Strategy of Collaborative Control Including the Effects of Controllable Parameters

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A chemical process plant is composed of several process units that work together in order to transform raw material into the desired final product. Additionally, the objective is to increase efficiency and decrease the effects that disturbances cause on the product quality. Disturbances motivate the implementation of control systems on chemical processes [1], which should be multivariable because processes have multiple input variables and multiple output variables (MIMO). In addition, control systems should consider the interactions of process dynamics.

There exist many multivariable control strategies. Each strategy has applicability in accordance to a particular process, because it can consider their relevant aspects. In this sense, the multivariable control strategies can consider: strong nonlinearities, the necessity of a short settling time, low overshoot, the importance of the error between the controlled variable and the set point. Despite of the large amount of control strategies, the effect of controllable parameters is not considered by any of them, except for direct manipulation of these parameters proposed by some authors. This is particularly important when additional degrees of freedom are required in the control system.

In this thesis an approach to collaborative and cooperative control definitions, highlighting their differences, are proposed. Usually in the literature, collaborative control and cooperative control are studied like the same techniquey, but there exist differences between them. Here, a collaborative control strategy including the effects of controllable parameters is proposed and applied. That strategy includes into the optimization procedure a term for considering the influence of one or more parameters that can be controlled using available control actions. To do this a mass transfer model for the aerated section in Benchmark Simulation Model No.1 (BSM1) is developed separating the effects of parameters kL y a. The behavior of collaborative control using such a separation is compared with traditional control structures using the integrated kLa parameter, all implemented over this benchmark.

Keywords: Collaborative control strategy, multivariable control strategies, controllable parameters.

Una planta de procesos químicos está compuesta por varias unidades de proceso, que juntas operan con el objetivo de transformar la materia prima en el producto deseado. Adicionalmente, el objetivo es incremetar la eficiencia del proceso y disminuir los efectos que causan las perturbaciones en la calidad del producto. Dichas perturbaciones, son las que motivan la implementación de sistemas de control en procesos químicos . Estos sistemas de control deben ser multivariables, ya que los procesos tienen múltiples variables de entrada y múltiples variables de salida (MIMO). Además, los sistemas de control deben considerar las interacciones dinámicas del proceso.

Existen muchas estrategias de control multivariable. Cada estrategia tiene importancia de acuerdo al proceso en particular, puesto que cada una puede considerar diferentes aspectos relevantes en el proceso. En este sentido, algunas estrategias de control multivariable pueden considerar: linealidades muy fuertes, la necesidad de un tiempo de respuesta corto, un bajo sobreimpulso, la importancia del error entre el valor de la variable de control y el punto de referencia o considerar el punto de referencia de otra dinámica. Pero ninguna estrategia de control incluye los efectos de los parámetros controlables. Este último aspecto es importante cuando es necesario adicionar grados de libertad al sistema de control. Algunos autores remplazan dicha necesidad con manipular directamente el parámetro de interés.

En esta tesis se presentan una aproximación a la definición de control colaborativo y control cooperativo, resaltando sus diferencias. Normalmente, en la literatura estas técnicas son estudiados como si fueran lo mismo, pero existen diferencias entre ellas. Aquí se propone y aplica una estrategia de control colaborativo incluyendo los efectos de los parámetros controlables. Esta estrategia incluye dentro del procedimiento de optimización un término que considera la influencia de uno o más parámetros que pueden ser controlados usando acciones de control disponibles. Para hacer esto, se desarrolla un modelo de la transferencia de masa para la sección aireada del BSM1, separando los efectos de los parámetros kL y a. El comportamiento del control colaborativo usando esta separación se compara con estructuras de control tradicionales que usan el parámetro kLa integrado, todas implementadas sobre el mencionado problema de referencia.

Palabras claves: Estrategia de control colaborativo, estrategias de control multivariable, parámetros controlables.

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CHAPTER 1 Introduction

Plantwide control (PWC) has been studied intensely during the last ten year because the PWC design because it promises important improvements to industrial processes [4]. This topic is relevant because the majority of chemical plants have many units and the dynamic behaviour is complex requiring a proper control structure [5]. The control structure selection includes the selection of manipulated and controlled variables, and the pairing of these variables if the controller is not multivariable. After that, the tuning of the controllers must be performed. These tasks are complex when a complete plant is considered as a whole. This thesis remarks the possibility of considering as controlled variables not only the states, but also the controllable parameters available in the process.

This thesis is focused on those process parameters with option of being controlled to improve the response of the total process. Moreover, this proposal increases the collaborative control strategy capabilities by including one or more process controllable parameters into the controller strategy. Particularly, the controllable parameters for the wastewater treatment process proposed in this thesis have been obtained increasing the degrees of freedom of the oxygen transfer process by separating the volumetric mass transfer coefficient into the liquid phase mass transfer coefficient and the specific area for mass transfer. Below, in the next section, motivation for this research, the main objective, specific objectives and finally, the main novelty are presented.

Motivation

Plantwide control (PWC) is a procedure in order to determinate the manipulated and controlled variables and control loops [6]. Moreover, the PWC must maintain the momentum, energy and mass balance of the plant [7]. For this reason, it is necessary a more complex control structure involving all the interesting dynamics, which is not possible using only PID controllers or other kind of controllers working individually, i.e. without communication among them.

Many control architectures have been developed and applied over the last 45 years ago [8]. Those control structures can be grouped on three families: centralized, decentralized and distributes control. Centralized control structure can be difficult to implement because of the computational complexity and robustness and reliability problems [8]. However, studies like [9] shows good results using them. On the other hand, decentralized structure has been used the last years and in [10] is presented a novel framework for decentralized structure. Finally, distributed structure is the most used on last years, many works use this structure, for example in [11] and [12] this structure is applied to control a system without a model of the

system.

