model.
- (c) As the core of the optimization problem, the process PBM is used with some mathematical transformations (explicit differentiation) but maintaining all its information about the process. In this way, information that was not directly available can be obtained and exploited for process control. In contrast, MPC controllers use the process model as an on-line simulation tool to select the control action by predicting process outputs within a prediction horizon, which increases its complexity when using a linear or a nonlinear process model.

Step 9: Establishment of Triggers for the Optimization. Some triggers can also be established for the optimization procedure because if no disturbance is affecting the system, changing the SeDs set points would not be necessary. These triggers include deviations on the value of the cost function (7) greater than 5%, for example deviations on the MaD set point greater than  $\epsilon > 0$ , when disturbances appear, or performing the optimization after a time  $t_I$ .

The optimization problem (7) should be solved using global optimization techniques in order to avoid local solutions that might be far from the desired behavior. This will provide the best values of SeDs set points that return the controlled variable (MaD) to its set point. It is worth clarifying that this procedure uses the steady-state sensitivities, thus avoiding the need for dynamic optimization procedures that would increase the

computational requirements of this layer. Also, despite using steady-state information, given that this optimization is carried out when one of the triggers is active, it results in a piecewise optimized trajectory since the process is optimized when significant changes on the process state or performance are found.

#### APPLICATION TO A BENCHMARK PROCESS PLANT

In this section the control of a plant for propylene glycol production is addressed. The considered process features a reactor and a flash column interconnected with a material recycle, known as reactor—separator—recycle (RSR) system, with a mixing point and a heat exchanger as shown in the process and instrumentation diagram (P&ID) of Figure 2. It is worth clarifying that the selection and design of the control loops therein depicted are explained further in this section.

**Stage 1: Process Analysis.** In this stage, steps 1-3 are performed.

Step 1: Development of a Process PBM. In this process, fresh feed is mixed with the condensed recycle gas stream from the flash tank. Then, the mixed stream passes through a heat exchanger where it is heated before entering the reactor. Inside the reactor, the catalytic hydrolysis of propylene oxide (A) in aqueous solution to produce propylene glycol (B) takes place  $(A + H_2O \rightarrow B)$ . The reaction is exothermic, and a cooling jacket allows the heat removal. Then, the propylene glycol is separated from all propylene oxide and the majority of the water in a flash separation column, where the product is removed on the liquid stream. The gas stream contains most of the remnant propylene oxide and water and is sent back to be mixed with fresh feed to the reactor.

The model presented is composed of (8)–(23). It consists of an ensemble of individual models for each process unit (reactor, <sup>47</sup> flash separator, <sup>48</sup> mixing point, and heat exchanger <sup>49</sup>). The aim

was to propose a simple benchmark for multivariable controller testing but maintain the process complexity of highly interacting dynamics in the chemical process. Here, each unit model will be presented independently for easier comprehension.

In the reactor, water is in excess with respect to the other reactive components, so a first-order reaction regarding the oxide concentration can be assumed.

$$\frac{dC_{A,r}}{dt} = \frac{F_{in}}{V_r} (C_{A,m} - C_{A,r}) - C_{A,r} k_0 e^{-E_a/RT_r}$$
(8)

$$\frac{dC_{H_2O,r}}{dt} = \frac{F_{in}}{V_r} (C_{H_2O,m} - C_{H_2O,r}) - C_{A,r} k_0 e^{-E_a/RT_r}$$
(9)

$$\frac{dC_{B,r}}{dt} = \frac{F_{in}}{V_r} (C_{B,0} - C_{B,r}) + C_{A,r} k_0 e^{-E_a/RT_r}$$
(10)

$$\frac{dT_{\rm r}}{dt} = \frac{F_{\rm in}}{V_{\rm r}} (T_{\rm in} - T_{\rm r}) - \frac{\Delta H k_0}{\rho C_p} C_{\rm A,r} e^{-E_a/RT_{\rm r}} - \frac{UA_s}{V_{\rm r} \rho C_p} (T_{\rm r} - T_{\rm j})$$
(11)

where  $C_{\text{A,r}}$ ,  $C_{\text{B,r}}$  and  $C_{\text{H}_2\text{O,r}}$  are propylene oxide, propylene glycol, and water concentrations in the reactor, respectively;  $T_{\text{r}}$  is the temperature inside the reactor;  $C_{\text{A,m}}$  and  $C_{\text{H}_2\text{O,m}}$  represent reactant and water concentrations in the mixing point, respectively;  $C_{\text{B,0}}$  is the initial product concentration; and  $F_{\text{in}}$  and  $T_{\text{in}}$  are the feed flow rate and temperature, respectively. Additionally,  $k_0$  is the frequency factor,  $E_{\text{a}}$  is the activation energy,  $\Delta H$  is the heat of reaction, R is the universal gas constant,  $T_{\text{j}}$  is the temperature inside the reactor jacket, and UA<sub>s</sub> is the product of the overall heat-transfer coefficient and the surface area in the reactor, respectively.  $V_{\text{r}}$  is the reactor volume,  $\rho$  is the density of the reactive mass, and  $C_p$  its heat capacity.

The separation in the flash column is considered to be isothermal. In addition, the separator pressure and level are controlled by vapor pressure and liquid level controllers. These two controllers were not included in the proposal due to their inherent decoupled behavior regarding the relevant dynamic behaviors in the process. Under this situation, a separation factor was deduced from relative volatility  $\alpha_{A,B}$  and equilibrium ratios, Ki, but compensating for nonideal operation. Normally  $\alpha_{A,B}$  and  $K_i$  are temperature-, pressure-, and compositiondependent. Considering pressure and liquid level controlled and a high difference in relative volatility, implying low propylene glycol vaporization, it is concluded that  $\alpha_{A,B}$  and  $K_i$ are only temperature-dependent. Therefore, the separation factor  $(y^*)$  is also just temperature-dependent. In (15), the vapor flow is directly related to the flash feed temperature. A correction to  $K_i$  was added in order to consider the effect of the residence time of fluids in the flash column on the separation efficiency. This correction included flash capacity and feed flow values in addition to a numeric value empirically adjusted. Assumptions about flash operations correspond to a common operative condition under automatic operation for the mentioned substances. It is worth clarifying that for other operating conditions or substances, a new parameter identification must be done.

