

*A DESIGN PROCEDURE FOR A SUPERVISORY
CONTROL STRUCTURE IN PLANTWIDE CONTROL*

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*A mi familia y amigos ...
incondicionales.*

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Abstract

This work presents a methodology for designing a supervisory control structure in Plant-wide Control (PWC). First, available PWC structures are discussed focusing on their drawbacks originated from the scarce flexibility and simplicity when implementing them in industrial environments. Additionally, the available control strategies involve decoupling of the process, losing all interactions information and therefore requiring more complex models inside the control structure to account for interactions among units. To overcome this, a hierarchical approach to PWC is proposed, introducing a two-layer control structure where dynamics on the regulatory layer are classified by hierarchical association considering that process dynamics and their set-points are optimized on the supervisory layer to achieve collaboration among Proportional-Integral-Derivative (PID) controllers in the regulatory layer. A 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 the decentralized proposal.

Resumen

Este trabajo presenta una metodología de diseño para estructuras de control supervisorio en control total de planta (CTP). Primero se discuten las estructuras de CTP resaltando sus limitaciones, como baja flexibilidad y simplicidad para su implementación industrial. Adicionalmente, estas estructuras involucran el desacople de las dinámicas del proceso, perdiendo la información sobre las interacciones del mismo y por ende, requiriendo modelos más complejos dentro de la estructura para dar cuenta de estas interacciones. Para superar estas limitaciones, se propone una estructura de control jerárquica, introduciendo una estructura de control con dos niveles, en la que las dinámicas en el nivel regulatorio son clasificadas jerárquicamente considerando el comportamiento dinámico del proceso y sus puntos de ajuste son optimizados en el nivel supervisorio alcanzando un esquema colaborativo entre los controladores Proporcional–Integral–Derivativo (PID) del nivel regulatorio. La jerarquía de dinámicas en el nivel regulatorio se establece por medio de la matriz de Hankel del proceso, que cuantifica el efecto de toda las variables de entrada sobre cada estado del proceso. Finalmente, la metodología propuesta se aplica para controlar un sistema Reactor–Separador–Reciclo para producción de propilenglicol, logrando un mejor desempeño usando la estructura jerárquica comparado con una estructura descentralizada.

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List of Symbols and Abbreviations

Latin Letters

Symbol	Description
A	System matrix
B	Input matrix
C	Output matrix
c_{ij}	Diagonal controller elements
d	Disturbances
D	Input related output matrix
\mathcal{D}	Decoupler matrix
d_{ij}	Decoupler matrix elements
f	State variables function vector
G	Transfer matrix
g_{ij}	Transfer matrix elements
H	Hamiltonian function
\mathcal{H}	Hankel matrix
III	Input impactability index
J	Cost functional/Objective function
K	MPC state-related function
l	Output variables vector dimension
L	MPC input-related function
m	Input variables vector dimension
n	State variables vector dimension
N_p	MPC prediction horizon
N_u	MPC control horizon
p	Matrix rank/Number of non-zero singular values
\mathcal{R}_t	Reachable set in time t
S	Constraint set for state variables
\mathcal{S}	Main dynamics sensitivity function
SII	State impactability index
t	Time
t_s	Output settling time
u	Manipulated variables vector
u(.)	Manipulated variables trajectory
U	SVD matrix composed by the left singular vectors
\mathcal{U}	Admissible input space
u_k	k -th manipulated variable
V	SVD matrix composed by the right singular vectors

Symbol	Description
\mathbf{w}	Reference trajectory vector
\mathbf{x}	State variables vector
$\mathbf{x}(\cdot)$	State variables trajectory
\mathcal{X}	State space
x_j	j -th secondary dynamics
x_k	k -th state variable
\mathbf{y}	Output variables vector
y_k	k -th output variable

Greek Letters

Symbol	Description	Unit
α	Main dynamics error weight	
β	Main dynamics sensitivities weight	
γ	Condition number	
δ	Output-related MPC tuning parameter	
Δ	Signal overshoot	
κ	Input-related MPC tuning parameter	
Λ	Relative Gain Array matrix	
λ	Lagrange multiplier	
λ_{ij}	Relative Gain Array elements	
Σ	Singular values matrix	
σ_{ii}	i -th singular value	
$\bar{\sigma}$	maximum singular value	
$\underline{\sigma}$	minimum singular value	
Ω	Input admissible set	
Ω_x	State admissible set	

Subscripts

Symbol	Description
a	Initial state
b	Final state
d	Discrete system
dec	Decentralized
$hier$	Hierarchical
max	Maximum value
min	Minimum value
s	Frequency domain system
sp	Set-point value
ss	Steady-state
$\mathbf{0}$	Initial condition

Superscripts

Symbol	Description
*	Main Dynamics
^	Predicted value
o	Optimal solution

Abbreviations

Abbreviation	Description
CN	Condition Number
CSTR	Continuous Stirred–Tank Reactor
DG	Directed graph
DPT	Deviation on Production Targets
IAE	Integral Absolute Error
IAU	Derivative action of the controller output
ITAE	Integral Time–weighted Absolute Error
ITAU	Time–weighted derivative action of the controller output
MaD	Main Dynamics
MIMO	Multi–Input/Multi–Output
MPC	Model Predictive Controllers
NI	Niederlinsky Index
PBM	Phenomenological–Based Models
P& ID	Process and instrumentation diagram
PID	Proportional–Integral–Derivative controllers
PO	Propylene oxyde
PPG	Propylene glycol
RL	Regulatory Layer
RSR	Reactor–Separator–Recycle system
SeD	Secondary Dynamics
SISO	Sulti–Input/Sulti–Output
SL	Supervisory Layer
SVD	Singular Value Decomposition

CHAPTER 1

Introduction

Plantwide control (PWC) strategies have been increasingly important given the mass and energy integration of chemical plants driven by economic, environmental and safety concerns [1]. This thesis stresses the importance and relevance of PWC, specially on industrial applications where highly interacting processes (complete plants or multivariable processes) are controlled separately by units, which do not necessarily guides the process towards its optimal operation. This problem has been a subject of interest in a plethora of research works, but their integration to industrial environments is delayed because of the complexity of the available solutions.

This work aims to propose a methodology for designing control structures that offer good performance with a simple architecture, so they can be practical for their industrial implementation. This chapter presents the background, motivation and statement of the research addressed in this thesis. Section 1.1 presents the motivating reasons for this work. The research problem and objectives to follow through with this thesis are addressed in Section 1.2 and 1.3. The main accomplishments of this work and dissemination of partial results are gathered in Section 1.4. Finally, Section 1.5 maps out the thesis outline.

1.1. Motivation

Plantwide control deals with regulation of large scale systems. The main characteristic of these systems is that they are composed by several interacting components, and thus PWC strategies can be applied to complete plants, sections of a plant or even individual processes with several coupled dynamics.

Over the last 40 years, different structures have been developed and applied for PWC, namely: centralized, distributed, hierarchical and decentralized [2; 3; 4]. However, the high computational cost associated with centralized control schemes, attributed to robustness and reliability problems and communication bandwidth limitations, is one issue that many times shades their good performance [2]. In contrast, decentralized control structures have been exhaustively studied and they represent a suitable way to design the control system in the lower layers of the structure [2; 5; 6]. However, they are not the best way of solely controlling a highly interactive process [7]. Distributed and hierarchical control 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 [2]. Distributed control systems involve exchange of information among local regulators and require a process model that includes interactions between units and uses it in each MPC controller composing the structure [7; 8; 9]. Therefore, they are subjected to uncertainty and

changes in the operating point, since they compute the control input by predicting the process output with a linearized model of the process in a single operating point. These characteristics also imply a high computational cost and high communication bandwidth requirements [10].

PWC is widely discussed in scholarly articles but is rarely found in industrial practice because of the high complexity of available structures, computational requirements and the inexistence of a simple yet formal approach to the problem [10; 11]. For these reasons, current industrial practice involves the use of local controllers with local control objectives for each component, being the integration of these objectives hardly ever possible [7]. These local controllers are often Proportional-Integral (PI) or Proportional-Integral-Derivative (PID) because of their simple structure and easy implementation [12]. Their reliability and practicality allow them to be easily operated without requiring expert personnel. However, as 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 unit outputs are disturbances for other units and viceversa [7; 12].

In order to overcome PID control issues, supervisory control strategies involve the implementation of advanced techniques (such as MPC and adaptive control). It has been applied in different industries generally to replace the use of PID controllers that, as mentioned before, can not satisfy some planning objectives [11; 13; 14; 15; 16]. Furthermore, the need for a coordination layer arises from the need for integrating upper layers in the control hierarchy (optimization, plant programming) with the control layer and thus reconciling the different models used in these layers to improve control quality [3; 11]. 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].

On the other hand, characteristics such as transparency and intuitiveness are important factors for operator acceptance and safe operation of the designed control structure [17] in an industrial environment. Therefore it is essential to find control layouts of easy implementation and tuning that at the same time use process knowledge [10; 11]. Thus, this work presents a methodology for designing control structures that offers good performance with a simple architecture, so they can be practical for industrial implementation.

Bearing in mind that an appropriate design of the lower layers can yield a good overall control performance without compromising the simplicity required for the system [4; 18], this methodology presents some criteria to assess the design of PID controllers used in the regulatory layer followed by the addition of a model-based supervisory layer that contributes to optimize the plant operation [15] by reflecting the rationale from the process design phase [17]. According to this, the model-based supervisory layer considers system performance criteria in opposition to the usual economic guided design [3; 19; 20].

Another relevant motivation for carrying out this research comes from the work of Alvarez Toro [18], in which the design of the control structure involves a controllability analysis and proposes a criteria based on Hankel matrix singular value decomposition for establishing input-output pairings in the regulatory layer according to the dynamic effect of input variables over each output of the process. Given the good performance shown by this approximation, it is taken as the departing point for the design of a supervisory layer.

Finally, Ramírez [21] suggests that a possible multivariable control structure for a coupled system could involve changes on set–points of non–critical variables on a process in an optimal way to facilitate the regulation of critical variables on their desired set–points. This idea changes the paradigm of uncoupling the dynamics on a system or regulating all of them for controlling the process, and it is the other significant motivation for this thesis, that aims to exploit this for complete plants.

1.2. Research problem

Interest on the design of control structures for PWC has grown increasingly over the last 40 years, supported on the appearance of more rigorous process design with high energetic and mass integration, represents a challenge for the control system designer since the dynamic behavior of the plant considerably increases its complexity with this integration.

Advances on PWC have focused on developing strategies for each level on the control hierarchy of a process plant: regulation, supervision, optimization and programming. So far, plantwide control design methodologies center on the structural decisions that must be taken on the regulatory layer [1; 5; 18; 22] or in the design of the optimization layer[3; 19; 23; 24], solving the control problem in the regulatory or supervisory layer with MPC controllers. These structures imply high computational loads when using the non–linear model of the process. Furthermore, its functioning is not transparent and the designer lack of knowledge of the process and its interactions is concealed by the optimization routine carried out in this controllers. Other drawbacks of MPC controllers are its high sensitivity to model uncertainties and the lack of tools for their tuning, which do not allow to clearly establish the importance and influence of each term on the objective function in controlling the process [25].

An important issue is the decomposition in operation units that must be carried out as part of the design of the control structure. This step represents large losses of information and there is no agreement on this procedure, existing several approaches but without any criteria to decide which is better for the application under investigation [10]. Additionally, available methodologies involving an optimization layer use economic criteria for optimizing the process, delegating process performance to the control layers which operate without major knowledge of the process and require the attention of experts for its operation.

Therefore, the need for a simple yet formal design procedure arises that strive away from the operating unit approach that is currently used in industrial practice [10]. This procedure must clarify all the decisions to be made when designing control structures and deal with the control problem as a whole, but operating in more efficient ways for process with high energy and mass integration [8], without using complex control structures that may be impractical in industrial applications.

In this way, the research question that conducts this work is:

How to formulate a systematic methodology for designing a supervisory control structure in PWC using the model of the process, that preserves the most information about the process while maintaining a simple architecture for its industrial implementation?

1.3. Objectives

1.3.1. General objective

Propose a design methodology for a multilevel supervisory control structure based on the dynamics classification in the regulatory level in regulation and tracking from a Phenomenological-Based Semiphysical Model (PBSM) of the process, and the application of a collaborative control scheme that uses an objective function based on the model of the process and the dynamics classification previously established.

1.3.2. Specific objectives

1. Recognize the design procedures used for the supervisory level in control structures for plantwide control.
2. Identify the design criteria used in the methodologies found for supervisory control structures, determining the strengths and limitations of the structures designed under these criteria.
3. Establish a criteria for unit partitioning on the regulatory level in regulation and tracking dynamics based on the process PBSM.
4. Formulate an objective function for the collaborative control in the supervisory level, based on the process PBSM and the dynamics classification, under stability constraints.
5. Develop a procedure for the design of supervisory control structures based on the dynamics classification and the optimization problem formulated.
6. Verify the effectiveness of the proposed methodology for the design of supervisory control structures on its application to an industrial process, based on the performance of the control system.

1.4. Major findings and dissemination of results

One of the main outcomes of this work is the usage of an index to determine a dynamics hierarchy and using it for establishing control objectives (not only control loop pairings), and controlling all the states of the process by model-based coordination of non-critical state variables to achieve the regulation of the main dynamics of the process. This represents a paradigm shift from the decoupling multivariable control strategies, since the dynamic interactions of every dynamics are profited for controlling the process.

The other main achievement of this work is the control of the main dynamics through 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 non-critical state variables based on the process performance with information gathered on-line from the process non-linear model and process sensors. This structure achieves control of highly-coupled multivariable process

and complete plants without needing sophisticated control strategies such as MPC, which is very important when considering the industrial implementation of these control strategies.

Partial results of this thesis were divulged on the following congress presentations:

H.M Moscoso y H. Alvarez. Applicability of multivariable hierarchical control strategies in chemical processes (In Spanish). In *XXVI Congreso Interamericano de Ingeniería Química*, volumen 57, p. 4. Montevideo, Uruguay, 2012.

H. M. Moscoso-Vasquez, G. M. Monsalve-Bravo, and H. Alvarez. Model-based hierarchical control of multivariable processes. In *XV Reunión de Trabajo Procesamiento de la Información y Control – RPIC 2013*, San Carlos de Bariloche, Río Negro – Argentina. ISBN 978-950-698-280-5.

H. M. Moscoso-Vasquez, G. M. Monsalve-Bravo, and H. Alvarez. An Approach to Total State Control in Batch Processes through a Distributed Control Structure. In *2013 AIChE Annual Meeting*, San Francisco, CA – United States, 2013.

1.5. Thesis outline

The main purpose of this thesis is to present a novel approach for supervisory control aiming towards a control structure with good performance yet simple for its industrial implementation. This approach is based on a two layer control structure, where dynamics on the regulatory level are classified hierarchically and their set points are optimized on the supervisory layer based on a cooperative scheme.

This thesis is organized as follows. Chapter 2 presents a review of the control structures currently available for plantwide control, identifying the approaches used for obtaining the structure and classifying the kind of structure obtained under these approaches, namely, decentralized, distributed, multi-layer (hierarchical) and centralized control structures. Selecting the hierarchical control structures, and towards the design of the coordinator on these structures, a review of available methods for multivariable process control is presented in Chapter 3 in order to select the strategy to be applied on the supervisory layer. In Chapter 4 the proposed model-based supervisory control structure is developed and presented in detail. In Section 4.4.1 the criteria for establishing the dynamics hierarchy is introduced. The design of the regulatory level is addressed in Section 4.3 and the formulation of the optimization problem to be solved by the supervisory level is described in Section 4.4.2. The methodology developed in Chapter 4 is then applied for control of a Reactor–Separation–Recycle system in Chapter 5 for assessing the control structure performance compared with the traditional approach.

CHAPTER 2

Plantwide control

The purpose of this chapter is to introduce the key concepts for the development of this research in order to establish the ground-basis for this work. In Section 2.1 plantwide control is defined. Then, the different approximations for control structure design and a classification of the available structures for plantwide control are presented in 2.2, analyzing their advantages and limitations. Finally, 2.3 gathers some concluding considerations of this chapter.

2.1. Plantwide control

Industrial chemical plants and processes usually involve many types of operations and numerous items of equipment operating at different concentrations, temperatures and pressures, often resulting in complex and large in size plants [8]. The safe and optimal operation of industrial plants require the maintenance of operating variables (temperatures, pressures and compositions) in optimal values and within safe limits under the influence of disturbances [8], demanding high reliability of the control system to achieve such operation. Moreover, chemical process design aims to minimize operating costs and maximize raw materials conversion. As a result of this, mass recycles and energetic integration are more frequent in industrial operation. These characteristics complicate the control task, and the need of designing the control system from the global process characteristics arises and originates PWC [18].

PWC refers to the synthesis and design of a control system for the complete plant considering all aspects such as throughput changes and interaction between units [8]. The interactions can either be: (i) dynamic, in the sense that the states and inputs of each subsystem influence the states of the ones to which it is connected, (ii) because of the fact that subsystems share common goals and constraints or (iii) both [26]. In this way, the dynamic behavior of one unit is subjected to other units dynamics and the relations become more complex with increasing mass recycles and energetic integration [18; 27]. This increases the complexity of the dynamic behavior of the plant and thus induces great variability on product quality and characteristics [28]. Interaction among units are intricate and thus the PWC problem should not be addressed as an extension of individual units control, since interconnections reduce the number of degrees of freedom and special care must be taken in not under or over specifying the control objectives of the process plant [29].

In PWC, the structural decisions and control law for the complete process plant are determined, instead of the design and tuning of the individual controllers. These decisions include [4; 5; 29]:

1. **Controlled variables selection:** variables whose set points are defined by the optimization layer (if existent) or by the process manager. For their selection, there are two main approaches (i) self-optimizing control [4] and (ii) according to the plantwide operation goal [30]. Regardless of the approach, the controlled variables must fulfill the following requirements [4]:
 - Its optimal value should be insensitive to disturbances.
 - It should be easy to measure and control accurately.
 - Its value should be sensitive to changes in the manipulated variables.
 - For cases with two or more controlled variables, they should not be closely correlated.
2. **Selection of manipulated variables:** inputs of the system, i.e., valves and pumps location or energy inputs to the process. They must be selected such as they guarantee process controllability, while having a significant and rapid effect over the controlled variables.
3. **Measured variables selection:** They depend on a balance between the measurement costs and the enhancement of the control system, and are ideally selected through a process observability analysis. However, on industrial environments they are selected mostly through heuristic approaches. Additionally, they should be related to the controlled variables.
4. **Controller configuration:** selection of the controller that connects the measured variables, set-points and manipulated variables [30]. This includes the control law that is going to be applied to the whole process. This structure is determined by vertical decomposition (hierarchical structures) or horizontal (decentralized structures) [2]. For complete PWC design, parameters of these feedback controllers, ratio or cascade control loops and so on also need to be specified. Complexity of PWC is then inferred from the numerous PID controllers in a typical process plant [8].

When dealing with process plants, the design of the control structure is a troublesome task given the high number of possibilities for selecting the controlled, manipulated and measured variables inherited from the size and complexity of the plant. As a way of simplifying this task, a system with enough size or natural hierarchical structure (such as process plants) can be decomposed in subsystems and be manipulated in a way that the plantwide objectives are accomplished. [23; 31; 32]. In these hierarchical structures some controllers have direct influence over the lower layers instead of having it over the process itself [32]. In this way, upper layers establish the set-points for the layers below them and also receive information from these layers as to have complete knowledge of the feasible regions for these set-points and the disturbances that influence the process [2].

If the plant is decomposed according to time scales, the following layers are obtained, as shown in Fig. 2.1 [2; 30].