Hierarchical control can be obtained for centralized or distributed structures because it is possible to consider a control structure with some kind of hierarchy. Then, a hierarchical control structure is composed of supervisory and regulatory level, independently of the control architecture. On this way, some works like [13] and [14] have been studied this scheme obtaining good results. On the other hand, [15], [16] and [17] show the possibility of including some kind of sensitivity terms in the cost function when the optimization of large-scale process is treated. In this sense, the main motivation of this work is [2] because it considers a supervisory hierarchical structure based on main dynamic including secondary to main dynamic sensitivities. In spite of the results presented in that work are satisfactory, in some processes there exist parameters with option of being controlled but mentioned procedure does not allow to include them. Those parameters like transport parameters and physico-chemical properties can be changed by input processes variables, directly affecting the main process dynamic. In this sense, if these parameters are maintained at good values they can help to a better control of the process.

Research problem

If a control system is multivariable, there are several control strategies useful for performing the control task. According to the scheme shown in Figure 2.1 on the Section 2.1, it is possible to choose among several control architectures. The control strategy of interest in this thesis is the collaborative control. This chosen is supported on [2] and [14], where authors show how this type of strategy works well in chemical process. Obviously, some improvements are possible to overcome uncover aspect of chemical processes.

Although the collaborative control has been succesfully applied in many chemical processes, the consideration of controllable parameters has not been considered yet. In this thesis, the architecture proposed by [2] is taken as the basis to include the effect of controllable parameters into the control strategy. That work uses the sensitivities of a process state against variations of another states, to determinate the effects on the main dynamic when changes on secondary dynamics take place. However, in chemical processes a state can also have variations according to changes in some process parameters. As it is evident from process model, the parameters affect the behavior of states through crossed effects between parameters and state variables. Parameter changes from one operation point to another can be directly regulated by some control actions. This kind of parameters are called in this research **controllable parameters**. In [2] the optimization cost function only includes the process states without considering the controllable parameters effects. The influence of controllable parameters over the process allows additional control actions (new degrees of freedom for control), which finally can improve the process performance. Thus, it is suitable to study the inclusion of controllable parameters in the cost function of collaborative control to increase the degrees of freedom in plantwide control.

In this sense, it is necessary to ask:

How to include the process **controllable parameters** effects in the cost function proposed by [2] to improve the system response through new control freedom degrees in a collaborative control structure?.

Objectives

The objectives that conduct this thesis are:

General objective: Develop a collaborative control strategy including the effects of process controllable parameters, by considering explicitly the sensitivity of the main dynamic with respect to changes in these parameters, in order to achieve good performance and disturbance rejection.

Specific objectives:

- Describe the multivariable control strategies more important and used in chemical process control. Additionally, describe the strategies more commonly used in wastewater treatment plant.
- Reconstruct a definition of collaborative and cooperative control allowing a comparation between them and giving knowledge about their capabilities.
- Define the term controllable parameter and characterize all its possible effects on chemical processes control.
- Reproduce some multivariable control strategies applied to wastewater treatment plants, found in the literature for comparison with the collaborative control strategy analyzed here.
- Formulate a mathematical expression including the effects of controllable parameters in the objective function of primary controller in a collaborative control strategy.
- Validate the performance of the proposed collaborative control strategy, when it is applied to the plantwide control of the wastewater treatment plant given in BSM1 compared to other multivariable control strategies documented in the literature.

Main novelty

The collaborative control structure has two layers, supervisory layer and regulatory layer. The main outcome of this thesis is to include the controllable parameters at the supervisory level, taking into account the sensitivity of main dynamic respect to controllable parameters. Another novelty is the development of a mass transfer model that represents the phenomenon in a wastewater treatment process, validated in the BSM1 benchmark.

Thesis outline

This thesis is organized in six chapters as follow. Chapter 2 introduces some plantwide control architectures, that are explained and compared. In that chapter a taxonomy of plantwide control is proposed. Chapter 3 presents the case of study where the methodology proposed is

tested. In this sense, the mathematical model of Benchmark Simulation Model No.1 (BSM1) is explained. Moreover, a formulation for the mass transfer model is developed. This model is applied to BSM1. On the other hand, Chapter 4 presents the strategy for collaborative control proposed in this thesis. The Section 4.1 deepens in controllable parameter where the definition of this term is presented. Moreover, the methodology proposed is detailed in that chapter and finish with a illustrative example. The Chapter 5 shows the results of methodology applied to BSM1. Finally, Chapter 6 presents conclusions about this thesis and future works that can be explored.

CHAPTER 2 Plantwide Control and Collaborative Control

The aim of this chapter is to highlight important topics and concepts for the development of this research. In this sense, the section dedicated to plant-wide control architectures describes different structures for plant-wide control and proposes a classification for them, according to information send to controllers and controller distribution in the plant. Next, the multivariable control strategies section describes the control strategies showed in Section 2.1. Then, the collaborative control strategy section explains that control strategy, taken as the base for the collaborative control strategy including the effect of controllable parameters as it is explained in Section 4. Finally, model predictive control section discusses this strategy in order to perform a comparison.

2.1. Plantwide control architectures

In chemical processes is very important to keep some variables at their set point, because the performance of the whole process depends on the interaction among them. Additionally, the processes are more complex due to interaction among the units caused by material and energy recycling [5]. In this sense, the implementation of a control strategy in the process facilitates to guarantee the desired behaviour of the global process. Plantwide control (PWC) links the systems and strategies necessaries to control an complete chemical plant that composed of many interacting unit operations [18]. Moreover, the structural decision of the control system should include what to control and how to pair the manipulated and controlled variables in order to form control loops [19]. The Figure 2.1 shows a proposed classification for control structures. This figure presents three structures of plantwide control: centralized, decentralized and distributed control. The classification is done in accordance to controllers distribution at the plant and the information sent to each controller or final control (FCE).