$$\frac{dC_{A,cl}}{dt} = \frac{1}{V_l} (F_{in}C_{A,r} - F_0C_{A,cl} - F_RC_{A,cv})$$
(12)

$$\frac{dC_{B,cl}}{dt} = \frac{1}{V_l} (F_{in}C_{B,r} - F_0C_{B,cl})$$
(13)

$$\frac{dC_{H_2O,cl}}{dt} = \frac{1}{V_l} (F_{in}C_{H_2O,r} - F_0C_{H_2O,cl} - F_RC_{H_2O,cv})$$
(14)

$$y^* = \frac{1.5V_{l}\alpha}{40F_{in}} \left( \frac{C_{A,cl}}{\alpha C_{A,cl} + C_{B,cl} + C_{H_2O,cl}} \right)$$
(15)

$$C_{A,cv} = \frac{10^6 y^* \rho_A \rho_{H_2O}}{y^* (MW_A \rho_{H_2O} - MW_{H_2O} \rho_A) + MW_{H_2O} \rho_A}$$
(16)

$$C_{\rm H_2O,cv} = \frac{10^6 (1 - \rho_{\rm A} y^*) \rho_{\rm H_2O}}{y^* MW_{\rm A} \rho_{\rm H_2O} + MW_{\rm H_2O} (1 - \rho_{\rm A} y^*)}$$
(17)

$$F_{\rm R} = \frac{T_{\rm r} - 273}{500} \tag{18}$$

In (12)–(17),  $C_{\text{A,cl}}$ ,  $C_{\text{B,cl}}$  and  $C_{\text{H}_2\text{O,cl}}$  are reactant, product, and water concentrations in the liquid stream exiting the flash column, respectively; and  $C_{\text{A,cv}}$  and  $C_{\text{H}_2\text{O,cv}}$  are the reactant and water concentrations in the gas stream of the flash column. Furthermore,  $y^*$  represents a separation factor, and  $\alpha$  is the relative volatility between the product and the reactant.  $V_1$  is the liquid volume in the column,  $F_R$  is the recycle flow rate, and  $F_0$  is the flow rate of the liquid stream, which is the same as the fresh feed flow rate.  $MW_A$ ,  $MW_{\text{H}_2\text{O}}$ ,  $\rho_A$ , and  $\rho_{\text{H}_2\text{O}}$  are the molecular weights and densities of reactant and water, respectively.

In the mixing point, the condensed gas stream from the flash column and fresh feed are combined instantaneously. The algebraic equations that describe this stage are presented in (19) and (20), where  $C_{\rm A,0}$  and  $T_{\rm 0}$  are the feed reactant concentration and temperature, respectively.

$$C_{A,m} = \frac{F_{R}C_{A,cv} + F_{0}C_{A,0}}{F_{in}}$$
(19)

$$T_{\rm m} = \frac{F_{\rm R}T_{\rm r} + F_0T_0}{F_{\rm in}} \tag{20}$$

$$C_{\rm H_2O,m} = \frac{F_{\rm R}C_{\rm H_2O,cv} + F_0C_{\rm H_2O,0}}{F_{\rm in}}$$
(21)

$$F_{\rm in} = F_{\rm R} + F_0 \tag{22}$$

In the heat exchanger, only reactor feed temperature is considered since no chemical reaction occurs in this unit.

$$\frac{\mathrm{d}T_{\rm in}}{\mathrm{d}t} = \frac{F_{\rm in}}{V_{\rm hx}} (T_{\rm m} - T_{\rm in}) + \frac{U_{\rm hx} A_{\rm hx}}{10^3 V_{\rm hx} \rho_{\rm hx} C_p} (T_{\rm cf} - T_{\rm in}) \tag{23}$$

where  $U_{\rm hx}$  is the overall heat-transfer coefficient in the heat exchanger;  $A_{\rm hx}$  and  $V_{\rm hx}$  are the heat-transfer area and volume of the heat exchanger, respectively;  $\rho_{\rm hx}$  and  $C_p$  are the process fluid density and heat capacity, respectively; and finally  $T_{\rm cf}$  is the temperature of the cooling fluid.

Step 2: Identification of Available Manipulated Variables. As indicated in Table 2, the system has eight state variables and seven input variables. Of these,  $T_0$ ,  $C_{\rm A,0}$ ,  $C_{\rm B,0}$ , and  $C_{\rm H_2O,0}$  correspond to the feed temperature and composition, respectively, and are considered disturbances. Therefore, the

Table 2. Operating Point of the Propylene Glycol Plant

variab	ole	value	span
$C_{A,r}$	$x_1$	645.9965 mol/m <sup>3</sup>	$0-4000 \text{ mol/m}^3$
$C_{\rm B,r}$	$x_2$	726.98127 mol/m <sup>3</sup>	$0-10^6 \text{ mol/m}^3$
$C_{\rm H_2O,r}$	$x_3$	49491.054 mol/m <sup>3</sup>	$0-4 \times 10^6 \text{ mol/m}^3$
$T_{\mathrm{r}}$	$x_4$	324.822 K	273-350 K
$C_{\mathrm{A,cl}}$	$x_5$	689.3169 mol/m <sup>3</sup>	$0-4000 \text{ mol/m}^3$
$C_{B,cl}$	$x_6$	1025.183 mol/m <sup>3</sup>	$0-10^6 \text{ mol/m}^3$
$C_{\rm H_2O,cl}$	$x_7$	47865.168 mol/m <sup>3</sup>	$0-4\times10^6~\text{mol/m}^3$
$T_{ m in}$	$x_8$	311.5025 K	273-400 K
$F_0$	$u_1$	$0.25267 \text{ m}^3/\text{min}$	$0-0.5 \text{ m}^3/\text{min}$
$T_{j}$	$u_2$	330 K	273-373 K
$T_{ m cf}$	$u_3$	290 K	275-373 K

available input variables are  $F_0$ ,  $T_{\rm j}$ , and  $T_{\rm cf}$ . In this step a controllability analysis is performed with the linear model of the process. The system verifies the full-rank condition of the controllability matrix.