On the *Plant programming and scheduling layer* the determination of plant objectives is set according to managerial and marketing decisions. The *Optimization layer* deals with the economic optimization (via Real Time optimization, RTO, or Dynamic Real Time Optimization, DRTO) of the plant, allowing the determination of the optimal values of the controlled variable when the operating conditions change, thus defining the controlled variables for the

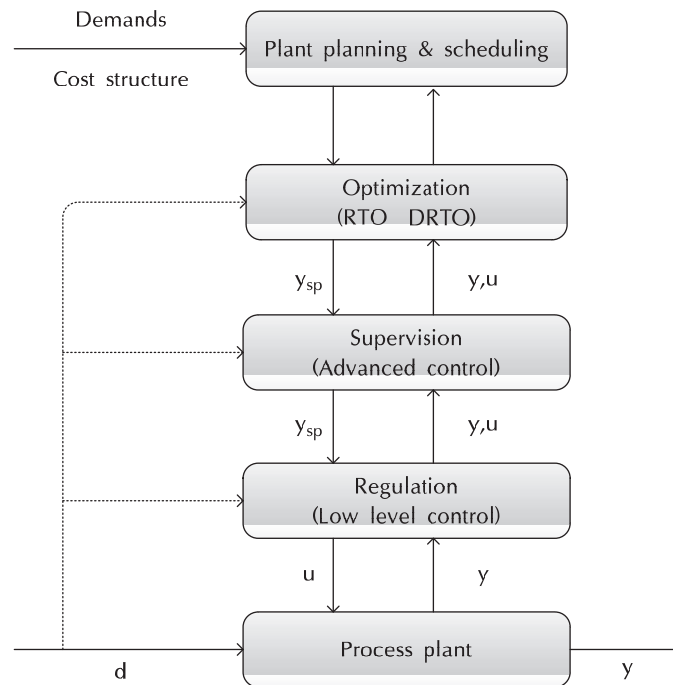


FIGURE 2.1. Control hierarchy in PWC.

supervisory layer and their set-points [3; 19]. The objective of the *Supervisory layer* is to control the outputs of the process using the set-points of the regulatory layer controllers as manipulated variables. Here, the usage of one or more Model Predictive Controllers (MPC) is frequent given the requirement of multivariable controllers in this layer [24]. This layer can also perform some simple optimization routines in specific parts of the plant [18] and this characteristic is exploited in this research work. The *Regulatory layer* normally consists of ubiquitous Proportional–Integral–Derivative (PID) controllers which directly manipulate mass and energy flow to the each operating unit [8; 33], and includes ratio or cascade controllers if they exist. Lately, the implementation of MPC controllers in this layer allows the usage of only one controller per each operating unit [34].

The control problem regarding to large, complex and networked systems is commonly solved splitting the problem and applying local modeling and control techniques to the smallest and more manageable subsystems [5; 20]. Such partitioning is not natural, and the subsystems should not necessarily exchange the proper information leading to an unexpected behavior [20].

Several approaches have emerged for process decomposition. The first is the *horizontal decomposition* in which the plant is partitioned in individual pieces of equipment. This approach has always been used in industry, and its main advantages are the many effective control schemes that have been established over the years for individual units. However it is highly inefficient when the level of mass and energy integration rises [5]. The second approach is the *hierarchical decomposition* in which the process partitioning is made under five possible patterns: different level of abstraction, complexity, capacity of decision-making, functional decomposition of the problem and based on temporal issues [20]. Despite the im-

portance of this critical issue, there is no unifying criteria for determining the best approach for decomposing a particular problem.

According to the configuration of the subsystems a different control structure can be obtained as will be described in the following section.

2.2. Classification of PWC strategies

PWC structures can be classified according to the configuration of the control system and the control law defined for the process under four large groups: *decentralized*, *distributed*, *hierarchical*, and *centralized* as shown in Fig. 2.2. These structures can be obtained from different approaches or methodologies: heuristic, mathematical, optimization-based and combined approaches.

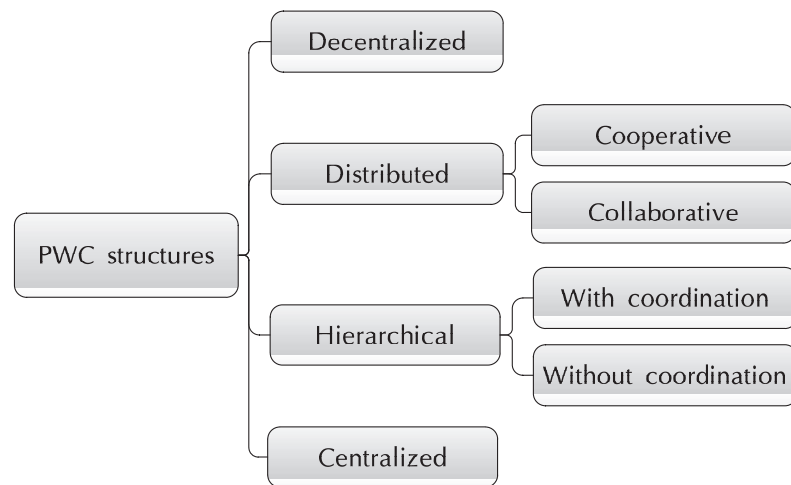


FIGURE 2.2. PWC control structures

On the *Heuristic approach* all structural decisions are given by the expertise of the designer. Although they are easy to understand and implement [8; 27], they are also highly dependent on the designer expertise since they include a detailed analysis of the importance of each control objective [27] and can also consider the influence of the mass and energy recycles over the process performance [1]. Therefore, if the knowledge of the process is deficient, a good performance of the control system can not be assured. The *mathematical approach* uses a model of the process (either dynamic or stationary) for the selection of the control structure by means of tools as the Relative Gain Array (RGA), Condition Number (CN), Niederlinski Index (NI) and Singular Value decomposition (SVD) [8].

Optimization-based approaches integrate both control and optimization tasks, using tools as Mixed Integer Linear Programming (MINLP) and Mixed Integer Non-Linear Programming (MINLP) for selecting the optimal structure with economic or process performance criteria [8; 35] either with a model of the process [22] or process data [36]. This approach is supported by the postulate of Morari et al. [29] and Skogestad [22]:

“We want to find a function c of the process variables which when held constant, leads automatically to the optimal adjustments of the manipulated variables, and with it, the optimal operating conditions...”

The main inconvenient with these approaches is that the optimization is performed with a given set of values for the disturbances and therefore the optimal solution only applies if the disturbance is within the interval considered, also requiring the measurement of the disturbances that enter the process. Among the methodologies developed in the last 10 years combined approaches are preferred, combining heuristic, mathematical and optimization tools to obtain more effective control structures.

As mentioned before, the control structures obtained by either one of these approaches can be classified in four groups which are described in the following subsections.

2.2.1. Decentralized

In these structures only the regulatory layer is present, and according to this it involves the employment of multiple PID controllers (C_i) for each controlled variable or process unit (PU_i) [3], as can be seen in Fig. 2.3. The main advantage of these structures is that they do not require a detailed model of the process.

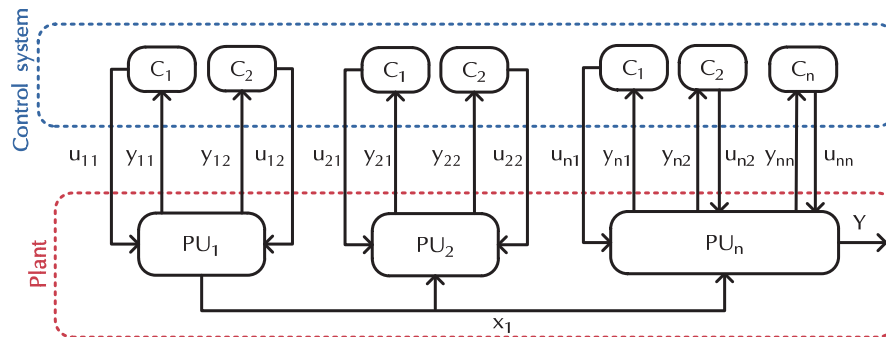


FIGURE 2.3. Decentralized control structures

Despite their simplicity, these structures are most recommended for processes with low interactions and with time-invariant constraints, which is not always the case of chemical processes. However, some processes can be decomposed in a family of independent problems with much simpler structure in a way that each sub-problem can be considered as a low interacting system, but preserving interactions among sub-problems through interaction variables.

Skogestad [4] and Alvarez Toro [18] suggest that an appropriate design of the lower layers would grant robustness to the upper layers of the structure, without compromising the simplicity required for the lower layers. According to this, it is not surprising to find many methodologies for determining the best set of controlled variables and the input-output pairings for controlling them, such as the proposals of Murty Konda et al. [1]; Alvarez Toro [18]; Skogestad [22]; Luyben et al. [27]; Zumoffen and Feroldi [37]. Recent approaches to decentralized process control use graph theory for determining the optimal input-output pairing by reducing the overall structural coupling of the process network [38].

2.2.2. Distributed

Unlike the decentralized control structures, the controllers in distributed control structures can communicate in order to control the complete plant. 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 its decisions about the local control actions and (iii) negotiate with the other controller which control action should be applied [7].

According to the communication protocol there are two alternatives for distributed control: *Cooperative* (see Fig.2.4) and *Collaborative* (see Fig. 2.4) [2; 39].

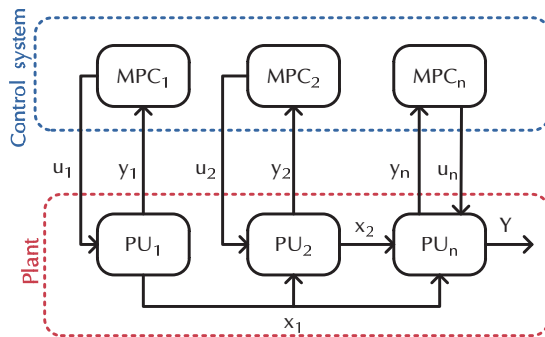


FIGURE 2.4. Cooperative distributed control structures.

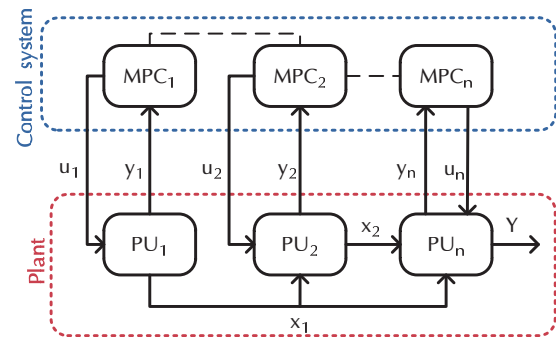


FIGURE 2.5. Collaborative distributed control structures.

Cooperative structures are based on cooperative game theory, in which all the players aim to a global goal but there is not actual communication between them [9]. For control systems, this means that each MPC controller optimizes the same objective function (global control objectives) but no information is shared between them. These systems consider the effect of the interactions over the whole process, which are included during the resolution of each controller's optimization problem. With these structures, the plant reaches a Pareto optimal [7], which yields a plant performance very close to that obtained with a centralized structure. However, the time required for the convergence of the optimization problem is very high, and thus the system reaches sub-optimal conditions that may not be suitable for the plant [40].

Based on the concept of non-cooperative games, in the *collaborative or coordinated structures* each MPC controller has a local objective function with communication between units through an interaction model inside the model of each MPC controller [3]. Interaction models can include the whole plant or a small neighborhood of each unit [9; 41]. These systems converge towards a Nash equilibrium point, which might be undesirable because it might generate an unstable closed-loop behavior of the system [7; 9]. Despite this fact, these kind of structures have been successfully applied to electrical and some chemical systems [7; 41; 42].

The key difference between cooperation-based and coordination-based distributed control is the introduction of a new element into the plant controller network, named a **coordinator** which aims to moderate the demands of individual controllers based on knowledge of the interactions among the operating units and, by an iterative procedure, to correctly find the optimal strategy for plantwide operation [8].

Three coordination policies are used in these structures [8]: (i) the *price-driven approach*, where the coordinator decides to allocate a price for the consumption of shared resources

by any individual controller and it is possible for each individual controller to get a different pricing structure for shared resources, (ii) the *resource allocation approach*, where the coordinator allocates the amount of shared resources that can be used by each individual controller, and (iii) the *prediction-driven coordination* where the constraint space of the plant is decomposed into local constraints for each individual controller such that each operating unit optimizes its own performance based on the resource consumption predicted by the other operating units. However, there is no complete interaction structure linking a subsystem with all others; rather, a subsystem interacts only with a few neighbors [42], and modeling the interactions between subsystems and exchanging trajectory information among their MPCs is insufficient to provide even closed-loop stability [39].

The works of Valencia Arroyave [7]; Giovanini [26]; Hu and El-Farra [41]; Scheu and Marquardt [42]; Heidarinejad et al. [43]; Liu and Mun [44]; Camponogara et al. [45]; Xu and Bao [46] are examples of these control structures, where it is worth highlighting that is a research field that has just begun to be explored in recent years.

2.2.3. Hierarchical

Hierarchical structures are feasible structures that reduce complexity of large-scale systems and improve the solution through decomposition, coordination and parallel processing. The basic principle of hierarchical control is decomposition of a given large-scale system into several smaller sub-systems, and coordination of the resulted sub-systems that lead to an optimal solution [47]. Generally, these structures involve an optimization level (RTO, DRTO) which determines the optimal values of the controlled variables to the control layer, comprised by MPC controllers [24; 39], as represented in Fig. 2.6. 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, as shown in Fig. 2.7. 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 a 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; 17]. Coordination generally involves plant economics criteria [15; 48], and can be achieved under Mesarovic et al. [32] principles, which can be applied to linear and non-linear models. This coordination principles are:

1. *Interactions prediction*, where process outputs are predicted and compared to the current outputs, updating the prediction error when it is out of tolerance bounds. Nowadays, this scheme is used in the supervisory control structures and is being implemented with MPC controllers.
2. *Balance of interactions*, in which the coordinator on the supervisory layer modifies the objective function of each MPC controller according to the difference between plant and controllers outputs, updating the objective function according to the capabilities of each controller. Generally, this approach is not widely used, but it can improve the system performance since it considers interactions among units [39].

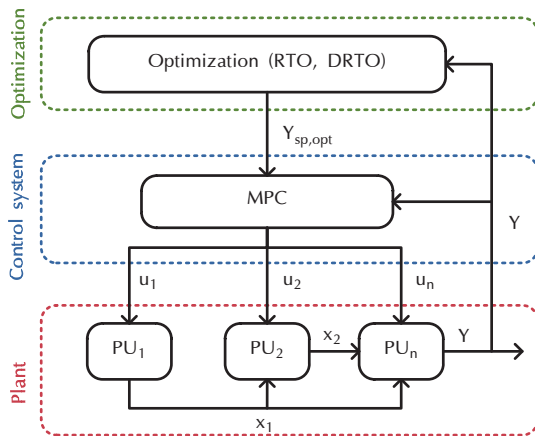


FIGURE 2.6. Hierarchical control structure without coordination.

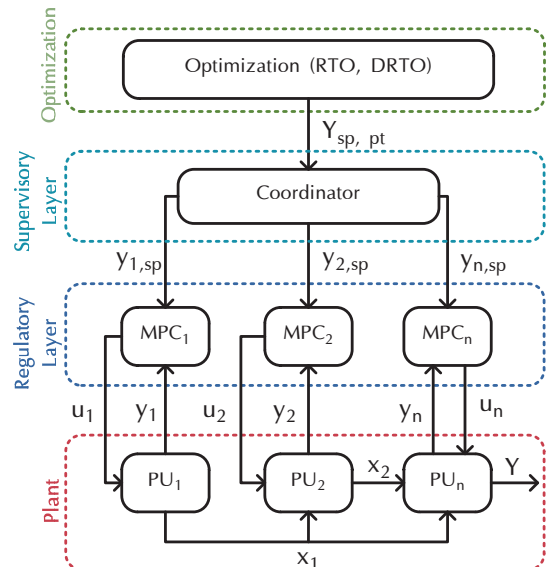


FIGURE 2.7. Hierarchical control structure with coordination.

The last principle is exploited in this work, where interactions between process dynamics are extracted from the process model, and consequently are used to optimize the regulatory layer controllers set-points. Additionally, aiming towards simpler control structures, the usual MPC controllers are replaced by PIDs, using a model in the supervisory layer to optimize the plant performance as to achieve the regulation of the plants output.

Another approach for the supervisory layer involve commutation principles, in which the regulatory layer controllers receive signals from the coordinator to enter or exit the feedback loop, and this allows an asymptotic regulation of the process [49]. However, this strategy requires of the decomposition of the process in subsystems, thus influencing the commutation between controllers policy. Also, it does not guarantee a smooth transition between controllers. Additionally, other strategies like the one proposed by Radhakrishnan [15] suggest replacing the MPC controllers on the regulatory layer and using PIDs instead, and optimizing the operation with a model-based coordinator. Similarly, Ochoa et al. [3] present a plantwide optimizing control strategy, in which the control layer consists of PID controllers whose set-points are directly determined by a DRTO layer. This structure exhibits good performance and uses simple controllers, nonetheless it has the requirement of a detailed dynamic model of the process for executing the optimization of an economic index. The computational cost is high because this structure executes an on-line dynamic optimization routine, which outranks all the advantages.

The works of Ochoa et al. [3]; Radhakrishnan [15]; Seki and Naka [17]; Marquez et al. [20]; Wolf et al. [50]; Hill et al. [51, 51]; Zheng et al. [52] present some examples of this kind of control structures applied to different chemical processes.

2.2.4. Centralized

In these structures, the process is controlled by means of a single multivariable controller, usually MPC, using a **complete** model of the plant [40]. The objective function is then a plantwide function that provides an optimal performance of the control structure since a larger set of possible control actions is used for the optimization [39]. The structure of these controllers is illustrated in Fig.2.8.

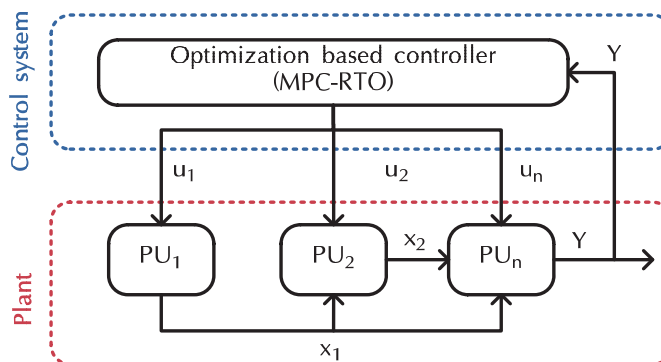


FIGURE 2.8. Decentralized control structures

These systems have a large computational load, but this has been solved by the increasing capacity of recent processors and more efficient optimization algorithms. Aske et al. [24]; Garrido et al. [53] have proposed centralized control structures, demonstrating their excellent performance in large-scale systems. Despite these facts and the good performance of these structures, the dangers on relying on a single controller for the operation are elevated, specially because possible fault situations can occur. Centralized schemes thus unfeasible for large-scale systems because they are considered impractical and inflexible [40].

2.3. Concluding remarks

In this chapter, the different architectures for addressing the PWC problem in chemical process and their correspondent theoretical background are reviewed. After analyzing the different PWC structures, the following aspects demand special attention:

- The complex nature of the plantwide control problem and the numerous decisions that must be taken have resulted in a plethora of approaches that can lead to different structures with the same performance, and criteria for selecting the best approach has not been developed yet.
- A critical aspect when designing distributed and hierarchical control structures is the process decomposition into smaller subsystems, and depending on where such partition is made there are significant information losses about process interactions. This situation is not favorable, since the dynamic behavior disregarded might generate instabilities under certain disturbances.
- Distributed and hierarchical structures represent good alternatives when dealing with plantwide control of chemical processes since they can include the interactions in the

system for its operation. However, the usage of MPC controllers in these structures require large investments accompanied with the care and attention from control experts. Also, the large computational load reduces their practicality in industrial environments thus raising the need for simpler structures that can achieve the same performance.