Figure 2.1. Classification of plant-wide control architectures.

According to the Figure 2.1, centralized control structure is based on just one coordinator controller, which sends information to other controllers or FCEs. In this sense, the centralized control structure can be pure or hierarchical. If the coordinator controller directly sends information about control actions (to FCE), the structure is pure centralized, like it is shown in Figure 2.2a where only one level of controller exist. On the other hand, if the coordinator controller decides the set point of other controller, it is a hierarchical centralized control structure and two layers exist in the control structure, like it is shown in the Figure 2.2b. The main level is the coordinator controller and the secondary level is a PID or a MPC controller, depending on behaviour of plant and its dynamic interactions. Optimal control and MPC are examples of pure centralized control structures. Note that the box marked with dashed line in the Figure 2.2 is the difference between pure a hierarchical centralized control structure, in this Figure PU represents process units.



As it was mentioned and shown in Figure 2.1, in a decentralized control structure there is no primary control level and communication among control loops. Then, only it is possible a pure decentralized control structure, where each controller is totally independent, like it is shown in the Figure 2.3, where it is evident that a main level does not exist. Multiloop control strategy uses this type of structure.



Figure 2.3. Decentralized control structure

On the other hand, in a distributed control structure the main level does not exist either, but the communication among the control loops is possible. As in centralized control structure, the distributed structure can be pure or hierarchical. In this sense, a pure distributed control structure takes the decisions about control actions in accordance to the information exchanged among the control loops. That information is about process variables including manipulated variables. Such a structure takes place when the set points change are performed by a main controller or coordinator controller, but the set point of coordinator controller can be changed according to the information sent by the other controllers. In this sense, the change of set point can be coordinated by some controller in the same level. Additionally, the exchange of information among controllers is possible, as it is shown in Figure 2.4b.



Figure 2.4. Distributed control structure.

Although the control structure is very important, to select the control strategy is relevant in order to accomplish the control objective, because it is possible to implement the same control structure with different control strategy or controllers (2.1) many strategies of control exist. The control strategy should ensure stability, be robust to disturbances and model errors, and be efficient, all with an easy implementation. For this reason, the control strategy should be selected in accordance to the process and the number of variables involved in it.

Depending on the number of variables, there are SISO controllers (single input and single output) and MIMO controllers (multiple input and multiple output). The first class is the simplest and common kind of control, in which one output is controlled by one control signal. Meanwhile, MIMO is a combination of two or more SISO control systems. In chemical processes the MIMO controllers are very frequent because two or more variables must be controlled to guarantee process objective. Temperature, concentration, pressure, concentration and level are typical variables in a chemical process, normally each one with its own one control loop. Therefore, the control strategy as a whole is called multivariable control.

The Figure 2.1 shows a classification for multivariable control structures, where it is possible to see the characteristic of centralized, decentralized and distributed architectures. In this sense, each control structure shown in Figure 2.1 is explained in the next section.

2.2. Multivariable control strategies

The Figure 2.1 shows the classification of plantwide control structures and lists examples of multivariable control strategies for each architecture. In this sense, an example of pure centralized multivariable control strategy is the optimal control and the model predictive control (MPC). Optimal control is a kind of control strategy where the trajectory of control actions for a dynamic system is found by minimizing a performance index or cost function, using different optimization methods depending on the cost function considered. The strategy can be stated in continuous or discrete time domain, and considering different type of constraints [20]. MPC control can be used in the pure centralized control strategy, because according to optimization problem shown in Section 2.4 it is possible to optimize the control action of the controllers in multivariable framework. Moreover, this is a typical control strategy used in the literature in order to control waste water treatment plants, but in this case it is important to take into account the dynamic of final control element (FCE) and its dynamic interaction with the rest of process elements. This is a requirement to guarantee that the process simulation is closer to the real process. In this sense, when the

process output is predicted for a given prediction horizon, the model of the FCE must be known.

On the other hand, the collaborative control strategy could not be on the family of pure centralized control structure, because the cross sensitivities explained in Section 4 are related to secondary dynamic or controllable parameters and the decision variables in the optimization problem are the set points. In this sense, if the coordinator controller decides control actions in the collaborative control strategy their structure would be very complicated, because they should relate the main dynamic with manipulated variables and this implies to know the phenomenological relationship between main dynamic and control actions. This relation is more complex that the relation between the main dynamic and secondary dynamics or the main dynamic and controllable parameters. In this way, collaborative control strategy is used in hierarchical centralized control structure because it permits a two level strategy. The first level is the supervisory layer where the coordinator controller is located and where the set points of the controllers are determined. The second level is the regulatory layer formed by the controllers receiving the information from main level. These local controllers normally are PID, each one related to one process unit doing the necessary control for a given variable. Obviously, each PID has its manipulated variable. The pairing from manipulated to controlled variable is obtained according to Hankel matrix [2]. Collaborative control strategy is treated in detail in the next section and Chapter 4.

Multiloop is a kind of decentralized control structure with two or more single loops, but without interaction among them. i.e. there is not information exchange. In multiloop control strategies the performance and the design are developed taking into account three main steps. The first one is the loop pairing, i.e. to decide the manipulated and controlled variable for every single loop. The second step is the controller tuning to achieve the desired performance. Finally, the third step is the system improvement according to PID loop shaping [1]. Evidently, this kind of multivariable control strategy is the simplest, but is less efficient in large-scale processes because each single-loop does not know the action of other single loops.