Step 3: Definition of the Process Operating Point and Span of State and Input Variables. Table 2 presents the operating point of the process and the span of state and input variables.

**Stage 2: Regulatory Layer Design.** On the regulatory level the individual controllers for process units are designed. Here, steps 4–6 take place.

Step 4: Establishment of Controller Configuration. As mentioned in the previous section, it is considered that all state variables are measured or estimated and that the available controllers are PIDs. For selecting the controlled variables, a control DoF analysis is carried out. Since there are only three available manipulated variables, the degrees of freedom of the system are three. Then three controlled variables must be chosen for designing the control structure. The importance of each state variable is considered, through the  $SII_{x_k}$  (see eq 5) for the selection of controlled variables, whose values are reported in Table 3.

Table 3. State Impactability Indexes for the Propylene Glycol Plant

variable	SII	variable
$C_{ m B,cl}$	0.6643	
$C_{ m B,r}$	0.5069	MaD
$C_{ m A,cl}$	0.5050	SeD
$T_{ m in}$	0.4986	SeD
$T_{ m r}$	0.4562	SeD
$C_{ m A,r}$	0.2741	SeD
$C_{ m A,r} \ C_{ m H_2O,cl}$	0.0026	SeD
$C_{\mathrm{H_2O,r}}$	0.0003	SeD

In this case,  $C_{\rm B,cl}$ ,  $C_{\rm B,r}$  and  $C_{\rm A,cl}$  are the most important variables and should be controlled. However, since there is no

vaporization of B in the column,  $C_{\rm B,cl}$  and  $C_{\rm B,r}$  can be considered as equivalent control objectives. Given that the column does not have a direct action of the control inputs,  $C_{\rm B,cl}$  is disregarded and only  $C_{\rm B,r}$  is controlled and  $T_{\rm in}$  is added as a controlled variable.  $T_{\rm r}$  is not considered since along with  $C_{\rm B,r}$  they are reactor outputs and are highly coupled with the available control action in the reactor  $(T_{\rm j};$  see (10) and (11)); contradictory effects are found if both variables are controlled independently. Thus, a cascade control is proposed with  $C_{\rm B,r}$  being the variable controlled in the master loop and  $T_{\rm r}$  the controlled variable in the slave loop.

Step 5: Selection of Input-Output Pairings for Each Process Unit. Since the controlled variables are the state variables selected in the previous step, input-output pairings are established through the  $SII_{x_k}$  and  $III_{u_k}$  defined by eq 3, which are found in Table 4.

Initially all variables are included and in this case (set A)  $T_r$  is paired with  $T_j$ . Then, these variables are eliminated obtaining set B, and according to  $\mathrm{SII}_{x_k}$  and  $\mathrm{III}_{u_k}$  values,  $C_{\mathrm{A,cl}}$  is paired with  $F_0$  and  $T_{\mathrm{in}}$  with  $T_{\mathrm{cf}}$  as can be seen from Figure 2. It is worth clarifying that the P&ID is the same for both approaches. For the decentralized approach it is the complete control system, and for the hierarchical control structure it represents the regulatory layer.

Step 6: Controller Tuning. PID tuning was made through simulation with the nonlinear model of the process, using as seed values the parameters obtained by the Ziegler—Nichols method. It is worth clarifying that PIDs for both structures have the same tuning parameters.

**Stage 3: Supervisory Layer Design.** In this final stage, steps 7–9 are performed.

Step 7: Dynamics Hierarchy. From Table 3 the state variable with the highest  $SII_{x_k}$  is  $C_{B,cl}$ . As mentioned before, since there is no product vaporization in the column, it is an equivalent control objective of  $C_{B,r}$  which has available control actions and is the state variable with the second highest  $SII_{x_k}$ . Therefore,  $C_{B,r}$  is selected as MaD and  $C_{A,cl}$  and  $T_{in}$  are the SeDs. The control structure for the process is presented in Figure 3. Despite the fact

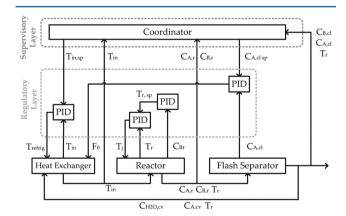


Figure 3. Hierarchical control structure for the RSR system.

Table 4. State and Input Impactability Indexes for the Propylene Glycol Plant

set A				set B			
variable	SII	variable	III	variable	SII	variable	III
$T_{ m r}$	0.2628	$F_0$	0.2494	$C_{ m A,cl}$	0.0742	$F_0$	0.1040
$C_{ m A,cl}$	0.0475	$T_{j}$	0.2577	$T_{ m in}$	0.1976	$T_{ m cf}$	0.1837
$T_{ m in}$	0.2474	$T_{cf}$	0.0617				

that the SeDs do not include all process state variables, they are needed in the supervisory level for the determination of the MaD sensitivity, as can be seen from Figure 3, and will be explained in further detail on the supervisory layer design.

Step 8: Coordinator Design. The coordinator on the supervisory layer is formulated based on (7). For this, the sensitivities of the MaD to each SeDs are required and obtained from the steady-state process model, which corresponds to (88)–(23) with all time derivatives equal to zero. Since  $C_{\rm B,r}$  is not a direct function of the secondary dynamics, a directed graph is used to determine the derivation path that allows one to obtain all sensitivity functions. A directed graph (DG) is a qualitative causal model which captures the information flow in the model and can be obtained from the nonlinear model of the process. The DG for the RSR process is presented in Figure 4, where the gray nodes indicate input variables and the black nodes indicate process variables (state and algebraic variables). State variables correspond to nodes with a curved arrow exiting the node and entering the same node.