- The possibility of achieving optimal plantwide performance through coordinated structures is a great motivation towards developing such structures. However, the increased computational complexity and the need to have the complete plant model (albeit distributed amongst the individual controllers) are major issues to be considered for the implementation of these structures. Also, for coordinated plantwide control, failure to incorporate the interactions into the overall control strategy may lead to sub-optimum plantwide operations. Today, there is increasing activity in research on distributed control structures driven by opportunities to achieve better computational performance and to remove possible communication bottlenecks [42].
- Despite PWC strategies have demonstrated good performance in simulation, much of the research in this area has not gained acceptance on industrial environments as to have profound influence. This reinforces the need for formalized but simple approaches for designing these systems, that result in practical control schemes for their installment in industrial applications.

CHAPTER 3

Control of multivariable processes

The need and desire to model, analyze and control systems with more than one input and one output is a recurrent topic in engineering. In fact, in hierarchical or distributed structures, a multivariable controller is part of unit supervision [54]. The plantwide sub-problem concerning the multivariable controller design is a very important issue since it defines the future dynamic closed-loop response [55]. Moreover, once the controlled and manipulated variables have been selected properly the control policy must be defined, for complete design of the control structure.

In order to identify the requirements of the supervisory control layer, in this chapter a review of the available control strategies for multivariable processes is made. First, a brief description of the main characteristics of multivariable processes is given in Section 3.1. Section 3.2 presents several tools for designing control systems for multiple loops, namely: Relative Gain Array, Condition Number, Niederlinski Index, decoupling control and Singular value decomposition (SVD) approaches. Then, multivariable control systems such as MPC and optimal control are addressed in Sections 3.3, focusing on the analysis of the objective functions applied for these controllers. Finally, Section 3.4 presents some concluding observations of this chapter.

3.1. Characteristics of multivariable processes

The objective of multivariable control is to simultaneously control several variables in a process that has more than one output variable which is controllable with more than one input variable. The most important characteristic of these Multi-Input/Multi-Output (MIMO) or multivariable systems is the existence of interactions between process inputs and outputs, which is expressed in the fact that any input can influence all outputs (high interactions) or just one of them (low interactions) [56]. Multivariable processes exhibit two different types of interactions: *Interference* or *Coupling*. On the first case, also known as forward interactions, some variables of one subsystem affect the variables on other subsystems in an unidirectional way. On the latter, cross paths of interactions exist which generates hidden feedback interference that if ignored, might cause instabilities on the closed loop behavior of the process.

There are several approaches for dealing with the multivariable control problem, as can be seen from Fig. 3.1: *multiloop control* in which several control loops are established in the process, and *multivariable control* where a single controller decides the values for all the manipulated variables in the process to maintain all the controlled variables in their set-points. The following sections describe the main characteristics of these strategies.

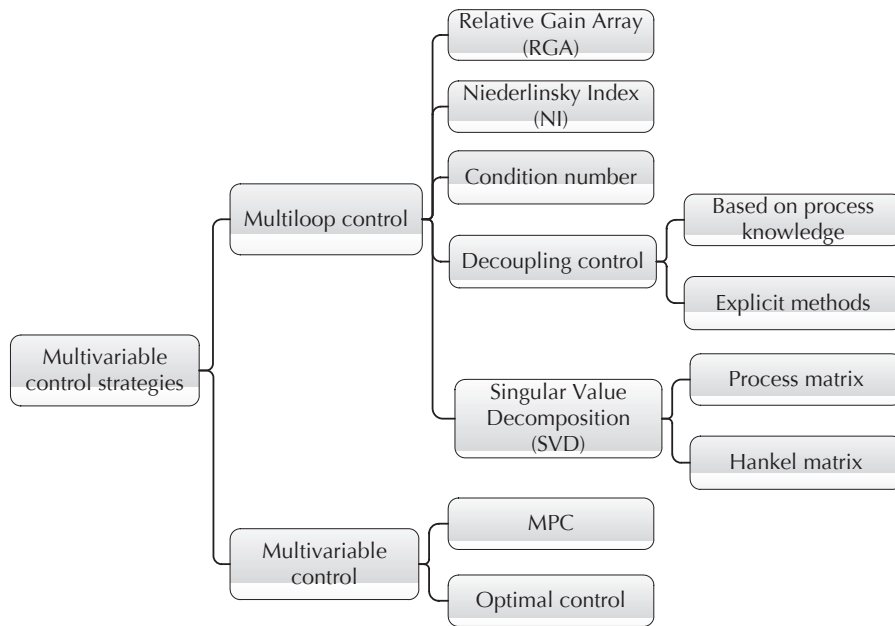


FIGURE 3.1. Multivariable control strategies. Adapted from [54; 57]

3.2. Multiloop control

Non-interacting systems can be regarded as a collection of distinct single-input/single-output systems, each of which can be controlled independently of the others [56]. Under these considerations, in multiloop control strategies the main problem is the design of the individual control loops and connecting them in a way that interactions are eliminated or reduced [54]. For this, the selection of the most adequate input–output pairings for independent control loops is critical, since it is not an intuitive task for multivariable processes. Although interactions are not considered for the design of the control loops, they have a major influence on the controllers performance and their tuning process.

Multiloop control strategies concerns with the selection of the most suitable input–output pairing based on plant controllability. The most popular strategies are: these structures the Relative Gain Array (RGA), Condition Number (CN), Niederlinski Index (NI), decoupling control and Singular Value Decomposition (SVD), and will be explained in further details in Subsections 3.2.1 to 3.2.5.

Once the input–output pairings are established, each controller must be tuned. Multiloop control strategies consider that interactions do not affect the admissible range for controller parameters values, so any tuning method can be used without inconveniences [54]. However, it is important to consider that the parameter range for which the system is stable is smaller than that of the non-interacting system. This represent the major drawback of these strategies, since not considering process interactions can lead to an inadequate selection of input–output pairings.

For these methods it is important to note that they are based on a process linear model. The system shown in (3.1) reflects the state–space representation of a linear model.

$$\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t), \quad \mathbf{x}(0) = \mathbf{x}_0 \quad (3.1)$$

$$\mathbf{y}(t) = \mathbf{C}\mathbf{x}(t) + \mathbf{D}\mathbf{u}(t)$$

where $\mathbf{x} \in \mathbb{R}^n$ is the process state vector with \mathbf{x}_0 being the initial state vector, and $\mathbf{u} \in \mathbb{R}^m$ and $\mathbf{y} \in \mathbb{R}^l$ describe the input and output vectors of the system at time t . Additionally, $\mathbf{A} \in \mathbb{R}^{n \times n}$, $\mathbf{B} \in \mathbb{R}^{n \times m}$, $\mathbf{C} \in \mathbb{R}^{l \times n}$ and $\mathbf{D} \in \mathbb{R}^{l \times m}$.

Other strategies are formulated the frequency domain, in which the process is represented through a transfer matrix $\mathbf{G} \in \mathbb{R}^{l \times m}$ obtained from the state–space linear model according to (3.3), which gives the process realization presented in (3.2).

$$\mathbf{y}_s(s) = \mathbf{G}(s)\mathbf{u}_s(s) \quad (3.2)$$

$$\mathbf{G}(s) = \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{B} + \mathbf{D} \quad (3.3)$$

\mathbf{G} is the matrix of steady–state process gains. It is important that the variables are scaled as they are seen by the controller, i.e., the sensors and manipulated variables should be scaled to 0–100%.

3.2.1. Relative Gain Array

The Relative Gain Array (RGA), $\boldsymbol{\Lambda} \in \mathbb{R}^{l \times m}$, is a matrix based on steady–state information of the process, and through this matrix the determination of (i) a measurement of process interactions and (ii) an input–output pairing is possible. The elements of this matrix, λ_{ij} represent the relations existent between the i -th process output y_i and the j -th manipulated variable, u_j , relating the steady–state gains when all the input variables are constant (open loop) and when all the process variables are constant (closed loop), according to (3.4) [18; 54].

$$\lambda_{ij} = \frac{\left(\frac{\partial y_i}{\partial u_j}\right)_u}{\left(\frac{\partial y_i}{\partial u_j}\right)_y} \quad (3.4)$$

Input–output pairings are then defined according to the following recommendations [18; 54]:

- $\lambda_{ij} < 0$: different signs on the numerator and denominator indicate unstable pairings. In this case, the system is subject to positive feedback and its control is complicated when the other control loops are established.
- $\lambda_{ij} = 0$: the input and output variables are not related, and therefore a different input variable would be needed to control the process variable.
- $\lambda_{ij} = 1$: this is the best possible scenario. Here, there is no interrelation with other control loops, and thus this loop can be designed without considering the others.

- $0 < \lambda_{ij} < 0.67$: there are strong interactions with the other control loops and negative feedback occurs. In this circumstance, a decoupling strategy is more suitable for the system.
- $0.67 < \lambda_{ij} < 1.5$: interactions with other loops are relatively small, which gives a reasonably proper performance to the control loop of interest.
- $2 < \lambda_{ij} < 10$: the interrelations among control loops annul the effect of the input variable over the controlled variable, therefore, the use of a decoupling strategy is recommended.

Some additional considerations must be taken into account regarding the RGA [57]:

- Λ is independent of input and output scaling.
- Plants with large RGA–elements are always ill–conditioned and are difficult to control because of sensitivity to input uncertainty.
- A relative change in an element of \mathbf{G} (3.3) equal to the negative inverse of its corresponding RGA–element, yields singularity.
- If the sum of elements in a column of RGA is small ($\sum_j \lambda_{ij} \ll 1$), then the corresponding input can be deleted since its impact on the process is very low. Furthermore, if all elements in a row of RGA are small ($\sum_i \lambda_{ij} \ll 1$), then the corresponding input cannot be controlled.

3.2.2. Niederlinski Index

The Niederlinski Index (NI) is a necessary condition for analyzing control configuration stability. This analysis involves the steady–state gains of the process, and if resulting in a negative NI the control loop would be unstable [18]. The NI is defined as:

$$NI = \frac{\det \mathbf{G}}{\prod_{i=1}^n g_{ii}} \quad (3.5)$$

Where \mathbf{G} is the $l \times m$ matrix of the system steady–state gains, in a way that the i -th controlled variable is paired with the i -th input variable. An advantage of this method is that it considers system stability. However, it does not consider the dynamic behavior of the process which is a major disadvantage of this method.

3.2.3. Decoupling Control

This method considers the interactions among process dynamics existent in the system. It works by eliminating them in a way that the controllers do not perceive them. For the system decoupling, the least relevant variables of the system are defined (generally under economic criteria) and the corresponding controllers are loosely tuned [54]. Other strategies for decoupling the system are [54]:

- **Decoupling based on process knowledge:** The system can be decoupled by redefining the manipulated or controlled variables. However, the good performance of this approach depends highly on the expertise of the designer and the particular system under investigation.
- **Explicit decoupling:** The multiloop scheme is maintained but a decoupling module $\mathcal{D} \in \mathfrak{R}^{l \times m}$ is added to the system. This module holds the information of the interactions in the process and modifies its transfer function \mathbf{G} in such a way that for the controller it is a diagonal matrix, i.e. a process without interactions, as illustrated in Fig. 3.2.

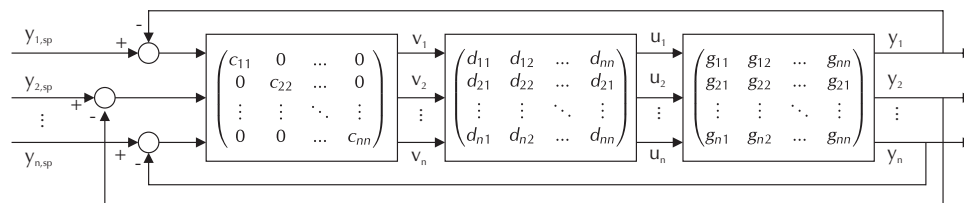


FIGURE 3.2. Block diagram of a decoupling control system [53].

For the particular case of a Two-Inputs/Two-Outputs (TITO) system, the decoupling module is given by (3.6).

$$\mathbf{D} = \begin{bmatrix} 1 & -\frac{g_{12}}{g_{11}} \\ -\frac{g_{21}}{g_{22}} & 1 \end{bmatrix} \quad (3.6)$$

Where g_{ij} correspond to the elements of \mathbf{G} (3.3).

Decoupling is very sensitive to modeling errors and uncertainties. Moreover, the requirement of decoupling and the use of an inverse-based controller may not be desirable for disturbance rejection.

Internal Model Control (IMC) is a design method based on a decoupling controller [57] and have recently been used for designing decentralized control structures [37]. This approach have been also explored for designing centralized control structures using a explicit decoupling scheme which allowed control of 2×2 and 3×3 systems with individual PID controllers reducing the interactions among them [53].

3.2.4. Singular Value Decomposition

The Singular Value Decomposition (SVD) quantifies process controllability and observability, allowing the determination of sensor location and input-output pairings in a process [54; 57]. SVD is generally applied to systems on the frequency domain, see Eq. (3.2) using the \mathbf{G} matrix, and it is a factorization of the form (3.7) [18]:

$$\mathbf{G} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T \quad (3.7)$$

Here, \mathbf{U} and \mathbf{V} are orthonormal matrixes where each column represents a singular vector of \mathbf{G} , and $\mathbf{\Sigma}$ is a diagonal matrix whose elements are the singular values of \mathbf{G} obtained as the non-negative squared roots of the eigenvalues of $\mathbf{G}\mathbf{G}^T$ [58]. Matrices \mathbf{U} and \mathbf{V} are orthonormal bases for the column space (output space) and row space (input space) of \mathbf{G} [18].

G singular values represent operating modes of a plant which refers to the ways a plant responds to different situations, it means that a given direction of input changes will generate a determinate direction on the plant outputs [18]. The direction of these movements is indicated by the sign of the singular vector components, where positive components represent an increment and negative ones a decrease whether on the plant inputs (components of vector V_i) or outputs (components of vector U_i) [18]. Higher singular values mean more probable operating modes and they are the first components of Σ matrix. Modes corresponding to small singular values are very difficult to achieve by any control system.

When applied to multivariable control problems, SVD provides physical insight into the nature of the problem, and each part of the decomposition can be understood in terms of some physical aspect of the process as follows [54]:

- The left singular vectors, U_i , indicate the best way in which to view the sensors (outputs). This means that U_1 is the best combination of sensors, i.e., the combination that is most easily influenced by changes in the manipulated variables. In this way, U_2 is the next easiest combination and so on.
- The right singular vectors, V_i , indicate the best way in which to view the manipulated variables (inputs). This means that V_1 is the best combination of manipulated variables that have the strongest effect on the process. V_2 is the next best combination and so on.
- Σ , the singular values matrix, indicates the decoupled gain of the open-loop process.

For input–output pairings, the main output variable (largest element of the first column of U_i) is paired with the main manipulated variable (largest element of the first column of V_i). This procedure is continued until all input–output pairings are determined [54]. This method has the advantage of quantifying process interactions and establish the input–output pairings according to them. However, it is based on a steady–state matrix of the process and is highly dependent on the selection of the unit system.

Another approach to input–output pairings selection is based on the SVD of Hankel matrix is proposed by Alvarez Toro [18], and differs on the previous one because it performs the SVD analysis in the time–domain. It overcomes the issues mentioned above for the SVD with the process matrix, since it integrates the dynamic behavior of the process through Hankel Matrix \mathcal{H} . Hankel matrix has been widely used for model reduction, systems identification and recently in controllers design for establishing input–output pairings [18; 59] and process scale–up [60]. This matrix represents the impulse–response of a system and can be obtained through the discrete form of the system (3.1), as shown in (3.8) [18].

$$\mathcal{H} = \begin{bmatrix} \mathbf{C}_d \\ \mathbf{C}_d \mathbf{A}_d \\ \dots \\ \mathbf{C}_d \mathbf{A}_d^{n-1} \end{bmatrix} [\mathbf{B}_d \quad \mathbf{B}_d \mathbf{A}_d^{n-2} \quad \dots \quad \mathbf{B}_d \mathbf{A}_d^{n-1}] \quad (3.8)$$

Where \mathbf{A}_d , \mathbf{B}_d , \mathbf{C}_d and \mathbf{D}_d matrices, represent the discrete–time model of the process (3.9).

$$\mathbf{x}(k + 1) = \mathbf{A}_d \mathbf{x}(k) + \mathbf{B}_d \mathbf{u}(k), \quad \mathbf{x}(0) = \mathbf{x}_0 \quad (3.9)$$

$$\mathbf{y}(k) = \mathbf{C}_d \mathbf{x}(k) + \mathbf{D}_d \mathbf{u}(k)$$

\mathcal{H} represents the input–output behavior of the system, considering that it relates a sequence of past inputs to future outputs [58]. Therefore Hankel matrix SVD 3.10 can be exploited to obtain a quantitative measure of the dynamic influence of each process variable and establish the input–output pairings accordingly [18]. Such quantitative measure involves the euclidean norm of the corresponding input and output entries of the singular vectors (V_i and U_i) with the singular values as given by (3.11) and (3.12) respectively.

$$\mathcal{H} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T \quad (3.10)$$

$$III_{u_k} = \sqrt{\sum_{i=1}^p \sigma_{ii}^2 \sum_{j=0}^{n-1} \mathbf{V}_{i,k+mj}^2} \quad (3.11)$$

$$SII_{y_k} = \sqrt{\sum_{i=1}^p \sigma_{ii}^2 \sum_{j=0}^{n-1} \mathbf{U}_{k+lj,i}^2} \quad (3.12)$$

where p represents the number of non–negative singular values, i.e., the rank of the system. The matrices \mathbf{U} and \mathbf{V} are the orthonormalized eigenvectors of $\mathcal{H}\mathcal{H}^T$ and $\mathcal{H}^T\mathcal{H}$ respectively. σ_{ii} are the non–negative square roots of the eigenvalues of $\mathcal{H}^T\mathcal{H}$, i.e. \mathcal{H} singular values. Furthermore, SII_{y_k} is the State Impactability Index of the k -th output variable and represents the impact of process manipulated inputs \mathbf{u} as a whole over the k -th output variable y_k . III_{u_k} is the impact of the k -th process manipulated input u_k over process outputs \mathbf{y} as a whole, called Input Impactability Index. It is important to take into account that the number of inputs m must be equal to the number of output variables l [18].

Once the SII and III of all input and output variables are computed, the input–output pairings are established by pairing the u_j with the highest III and the y_i with the highest SII . The procedure continues by eliminating the set of variables already paired and repeating until all the variables are paired.

This strategy presents a good performance compared with the \mathbf{G} matrix SVD or RGA, but has the following drawbacks [18]

- Only individual pairings are considered. Despite the SVD procedure can be applied to non–squared matrices, for assigning a specific pairing, the system must have the same number of input and output variables.
- Although observability and controllability of the process are considered for computing Hankel matrix the procedure assumes the process is stable. Therefore, the system must be stable or stabilized before following this methodology.
- SVD is sensitive to scaling. Therefore, the results are properly interpreted only if the gain matrix is scaled as the process is perceived by the controller [54].

3.2.5. Condition Number - CN

For evaluating a set of input and outputs, the condition number γ of the process matrix in the frequency domain, \mathbf{G} , can be used. The CN of a matrix can be computed as the ratio between the maximum and minimum singular values [57]:

$$\gamma(\mathbf{G}) \triangleq \frac{\bar{\sigma}(\mathbf{G})}{\underline{\sigma}(\mathbf{G})} \quad (3.13)$$

where $\underline{\sigma}$ is the lowest singular value of \mathbf{G} and $\bar{\sigma}$ is the highest singular value.

A system whose condition number is large is a system hard to control, because there are operating modes difficult to maintain and hence the process operation is also difficult. For this reason, a set of input and output variables that result in a small γ is preferred [54], and this also provides the system with robustness to disturbances [57]. It is worth noticing that the condition number depends strongly on the scaling of the inputs and outputs, so it must be carefully calculated before disregarding a feasible set of variables.