The pure distributed control structure considered in Figure 2.1 comprises MPCs and PID controllers. These strategies keep a pure distributed architecture because the controllers installed on the plant can be MPCs or PIDs with communication among them and according to this information the decision about the manipulated variables is taken [2], [14]. Another multivariable control strategy presented in Figure 2.1 is the cascade control. This strategy is actually a distributed hierarchical control because there exist a primary controller and a slave controller. Between these two controllers there exists communication. A cascade control can enhance a single loop, because it has extra information about some process measurements and this information assists the control system. The selection of process measurements variables are made in accordance to more commons disturbances and real process dynamic response. Finally, cooperative strategy is listed, but its definition is scattered of this strategies is scattered in the literature. Usually, this strategy is confused with collaborative strategy. For example, [21] studied the collaborative control general characteristics, but they never do an explicit definition of it. Even though in robotic cooperative and collaborative control strategies are very frequent, it is important to highlight the difference between them.

2.3. Collaborative control strategy

Before studying collaborative control it is necessary to state its definition and point out the difference between collaborative control and cooperative control. According to Royal Spanish Academy (RAE), to collaborate is to work with one or more persons in the development of an activity. On the other hand, to cooperate is defined as working together to achieve a common goal. Both terms are used in biology, where cooperation is the association between two or more individuals of the same species, where all of them are beneficiaries by a collective action. Furthermore, mutualism is defined as a symbiotic relationship between individuals of different species in which both individuals benefit from the association, thus they collaborate [22]. The collaboration concept is used in different knowledge areas. For example, [23] speaks about measuring collaborative intelligence in knowledge based service planning. The authors identify measures in order to achieve the best collaboration between different enterprises. These authors define the collaborative intelligence as a combination of communication, collective, cumulative and cooperative intelligence.

On the other hand, [24] studied the performance of collaborative control for a robotic wheelchair. In this work, a collaborative control mechanism that assists users when they require help is proposed. Basically, the system uses a multi-hypothesis method to predict the driver intention and if it is necessary, to adjust the control signals to achieve the desired goal safely. Another work is [21], where a collaborative control is applied in teleoperation systems. They have the hypothesis that teleoperation can be significantly improved by modeling the human as a collaborator rather than the controller. They say that in "collaborative control model a human operator and robot are peers who work together, collaborating to perform tasks and to achieve common goals". This concept is not commonly adopted in chemical processes, but [2] proposes a structure of collaborative control, where there exist communication between the process units and a coordinator controller. Furthermore, this work describes a cooperative structure based on cooperative game theory in which all the players aim a global goal but there is not actual communication between them. In this way, this author according to the communication protocol proposes two structures of control: cooperative and collaborative control. Note that the mentioned work presents a classification based only on communication. Next definition extends those definitions.

Definition 2.1. Collaborative control. This is a kind of multivariable control strategy used when the dynamic effects in the process are different. In this strategy all control systems work together, contributing from its individual capability to achieve a common goal. Even though each control loop has different functions and dynamic behavior, they are coupled with the general behavior of the process and share the same physical space. Based on this fact, there exists two kinds of communication among the control system: inherent communication due to their interaction through the process dynamics and control communication through their local controller signals. Last one communication permits the complete control coordination.

Definition 2.2. Cooperative Control. This is a kind of multivariable control strategy that unlike the collaborative control is utilized when the dynamics of the process are similar. Then, each control loop has the same function and dynamic behavior in the process, for this reason, they have the same contribution to the process objective. Therefore, if any controller fails is possible to replace it with another controller acting over the process. In this sense, the process dynamic should not be coupled or they should be loosely coupled. This kind of control system

is typically used in robot teams.

The conditions for implementing a collaborative control strategy are frequent in chemical processes, where each equipment (production, separation, transportation, etc.) work for a common goal, the final product, but their dynamics are different, because temperature dynamic is different to concentration or level dynamic, for example. Meanwhile, in robotics is more common the cooperative control. For example, a team of robots work for a common goal, being all of them similar machines and having similar objective and dynamic behavior.

As it was mentioned previously, collaborative control strategy is a hierarchical centralized control structure, because there are several control loops in the system communicated by a coordination mechanism, external to the controllers [2]. In collaborative control strategy there are two levels: supervisory layer and regulatory layer. The first level, named primary or main controller too, calculates the changes in manipulated variables or set points of individual controllers on second level. A classification of process dynamics in main dynamic and secondary dynamics is done. The optimization of the set points of those controllers driving secondary dynamics is done to reduce the control efforts for the main dynamic loop. On the other hand, the regulatory layer comprises the individual controllers for secondary dynamics of the process. In this sense, in a collaborative control strategy with n total control loops, n-1 control loops are passed from regulation mode to tracking mode leaving only the control loop of main dynamic in regulation mode. This strategy is contrary to chemical process design traditional principle, which requires to fix set point values for all variables in a continuous process.

The collaborative control strategy is studied in [2] and a novel methodology for plantwide control structure design is proposed there. The Figure 2.5 shows the structure of control strategy proposed by [2]. Where x_n represent states, y_{nn} outputs, u_{nn} inputs and $x_{nn,sp}$ the set points. The plant is represented by three blocks or equipment (PU_1 , PU_2 and PU_n). Regulatory layer is conformed by PID controllers (PID_{11} , PID_{nn}) and finally supervisory layer is the coordinator controller. The design procedure for collaborative control strategy is presented in Figure 2.6.



Figure 2.5. Hierarchical control architecture proposed by [2].



Figure 2.6. Plant-wide control structure design procedure proposed by [2].