From the DG it is possible to identify the following paths for each sensitivity:

(1)  $S_1$ , i.e., the sensitivity of  $C_{\rm B,r}$  to  $T_{\rm in}$ , is found according to eq 24, corresponding to the path marked by the bold dashed lines in Figure 4.

$$S_{1} = \frac{\partial C_{B,r}}{\partial T_{in}} = \frac{\partial C_{B,r}}{\partial T_{r}} \frac{\partial T_{r}}{\partial T_{in}}$$
(24)

where

$$\frac{\partial C_{\text{B,r}}}{\partial T_{\text{r}}} = \frac{500V_{\text{r}}k_{0}C_{\text{A,r}}e^{-E_{\text{a}}/RT_{\text{r}}}[E_{\text{a}}(500F_{0} + T_{\text{r}} - 273) - RT_{\text{r}}^{2})}{RT_{\text{r}}(500F_{0} + T_{\text{r}} - 273)^{2}} + \frac{500V_{\text{r}}k_{0}C_{\text{A,r}}e^{-E_{\text{a}}/RT_{\text{r}}}}{500F_{0} + T_{\text{r}} - 273}\frac{\partial C_{\text{A,r}}}{\partial T_{\text{r}}} \tag{25}$$

$$\frac{\partial C_{A,r}}{\partial T_r} = \frac{RC_{A,m}T_r(1+k_0e^{-E_a/RT_r}) - 500C_{A,m}k_0E_ae^{-E_a/RT_r}(500F_0+T_r-273)}{500V_rRT_r^2(1+k_0e^{-E_a/RT_r})} + \frac{500F_0+T_r-273}{500V_r(1+k_0e^{-E_aRT_r})} \frac{\partial C_{A,m}}{\partial T_r} \tag{26}$$

$$\frac{\partial C_{m,r}}{\partial T_r} = -\left(\frac{1}{C_{A,cl}\left(Mw_A\rho_{H_2O} - Mw_{H_2O}\rho_A\right) + Mw_{H_2O}\rho_A\left(\alpha C_{A,cl} + C_{B,cl} + C_{H_2O,cl}\right)}\right) \\
\left(\frac{75 * 10^6 V_1 \alpha C_{A,cl}}{\left(500F_0 + T_r - 273\right)^3}\right) - \frac{500F_0 C_{A,0}}{\left(500F_0 + T_r - 273\right)^2}$$
(27)

$$\frac{\partial T_{\rm r}}{\partial T_{\rm in}} = \frac{500F_0 + T_{\rm r} - 273}{500F_0 + T_{\rm r} - 273 + \frac{500V_r k_0 C_{\rm A,r} \Delta H k_0}{\rho C_p} e^{-E_{\rm a}/RT_{\rm r}} - T_{\rm in} + T_{\rm r}}$$
(28)

(2)  $S_2$ , i.e., the sensitivity of  $C_{B,r}$  to  $C_{A,cl}$ , is computed with (29). Here it is worth noticing that this derivation path corresponds to the effect of the recycle stream on the reactor product concentration and is indicated by the solid bold lines in Figure 4.

$$S_{2} = \frac{\partial C_{B,r}}{\partial C_{A,cl}} = \frac{\partial C_{B,r}}{\partial T_{r}} \frac{\partial T_{r}}{\partial C_{A,r}} \frac{\partial C_{A,r}}{\partial C_{A,m}} \frac{\partial C_{A,m}}{\partial C_{A,cv}} \frac{\partial C_{A,cv}}{\partial C_{A,cl}}$$
(29)

Obtaining these derivatives from the process model, it is found

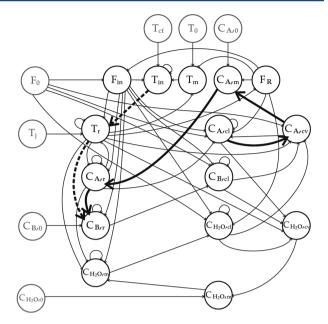


Figure 4. Directed graph for the RSR.

$$\frac{\partial C_{\text{B,r}}}{\partial C_{\text{A,r}}} = \frac{\frac{500V_r \Delta H k_0^2 e^{-2E_a/RT_r}}{\rho C_p (500F_0 + T_r - 273)}}{\frac{500F_0 + T_r - 273}{500V_r} - \frac{\Delta H k_0 E_a C_{\text{A,r}} e^{-E_a/RT_r}}{R \rho C_p T_r^2} - \frac{UA}{V_r \rho C_p}}$$
(30)

$$\frac{\partial C_{A,r}}{\partial C_{A,m}} = \frac{500F_0 + T_r - 273}{500F_0 + T_r - 273 + 500V_r e^{-E_a/RT_r}}$$
(31)

$$\frac{\partial C_{\text{A,m}}}{\partial C_{\text{A,cv}}} = \frac{T_{\text{r}} - 273}{500F_0 + T_{\text{r}} - 273}$$
(32)

and finally

I

$$\frac{\partial C_{A,cv}}{\partial C_{A,cl}} = \left( \frac{75 \times 10^6 V_{l} \alpha}{4(500 F_0 + T_r - 273)(\alpha C_{A,cl} + C_{B,cl} + C_{H_2O,cl})^2} \right) \times \left( \frac{1 - \frac{y * (MW_A \rho_{H_2O} - MW_{H_2O} \rho_A)}{\rho_A \rho_{H_2O}}}{\left( \frac{y * (MW_A \rho_{H_2O} - MW_{H_2O} \rho_A)}{\rho_A \rho_{H_2O}} + \frac{MW_{H_2O}}{\rho_{H_2O}} \right)^2} \right) \tag{33}$$

In (25)–(33)  $T_r$ ,  $C_{\rm B,cl}$  and  $C_{\rm H_2O,cl}$  are the current values of these state variables, measured or estimated.  $F_0$  also corresponds to the current value of the fresh feed flow rate, and it should not be expressed with the PID control law in order to avoid effects of the controller tuning over the objective function.

Once the sensitivities are determined, the constraints for the SeDs must be found. These are extracted from the reachable set of the process. The obtained set is  $\mathcal{R}_{3000}$  which considers all of the x  $\epsilon$   $\chi$  that can be reached from the operating point in Table 2 in 3000 min. For obtaining this set, a Monte Carlo approach was used, considering the admissible control inputs with a uniform distribution and taking 35000 samples to guarantee that all of the admissible combinations of inputs are covered. It is worth clarifying that this task is only performed off-line during the design of the supervisory layer. Since the system has eight state variables, a graphic representation of the reachable set is not possible and only the values regarding the MaD and

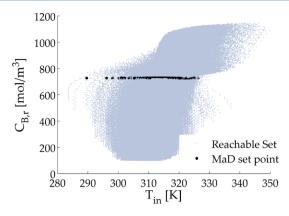


Figure 5. Reachable set for the RSR system:  $C_{B,r}$  vs  $T_{in}$ .