3.3. Multivariable Control

As mentioned in Section 3.1, multivariable control strategies use all the measurements simultaneously to compute all the values for the manipulated variables [54]. Under this approach, Model Predictive Control (MPC) and optimal control strategies are found as the main options.

3.3.1. Model Predictive Control

The term Model Predictive Control (MPC) designates a wide range of control methods that make use of a model of the process to obtain the control signal via minimization of an objective function. The basic ideas in the predictive control approach are: (i) explicit use of a model to predict the process output at future time instants (prediction horizon), (ii) calculation of a control sequence minimizing an objective function; and (iii) receding strategy, so that at each instant the prediction horizon is displaced towards the future, which involves the application of the first control signal of the sequence calculated at each step [61].

The methodology of all MPC controllers is based on the following strategy, depicted in Fig. 3.3 [61]:

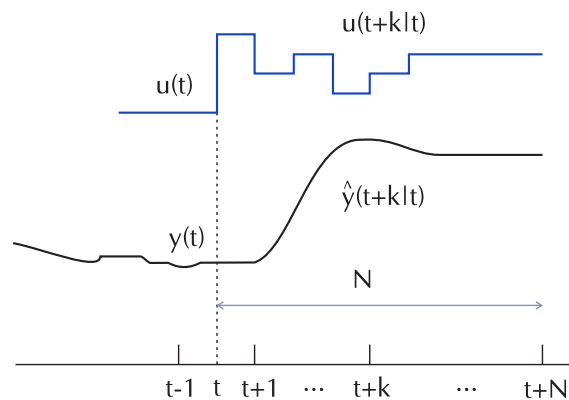


FIGURE 3.3. MPC strategy

1. The future outputs for a determined horizon N , called the prediction horizon, are predicted at each instant t . A model is used to predict the future plant outputs ($\hat{\mathbf{y}}(t + k|t)$ for $k = 1 \dots N$) based on past and current values of inputs and outputs, and on the future control signals ($\mathbf{u}(t + k|t)$ for $k = 0 \dots N - 1$), which are those to be sent to the system and calculated. Here, the notation $\hat{\mathbf{y}}(t + k|t)$ indicates y value at the instant $t + k$ calculated at instant t .
2. The set of future control signals is calculated by optimizing a determined criterion to keep the process in its reference trajectory $\mathbf{w}(t + j)$. This criterion (objective function) includes the deviation between the predicted output and its set point or reference trajectory, and the control efforts, $\Delta\mathbf{u}$, required to achieve that objective. A general form of the objective function J is presented in (3.14).

$$J(N_p, N_u) = \sum_{k=1}^{N_p} \delta(j) [\hat{\mathbf{y}}(t + k|t) - \mathbf{w}(t + j)]^2 + \sum_{k=1}^{N_u} \kappa(j) [\Delta\mathbf{u}(t + k - 1)]^2 \quad (3.14)$$

where N_p and N_u are the prediction and control horizons respectively. Additionally, the coefficients $\delta(j)$ and $\kappa(j)$ are the tuning parameters of the MPC and are selected according to the desired response of the controller. Usually, an exponential weight of $\delta(j)$ is used, and it is defined by (3.15):

$$\delta(j) = \alpha^{N_p - j} \quad (3.15)$$

In this way, selecting a value of $0 < \alpha < 1$ will give a smoother response with lower efforts, and $\alpha > 1$ will provoke a tighter control since the first errors will be more penalized.

3. The control signal $\mathbf{u}(t|t)$ is applied to the process. The other computed control signals are rejected, and at the next sampling instant $y(t + 1)$ step is repeated with this new value and all sequences are updated. In this way, $\mathbf{u}(t + 1|t + 1)$ is different from $\mathbf{u}(t + 1|t)$ since new information is available.

This strategy has many advantages. Given that the prediction model of the process usually is either an impulse–response, step–response or empirical model, a limited knowledge of the process would be enough for achieving its control [62]. It also has intrinsic compensation for dead times and known disturbances [61]. MPC can also manage the strong interaction between the states in large scale and networked systems, a particular characteristic in multivariable control that is difficult to handle [20].

However, the derivation of the control law, see (3.14), is more complex than that of the classical PID controllers and its computation must be performed in every sampling time. Also, when constraints are considered the required computation time is even higher [61]. The major drawback of this strategy is the explicit usage of the model for the optimization routine, since it is highly sensitive to modeling errors and the results will be highly affected for the discrepancies between the real process and the model used. This is usually solved by using a phenomenological model of the process, however, it increases the computational requirements of this control systems, specially when aiming towards its implementation on industrial Programmable Logic Controllers (PLC) or other small industrial computing units.

Among other important drawbacks of the MPC controllers are the lack of criteria for its tuning and the usage of a linear model of the process. This reduces the application of the model to a small neighborhood of the linearization point, and if disturbances drive the process away from this point, the model no longer represents the process, leading to erroneous predictions and therefore inadequate process control [62].

3.3.2. Optimal Control

The objective of optimal control is to generate an optimal control input that allows the obtainment of a minimum or maximum of a performance measure, subject to the dynamics of the system under study with various design specifications and constraints [47]. In an optimal control problem, the goal is to find an admissible control trajectory $\mathbf{u} : [t_a, t_b] \rightarrow \Omega \subseteq \mathfrak{R}^m$ such that the dynamic system described by the non-linear state-space model (3.16)

$$\dot{\mathbf{x}} = f(\mathbf{x}(t), \mathbf{u}(t), t) \quad (3.16)$$

is transferred to the initial state $\mathbf{x}(t_a) = \mathbf{x}_a$ into an admissible final state $\mathbf{x}(t_b) \in S \subseteq \mathfrak{R}^n$, and such that the corresponding state trajectory $\mathbf{x}(\cdot)$ satisfies the state constraint $\mathbf{x}(t) \in \Omega_x(t) \subseteq \mathfrak{R}^n$ at all times $t \in [t_a, t_b]$ and such the cost functional $J(\mathbf{u})$ given by (3.17) is minimized [63].

$$J(\mathbf{u}) = K(\mathbf{x}(t_b), t_b) + \int_{t_a}^{t_b} L(\mathbf{x}(t), \mathbf{u}(t), t) \quad (3.17)$$

Here, t_a and t_b are the initial and final time of the time interval of interest respectively, $\mathbf{x}(t_a) = \mathbf{x}_a$ and $\mathbf{x}(t_b) = \mathbf{x}_b$ are the initial and final states of the process respectively, and Ω_x and Ω are the admissible sets for the state and input variables respectively. The functions f , K , and L are assumed to be C^1 with respect to all of their arguments, and are dependent of the problem of interest. Finally, S is an specific target set which can be a constraint for the final state.

Depending on the characteristics of the problem, there are four different types of optimal control problems: (i) the final state is fixed $\mathbf{x}^\circ(t_b) = \mathbf{x}_b$, where the superscript indicates the optimal solution, (ii) the final state is free, (iii) the final state is constrained to lie in a specified target set S and (iv) the states are subject to $\mathbf{x}^\circ(t) \in \Omega_x(t)$ at all times additional to the constraint of the final state belonging to a set S . It is worth clarifying that each of the four problem types is divided in two subtypes depending on whether the final time t_b is fixed or free (i.e., to be optimized) [63].

An optimal control problem can be solved using Pontryagin's Minimum Principle, which typically proceeds as in the following steps [63]:

1. Formulate the optimal control problem, see (3.17).
2. Determine whether the problem can have a solution (existence proof).
3. Formulate the necessary conditions of Pontryagin's Minimum Principle, based on the definition of the Hamiltonian function H given by (3.18) [63]:

Definition 3.1. Hamiltonian function Is a function $H : \mathfrak{R}^n \times \Omega \times \mathfrak{R}^n \times 0, 1 \times [t_a, t_b] \rightarrow \mathfrak{R}$ where:

$$H(\mathbf{x}(t), \lambda(t), \lambda_0, t) = \lambda_0 L(\mathbf{x}(t), \mathbf{u}(t), t) + \lambda^T(t) f(\mathbf{x}(t), \mathbf{u}(t), t) \quad (3.18)$$

where $\lambda \in \mathfrak{R}^n$ are the Lagrange multipliers of the system.

The Pontryagin's Minimum Principle lays the conditions that must be fulfilled by the optimal solution $\mathbf{u}^\circ : [t_a, t_b] \rightarrow \Omega$ and $\lambda^\circ \in \mathfrak{R}^n$. A detailed formulation of this principle is found in [63].

4. Globally minimize the Hamiltonian function H for all $t \in [t_a, t_b]$:

$$\mathbf{u}^\circ(\mathbf{x}^\circ(t), \lambda^\circ(t), \lambda_0^\circ, t) = \arg \min_{\mathbf{u} \in \Omega} H(\mathbf{x}^\circ(t), \lambda^\circ(t), \lambda_0^\circ, t) \quad (3.19)$$

5. Determine whether the problem can have a singular solution, i.e., verify if one of the following conditions is met:
 - $\lambda_0^\circ = 0$
 - $H \neq H(\mathbf{u})$ for $t \in [t_a, t_b]$
6. Solve the two-point boundary value problem for $\mathbf{x}^\circ(\cdot)$ and $\lambda^\circ(\cdot)$. This problem results from replacing the control law $\mathbf{u}^\circ(t)$ in the differential equations (3.16).
7. Eliminate locally optimal solutions.
8. If possible, convert the optimal open-loop control $\mathbf{u}^\circ(t)$ into an optimal closed-loop control $\mathbf{u}^\circ(\mathbf{x}^\circ(t), t)$ using state feedback.

There are various algorithms that can be used for solving non-linear optimal control problems. These algorithms can be divided into three categories: indirect, direct and dynamic programming approaches. However, the common point in all these schemes is that for a large-scale system that consists of many states and inputs, a tremendous number of equations need to be solved simultaneously. As a result, there is a high computational and numerical complexity in solving such a problem [47]. Additionally, for obtaining the optimal closed-loop control law a complete state feedback is required, either measured or estimated through a state observer. This step is very important, since if such feedback is not present, the control policy lies in open-loop and disturbances will not be considered. Thus, the control system might drive the process to undesired operating points.

3.4. Concluding remarks

In this chapter, the different control strategies available for multivariable processes are analyzed. Also, some examples of the application of these strategies in hierarchical, distributed or centralized control structure are presented. Here, it is worth considering:

-
- Multiloop control strategies, thought suitable for process with low interactions, can be applied for the design of the regulatory layer under either decentralized or distributed approaches, when the selection of controlled and manipulated variables is not straightforward.
 - The effect of disturbances is not included in an optimal control problem, and therefore it is necessary to convert the open-loop optimal policy to a closed loop which may not be always possible. Also, the development of an optimal control policy for a process is not intuitive and requires a strong knowledge for this task. Therefore, despite offering very good performances and optimal plant operation, its industrial implementation would not be an easy task.
 - Although MPC-based structures allow the integration of dynamic interactions in the process for its control, the usage of linear models inside these structures restrict their operation to a close vicinity of the operating point in which the process model was linearized. These is not desirable considering that disturbances may lead the process far from the operating point, and in this circumstances, the model does not represent the process correctly and predictions made over this model will be away from the real behavior of the process.

CHAPTER 4

Design procedure for model–based supervisory control structures

This chapter presents the development of the model–based supervisory control structure, detailing the design criteria for each level of the structure. An overall description of the procedure is presented on Section 4.1. Then, a first stage of process analysis before designing regulatory and supervisory layers is described on Section 4.2, including the procedure for obtaining phenomenological–based models which is a fundamental tool for the development of the design procedure proposed in this thesis. On Section 4.3 the requirements for the regulatory level are described, and an assessment criteria for the input–output pairings available in the plant is presented. The establishment of the dynamics hierarchy of the process, the formulation of the optimization problem to be solved by the coordinator of the supervisory level and the triggers for such optimization is addressed in Section 4.4. Then, on Section 4.5 the procedure is applied for controlling a Continuous Stirred Tank Reactor in order to verify its effectiveness. Finally, some closing remarks for this chapter are presented in Section 4.6.

4.1. Procedure overview

As mentioned in Chapter 2, the major drawbacks of the available plantwide control (PWC) structures are their complex structure, communication demands and high computational requirements. The design procedure proposed here aims to obtain a control structure with a good performance but with a simple structure for its implementation on industrial environments.

In order to reduce control efforts when controlling 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 characteristics and process objective, and is the dynamic behavior that must be controlled in order to guarantee product quality; and *(ii)* Secondary or Non-critical Dynamics (SeDs). This classification has the advantage of *(i)* requiring lower control efforts if 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, so the regulation of the MaD is achieved in an easier way. This approach is inspired by collaborative structures in distributed MPC, in which controllers are coordinated optimally to achieve regulation of the whole plant [2; 47].

Table 4.1 presents the procedure for obtaining a supervisory control structure that can be applied for either multivariable or plantwide control problems. It is based on the procedure

proposed by Skogestad [22], and a modification on the bottom-up analysis is made for including the design of the supervisory level. Each step will be explained in detail in the following sections.

TABLE 4.1. Proposed plantwide control structure design procedure.

Step	Analysis tools and comments	Model Requirements
Process analysis		
1	Development of a process Phenomenological-Based Model (PBM)	–
2	Identification of available manipulated variables and states of the process	Linear model / non-linear
3	Definition of the process operating point and span of state and input variables	–
Regulatory layer		
4	Establishment of controllers configuration	PID (simple structure of easy implementation)
5	Selection of input-output pairings for each process unit	Pairing analysis: RGA, NI, CN, SVD, SVD of Hankel Matrix
6	Controller tuning	Single-loop PID controllers. Possible ratio or cascade control.
Supervisory layer		
7	Determination of dynamics hierarchy	SVD of the Hankel matrix: SII_{x_k} . Selection of Main Dynamics (regulatory control) and Secondary Dynamics (tracking control)
8	Formulation of the optimization problem	Determination of MaD sensitivities to SeDs
9	Establishment of triggers for the optimization on the supervisory level	Selected according to the designers desire. Possible triggers: time frame, deviations on Main Dynamics, deviations on cost functional, J .

The control structure obtained with the proposed procedure is a hierarchical control structure with two layers, as can be seen from Fig. 4.1: (i) *Regulatory layer (RL)* which deals with MaD and SeDs control, and (ii) *Supervisory layer (SL)* where set-points of SeDs controllers are optimized based on the non-linear model of the process, minimizing the deviation on the MaD and reducing the control efforts on the MaD control loop. Although hierarchical control structures normally include an optimization level, its design is out of the scope of this thesis.

Ochoa et al. [3]; Marquez et al. [20]; Dang and Banjerdpongchai [64] introduce various criteria for obtaining this layer within their works.

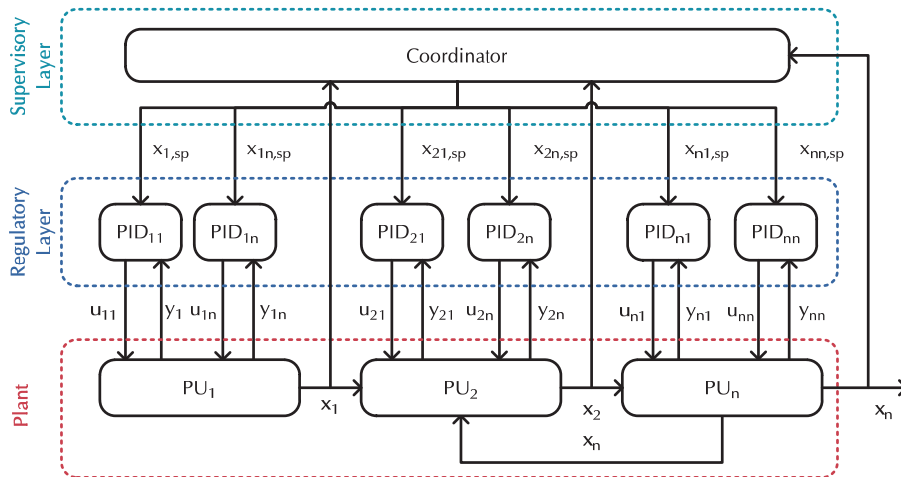


FIGURE 4.1. Proposed supervisory control structure.

4.2. Process analysis

As consequence of chemical processes complexity, modeling has become a necessary and useful tool for understanding and designing processes. Considering the final use of a model determines its structure, for control purposes, the model must be insensitive to parameter changes, finding that Phenomenological-based model (PBM) matches the requirements for control structure design [22]. This kind of model is a non-linear state-space model based on mass and energy balances that uses constitutive equations that can be either empirical or phenomenological. Alvarez et al. [65] presents a methodology for obtaining PBMs which can be summarized as:

1. Elaborate a verbal description and a complementary process flow diagram (PFD).
2. Establish the resolution and objectives of the model according to its application.
3. Define as many process systems as required for achieving the desired resolution and propose a modeling hypothesis.
4. Obtain the differential equations for the process through mass and energy balances, and the necessary equations for the unknown parameters.
5. Validate the model for different conditions and evaluate its performance.

The proposed procedure takes advantage of this type of model for the control structure design. Here, the PBM is not explicitly used on-line, so the proposed control structure only requires the information regarding dynamic interactions that must be represented as accurately as possible for the proper performance of the resulting control structure. On the other hand, for controller design of each individual unit a PBM of each process unit is used in its linear form for the controller tuning. In this sense, accuracy on the model parameters is also desired so the deviations between the model and the real system will be negligible and thus the control system will have a proper response.

Once the process model is obtained, the available manipulated variables \mathbf{u} are determined along with the state variables \mathbf{x} of the process. In this procedure, the aim is to achieve Total State Control (TSC) of the process, and therefore all the decisions regarding controlled variables are made over the state variables of the process, assuming that the process state is completely measured or estimated which makes $\mathbf{y} = \mathbf{x}$.

Finally, a controllability analysis is also required to evaluate whether the state behavior can be affected by process inputs [66]. This analysis performed with either graph theory [67], set theory [66; 68], or using the condition number or the singular value decomposition of the process matrix [22]. This property should be considered before the control system is designed [67].

4.3. Regulatory layer

On the regulatory level the individual controllers for process units are found. Here, the selection of: (i) controlled variables, (ii) measured variables, (iii) manipulated variables, and (iv) control configuration [22] is made. For this layer, it is assumed that it is already available from the control system installed in the real process plant, so the criteria given in this section can be used as performance assessment tools to verify if the existent structure is suitable for the process under analysis. It is worth highlighting that no decomposition of the plant is required for this procedure, and all plant dynamics are considered for the design of the control structure.

4.3.1. Controller configuration

PID controllers are the most used in industrial practice thanks to their simple structure and ease of implementation. This selection is not changed by this procedure, considering that current industrial practice aims toward fewer new designs and operation of the existing facilities in new ways [10] and that tuning rules for PID controllers are widely available [6; 69; 70; 71]. It is a well-known fact that despite its simplicity, it has major drawbacks in terms of performance and stability respect to other types of controllers such as MPC, and that most of industrial PID controllers are poorly tuned, operating in manual mode or even in automatic mode with default settings [12]. However, the task of overcoming these drawbacks corresponds to the model-based supervisory layer [15] and it is also highly recommended to assess the status of the available PID controllers (pairing and tuning) before proceeding to the design of the supervisory layer.

4.3.2. Controlled and manipulated variables

Any of the multiloop control strategies discussed in Section 3.2 can be used for determining the input-output pairings for the process. Of these strategies, the SVD of Hankel matrix has proved to have good results, since it considers the dynamic behavior of the process [18]. 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. Here, if there are insufficient control inputs (less

than the state variables), MaD can be left without controller and thus be regulated only with SeD set-points as manipulated variables [59].