In order to implement this methodology the first task is to analyse the process. For this reason, it is important to develop a phenomenological based semi-physical model (PBSM) of the process to be controlled. This activity can be developed according to the methodology proposed by [25]. The methodology includes to elaborate a verbal description and a process flow diagram in order to complement the verbal description. Then, the objectives and hypothesis of model must be established. After that, the differential equations are obtained according to mass and energy balances. Additionally, the necessary constitutive equations are obtained in order to calculate model parameters. Finally, the model must be solved and

validated for different conditions or general performance [2], [25],.

The second step is to identify the process states and available manipulated variables. This activity can be performed according to different procedures and assumptions. For example, full state measurement can be assumed available and then to analyse the controllability with either graph theory, set theory, singular values analysis, etc. Additionally, the set points or operation points, input variables and span are specified in the third step. This is done according to the process knowledge.

The second part of the methodology is related to the regulatory and supervisory level shown in the Figure 2.5 in the blue and orange box. The regulatory layer is the secondary level of collaborative control strategy. For this reason PID controllers are located at this level. In this sense, the first task of this part is to establish the controller configurations and then the input-output pairing is analysed for each control loop. The last step can be done according to different methodologies, for example pairing analysis by RGA (relative gain array), SVD (singular value decomposition) or SVD using Hankel Matrix. Finally, the controllers should be tuned before their use in the process.

The last part of the methodology proposed by [2] is related to the supervisory level design. In this way, the supervisory layer is associated with the optimization problem shown in Equation 2.1. The objective is calculating the set points of controllers located at the regulatory level, for this reason, the set points are the decision variables in this optimization. The used restrictions are related to operations points and feasible movements of control actions or set points span with guaranteed stability.

$$\min_{x_{1,sp},\dots,x_{j,sp}} J = \alpha (x_{ss}^* - x_{sp}^*)^+ \sum_{i=0}^j \beta_i \frac{1}{S_i}$$

$$S. t. \ x_{j,sp_{min}} \le x_j \le x_{j,sp_{max}}$$

$$\Delta x_{j,sp_{min}} \le \Delta x_j \le \Delta x_{j,sp_{max}}$$

$$(2.1)$$

Where $x_{j,sp}$ represent the set points of *j*-th secondary dynamic to be calculated by the optimization, α and β_i are weights acting as tuning factors, x_{sp}^* is the set point of the main dynamic (x^*) , x_{ss}^* corresponds to the x^* steady-state value that would be achieved if the system should reach steady-state with the $x_{j,sp}$ values determined during the optimization. S_i is the sensitivity of main dynamic to changes on i - th secondary dynamic at the current values of the process state, $x_{j,sp_{min}}$ and $x_{j,sp_{max}}$ are the limit values for secondary dynamics set points guaranteeing process stability, $\Delta x_{j,sp_{min}}$ and $\Delta x_{j,sp_{max}}$ are the maximum and minimum changes possible in the set points of secondary dynamics.

As it is evident, to determinate the dynamic hierarchy is crucial because the first term of the Equation 2.1 is related to the main dynamic, but this dynamic is not evident in the majority of processes. In that work, the SVD of the Hankel Matrix is used to determine the main dynamic. More precisely, the state impactability index (SII_{xk}) , Equation 2.2. The main dynamic is the state (x_k) with the highest SII_{xk} and the rest are secondary dynamics.

$$SII_{xk} = \sqrt{\sum_{i=1}^{p} \sigma_{ii}^2 \sum_{j=0}^{n-1} \mathbf{U}_{k+nj,i}^2}$$
(2.2)

Where σ_{ii}^2 and **U** are found according to the SVD of the Hankel matrix H of the model. p is the number of non-negative singular values, n is the number of state variables, σ_{ii} are the *i*-th singular value and U are the orthonormalized eigenvectors HH^T .

The last term in the Equation 2.1 is the summation of the sensitivities of main dynamic respect to secondary dynamics. These terms are calculated according to the Equation 2.3 using the knowledge contained in the PBSM of the process about the effect that each secondary dynamics has over the main dynamic.

$$S_i(\mathbf{x}(t), \mathbf{u}(t)) = \frac{\partial x^*}{\partial x_i} \Big|_{x_i \neq i}$$
(2.3)

Where x_i represents the *i*-secondary dynamics, with i = 1, ..., n - 1. At each sampling time, the set-points of secondary dynamics are the result of the optimization problem described for the Equation 2.1.

2.4. Model predictive control (MPC)

MPC or receding horizon control (RHC) is a control strategy in which the control action is obtained on line by solving an optimal control problem with constraints at each sampling time. The optimization yield an optimal control sequence and the first control of this sequence is applied to the plant. The general optimization problem of MPC control is shown in the equation 2.4.

$$\min_{\Delta \mathbf{u}(k+i|k)} V(k) = \sum_{i=H_w}^{H_p} \| \mathbf{y}(k+i|k) - \mathbf{r}(k+i) \|_{\mathbf{Q}}^2 + \sum_{i=0}^{H_c-1} \| \Delta \mathbf{u}(k+i|k) \|_{\mathbf{R}}^2 + \| \mathbf{y}(k+H_p|k) - \mathbf{r}(k+H_p) \|_{\mathbf{P}}^2$$
(2.4)

S. t.
$$\mathbf{u}_{min} \leq \mathbf{u}(k+1 \mid k) \leq \mathbf{u}_{max}$$
 $i = 0, ..., H_c - 1$
 $\mathbf{y}_{min} \leq \mathbf{y}(k+1 \mid k) \leq \mathbf{y}_{max}$ $i = H_w, ..., H_p$
 $\Delta \mathbf{u}_{min} \leq \Delta \mathbf{u}(k+1 \mid k) \leq \Delta \mathbf{u}_{max}$ $i = 0, ..., H_c - 1$

Where **y** is the vector of controlled outputs, **u** is the vector of manipulated variables, **r** is the set points vector, **P** is the terminal penalty weight matrix, **Q** is the output weighting matrix, **R** is the move suppression weigh matrix, H_c is the control horizon, H_w and H_p are the initial and final prediction horizons, u_{min} and u_{max} are the lower and upper bounds for the manipulated variables, Δu_{min} and

 Δu_{max} are the lower and upper bounds for the control action movements [26].