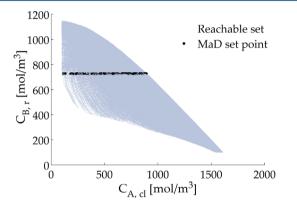


Figure 6. Reachable set for the RSR system:  $C_{B,r}$  vs  $C_{A,cl}$ .

SeDs are shown. The SeDs bounds are then determined by means of Figures 5 and 6, where the black dots represent the values of the MaD set point. Here, the scattered regions of the set  $\mathcal{R}_{3000}$  are not considered to avoid uncertainty over unstable or uncontrollable regions, and thus, the boundaries for each secondary dynamics at  $C_{\text{B,rsp}} = 726.98 \text{ mol/m}^3$  are 310 K  $\leq T_{\text{in}} \leq 320 \text{ K}$  and 500 mol/m $^3 \leq C_{\text{A,cl}} \leq 900 \text{ mol/m}^3$ .

Therefore, the optimization problem to be solved by the supervisory layer is given in (34), also considering as constraints on the SeDs changes the maximum heating rate in the heat exchanger (2 K/min) and maximum changes of 1.5% on  $C_{\rm A,cl}$  per minute, determined by inherent conditions of the process such as valve selection.

$$\min_{T_{\text{in}}, C_{\text{A,cl}}} J = \alpha (C_{\text{Br,ss}} - C_{\text{Br,sp}}) + \beta_1 \frac{1}{S_1} + \beta_2 \frac{1}{S_2}$$
s.t.  $310 \text{ K} \le T_{\text{in}} \le 320 \text{ K}$ 

$$500 \text{ mol/m}^3 \le C_{\text{A,cl}} \le 900 \text{ mol/m}^3$$
 $0 \le \Delta T_{\text{in}} \le 2 \text{ K/min}$ 
 $0 \le \Delta C_{\text{A,cl}} \le 0.015 C_{\text{A,cl}} \text{ mol/m}^3$ 

In this case,  $\alpha=10$ ,  $\beta_1=0.025$ , and  $\beta_2=1$  and were determined by reducing  $\beta_1$  if the response on either  $T_{\rm in}$  or  $T_{\rm cf}$  was too oscillatory using the same criteria as when adjusting  $K_{\rm p}$  in a PID controller. This optimization problem is then solved by a global optimization method, in this case, a genetic algorithm. The optimization is carried out using Matlab's genetic algorithm for constrained optimization. For this, a maximum of 100 generations were considered, migrating 20% of individuals every

20 generations and a doublevector population for constraint handling.

Step 9: Establishment of Triggers for the Optimization. In this case, the presence of disturbances and deviations greater than 3% on the MaD were defined as optimization triggers.

#### RESULTS

The proposed control structure is compared to the traditional decentralized approach when disturbances on feed concentration appear. First, at 50 min it is reduced on 9.5% of its nominal value, and at 700 min it is increased to 30% of its nominal value. The subscripts dec and hier in Figures 7-13

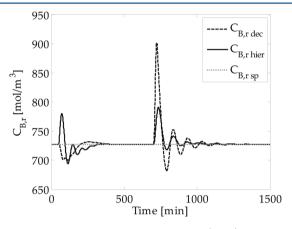


Figure 7. Product concentration in the reactor (MaD).

represent the decentralized (independent PIDs) and hierarchical (obtained with this proposal) approaches, respectively. The main dynamics response is presented in Figure 7 using both approaches. For the hierarchical approach, it can be seen that a lower magnitude overshoot of  $C_{\rm B,r}$  is obtained with a less oscillatory behavior and a faster return to its set point after both disturbances.

For the first disturbance, it is worth noticing that the direction of the response through both approaches is different: with the decentralized approach  $C_{\rm B,r}$  tends to diminish while with the hierarchical approach it tends to increase. This behavior can be attributed to the different set point determined for  $C_{\rm A,cl}$  by the hierarchical approach in which it reduces. This reduction increases the amount of A in the recycle stream entering to the reactor, producing more B. On the other hand, in the decentralized approach, the amount of A recirculated drops and, therefore, B production in the reactor must decrease.

Reactor temperature set points and its response with both approaches are presented in Figures 8 and 9. Recalling that  $T_r$  is the manipulated variable for  $C_{\rm B,r}$  lower control efforts for controlling the MaD are required since smaller changes on  $T_{\rm r}$  are required. Additionally, a faster return to the MaD is achieved as evidenced by the less oscillatory behavior  $T_{\rm r}$  compared to the decentralized approach, which is a desirable response for safety and security reasons. This is also supported by the performance indexes for  $C_{\rm B,r}$  control loop presented in Table 5, where it can be seen that with the hierarchical approach a reduction of 40% on the absolute error of the MaD is obtained, with a reduction of the control efforts of 35% compared with the decentralized approach.

The response of jacket temperature,  $T_{\rm r}$  manipulated variable in this cascade loop, is shown in Figure 10. It can be seen that the usage of the final control element is higher in the

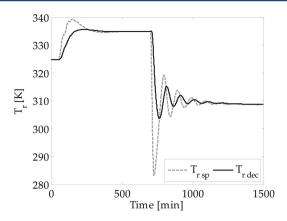
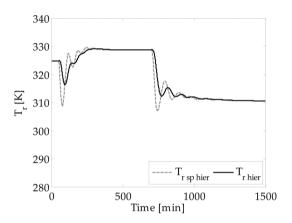


Figure 8. Reactor temperature response with the decentralized approach.