4.4. Supervisory layer

As mentioned in Section 4.1, on the supervisory level the optimization of SeD controllers set-points is carried out so the control efforts for the MaD control loop are reduced.

For supervisory control a model of the process and an adequate objective function are required [15]. According to the discussion of Section 2.2, the available cost functions for coordination in distributed or hierarchical control structures are based on optimal or MPC control policies, which lead to high computational costs. In order to maintain the simplicity of the control structure, this section presents the development of the objective function to be minimized with the SeD set-points as degrees of freedom, based on the PBM of the process.

4.4.1. Dynamics hierarchy

Considering that the control objective on a process is mostly a product quality related variable, the other process variables can be maintained on nominal values that admit tolerances, and therefore the required control efforts can be reduced if only the quality-related variable is controlled on its desired set-point. However, the determination of such variable is a key step when designing control loops and until now it is highly subject to expertise [8].

For determining this variable, a dynamics hierarchy of the process is established from process knowledge considering that if the SVD of the process matrix gives a measurement of the importance of a variable inside the system [54], the SVD of process Hankel matrix provides the same information but including the dynamic behavior of the process. Here, the State Impactability Index (SII_{x_k}) defined by Eq. (4.1) [18] is used to determine the most important state variable within the process and thus define the control objective.

$$SII_{x_k} = \sqrt{\sum_{i=1}^p \sigma_{ii}^2 \sum_{j=0}^{n-1} \mathbf{U}_{k+nj,i}^2} \quad (4.1)$$

Here, \mathbf{U} and σ are found by the SVD of Hankel matrix, where p is the number of singular values (σ), \mathbf{U} matrix are the orthonormalized eigenvectors of $\mathbf{H}\mathbf{H}^T$ 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 the Main Dynamics (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, so there are no losses of process information in opposition on what happens on decentralized or distributed control schemes without requiring any heuristic decisions.

4.4.2. Optimization of SeDs set-points

On the strategy herein proposed, 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 can be easily regulated. Here, the effect of every SeDs over the MaD is exploited and explicitly extracted from the process non-linear model with some mathematical transformations. In this way, a sensitivity-driven coordination criteria is proposed in this procedure without requiring the solution of an optimal control problem. Here, *sensitivity* refers to a certain function $\mathcal{S}_i(\mathbf{x}(t), \mathbf{u}(t)) : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}$ that relates the influence of the secondary dynamics over the main dynamics. Such function is obtained directly from the process model by differentiating the MaD over each SeD from its corresponding equation on the steady-state model of the process. In this way, the sensitivity function of the MaD to changes in the i -th SeD x_i , \mathcal{S}_i , is given by (4.2).

$$\mathcal{S}_i(\mathbf{x}(t), \mathbf{u}(t)) = \left. \frac{\partial x^*}{\partial x_i} \right|_{x_j \neq i} \quad (4.2)$$

where x^* represents the MaD and x_j represents the j -th SeD, with $j \neq i = 1, \dots, n-2$. SeD set-points are the result of solving the optimization problem described by (4.3),

$$\begin{aligned} \min_{x_{1,sp}, \dots, x_{j,sp}} \quad & J = \alpha (x_{ss}^* - x_{sp}^*) + \sum_{i=0}^j \beta_i \frac{1}{\mathcal{S}_i} \quad (4.3) \\ \text{s.t.} \quad & x_{j,spmin} \leq x_j \leq x_{j,spmax} \\ & \Delta x_{j,spmin} \leq \Delta x_{j,sp} \leq \Delta x_{j,spmax} \end{aligned}$$

Here:

- x_{ss}^* corresponds to x^* steady-state value that would be achieved should the system reach steady-state with the $x_{i,sp}$ values determined during the optimization. This is extracted from the non-linear steady-state model of the process.
- \mathcal{S}_i corresponds to the sensitivity of MaD to changes on the i -th SeD at the current values of the process state. This intends to drive the optimization problem towards the SeDs values that help achieving the fastest return of the MaD to its required value.
- $x_{n,spmin}$ and $x_{n,spmax}$ are the limiting values for SeDs set-points that allow the obtainment of the desired value of the MaD and are extracted from the reachable set \mathcal{R}_x of the process, that will be defined later.
- $\Delta x_{j,spmin}$ and $\Delta x_{j,spmax}$ are the maximum and minimum changes possible in the SeDs set-points, limited by the actual admissible change of the manipulated variables $\Delta \mathbf{u}$ by the installed final control element.
- α corresponds to the weight of MaD error and is selected according the designers criteria. β_i are scaling constants such as all \mathcal{S}_i are on the same order of magnitude. Although there appear to be multiple parameters to be tuned, the determination of each β_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 β_i is recommended to be $\beta_i = 1$ for the \mathcal{S}_i with the lowest magnitude order.

In order to define the reachable set, the definition of *reachability* is required [72].

Definition 4.1. Reachability in time t . $\mathbf{x}_R \in \mathcal{X}$ is said to be reachable from $\mathbf{x}_0 \in \mathcal{X}$ in a time t if there exists a control input $\mathbf{u} : [0, t] \in \mathcal{U}$ such as $f(t, \mathbf{x}, \mathbf{u}) = \mathbf{x}_R$. Equivalently, \mathbf{x}_0 can be controlled to \mathbf{x}_R in time t

Here, \mathcal{X} represents the process state-space and \mathcal{U} the admissible inputs of the process and f is the process state-transition function, see (3.16). The notation $\mathbf{x}_0 \xrightarrow[t]{} \mathbf{x}_R$ indicates that \mathbf{x}_R can be reached from \mathbf{x}_0 , or equivalently, \mathbf{x}_0 can be controlled from \mathbf{x}_R . The reachable set \mathcal{R}_t is thus defined by Sontag [72] as follows:

Definition 4.2. Reachable set from \mathbf{x}_0 in time t . The set \mathcal{R}_t containing all $\mathbf{x} \in \mathcal{X}$ that the process can reach from \mathbf{x}_0 in a time t .

$$\mathcal{R}_t(\mathbf{x}_0) = \left\{ \mathbf{x} \in \mathcal{X} : \mathbf{x}_0 \xrightarrow[t]{} \mathbf{x} \right\} \quad (4.4)$$

This means that the reachable set are all the points in the state-space to which the system can be taken from its operating point through the available control inputs [73]. The constraint related to this set is then a way to ensure the possibilities of the control system being able to drive the process towards new admissible set-points in which the system can be stabilized. In this way, controllability and stability of the process are considered in the supervisory layer.

The optimization problem (4.3) must then be solved using global optimization techniques in order to avoid local solutions that might be far from the desired behavior. This will give the best values of the controlled variables for a given set of process SeDs. These values of the SeDs are the set-points to the controllers in the lower level of process regulation. 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 during a sampling time it results in a piece-wise optimized trajectory since each step of the process is optimized, one time-step at a time.

Regarding the objective function (4.3) some characteristics are worth highlighting:

- Contrary to the optimization performed by MPC and optimal controllers, the effect of the disturbances over the process is known since it uses current state measurements of the process to compute the sensitivities \mathcal{S}_i .
- Since steady-state sensitivities are computed with current measurements, they are updated to account for the dynamic evolution of the system and considers this to optimize the next step for the process.
- For obtaining the MaD sensitivities and therefore as the core of the optimization problem, the process model is used with some mathematical transformations (explicit differentiation) but maintaining its information about the process to obtain and exploit new

information that is not available from the original model. On the other hand, MPC uses the process model indirectly for output prediction.

Some triggers can also be established for the optimization procedure, 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 (4.3) greater than, for example, 5%, deviations on the MaD set-point greater than $\epsilon > 0$, or performing the optimization after a time t_j .

4.5. Illustrative example

In this section, the design procedure for a supervisory control structure developed throughout this chapter is applied to Continuous Stirred Tank Reactor (CSTR) as a test-bed for the supervisory control strategy developed in Section 4.4.

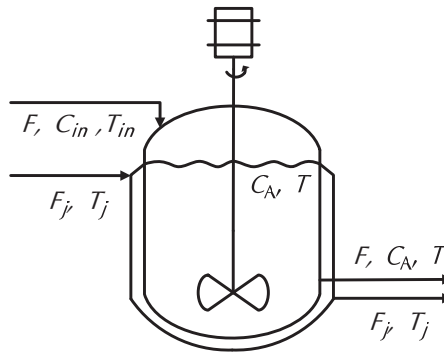


FIGURE 4.2. Process flow diagram for the CSTR.

Two different control approaches are analyzed for the CSTR shown in Fig. 4.2: (a) Decentralized, in which only individual PIDs are used for controlling the process and (b) Hierarchical, obtained by applying the design procedure proposed in this work. This process has been perhaps the most widely studied unit operation, from both dynamic analysis and control perspectives. Despite its apparent simplicity (only two state variables are considered), its interesting nature lies on the existence of exotic behavior, which increases the complexity of the control task for the reactor combined with a low availability of the control actions [74].

In this reactor, propylene glycol (PPG) is produced by the hydrolysis of propylene oxide (PO) with sulfuric acid as a catalyst ($PO + H_2O \rightarrow PPG$). Since water is supplied in excess, the reaction is first-order in propylene oxide concentration. The reaction is exothermic, so the reactor has a jacket for removing the excess of heat. Following the procedure described in Table 4.1, the first step is to obtain a phenomenological-based model of the process. For this process, the model developed by Bequette [74], presented in (4.5) and (4.6), is used.

$$\frac{dC_A}{dt} = \frac{F}{V} (C_{in} - C_A) - k_0 C_A e^{-E_a/RT} \quad (4.5)$$

$$\frac{dT}{dt} = \frac{F}{V} (T_{in} - T) - \frac{\Delta H k_0}{\rho C_p} C_A e^{-E_a/RT} - \frac{UA_j}{V \rho C_p} (T_j - T) \quad (4.6)$$

where V is the reactor volume, F the volumetric feed flow rate, C_{in} feed concentration, T_{in} feed temperature, C_A reactive concentration inside the reactor, T and T_j are the temperatures inside the reactor and in reactor jacket respectively. Also, ρ and C_p are the reactive mass density and heat capacity respectively, ΔH is the heat of reaction, E_a the activation energy, k_0 the frequency factor, both from Arrhenius law, and UA_j the product of the overall heat-transfer coefficient and the reactor heat transfer area. Values for these parameters can be found in [74].

On the second step, the operating point is defined, selecting the available manipulated variables. In this case, the control inputs are F and T_j . C_A and T as the states of the process, and the operating point is established in Table 4.2.

TABLE 4.2. Operating point of the CSTR.

Variable	Value	Span
C_A x_1	1146 mol/m ³	0 – C_{in}
T x_2	310.1 K	293.15 – 373.15 K
F u_1	0.18 m ³ /min	0–0.2286 m ³ /min
T_j u_2	280.2 K	0 – 298.15 K

Then, the design of the regulatory level takes place. On the third step, the input–output pairings of the process are selected. As stated in Section 4.3.2, they are established from the SVD of Hankel matrix. The values for the S_{II} of each state variable and the III of each input variable are reported on Table 4.3, according to which C_A is paired with F and T with T_j .

TABLE 4.3. State and Input Impactability indexes for the CSTR.

Variable	S_{II}	III
x_1	385.5	–
x_2	3.8	–
u_1	–	385.0
u_2	–	21.1

The fourth step involves controller tuning, which for this process is carried out through minimization of ITAE and IAE indexes by simulation with the non-linear model of the process. The dynamics hierarchy of the process is then established as indicated in Section 4.4.1. From Table 4.3, C_A is selected as MaD and T as the SeD. The control structure for the process and the closed-loop Process and Instrumentation Diagram (P& ID) are presented in Figures 4.3 and 4.4 respectively.

Finally, the coordinator in the supervisory layer is formulated based on (4.3). First, the value of the MaD that would be achieved should the system reach a steady-state is given by (4.7). Second, the C_A sensitivity to changes in T_r , \mathcal{S}_1 , is found by differentiating (4.5) from which (4.8) is obtained.

$$C_{A,ss} = \frac{FC_{in}/V}{F/V + k_0 e^{-E_a/RT}} \quad (4.7) \quad \mathcal{S}_1 = \frac{\partial C_A}{\partial T} = \frac{Vk_0 C_A e^{-E_a/RT}}{FT - k_0 T e^{-E_a/RT}} \quad (4.8)$$

As a last step, the constraints must be established. The values of T that achieve the set-point value for C_A are extracted from the steady-state map of the process (see Fig. 4.5) and will be used as constraints for the optimization problem in this layer. The steady-state map is

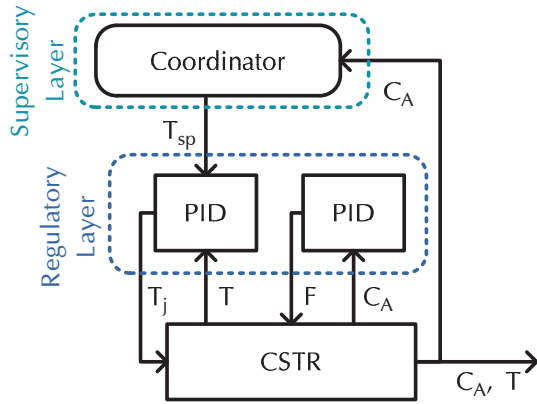


FIGURE 4.3. Hierarchical control structure for the CSTR.

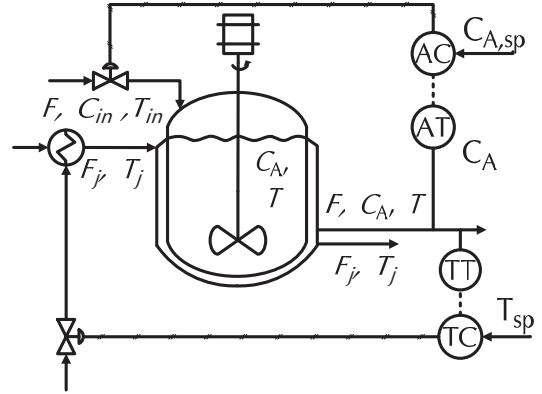


FIGURE 4.4. Closed-Loop P&ID for the CSTR.

a reachable set in infinite time \mathcal{R}_∞ , since the system is allowed to reach the steady-state to compute this set. Despite there is a void space in Fig. 4.5, it is attributed the numerical solution of Eqs.(4.5) and (4.6), since it was demonstrated that they are feasible steady-states of the process.

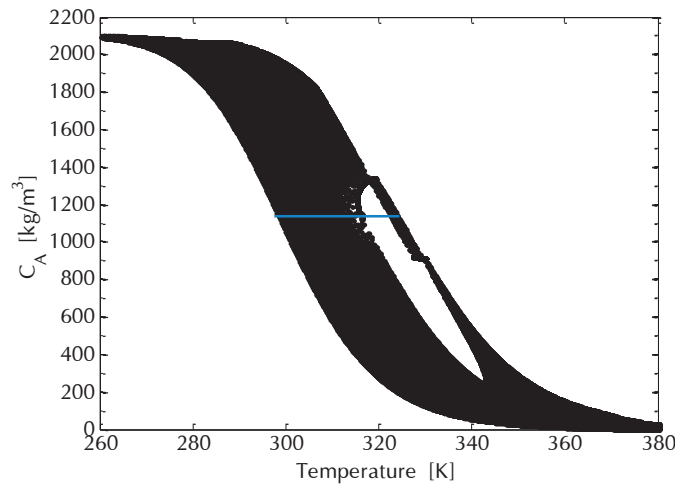


FIGURE 4.5. Steady-state map for the CSTR.

The optimization problem to be solved in the supervisory level is thus given by (4.9).

$$\min_{T_{sp}} \alpha (C_{A,ss} - C_{A,sp}) + \frac{1}{S_1} \quad (4.9)$$

$$\begin{aligned} \text{s.t. } & 285.3 \leq T_{sp} \leq 308.3 \\ & 0 \leq \Delta T_{sp} \leq 3 \text{ K} \end{aligned} \quad (4.10)$$

This problem is then solved using restricted enumeration optimization over a discrete set of feasible values for reactor temperature established by the inequality constraints. The solution method determines temperature optimal value as by means of an enumerative search over that set [75]. This is a global optimization technique, so the solution of the problem can be considered as the global minimum of the objective function. It is worth clarifying that this optimization is solved at each sample time, supporting the selection of an stochastic

optimization method, since deterministic methods demand a computation time greater than the sampling time of the control system.

Both control schemes are compared when disturbances on feed temperature and concentration appear. PIDs for both structures have the same tuning obtained in a previous step of the design procedure. The feed concentration is reduced on a 25% of its nominal value at 50 minutes, is taken again to its nominal value (2115.696 mol/m^3) at 150 minutes, and finally increased in 20% at 250 minutes. The response of the MaD, C_A is presented in Fig. 4.6. For every disturbance, it can be seen that by the hierarchical approach a lower magnitude overshoot Δ of C_A is obtained ($\Delta_{hier,max} = 25 \text{ mol/m}^3$ vs $\Delta_{dec,max} = 30 \text{ mol/m}^3$) and a faster return to its set-point is possible ($t_{shier,max} = 15$ vs $t_{sdec,max} = 40$). This is advantageous since it implies less product that can be out of specifications.

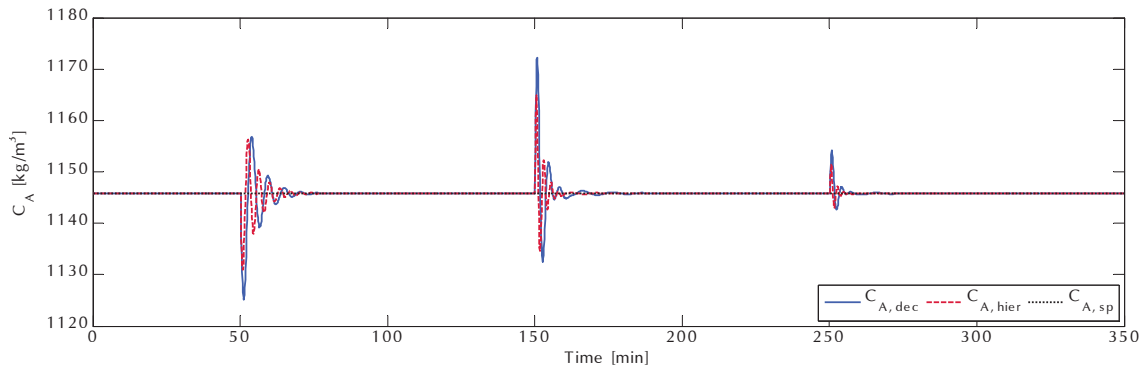


FIGURE 4.6. C_A response for disturbances on C_{in} . The subscripts *dec* and *hier* represent the decentralized (individual PID) and hierarchical approaches respectively.

When comparing the feed flowrate from Fig. 4.7, i.e., the manipulated variable for C_A , it exhibits less oscillatory behavior with the hierarchical structure, representing less control efforts and a smoother response as it was desired for the MaD control loop.

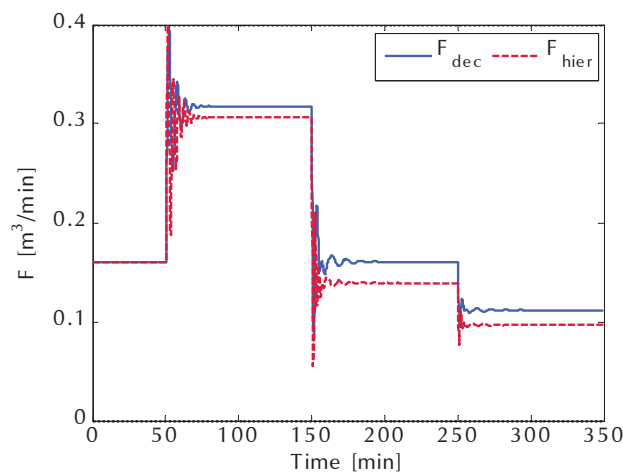


FIGURE 4.7. Feed flow rate response for disturbances on C_{in} . The subscripts *dec* and *hier* represent the decentralized (individual PID) and hierarchical approaches respectively.