MPC has some specially characteristics the main one is the use of an internal model for predicting the future process outputs. Then, the control actions are calculated with the purpose of minimizing a cost function that includes tracking of a reference and control efforts. Finally, MPC has a sliding strategy, because the horizon is displaced in the future after each control action application. Figure 2.7 represents the methodology of MPC. Before to time t, the control action is constant and y(t) is the output system according to u(t) value. At time t the control actions for a future control horizon are calculated and the first one control action is applied. After a time step, the same procedure is repeated using the new available measurements. The typical MPC structure is shown in Figure 2.8.



Figure 2.7. Predictive Control Methodology.



Figure 2.8. Predictive Control Structure.

This strategy is very popular but requires a lot of computation because each time step the optimization should solve the model into the optimization problem.

2.5. Remarks

In this chapter, different plantwide control architectures were presented. These control architectures are relevant for chemical processes because this kind of process present great complexity. The complexities are evident when it is necessary to control a chemical process. According to these control strategies it is important to highlight some aspects:

- The taxonomy proposed is important in order to identify the relevance of each strategy in different processes. In this sense, the taxonomy permits to find quick and easily the control structures useful for different processes. Onward, multivariable control strategies and control structures are classified in accordance to this taxonomy.
- The possibility of pure and hierarchy structure would be considered and studied. This aspect determines existence of information flow and the kind of available information. In this sense, when the control structure is decided, the decisions of controllers would be determined.
- MPC is a control strategy that can be adjust to many processes because it is robust respect to process complex. It should be noted that MPC would solve the process model at each iteration and this can be a disadvantage for computational burden.
- Collaborative control strategy presented in this chapter is the basis for the thesis development. In this sense, [2] proposes a methodology where the dynamic hierarchy is included, this aspect is very important in this work. However, [2] do not include the possibility of control parameters, just secondary dynamics. This aspect is relevant in this thesis.

CHAPTER 3 Processes Modelling: Case of Study

This chapter shows the mathematical model of wastewater treatment plant to be used used as a benchmark in this thesis. It is important to highlight that a model is a representation of a system. This representation can be material or mathematical. The models, can be of three types: white box or phenomenological, black box o empirical and gray box, that is a mixture of white and black box models. This section describe the BSM1 model and the mass transference in aerobic section. These models are phenomenological based semi-physical models (PBSM), because they are based in conservation principles and complemented with constitutive equations [25]. These models are important because the control strategy is based on these kind of models. In this sense, the first section shows the BSM1 model and second section shows mass transfer model. The last model was developed in this thesis and it is important because it takes into account the controllable parameters explained in the next chapter.

3.1. BSM1 model

A wastewater treatment plant is compound by three stages. The first one is the primary treatment. This stage is in order to reduce suspended solids and to condition residual water for secondary treatment. The second stage or secondary treatment is the activated sludge process, where aerobic and anoxic processes take place. Finally, in the tertiary treatment or advanced treatment the effluent quality is improved [27]. As it was mentioned the activated sludge process is part of secondary treatment and the BSM1 describe this process. The BSM1 model is a standardized mathematical model for the activated sludge process in a wastewater treatment plant, including also different set of disturbances (different influents for dry, storm and rain weather) and performance index. As it is shown in Figure 3.1, the plant has five reactors. The first and second reactors are anoxic (no dissolution oxygen, but it is possible the presence of bonded oxygen) and the other three are aerobics. Finally, there is a settler used to separate sludge and clean water [28], [3].



Figure 3.1. Process Flow Diagram for a wastewater treatment plant using activated sludge process.

The aerobic tanks have aerators to provide the necessary oxygen in nitrification process. The design of aeration system is important, because it represents 70% of energetic costs in the plant [3]. Additionally, the aeration is important in determination of metabolic route that microorganisms must follow to degrade pollutants. So, it is necessary to keep the oxygen concentration at a good level. This concentration depends on oxygen transfer rate from gas bubbles to sludge and the consumption rate of oxygen by microorganisms. Moreover, it is important highlight that oxygen transfer rate depends on reactor geometry, aerators design, properties of sludge, air flow, stirred rate and other factors.

The compounds considered in the activated sludge process, according to the Activated Sludge Model No.1 (ASM1), are the following:

- 1. Soluble inert organic matter, S_I
- 2. Readily biodegradable substrate, S_S
- 3. Particulate inert organic matter, X_I
- 4. Slowly biodegradable substrate, X_S
- 5. Active heterotrophic biomass, X_{BH}
- 6. Active autotrophic biomass, X_{BA}
- 7. Particulate products arising from biomass decay, X_P
- 8. Oxygen, S_O
- 9. Nitrate and nitrite nitrogen, S_{NO}
- 10. $NH_4^+ + NH_3$ nitrogen, S_{NH}
- 11. Soluble biodegradable organic nitrogen, S_{ND}
- 12. Particulate biodegradable organic nitrogen, X_{ND}

Additionally, it is considered the alkalinity (S_{ALK}) is considered like a state.