**Figure 9.** Reactor temperature response with the proposed hierarchical approach.

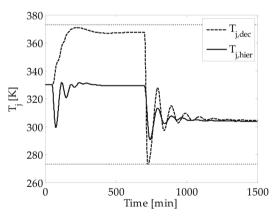


Figure 10. Jacket temperature response.

decentralized approach and it lies closer to the saturation limits than the hierarchical approach. Also, less oscillatory behavior is obtained with the hierarchical strategy which means that the associated control valve will not deteriorate as much as with the decentralized approach.

Reactor input temperature is presented in Figure 11 with both approaches. Given that  $T_{\rm in}$  is a SeD, with the hierarchical approach its set point is changed with respect to its nominal value to a higher temperature which aids in reactor temperature regulation as depicted in Figure 10. For both disturbances the decentralized approach is not able to maintain  $T_{\rm in}$  on its nominal value, demanding higher control efforts as can also

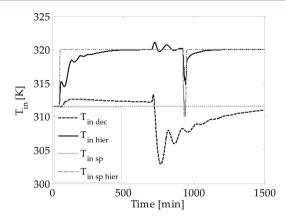


Figure 11. Reactor input temperature (SeDs) response.

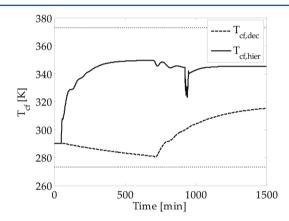


Figure 12. Cooling fluid temperature response.

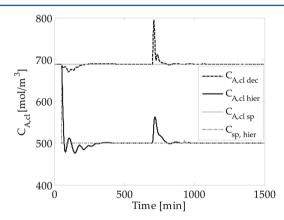


Figure 13. Reactant concentration in liquid phase from the separation column (SeDs).

be seen from Table 5. On the other hand, the hierarchical approach is able to regulate  $T_{\rm in}$  in its new set point.

Here, the property of speeding up the controllers' response of the hierarchical approach is evidenced in Figure 12 since the manipulated variables reach their stationary state faster than they do with the decentralized approach. Additionally, by relaxing the  $T_{\rm in}$  set point, lower performance indexes are obtained for this loop, with lower integral of absolute error (IAE) and time-weighted absolute error (ITAE) indexes, as shown in Table 5. Despite the fact than the IAU index indicates a greater variability of the control action in the hierarchical approach, its time-weighted integral (ITAU) is lower compared to the decentralized approach.

Table 5. Performance Indexes for the Propylene Glycol Plant

controller	index	decentralized	hierarchical	% difference
$C_{\mathrm{B,r}}$	IAE	$12.2 \times 10^{3}$	$7.32 \times 10^{3}$	-40.0
	ITAE	$7.8 \times 10^{6}$	$3.5 \times 10^{6}$	-55.2
	IAU	148.7	95.8	-35.5
	ITAU	$104.1 \times 10^3$	$41.4 \times 10^{3}$	-60.2
$T_{ m r}$	IAE	$3.0 \times 10^{3}$	$1.48 \times 10^{3}$	-50.6
	ITAE	$19 \times 10^{5}$	$7.06 \times 10^{5}$	-62.9
	IAU	275.6	178.2	-35.3
	ITAU	$187.9 \times 10^{3}$	$77.9 \times 10^{3}$	-58.5
$T_{ m in}$	IAE	$26 \times 10^{2}$	$8.6 \times 10^{2}$	-66.9
	ITAE	$22 \times 10^{5}$	$3.4 \times 10^{5}$	-84.6
	IAU	44.9	77.4	72.4
	ITAU	$36.7 \times 10^{3}$	$11.5 \times 10^{3}$	-68.7
$C_{A,cl}$	IAE	$3.8 \times 10^{3}$	$6.9 \times 10^{3}$	83.1
	ITAE	$1.8 \times 10^{6}$	$2.6 \times 10^{6}$	42.8
	IAU	$11 \times 10^{-1}$	$5.43 \times 10^{-1}$	-50.7
	ITAU	536.4	198.9	-62.9
plantwide performance	DPT	$309.1 \times 10^3$	$137.4 \times 10^3$	-55.6

The response of  $C_{A,cl}$  with both approaches is presented in Figure 13, where a displacement to lower values of the  $C_{A,cl}$  set point is again achieved with the hierarchical approach. However, as evidenced from IAE and ITAE indexes in Table 5 the difference between  $C_{A,cl}$  and its set point is greater with the hierarchical approach. Additionally, lower control efforts for the  $C_{A,cl}$  control loop are obtained with the hierarchical approach, but this was an expected result given the loosened regulation of the variable. Here, the hierarchical approach exhibits an advantageous behavior since a lower usage of the final control element is achieved, as shown in Figure 14. After the first

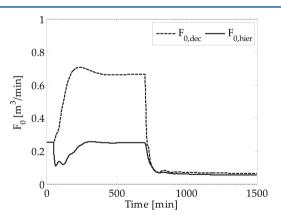


Figure 14. Fresh feed flow rate.

disturbance, in the distributed approach the flow rate required to maintain  $C_{A,cl}$  is higher so there would be a smaller margin of variation should other disturbance on the same direction appear.

Finally, performance indexes for all control loops with both approaches are presented in Table 5. For almost all control loops, reductions of more than 50% on IAE, ITAE, IAU, and ITAU are obtained, which implies a much better performance of the hierarchical control structure than the decentralized approach.

Of these results, two points are worth highlighting. First, is that both SeDs set points were changed by the supervisory

layer, relaxing the demands over these controllers and obtaining better performance indexes. Second, the regulation of the MaD was achieved in a faster way with lower control efforts, aided by the variation of the SeDs set points, as seen from the performance indexes of Table 5. This was also obtained despite the higher absolute error of one of the SeDs, revealing that not every dynamics in a process must be regulated for achieving the control objective. Therefore, compared to the decentralized approach where interactions in the process are not fully integrated to its control, by means of the proposed procedure the dynamic response of the MaD controller was improved by including said interactions in the SeDs set-points determination.