Temperature dynamic response with both approaches is shown in Fig. 4.8. Here, T_r set point is displaced to a new value with the hierarchical approach and it is successfully regulated in

this new value. On the contrary, the decentralized approach is not able to regulate T_r after the first disturbance. Moreover, with the hierarchical approach it is evidenced that it is not necessary to regulate reactor temperature in a fixed value since its set-point changes from 310.1 K (nominal value) to 308.6 K (optimized value), and still C_A is maintained.

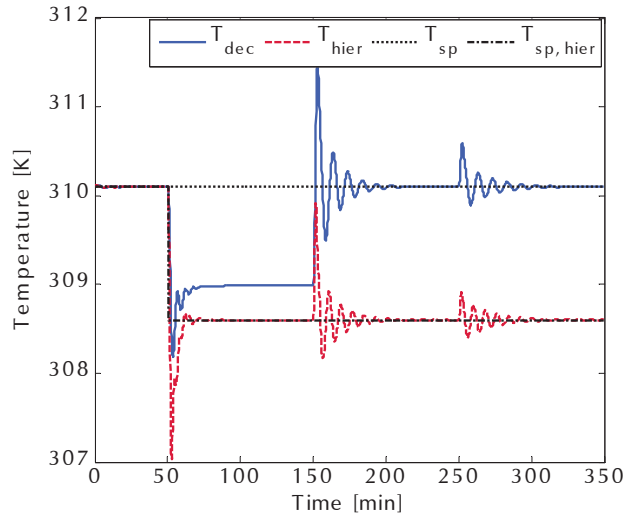


FIGURE 4.8. T response for disturbances on C_{in} . The subscripts *dec* and *hier* represent the decentralized (individual PID) and hierarchical approaches respectively.

The response of the jacket temperature, manipulated variable for T_r , is shown in Fig. 4.9. It can be seen that after the first disturbance, T_j reaches its maximum value in both cases but it remains less time on this situation with the hierarchical approach (10 minutes vs. 100 minutes with the decentralized approach). This is an advantage of the hierarchical approach, since any possible disturbance during this time could lead the decentralized system to undesired operating points, also considering that with the decentralized approach reactor temperature does not return to its nominal value after the first disturbance despite this saturation condition.

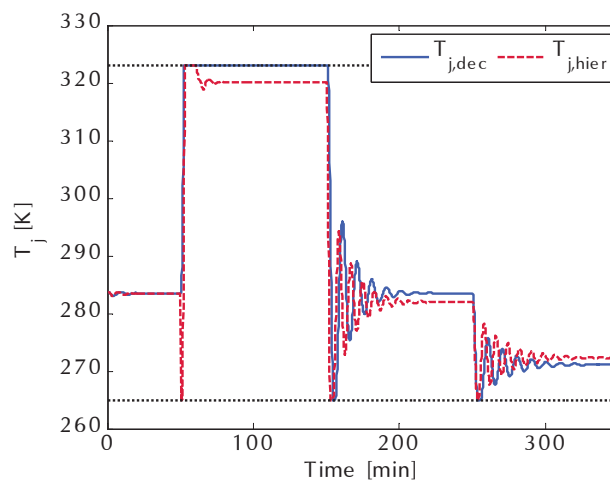


FIGURE 4.9. T_j response for disturbances on C_{in} . The subscripts *dec* and *hier* represent the decentralized (individual PID) and hierarchical approaches respectively.

In Table 4.4 control performance indexes (IAE, ITAE, IAU and ITAU) are presented for temperature and concentration control loops under both control schemes. The performance index

related to the control efforts (IAU) is modified to consider the temporal effect of the control action, resulting on the ITAU given by (4.11).

$$ITAU = \int_0^{\infty} t|u(t)| dt, \quad (4.11)$$

TABLE 4.4. Performance indexes for disturbances on feed concentration.

Index	$C_{A,dec}$	$C_{A,hier}$	T_{dec}	T_{hier}
IAE	158.5	99.32	128.58	18.30
ITAE	18296.45	10616.97	1401.10	2524.67
IAU	0.16	0.23	285.85	61.865
ITAU	9939.07	8951.08	17390715	17358724

From Table 4.4, it can be concluded that a better performance of the control system is achieved by the hierarchical approach since a decrease on the performance indexes is attained. This reduction is particularly greater for C_A control loop, where lower errors are obtained with the hierarchical approach. This, combined with the lower overshoots provides a better dynamic behavior of the control system, considering also the reduced control efforts (as quantified by IAU and ITAU) which indicates that the hierarchical control structure can attenuate the effects of that disturbance with relatively minimal control effort. A significant reduction on the IAE, ITAE and IAU for T control loop is also achieved, considering that it does not have the strong regulation requirement of the decentralized scheme, but still has its stability guaranteed.

Additionally, disturbances in feed temperature are applied to the system. First, it is reduced on a 5% of its nominal value at 50 minutes, then is taken again to its nominal value (295.22 K) at 150 minutes, and finally it is increased in 2% at 250 minutes. From Fig. 4.10, it can be seen that disturbances on feed temperature do not have a high impact on C_A with the hierarchical structure, but they do on the decentralized case. Furthermore, the overshoots are smaller and the stabilization time is lower with the hierarchical control scheme, considering that there also are less variations on the feed flow rate which reduces control efforts (see Fig. 4.11). These facts can be verified from the concentration loop performance indexes shown in Table 4.5.

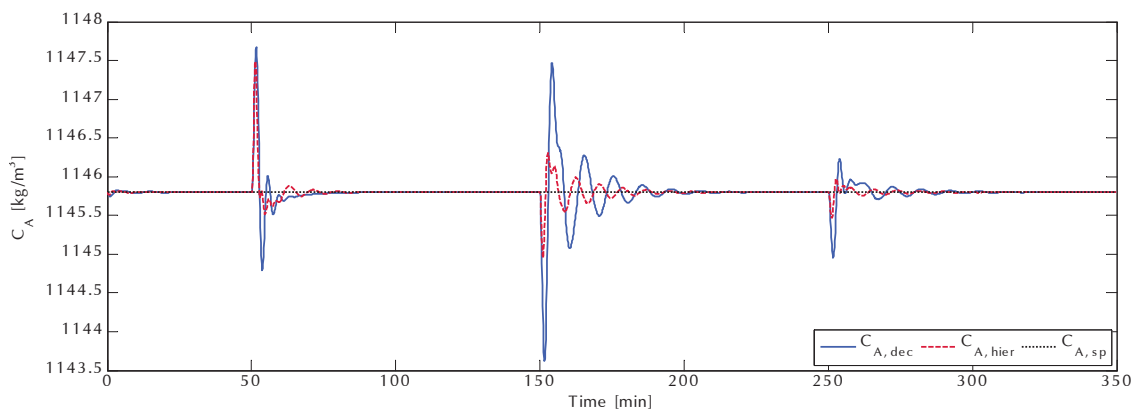


FIGURE 4.10. C_A response for disturbances on T_{in} . The subscripts *dec* and *hier* represent the decentralized (individual PID) and hierarchical approaches respectively.

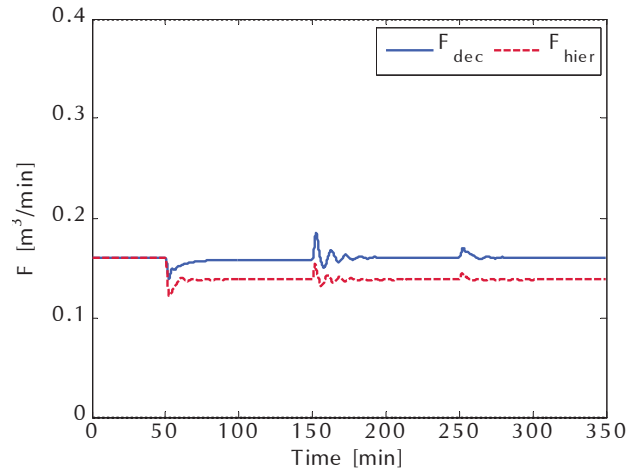


FIGURE 4.11. Feed flowrate response for disturbances on T_{in} . The subscripts *dec* and *hier* represent the decentralized (individual PID) and hierarchical approaches respectively.

Regarding reactor temperature, after the first disturbance the decentralized approach is not able to return to its nominal value (see Fig.4.12), while the hierarchical approach by displacing its set-point gets to regulate reactor temperature with lower control efforts, as evidenced in Table 4.5.

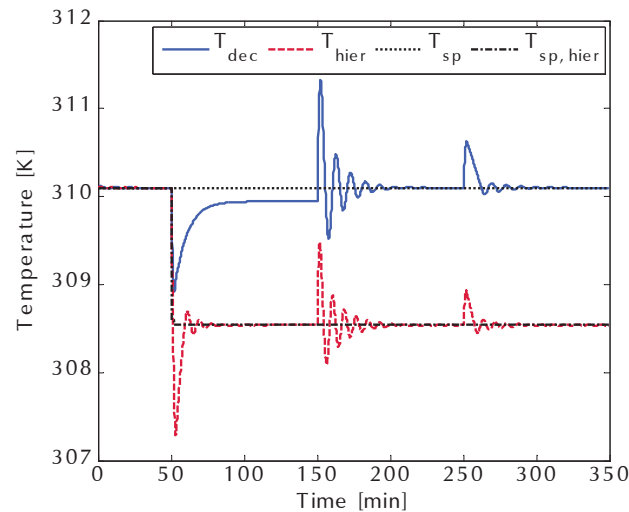


FIGURE 4.12. T response for disturbances on T_{in} . The subscripts *dec* and *hier* represent the decentralized (individual PID) and hierarchical approaches respectively.

Although after the first and last disturbances both systems reach T_j upper saturation bound (See Fig.4.13), the hierarchical approach remains less time in that situation compared to the decentralized one, which gives the former a great advantage over the latter as discussed previously. Moreover, after the last disturbance gets rejected, the decentralized system ends closer to the lower saturation limit than the hierarchical system, which places the decentralized one under a more vulnerable situation.

By comparing the performance indexes of both structures presented in Table 4.5, it is found that the hierarchical approach deals better with disturbances in T_{in} . Also, by obtaining lower

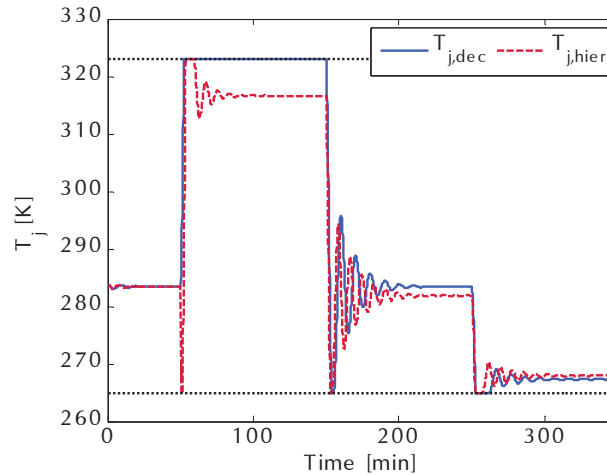


FIGURE 4.13. T_j response for disturbances on T_{in} . The subscripts *dec* and *hier* represent the decentralized (individual PID) and hierarchical approaches respectively.

TABLE 4.5. Performance indexes for disturbances on feed temperature.

Index	$C_{A,dec}$	$C_{A,hier}$	T_{dec}	T_{hier}
IAE	24.95	10.16	39.63	16.90
ITAE	3772.12	1362.99	4825.97	2231.69
IAU	0.0253	0.0232	88.29	57.39
ITAU	9801.88	8497.05	17270494	17192601

indexes than those on the case of disturbances on feed concentration, it can be concluded that disturbances affecting other dynamics can be easily rejected by redefining the remaining dynamics set-points which handle the effect of those disturbances before they can affect the concentration in the reactor in a significant way.

4.6. Concluding remarks

In this chapter the procedure for designing supervisory control structures was described and applied to a CSTR. Here, it is worth highlighting:

- The usage of an index for determining a dynamics hierarchy of the process and using it for establishing control objectives in addition to input-output pairings. This hierarchy allows to control a process by model-based coordination of non-critical state variables to achieve the regulation of the main dynamic of the process.
- 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 non-critical state variables. This optimization is based on the process interactions extracted from its model, and uses information gathered on-line from the process non-linear model and process sensors.
- By means of the proposed hierarchical approach, control of highly-coupled multivariable process can be achieved without needing sophisticated control strategies such as

MPC, which is very important when considering the industrial implementation of these control strategies.

- The proposed hierarchical control structure is applied to a CSTR in comparison to a decentralized structure. It is found that for disturbances on process inputs the hierarchical approach has a better performance based on performance index criteria. It is demonstrated that by only regulating the MaD and using SeD set-points to help regulate the MaD, a better performance of the control system is achieved with lower control efforts. It is also evidenced that not every disturbance on the process must be rejected since the SeD set-point changes can deal with them before they affect the MaD in a significant way.

CHAPTER 5

Case of Study: Reactor–Separator–Recycle system for Propylene glycol production

In this chapter, the control of a plant for propylene glycol production is addressed. In Section 5.1, the plant layout considered and the model of the process are presented. Then, the controllers available in the regulatory layer are described in Section 5.2. The design of the supervisory layer can be found in Section 5.3. Section 5.4 presents a comparison between the hierarchical and decentralized control structures for some disturbances on the plant. Finally, some concluding remarks of this chapter are drawn in Section 5.5.

5.1. Process model

The process considered features a reactor and a flash column interconnected with a material recycle, known as Reactor–Separator–Recycle (RSR) systems, with a mixing point and a heat exchanger as shown in Fig. 5.1. In this process, fresh feed is mixed with the 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 water and propylene oxide 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 is sent back to be mixed with fresh feed to the reactor.

The process model was obtained by following the methodology proposed in [65] and was developed by Calderón [68] considering the dynamic behavior of the pipelines. The phenomenological–based model is composed by (5.1)-(5.16). Here, transport delays in the pipelines are neglected. Values for all model parameters can be found in Table 5.1.

TABLE 5.1. Parameters of the propylene glycol plant.

Parameter	Value	Units	Description
D_r	2.4	m	Reactor diameter
D_c	1.568	m	Column diameter
V_{hx}	0.5	m ³	Heat exchanger volume
V_r	18.46	m ³	Reactor volume
k_0	2.83E+10	1/min	Frequency factor
E_a	75361.14	J/mol	Activation energy
ΔH	-4.07E+04	J/mol	Heat of reaction

Parameter	Value	Units	Description
R	8.3174	$\text{m}^3\text{Pa}/\text{molK}$	Universal gas constant
ρC_p	3571300	J/m^3	Product of propyleneglycol density and heat capacity
U	$4.56\text{E}+04$	$\text{J}/\text{m}^2\text{min}$	Reactor overall heat transfer coefficient
A	27.1434	m^2	Reactor heat transfer area
C_v	4071	J/kgK	Heat capacity of the cooling fluid in the heat exchanger
MW_A	58.08	kg/kmol	Reactant molecular weight
MW_B	76.09	kg/kmol	Product molecular weight
ρ_A	0.83	kg/m^3	Reactant density
ρ_B	1.036	kg/m^3	Product density
$MW_{\text{H}_2\text{O}}$	18	kg/kmol	Water molecular weight
$\rho_{\text{H}_2\text{O}}$	1	kg/m^3	Water density
$C_{B,0}$	0	mol/m^3	Product concentration in the fresh feed
T_0	310.22	K	Fresh feed temperature
U_{hx}	$8.00\text{E}+04$	$\text{J}/\text{m}^2\text{min}$	Heat exchanger overall heat transfer coefficient
A_{hx}	2.5	m^2	Heat exchanger heat transfer area
α	6	–	Product/Reactant relative volatility

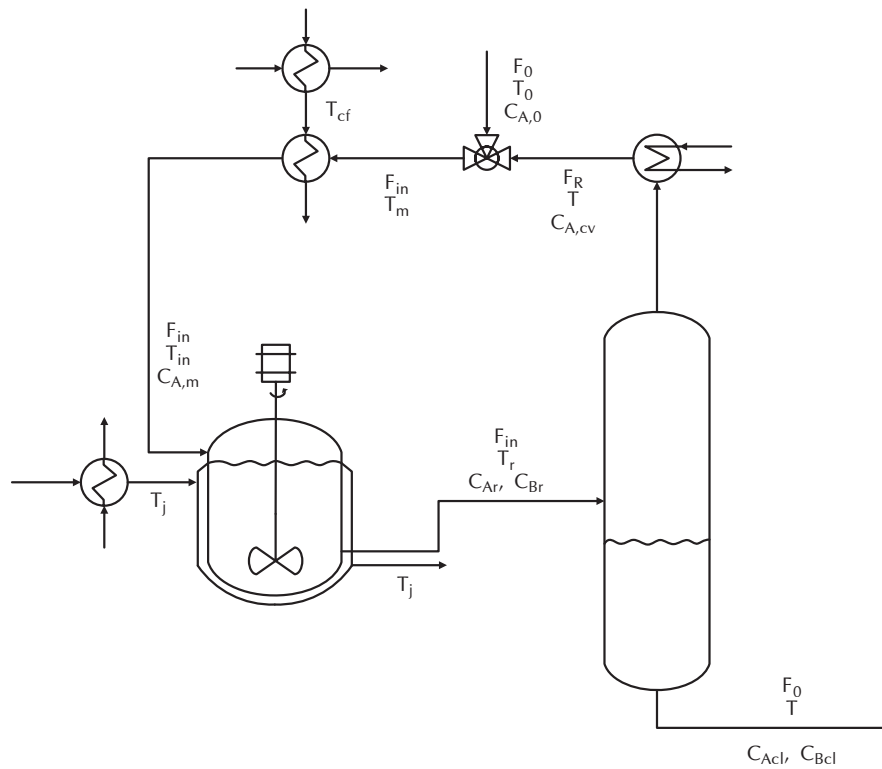


FIGURE 5.1. Process Flow Diagram for propylene glycol production.

The model for the whole process consists of the models for each operating unit (reactor, flash separator, mixing point and heat exchanger). Each units model will be presented independently for easier comprehension.

REACTOR: Considering the aqueous solution, water is present in excess respect to the reactive components, so the reaction can be assumed as a first order reaction regarding the oxide concentration. The reaction is considered as an irreversible reaction.

$$\frac{dC_{A,r}}{dt} = \frac{F_{in}}{V_r} (C_{A,m} - C_{A,r}) - C_{A,r}k_0e^{-E_a/RT_r} \quad (5.1)$$

$$\frac{dC_{H_2O,r}}{dt} = \frac{F_{in}}{V_r} (C_{H_2O,m} - C_{H_2O,r}) - C_{A,r}k_0e^{-E_a/RT_r} \quad (5.2)$$

$$\frac{dC_{B,r}}{dt} = \frac{F_{in}}{V_r} (C_{B,0} - C_{B,r}) + C_{A,r}k_0e^{-E_a/RT_r} \quad (5.3)$$

$$\frac{dT_r}{dt} = \frac{F_{in}}{V_r} (T_{in} - T_r) - \frac{\Delta Hk_0}{\rho C_p} C_{A,r}e^{-E_a/RT_r} - \frac{UA_s}{V_r\rho C_p} (T_r - T_j) \quad (5.4)$$

where $C_{A,r}$, $C_{B,r}$ and $C_{H_2O,r}$ are propylene oxide, propylene glycol and water concentration in the reactor respectively; T_r is the temperature inside the reactor, $C_{A,m}$ and $C_{H_2O,m}$ represent reactant and water concentration in the mixing point respectively; $C_{B,0}$ is the initial product concentration and F_{in} and T_{in} are the feed flow rate and temperature respectively. Additionally, k_0 is the frequency factor, E_a is the activation energy, ΔH is the heat of reaction, R is the universal gas constant, T_j is the temperature inside the reactor jacket, and UA_s is the product of the overall heat-transfer coefficient and the surface area in the reactor respectively. V_r is the reactor volume, ρ is the density of the reactive mass and C_p its heat capacity.