It should be noted that nitrate and nitrite nitrogen is considered one state for simplicity in modelling, and is produced by aerobic growth of the autotrophic bacteria and removed during anoxic growth of heterotrophic biomass, it has been assumed that nitrate is the only oxidized form of nitrogen present [28]. Note that each concentration depends on meteorological conditions. During rainy weather the concentration decreases and for dry weather it increases. The temperature is also important, because of its influence in oxygen transfer. The flow Q_{int} coming from the last reactor has the purpose to recirculate nitrate, which is the product of nitrification process but it is used as reactive in denitrification process. For the purpose of keeping the microbiological population at a correct level it is used the external recycling flow called Q_r , which comes from the bottom of the settler. In addition, a purge is required to remove some sludge and prevent accumulation in the system.

In the anoxic tanks, the denitrification process takes place. Denitrification consists of a reduction reaction that converts nitrate to nitrogen gas, where the energy source is organic matter and the electron acceptor is nitrogen. If there would be dissolved oxygen available, this element would accept the electrons and the conversion to nitrogen gas would not be possible. Bacteria that are responsible for this are heterotrophic facultative.

Meanwhile, in the next three tanks there exist aeration permitting the nitrification process. The objective is remove nitrogen present in the water. This process takes place in two steps, the first is the conversion of ammonium to nitrite and the second is the conversion of nitrite to nitrate. In this reaction, the electron donor is ammonia nitrogen, for this reason if there are organic matter able to donor electrons, a competition between the two donors occurs and it is possible that does not occur the transformation from ammonium to nitrite and much less to nitrate. Electrons are accepted by dissolved oxygen present in the ambient. Nitrification process is executed with the help of autotrophic bacteria, the first part by Nitrosomonas bacteria and the second part by Nitrobacter bacteria. The next reactions describe the two process.

Denitrification process:

$$24NO_3^- + 5C_6H_{12}O_6 + 24H^+ \rightarrow 12N_2 + 24H_2O + 30CO_2 \tag{3.1}$$

Nitrification process:

$$NH_4^+ + (3/2)O_2 \to NO_2^- + 2H^+ + H_2O$$
 (3.2)

$$NO_2^- + (1/2)O_2 \to NO_3^-$$
 (3.3)

In each reactor different biological processes take place involving the compounds listed previously. Firstly, there are two non-biodegradable organic matter compounds, which are biologically inert. They can be found in two forms: soluble (S_I) or particulate (X_I) . Although these compounds are not involved in conversion process, they are important for developing the biological process. On the other hand, biodegradable organic matter can be classified in readily biodegradable (S_S) and slowly biodegradable (X_S) . Readily biodegradable substrate can be taken by heterotrophic bacteria and used for cellular growth. This process can occur in aerobic or anoxic conditions, i.e. in any reactor of the plant. Moreover, slowly

biodegradable substrate transform into readily biodegradable substrate through hydrolysis, which occurs in anoxic conditions and it is slower that using S_S . Additionally, X_S can be formed by death of autotrophic and heterotrophic bacteria. It is necessary highlight that autotrophic bacteria (X_{AH}) have as carbon source inorganic matter. These bacteria grow in aerobic ambient. Meanwhile, heterotrophic bacteria (X_{BH}) have as carbon source organic matter and they can grow in aerobic and anoxic conditions. Both types of bacteria disappear by death or decay and this form three types of particulates: X_P , X_S and X_{ND} .

Oxygen (S_O) is used for the growth of autotrophic and heterotrophic bacteria, because this element is electron acceptor in nitrification process. Oxygen is demanded in the oxidation from ammonium to nitrate. This oxygen is supplied in the last three reactors by aerators. In these tanks the oxygen transference is only function of temperature. The S_{NO} represents the nitrate produced in nitrification process, which is removed by growth of heterotrophic bacteria and denitrification process. Ammonium (S_{NH}) is formed by ammonification of soluble biodegradable organic nitrogen and is removed by growth of biomass. Also, soluble biodegradable organic nitrogen (S_{ND}) is formed by hydrolysis of soluble biodegradable organic nitrogen (X_{ND}) that is formed by decay of autotrophic and heterotrophic bacteria is removed by ammonification. Now, the particulated biodegradable organic nitrogen (X_{ND}) that is formed by decay of autotrophic and heterotrophic bacteria is removed by ammonification. Finally, the alkalinity (S_{ALK}) must be considered because in the process there exist a constant flow of electrons, so there is a change in the protons of species and that can be interpreted as pH variations.

Compound	Formed by	Removed by
S_I	Compound soluble biologically inert	
S_S	Hydrolysis of X_S	Cellular growth
X_I	Particulate bio	ologically inert
X_S	Death of autotrophic and het-	Hydrolysis to S_S
	erotrophic bacteria	
X_{BH}	Growth in aerobic and anoxic	Decay to X_{ND} and death to
	conditions	X_S and X_P
X_{BA}	Growth in aerobic conditions	Decay to X_{ND} and death to
		X_S and X_P
X_P	Death of autotrophic and het-	Physical separation in the set-
	erotrophic bacteria	tler
S_O	Supplied by aerators	Growth of autotrophic and het-
		erotrophic bacteria
S_{N0}	Nitrification process (growth of	Denitrification process (growth
	X_{BA})	of X_{BH})
S_{NH}	Ammonification of S_{ND}	Growth of biomass and nitrifi-
		cation process
S_{ND}	Hydrolysis of X_{ND}	Ammonification to S_{NH}
X_{ND}	Decay of biomass	Ammonification to S_{ND}
S_{ALK}	ALK Represents pH variations	

All previously discussed chemical and biochemical interactions are listed in Tabla 3.1.