An additional index for plantwide performance was considered within this work, called the deviation on production target (DPT), which compares the actual production target with the nominal one at all times.<sup>2</sup> Considering that under the effect of disturbances it is desired that the production is not highly deviated from the desired value, this index includes performance and economic considerations, becoming very good criteria for assessing plantwide performance of a control structure.<sup>2</sup> In this case, the production target is the propylene glycol production on the liquid stream of the flash column, from which the DPT is found by means of (35).

$$DPT = \int_{t=0}^{t_s} ((F_0 C_{B,cl})_t - (F_0 C_{B,cl})_{SS}) dt$$
(35)

From Table 5 it can be seen that a significantly lower DPT is obtained through the hierarchical control structure, which reinforces the already discussed advantages of this structure.

#### CONCLUSION

In this work, a hierarchical control structure for controlling multivariable processes is proposed. One of the main contributions of this work is the usage of an index to determine a dynamics hierarchy and establish control objectives (not only control loop pairings) considering the dynamic behavior of the process. This dynamics classification inside the process is then profited for model-based coordination of noncritical state variables is to achieve the regulation of the main dynamic of the process. This represents a paradigm shift from the decoupling multivariable control strategies, since the dynamic interactions of all process dynamics are profited for its control.

Control of the main dynamics is achieved by a two-layer control structure where the regulatory layer deals with direct control of the process and the supervisory layer optimizes the set points of the noncritical state variables. This optimization is based on the process interactions extracted from its model using information gathered off-line from the process nonlinear model and on-line from process sensors. This approach allows one to control highly coupled multivariable processes improving MaD control by adaptation of the SeDs compared to decentralized control structures, as supported by controller performance indexes.

The usage of PID controllers in the regulatory layer of the proposed control structure evidences its huge potential for being implemented in already existing facilities without major resource investment. This approach arises as a possibility for controlling large-scale processes without requiring sophisticated control strategies such as MPC and promotes the possible industrial implementation of this control structure, considering that it can be easily operated and tuned using intuitive criteria by both operators or control experts. However, the appropriate

tools for solving the nonlinear optimization problem of the supervisory layer is the main challenge of implementing this strategy.

The proposed hierarchical control structure is applied to a RSR system for propylene glycol production in comparison to a decentralized structure. It is found that for disturbances on process inputs the hierarchical approach has a better outcome based on plantwide performance index criteria, obtaining lower control efforts than those required from each individual PID controller. This demonstrates that not every dynamics in a process must be regulated for achieving the control objective in a more efficient way.

#### AUTHOR INFORMATION

# **Corresponding Author**

\*E-mail: hdalvare@unal.edu.co. Tel.: +57(4) 4255332. Fax: +57(4) 2341002.

### **Notes**

The authors declare no competing financial interest.

#### REFERENCES

- (1) Murty Konda, N. V. S. N.; Rangaiah, G. P.; Krishnaswamy, P. R. Plantwide Control of Industrial Processes: An Integrated Framework of Simulation and Heuristics. *Ind. Eng. Chem. Res.* **2005**, *44*, 8300–8313.
- (2) Rangaiah, G., Kariwala, V., Eds. *Plantwide control: Recent developments and applications*; John Wiley & Sons: Chichester, England, 2012; p 478.
- (3) Downs, J. J.; Skogestad, S. An industrial and academic perspective on plantwide control. *Annu. Rev. Control* **2011**, *35*, 99–110.
- (4) Skogestad, S. Control structure design for complete chemical plants. *Chem. Eng.* **2004**, 28, 219–234.
- (5) Larsson, T. Studies on plantwide control. Ph.D. Thesis, Norwegian University of Science and Technology, Trondheim, Norway, 2000.
- (6) Alvarez, L.; Espinosa, J. Methodology based on SVD for control structure design. *Lat. Am. Appl. Res.* **2012**, *42*, 245–250.
- (7) Ochoa, S.; Wozny, G.; Repke, J. Plantwide Optimizing Control of a Continuous Bioethanol Production Process. *J. Process Control* **2010**, 20, 983–998.
- (8) Adetola, V.; Guay, M. Integration of real-time optimization and model predictive control. *J. Process Control* **2010**, 20, 125–133.
- (9) Aske, E. M. B.; Strand, S.; Skogestad, S. Coordinator MPC for maximizing plant throughput. *Comput. Chem. Eng.* **2008**, 32, 195–204.
- (10) Engell, S.; Harjunkoski, I. Optimal operation: Scheduling, advanced control and their integration. *Comput. Chem. Eng.* **2012**, *47*, 121–133
- (11) Lehouche, H.; Guéguen, H.; Mendil, B. Set-Point Supervisory Control Methodology for a Nonlinear. *Arabian J. Sci. Eng.* **2012**, *37*, 831–849.
- (12) Valencia Arroyave, F. Game theory based distributed model predictive control: An approach to large-scale systems control. Ph.D. thesis, Universidad Nacional de Colombia, Medellín, Colombia, 2012.
- (13) Ogunnaike, B. A.; Mukati, K. An alternative structure for next generation regulatory controllers Part I: Basic theory for design, development and inplementation. *J. Process Control* **2006**, *16*, 499–509.
- (14) Radhakrishnan, V. R. Model based supervisory control of a ball mill grinding circuit. *J. Process Control* **1999**, *9*, 195–211.
- (15) Skogestad, S. Plantwide control: The search for the self-optimizing control structure. *J. Process Control* **2000**, *10*, 487–507.
- (16) Seki, H.; Naka, Y. A Hierarchical Controller Design for a Reactor/Separator System with Recycle. *Ind. Eng. Chem. Res.* **2006**, 45, 6518–6524
- (17) Marquez, A.; Gomez, C.; Deossa, P.; Espinosa, J. J. Hierarchical control of large scale systems: A zone control approach. 13th IFAC Symposium on Large Scale Complex Systems: Theory and Applications,