FLASH SEPARATOR: The separation in this column is considered to be isothermal. In addition, the separator pressure is assumed to be kept constant, controlled by the overhead condenser so the separation factor is only temperature-dependent and the gas flow obtained is directly related to the feed temperature. Furthermore, given the difference on volatilities, the amount of product vaporized is neglected. Equilibrium between liquid and gas phases is modeled considering the residence time in the column and the relative volatilities between the product and reactant.

$$\frac{dC_{A,cl}}{dt} = \frac{1}{V_l} (F_{in}C_{A,r} - F_0C_{A,cl}) - F_R C_{A,cv} \quad (5.5)$$

$$\frac{dC_{H_2O,cl}}{dt} = \frac{1}{V_l} (F_{in}C_{H_2O,r} - F_0C_{H_2O,cl}) - F_R C_{H_2O,cv} \quad (5.6)$$

$$\frac{dC_{B,cl}}{dt} = \frac{1}{V_l} (F_{in}C_{B,r} - F_0C_{B,cl}) \quad (5.7)$$

$$y^* = \frac{1.5V_l\alpha}{40F_{in}} \left(\frac{C_{A,cl}}{\alpha C_{A,cl} + C_{B,cl} + C_{H_2O,cl}} \right) \quad (5.8)$$

$$C_{A,cv} = \frac{1 \times 10^6 y^*}{y^* (Mw_A \rho_{H_2O} - Mw_{H_2O} \rho_A) / \rho_A \rho_{H_2O} + Mw_{H_2O} / \rho_{H_2O}} \quad (5.9)$$

$$C_{H_2O,cv} = \frac{1 \times 10^6}{y^* Mw_A / (1 - y^* \rho_A) + Mw_{H_2O} / \rho_{H_2O}} \quad (5.10)$$

$$F_R = \frac{T_r - 273}{500} \quad (5.11)$$

In (5.5)–(5.10), $C_{A,cl}$, $C_{B,cl}$ and $C_{H_2O,cl}$ are reactant, product and water concentrations in the liquid stream exiting the flash column respectively, $C_{A,cv}$ and $C_{H_2O,cv}$ are the reactant and water concentration in the gas stream of the flash column. Furthermore, y^* represents a separation factor and α is the relative volatility between the product and the reactant. V_l is the column volume, 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_{H_2O} , ρ_A , ρ_{H_2O} are the molecular weights and densities of reactant and water respectively.

MIXING POINT: The condensed gas stream from the flash column and fresh feed are mixed instantaneously. The arithmetic equations that describe this process are presented in (5.12)–(5.14), where $C_{A,0}$ and T_0 are the feed reactant concentration and temperature respectively.

$$C_{A,m} = \frac{F_R C_{A,cv} + F_0 C_{A,0}}{F_{in}} \quad (5.12)$$

$$C_{H_2O,m} = \frac{F_R C_{H_2O,cv} + F_0 C_{H_2O,0}}{F_{in}} \quad (5.13)$$

$$T_m = \frac{F_R T_r + F_0 T_0}{F_{in}} \quad (5.14)$$

$$F_{in} = F_R + F_0 \quad (5.15)$$

HEAT EXCHANGER: Here, only reactor feed temperature is considered, since no chemical reaction occurs in this equipment.

$$\frac{dT_{in}}{dt} = \frac{F_{in}}{V_{hx}} (T_m - T_{in}) + \frac{U_{hx} A_{hx}}{1 \times 10^3 V_{hx} \rho_{hx} C_p} (T_{cf} - T_{in}) \quad (5.16)$$

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

The operating point of the process is then defined as indicated on Table 5.2. The system has eight state variables and three input variables.

5.2. Regulatory layer

For the design of the regulatory level, input–output pairings must be established. However, the SVD methodology proposed in [18] has the requirement of having the same number of state and input variables and therefore it can not be used. To overcome this, the controllers in this layer are designed considering the *SII* for the selection of controlled variables, whose values are reported on Table 5.3.

In this case, $C_{B,cl}$, $C_{B,r}$ and $C_{A,cl}$ are the most important variables and should be controlled. However, since there is no vaporization of B in the column, $C_{B,cl}$ and $C_{B,r}$ can be considered as equivalent control objectives. Given that the column does not have a direct action of the

TABLE 5.2. Operating point of the propylene glycol plant.

Variable		Value	Span
$C_{A,r}$	x_1	645.9965 mol/m ³	0 – 4000 mol/m ³
$C_{B,r}$	x_2	726.98127 mol/m ³	0 – 1×10^6 mol/m ³
$C_{H_2O,r}$	x_3	49491.054 mol/m ³	0 – 4×10^6 mol/m ³
T_r	x_4	324.822 K	273 – 350 K
$C_{A,cl}$	x_5	689.3169 mol/m ³	0 – 4000 mol/m ³
$C_{B,cl}$	x_6	1025.183 mol/m ³	0 – 1×10^6 mol/m ³
$C_{H_2O,cl}$	x_7	47865.168 mol/m ³	0 – 4×10^6 mol/m ³
T_{in}	x_8	311.5025 K	273 – 400 K
F_0	u_1	0.25267 m ³ /min	0–0.5 m ³ /min
T_j	u_2	330 K	273 – 373 K
T_{cf}	u_3	290 K	275 – 373 K

TABLE 5.3. State and Input Impactability indexes for the propylene glycol plant.

Variable	<i>SII</i>
$C_{B,cl}$	0.6643
$C_{B,r}$	0.5069
$C_{A,cl}$	0.5050
T_{in}	0.4986
T_r	0.4562
$C_{A,r}$	0.2741
$C_{H_2O,cl}$	0.0026
$C_{H_2O,r}$	0.0003

control inputs, $C_{B,cl}$ is disregarded and only $C_{B,r}$ is controlled and T_{in} is added as controlled variable. T_r is not considered since along $C_{B,r}$ they are reactor outputs and are highly coupled with the available control action in the reactor (T_j) (see (5.3) and (5.4)) contradictory effects are found if both variables are controlled independently. Thus, a cascade control is proposed with $C_{B,r}$ being the variable controlled in the master loop and T_r the controlled variable in the slave loop.

Having now equal number of state and manipulated variables, input–output pairings can be established through the SVD of Hankel matrix, where values of the *SII* and *III* are found in Table 5.4. Initially all variables are included and in this case (set A) T_r is paired with T_j . Then, this variables are eliminated, obtaining set B and according to *SII* and *III* values, $C_{A,cl}$ is paired with F_0 and T_{in} with T_{cf} . In this way, the closed–loop P& ID of the plant is presented in Fig. 5.2.

TABLE 5.4. State Impactability indexes for the propylene glycol plant.

Set	Variable	<i>SII</i>	Variable	<i>III</i>
A	$C_{B,r}$	0.2628	F_0	0.2494
	$C_{A,cl}$	0.0475	T_j	0.2577
	T_{in}	0.2474	T_{cf}	0.0617
B	$C_{A,cl}$	0.0742	F_0	0.1040
	T_{in}	0.1976	T_{cf}	0.1837

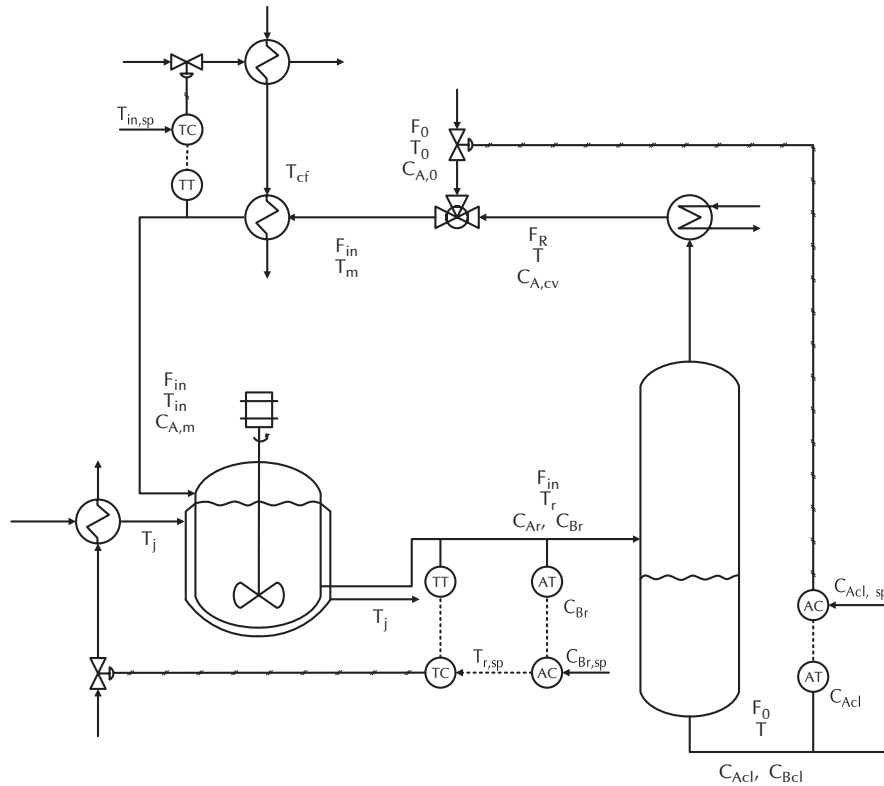


FIGURE 5.2. Closed-Loop diagram for the RSR system.

5.3. Supervisory layer

In this section, the design of the supervisory layer is detailed. Here, the establishment of the dynamics hierarchy of the whole plant and the formulation of the optimization problem for SeDs set-points is presented.

5.3.1. Dynamics hierarchy

The dynamics hierarchy of the process is determined as indicated in Section 4.4.1. According to the *SII* from Table 5.4, $C_{B,r}$ is selected as MaD and thus, $C_{A,cl}$ and T_{in} are the SeDs. The control structure for the process is presented in Fig. 5.3. Despite 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 Fig. 5.3, and will be explained in further detail on the supervisory layer design.

5.3.2. Coordinator design

The coordinator on the supervisory layer is formulated based on (4.3). For this, the sensitivities of the MaD to SeD are required and obtained from the steady-state process model, which corresponds to (5.1)-(5.16) with all time derivatives equal to zero. As $C_{B,r}$ is not a direct function of the secondary dynamics, it is necessary to use a directed graph to determine derivation

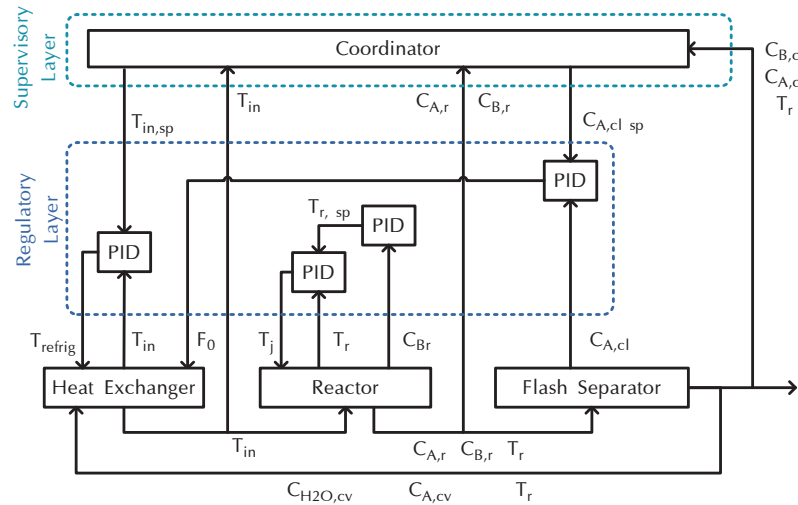


FIGURE 5.3. Hierarchical control structure for the RSR system.

path that allows the sensitivities determination. A Directed Graph (DG) is a qualitative causal model which captures the information flow in the model [76], and can be obtained from the non-linear model of the process. The DG for the Reactor-Separator-Recycle process is presented in Fig. 5.4, 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.

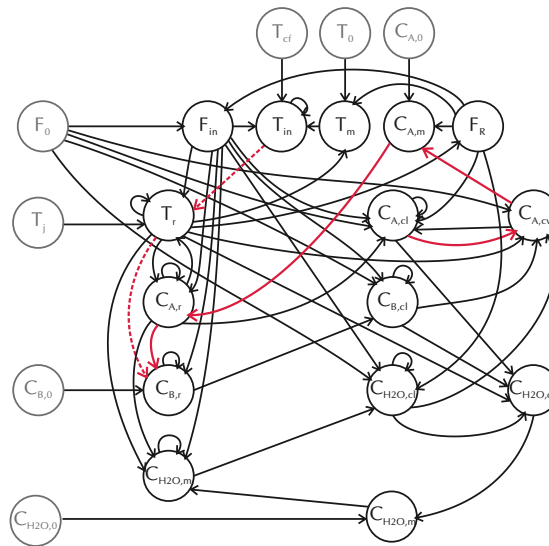


FIGURE 5.4. Directed graph for the RSR.

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

1. S_1 , i.e., the sensitivity of $C_{B,r}$ to T_{in} is found according to Eq. (5.17), corresponding to the path marked by the red dashed lines.

$$S_1 = \frac{\partial C_{B,r}}{\partial T_{in}} = \frac{\partial C_{B,r}}{\partial T_r} \frac{\partial T_r}{\partial T_{in}} \tag{5.17}$$

where:

$$\frac{\partial C_{B,r}}{\partial T_r} = \frac{500V_r k_0 C_{A,r} e^{-E_a/RT_r} (E_a/RT_r - 1)}{(500F_0 + T_r - 273)^2} \quad (5.18)$$

and

$$\frac{\partial T_r}{\partial T_{in}} = \frac{500F_0 + T_r - 273}{500F_0 + T_r - 273 + \frac{500V_r k_0 C_{A,r} \Delta H k_0}{\rho C_p} e^{-E_a/RT_r} - T_{in} + T_r} \quad (5.19)$$

2. S_2 , i.e., the sensitivity of $C_{B,r}$ to $C_{A,cl}$ is computed with (5.20). Here 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 red lines.

$$S_2 = \frac{\partial C_{B,r}}{\partial C_{A,cl}} = \frac{\partial C_{B,r}}{\partial C_{A,r}} \frac{\partial C_{A,r}}{\partial C_{A,m}} \frac{\partial C_{A,m}}{\partial C_{A,cv}} \frac{\partial C_{A,cv}}{\partial C_{A,cl}} \quad (5.20)$$

Here,

$$\frac{\partial C_{B,r}}{\partial C_{A,r}} = \frac{\partial C_{B,r}}{\partial T_r} \frac{\partial T_r}{\partial C_{A,r}} \quad (5.21)$$

then,

$$\frac{\partial C_{B,r}}{\partial C_{A,r}} = \frac{\frac{500V_r \Delta H k_0^2 e^{-2E_a/RT_r}}{\rho C_p (500F_0 + T_r - 273)}}{\frac{500F_0 + T_r - 273}{500V_r} - \frac{\Delta H k_0 E_a C_{A,r} e^{-E_a/RT_r}}{R \rho C_p T_r^2} - \frac{UA}{V_r \rho C_p}} \quad (5.22)$$

Additionally, from (5.1) and (5.12) it is found:

$$\frac{\partial C_{A,r}}{\partial C_{A,m}} = \frac{500F_0 + T_r - 273}{500F_0 + T_r - 273 + 500V_r e^{-E_a/RT_r}} \quad (5.23)$$

$$\frac{\partial C_{A,m}}{\partial C_{A,cv}} = \frac{T_r - 273}{500F_0 + T_r - 273} \quad (5.24)$$

and finally, from (5.9)

$$\frac{\partial C_{A,cv}}{\partial C_{A,cl}} = \left(\frac{75e6V_I \alpha}{4(500F_0 + T_r - 273) (\alpha C_{A,cl} + C_{B,cl} + C_{H_2O,cl})^2} \right) \left(\frac{1 - \frac{y^* (Mw_A \rho_{H_2O} - Mw_{H_2O} \rho_A)}{\rho_A \rho_{H_2O}}}{\left(\frac{y^* (Mw_A \rho_{H_2O} - Mw_{H_2O} \rho_A)}{\rho_A \rho_{H_2O}} + \frac{Mw_{H_2O}}{\rho_{H_2O}} \right)^2} \right) \quad (5.25)$$

In (5.18)–(5.25) T_r , $C_{A,r}$, $C_{B,cl}$, $C_{H_2O,cl}$ 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 plant, as indicated in Section 4.4.2. The obtained set is \mathcal{R}_{3000} which considers all the $\mathbf{x} \in \mathcal{X}$ that can be reached from the operating point in Table 5.2 in 3000 minutes. This was performed by using the admissible control inputs with an uniform

distribution and taking 35000 samples to guarantee that all the admissible combination of inputs is covered.

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 SeDs are shown. Figure 5.5 presents the reachable set with $C_{B,r}$ (MaD) as a function of T_{in} and $C_{A,cl}$ (the SeDs).

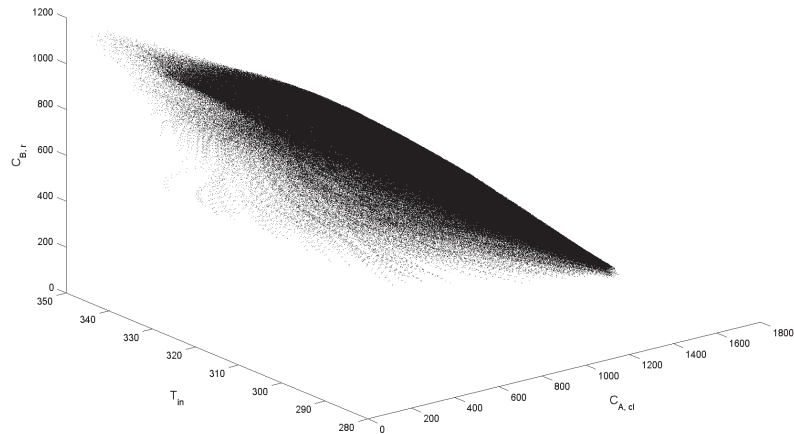


FIGURE 5.5. \mathcal{R}_{3000} for the RSR system.

The SeDs bounds are then determined by means of Figures 5.6 and 5.7 where the red dots represent the values of the MaD set–point. Here, the scattered regions of the set \mathcal{R}_{3000} are not considered in order to avoid unstable or uncontrollable regions, and thus, the boundaries for each secondary dynamics are $310K \leq T_{in} \leq 320 K$ and $500 \text{ mol/m}^3 \leq C_{A,cl} \leq 900 \text{ mol/m}^3$.

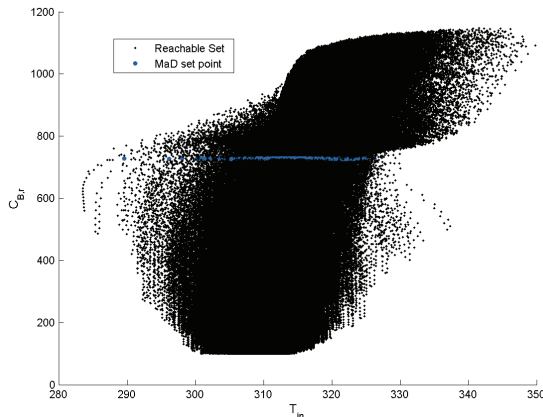


FIGURE 5.6. Reachable set for the RSR system:
 $C_{B,r}$ vs T_{in} .