- Shanghai, China; International Federation of Automatic Control: Laxenburg, Austria, 2013; pp 438–443.
- (18) Scattolini, R. Architectures for Distributed and Hierarchical Model Predictive Control—A Review. J. Process Control 2009, 19, 723-731.
- (19) Skogestad, S. Simple analytic rules for model reduction and PID controller tuning. *J. Process Control* **2003**, *13*, 291–309.
- (20) Luyben, M. L.; Tyreus, B. D.; Luyben, W. L. Plantwide control design procedure. *AIChE J.* **1997**, *43*, 3161–3174.
- (21) Zumoffen, D.; Feroldi, D. Exploring alternatives for decentralized plant-wide control. XV Reunión de Trabajo Procesamiento de la Información y Control, Bariloche, Argentina; Universidad Nacional de Rio Negro: San Carlos de Bariloche, Argentina, 2013; pp 31–36.
- (22) Erickson, K. T.; Hedrick, J. L. *Plantwide process control*; John Wiley & Sons: New York, NY, USA, 1999; p 547.
- (23) Skogestad, S.; Postlethwaite, I. Multivariable feedback control; John Wiley & Sons: Chichester, England, 1996; p 559.
- (24) Stewart, B. T.; Venkat, A. N.; Rawlings, J. B.; Wright, S. J.; Pannocchia, G. Cooperative distributed model predictive control. *Syst. Control Lett.* **2010**, *59*, 460–469.
- (25) Rawlings, J. B.; Stewart, B. T. Coordinating multiple optimization-based controllers: New opportunities and challenges. *J. Process Control* **2008**, *18*, 839–845.
- (26) Garrido, J.; Vázquez, F.; Morilla, F. Centralized multivariable control by simplified decoupling. *J. Process Control* **2012**, 22, 1044–1062.
- (27) Venkat, A. N. Distributed model predictive control: Theory and applications. Ph.D. thesis, University of Wisconsin—Madison, Madison, WI, USA, 2006.
- (28) Scheu, H.; Marquardt, W. Sensitivity-based coordination in distributed model predictive control. *J. Process Control* **2011**, 21, 715–728.
- (29) Sadati, N.; Ramezani, M. H. Novel interaction prediction approach to hierarchical control of large-scale systems. *IET Control Theory Appl.* **2010**, *4*, 228–243.
- (30) Mcavoy, T. J. A methodology for screening level control structures in plantwide control systems. *Comput. Chem. Eng.* **1998**, 22, 1543–1552.
- (31) Mesarovic, M.; Macko, D.; Takahara, Y. Two coordination principles and their application in large scale systems control. *Automatica* 1970, 6, 261–270.
- (32) Camacho, E. F.; Bordons, C. Model predictive control, 2nd ed.; Springer: London, England, 2007; p 422.
- (33) Wojsznis, W.; Gudaz, J.; Blevins, T.; Mehta, A. Practical approach to tuning MPC. *ISA Trans.* **2003**, 42, 149–162.
- (34) Darby, M. L.; Nikolaou, M. MPC: Current practice and challenges. *Control Eng. Pract.* **2012**, 20, 328–342.
- (35) Dang, P. X.; Banjerdpongchai, D. Design of integrated real-time optimization and model predictive control for distillation column. *Proceedings of 2011 8th Asian Control Conference (ASCC)*, Kaohsiung, Taiwan; Institute of Electrical and Electronics Engineers: Piscataway, NJ, USA, 2011; pp 988–993.
- (36) Alvarez, H.; Lamanna, R.; Revollar, S. Methodology for obtaining phenomenological-based semiphysical models applied to a sugar cane sulphitation process (in Spanish). *Rev. Iberoam. Autom. Inform. Ind.* **2009**, *6*, 10–20.
- (37) Lee, B.; Kim, Y.; Shin, D.; Yoon, E. S. A study on the evaluation of structural controllability in chemical processes. *Comput. Chem. Eng.* **2001**, *25*, 85–95.
- (38) Sontag, E. Mathematical control theory: Deterministic finite-dimensional systems; Springer-Verlag: New York, NY, USA, 1998; p 544.
- (39) Kerrigan, E. C.; Maciejowski, J. M. Invariant sets for constrained nonlinear discrete-time systems with application to feasibility in model predictive control. *Proceedings of the 39th IEEE Conference on Decision and Control*; Institute of Electrical and Electronics Engineers: Piscataway, NJ, USA, 2000; pp 4951–4956.

- (40) Monsalve-Bravo, G. M.; Moscoso-Vasquez, H. M.; Alvarez, H. Scale-up of continuous reactors using phenomenological-based models. *Chim. Oggi (Chem. Today (Milano, Italy))* **2014**, *32*, 20–27.
- (41) Ruiz, A. A.; Alvarez, H. Scale-up of Chemical and Biochemical Processes Using a Phenomenological Model (in Spanish). *Inf. Tecnol.* **2011**, 22, 33–52.
- (42) Åström, K.; Hägglund, T. Revisiting the Ziegler–Nichols step response method for PID control. *J. Process Control* **2004**, *14*, 635–650
- (43) Cominos, P.; Munro, N. PID controllers: Recent tuning methods and design to specification. *IET Control Theory Appl.* **2002**, 19, 46–53.
- (44) Rivera, D.; Morari, M.; Skogestad, S. Internal Model Control. 4: PID Controller Design. *Ind. Eng. Chem. Proc. Des. Dev.* **1986**, 25, 252–265
- (45) Yin, H.; Zhu, Z.; Ding, F. Model order determination using the Hankel matrix of impulse responses. *Appl. Math. Lett.* **2011**, *24*, 797–802
- (46) Alzate, A. Metodology for simultaneous process and robust control design (in Spanish). M.Sc. thesis, Universidad Nacional de Colombia, Medelln, Colombia, 2013.
- (47) Bequette, B. W. Behavior of a CSTR with a recirculating jacket heat transfer system. Proceedings of the 2002 American Control Conference (ACC), Anchorage, AK, USA; Institute of Electrical and Electronics Engineers: Piscataway, NJ, USA, 2002; pp 3275–3280.
- (48) Henley, E. J.; Seader, J. D.; Roper, D. K. Separation process principles; John Wiley & Sons: Hoboken, NJ, USA, 2011.
- (49) Kuppan, T. Heat exchanger design handbook; Marcel Dekker: New York, 2000; Vol. 126.
- (50) Maurya, M. R.; Rengaswamy, R.; Venkatasubramanian, V. A Systematic Framework for the Development and Analysis of Signed Digraphs for Chemical Processes. 1. Algorithms and Analysis. *Ind. Eng. Chem. Res.* **2003**, 42, 4789–4810.