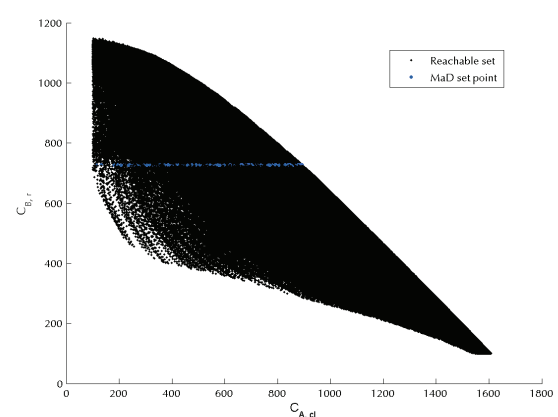


FIGURE 5.7. Reachable set for the RSR system:
 $C_{B,r}$ vs $C_{A,cl}$.

Therefore, the optimization problem to be solved by the supervisory layer is given in (5.26), 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 $C_{A,cl}$ per minute.

$$\begin{aligned} \min_{T_{in}, C_{A,cl}} J &= \alpha (C_{Br,ss} - C_{Br,sp}) + \beta_1 \frac{1}{S_1} + \beta_2 \frac{1}{S_2} \\ \text{s.t. } 310 \text{ K} &\leq T_{in} \leq 320 \text{ K} \\ 500 \text{ mol/m}^3 &\leq C_{A,cl} \leq 900 \text{ mol/m}^3 \\ 0 &\leq \Delta T_{in} \leq 2 \text{ K/min} \\ 0 &\leq \Delta C_{A,cl} \leq 0.015 C_{A,cl} \text{ mol/m}^3 \end{aligned} \quad (5.26)$$

In this case, $\alpha = 10$, $\beta_1 = 0.8$ and $\beta_2 = 1$ and where determined reducing β_1 if the response on either T_{in} or T_{cf} was too oscillatory using the same criteria as when adjusting K_p in a PID controller. This optimization problem is then solved by a global optimization method, in this case, a genetic algorithm was selected.

5.4. Results

Both control schemes are compared when disturbances on feed concentration appear. First, at 50 minutes it is reduced on a 9.5% of its nominal value and at 700 minutes it is increased to a 30% of its nominal value. PIDs for both structures have the same tuning obtained in a previous step of the design procedure. The subscripts *dec* and *hier* in Figures 5.8 to 5.14 represent the decentralized (independent PIDs) and hierarchical approaches respectively.

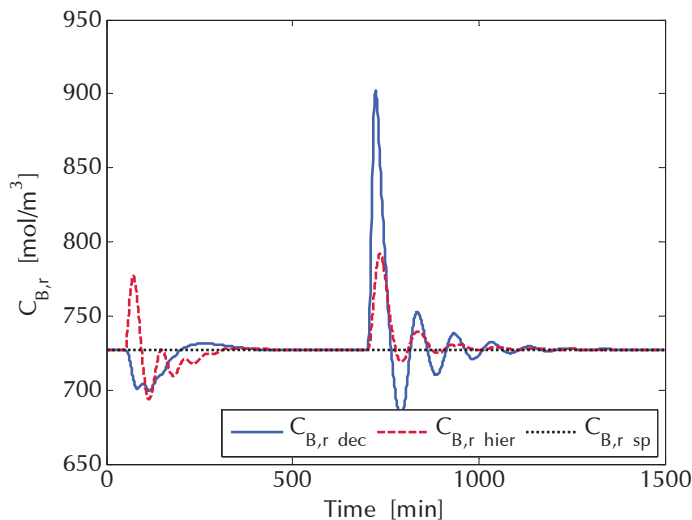


FIGURE 5.8. Product concentration in the reactor.

The Main Dynamics response is presented in Fig. 5.8 with both approaches. For the hierarchical approach it can be seen that a lower magnitude overshoot of $C_{B,r}$ is obtained with a less oscillatory behavior and a faster return to its set–point. For the first disturbance, it is worth noticing that the direction of the response through both approaches is different: with the decentralized approach $C_{B,r}$ tends to diminish whilst with the hierarchical approach it tends to increase. This behavior can be attributed to the different set–point determined for $C_{A,cl}$ by the hierarchical approach in which it reduces. This reduction causes that the amount of A in the recycle stream entering to the reactor increases and therefore more B is produced. On the other hand, the decentralized approach by keeping $C_{A,cl}$ in a higher value, 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 is presented in Figures 5.9 and 5.10. Recalling that T_r is the manipulated variable for $C_{B,r}$ lower control efforts are required since after the first disturbance the hierarchical approach demands a lower temperature in the reactor, which gives a less aggressive response, which is supported by the performance indexes for $C_{B,r}$ control loop presented in Table 5.5. Additionally, after the second disturbance the oscillations of reactor temperature are higher with the decentralizes approach, which is also an undesirable response.

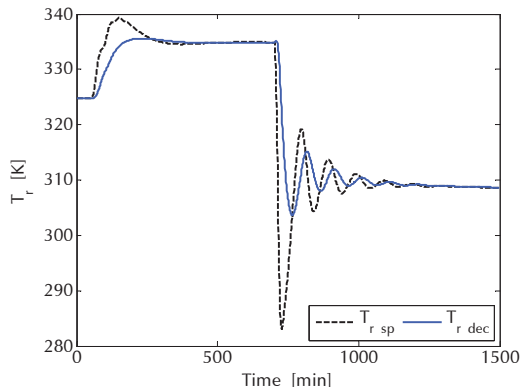


FIGURE 5.9. Reactor temperature response with the decentralized approach.

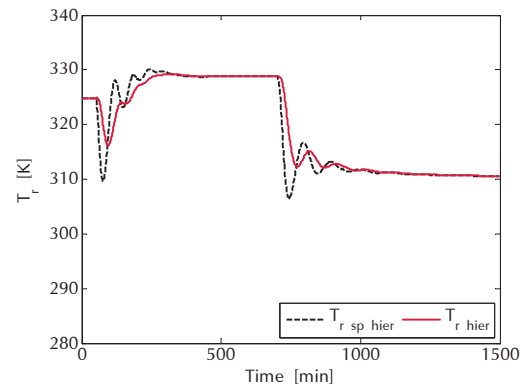


FIGURE 5.10. Reactor temperature response with the proposed hierarchical approach.

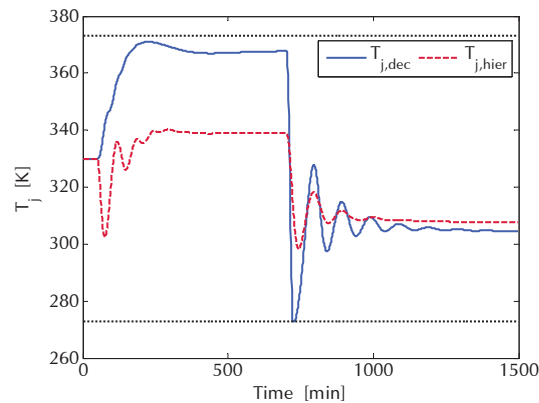


FIGURE 5.11. Jacket temperature response.

The dynamic response of jacket temperature, the manipulated variable for T_r , is presented in Fig. 5.11. Here, the usage of the final control element is bigger through the decentralized approach and it lies closer to the saturation limits than the hierarchical approach. Also, less oscillatory behavior is obtained with the hierarchical which means that the control valve associated will not deteriorate as much as with the decentralized approach.

Reactor input temperature is presented in Fig.5.12 with both approaches. Given that T_{in} is a SeD, with the hierarchical approach its set–point is changed respect to its nominal value to a lower temperature which aids on reactor temperature regulation as was evidenced in Fig. 5.11. It can be seen that after the first disturbance both approaches cannot successfully regulate T_{in} on each set–point.

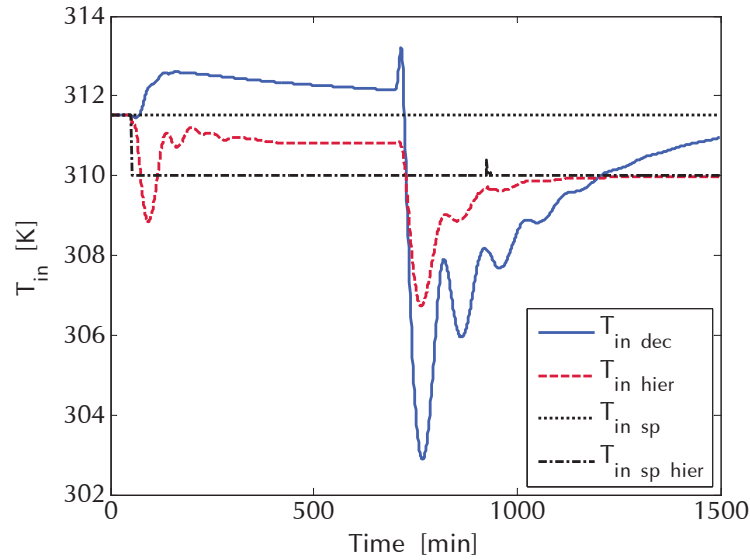


FIGURE 5.12. Reactor input temperature response.

However, it reaches the desired set–point faster with the hierarchical approach despite the saturation on T_{cf} (see Fig. 5.13) and remains on the required range for T_{in} . After the second disturbance, the hierarchical approach recovers from the saturation state and T_{in} is regulated in the new set–point determined by the supervisory layer. For both disturbances the decentralized approach is not able to maintain T_{in} on its nominal value, demanding higher control efforts as can be seen from Table 5.5. Additionally, the property of the proposed hierarchical approach of speeding up the controllers response is evidenced in Fig. 5.13 since the manipulated variables stabilize faster than they do with the decentralized approach, which tends to increase the cooling fluid temperature above the required for the hierarchical approach.

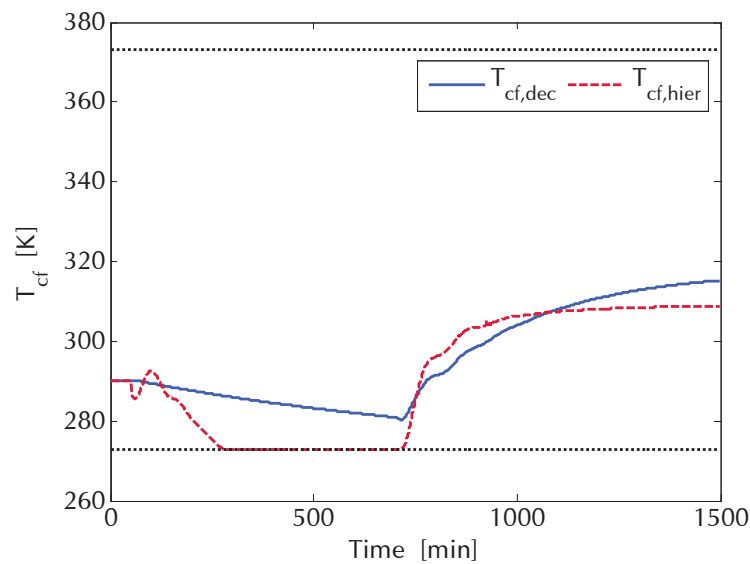


FIGURE 5.13. Cooling fluid temperature response.

For the other SeD, i.e., $C_{A,cl}$ the response with both approaches is presented in Fig. 5.14, 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 5.5 the

difference between $C_{A,cl}$ and its set–point is greater with the decentralized approach. As a consequence of this, lower control efforts are achieved and also it is evidenced that not every dynamics in a process must be regulated for achieving the control objective, since despite this difference, with the hierarchical approach $C_{B,r}$ is kept on its set–point in a more efficient way.

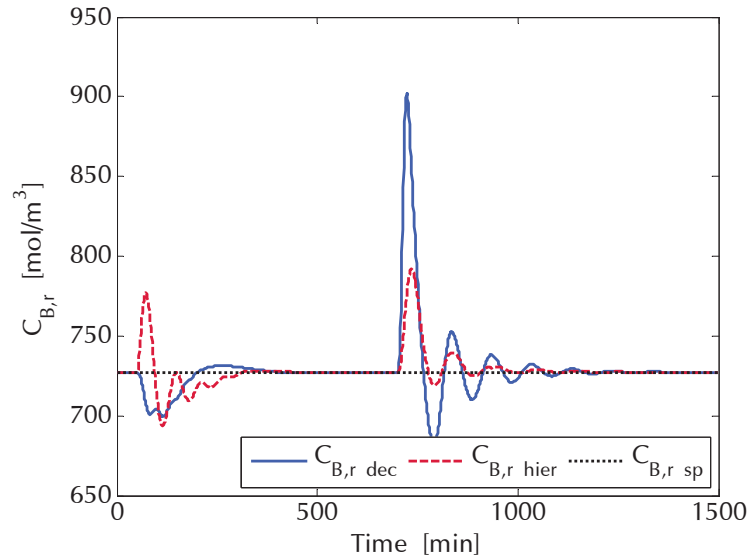


FIGURE 5.14. Reactant concentration in liquid phase from the separation column.

As mentioned before, 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. Despite this fact, the hierarchical approach exhibits an advantageous behavior since a lower usage of the final control element is achieved as shown in Fig. 5.15. After the first disturbance, in the distributed approach the flow–rate required to maintain $C_{A,cl}$ is higher so there would be a smaller margin of freedom or variation should other disturbance on the same direction appear.

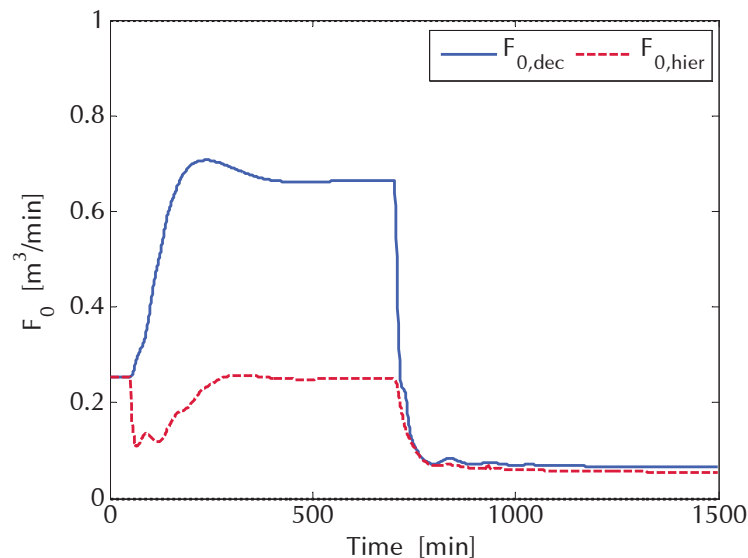


FIGURE 5.15. Fresh feed flowrate.

Finally, performance indexes for all control loops with both approaches are presented in Table 5.5. For almost all control loops, reduction of more than 50% on IAE, ITAE, IAU and ITAU are obtained, which implies a much better performance of the hierarchical control structure than that of the decentralized approach. The differences on the $C_{A,cl}$ control loop were discussed above. For T_{in} control loop, despite a greater control effort is obtained (IAU) if the temporal variation of the manipulated variable is considered (ITAU) it is better for the hierarchical control structure.

An additional index for plantwide performance is called *Deviation on Production Target* (DPT) and considers the actual production target with the nominal one at all times [8], and is defined by (5.27).

$$DPT = \int_{t=0}^{t_s} ((\text{Production rate})_{current} - (\text{Production rate})_{SS}) dt \quad (5.27)$$

It is desired that, under the effect of disturbances, the production is not highly deviated from the desired value. This index represents more robustness to the disturbances and includes economic considerations, which makes it a very good criteria for assessing plantwide performance of a control structure [8].

In this case, the production target is B production on the liquid stream of the flash column (product of interest), and therefore, the DPT is found by means of (5.28).

$$DPT = \int_{t=0}^{t_s} ((F_0 C_{B,cl})_t - (F_0 C_{B,cl})_{SS}) dt \quad (5.28)$$

From Table 5.5 it can be seen that a significantly lower DPT is obtained through the hierarchical control structure, which reinforces the advantages already discussed of this structure.

TABLE 5.5. Performance indexes for the propylene glycol plant.

Controller	Index	Decentralized	Hierarchical	% Difference
$C_{B,r}$	IAE	12165	7217.30	40.7
	ITAE	7764100	3444100	55.6
	IAU	148.69	94.00	36.8
	ITAU	104140	40361	61.2
T_r	IAE	2978	1534.90	48.5
	ITAE	1851100	717830	61.2
	IAU	275.56	174.00	36.9
	ITAU	187940	74966	60.1
T_{in}	IAE	2606.50	926.89	64.4
	ITAE	2195500	510760	76.7
	IAU	44.90	69.18	-54.1
	ITAU	36714	35174	4.2
$C_{A,cl}$	IAE	3754.10	7053.80	-87.9
	ITAE	1777400	2665700	-50.0
	IAU	1.14	0.56	51.3
	ITAU	536.36	211.35	60.6
Plantwide performance	DPT	309060	137610	55.5

5.5. Concluding remarks

In this chapter the proposed hierarchical control scheme has been successfully 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. Here, some aspects are important to highlight:

- The dynamics hierarchy of the plant allows the determination of control objectives for the complete plant for non–squared systems.
- Overall, lower control efforts are required from each individual PID controllers, which also demonstrates that not every dynamics in a process must be regulated for achieving the control objective in a more efficient way by relaxing the control requirements of the SeDs control loops.
- The proposed hierarchical approach arises as a possibility for controlling large–scale processes without requiring sophisticated control strategies such as MPC, thus promoting the possible industrial implementation of this control structure.

Conclusions

This work presents a methodology for obtaining a model-based supervisory control structure in which (i) a dynamics hierarchy of the process is established to determine control objectives and classify process dynamics in Main Dynamics (MaD) and Secondary Dynamics (SeDs), and (ii) a supervisory layer optimizes a process performance function obtained from the non-linear model of the process to determine the SeDs set-points that achieve a good regulation of the MaD with lower control efforts and a simple control layout by using PID controllers in the regulatory layer.

The establishment of the dynamics hierarchy allows the design of the control structure considering the dynamic behavior of the whole plant. This represents a paradigm shift from the decoupling multivariable control strategies, since instead of decomposing the problem in smaller ones, all the dynamic interactions of the process are profited for its control.

Regulatory layer PID coordination is achieved in the supervisory layer by optimizing SeDs set points. The optimization is carried out over a performance function that does not need to predict over the process model, but uses current state measurements of the process to compute the sensitivities S_j . The optimal values for the SeDs set-points are thus determined in each sampling time which results in a piece-wise optimized trajectory for the SeDs. Also, by constraining the search region to the reachable set of the process controllability and stability of the process are considered in the supervisory layer.

The proposed design procedure was successfully applied to a multivariable process (CSTR) and a plantwide process (RSR) in comparison to a decentralized structure. Based on the improved performance of the individual and plantwide performance indexes, the effectiveness of this methodology in both small and large-scale problems is verified.

This approach emerges as a potentially feasible plantwide control structure for industrial implementation since despite an adequate process model is required, the necessary tools for obtaining the control structure and optimizing SeDs set-points are not utterly complex and process knowledge is directly used for the operation of the control system. Once the control structure is obtained, it can be easily operated and tuned using intuitive criteria by both operators or control experts.

Future Work

After completing this work, the following aspects must be revised or explored towards complementing the outcome of this thesis:

- Evaluate the performance of the proposed control structure in other large-scale processes, in order to evaluate its performance in different problems and thus prove its generality.
- Design of the PLC module for the global optimization required in the supervisory layer proposed in this methodology for implementing this strategy in a real process in order to evaluate the actual performance of the control structure.
- Evaluate the usage of dynamic sensitivities in the optimization of the secondary dynamic set-points instead of the stationary sensitivities. It should be determined whether the possible performance improvement is justified from the additional computational requirements that dynamic sensitivities demand.
- The methodology herein proposed considers that the process is observable and therefore data of the process state is available. Further works should aim to study the influence of not having full state measurement (or estimation) over the performance of the control system.

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