Table 3.1. Process summary

Mathematical Description

The BSM1 model wants to answer the following question, how do change the concentration of all components respect to time in each equipment? specially how do change ammonium concentration and total suspend solids concentration in the effluent?, how change nitrate concentration in reactor 2? and how do change oxygen concentration in the reactor five?. In order to answer these questions, seven process systems are considered as it is shown in Figure 3.2.



Figure 3.2. Diagram of Process Systems

The result of applying conservation principles are balances per component at each system and they are presented below. In this expressions, the subindex *i* represents the component listed before, the second subindex is the current name, *w* is mass fraction, \dot{m} is mass flow, *V* is tank volume, S_O is oxygen concentration, S_O^* is oxygen saturation concentration, *r* is reaction rate and M_i is total mass of component *i*:

- First anoxic reactor (S_I)
 - Balance per component (different to oxygen)

$$\frac{dM_{i,1}}{dt} = w_{i,0} * \dot{m_0} + w_{i,int} * \dot{m_{int}} + w_{i,r} * \dot{m_r} + r_{i,1} * V_1 - w_{i,1} * \dot{m_1}$$
(3.4)

- Balance of oxygen

$$\frac{dS_{O,1}}{dt} = S_{O,0} * \dot{m_0} + S_{O,int} * \dot{m_{int}} + S_{O,r} * \dot{m_r} + r_{O,1} * V_1 + K_L a_1 * V_1 * (S_O^* - S_{O,1}) - S_{O,1} * \dot{m_1}$$
(3.5)

- Second anoxic reactor (S_{II})
 - Balance per component (different to oxygen)

$$\frac{dM_{i,2}}{dt} = w_{i,1} * \dot{m_1} + r_{i,2} * V_2 - w_{i,2} * \dot{m_2}$$
(3.6)

- Balance of oxygen

$$\frac{dS_{O,2}}{dt} = S_{O,1} * \dot{m_1} + r_{O,2} * V_2 + K_L a_2 * V_2 * (S_O^* - S_{O,2}) - S_{O,2} * \dot{m_2}$$
(3.7)

- First aerobic reactor (S_{III})
 - Balance per component (different to oxygen)

$$\frac{dM_{i,3}}{dt} = w_{i,2} * \dot{m_2} + r_{i,3} * V_3 - w_{i,3} * \dot{m_3}$$
(3.8)

- Balance of oxygen

$$\frac{dS_{O,3}}{dt} = S_{O,2} * \dot{m_2} + r_{O,3} * V_3 + K_L a_3 * V_3 * (S_O^* - S_{O,3}) - S_{O,3} * \dot{m_3}$$
(3.9)

- Second aerobic reactor (S_{IV})
 - Balance per component (different to oxygen)

$$\frac{dM_{i,4}}{dt} = w_{i,3} * \dot{m_3} + r_{i,4} * V_4 - w_{i,4} * \dot{m_4}$$
(3.10)

- Balance of oxygen

$$\frac{dS_{O,4}}{dt} = S_{O,3} * \dot{m_3} + r_{O,4} * V_4 + K_L a_4 * V_3 * (S_O^* - S_{O,4}) - S_{O,4} * \dot{m_4} \quad (3.11)$$

- Third aerobic reactor (S_V)
 - Balance per component (different to oxygen)

$$\frac{dM_{i,5}}{dt} = w_{i,4} * \dot{m_4} + r_{i,5} * V_5 - w_{i,5} * \dot{m_5} - w_{i,int} * \dot{m_{int}}$$
(3.12)

- Balance of oxygen

. ~

$$\frac{dS_{O,5}}{dt} = S_{O,4} * \dot{m_4} + r_{O,5} * V_5 + K_L a_5 * V_5 * (S_O^* - SO, 5) - S_{O,5} * \dot{m_5} - S_{O,int} * \dot{m_{int}}$$
(3.13)

- Settler
 - Balance per component

$$\frac{dM_{i,6}}{dt} = w_{i,5} * \dot{m_5} - w_{i,e} * \dot{m_e} - w_{i,6} * \dot{m_6}$$
(3.14)

• Delivery point

$$\dot{m_6} = \dot{m_r} + \dot{m_w} \tag{3.15}$$

Now, in order to complete the mathematical model that describe the process it is necessary to provide the model with some constitutive equations. The main constitutive equation are reaction rates for all components. These expressions are listed in Table 3.2.

Component	Process rate
S_I (i=1)	$r_1 = 0$
S_S (i=2)	$r_2 = rac{1}{Y_H} * ho_1 - rac{1}{Y_H} * ho_2 + ho_7$
X_I (i=3)	$r_{3} = 0$
X_S (i=4)	$r_4 = (1 - f_p) * \rho_4 + (1 - f_p) * \rho_5 - \rho_7$
<i>X_{BH}</i> (<i>i</i> =5)	$r_5 = \rho_1 + \rho_2 - \rho_7$
X_{BA} (i=6)	$r_6 = \rho_3 - \rho_5$
X_P (i=7)	$r_7 = f_p * \rho_4 + f_p * \rho_5$
S _O (i=8)	$r_8 = -rac{1-Y_H}{Y_H}* ho_1 - rac{4.57-Y_A}{Y_A}* ho_3$
S_{NO} (i=9)	$r_9 = -rac{1-Y_H}{2.86*Y_H}* ho_2 + rac{1}{Y_A}* ho_3$
S_{NH} (i=10)	$r_{10} = -i_{XB} * \rho_1 - i_{XB} * \rho_2 - (-i_{XB} + \frac{1}{Y_A}) * \rho_3 + \rho_6$
S_{ND} (i=11)	$r_{11} = -\rho_6 + \rho_8$
X_{ND} (i=12)	$r_{12} = (i_{XB} - f_p * i_{XB}) * \rho_4 + (i_{XB} - f_p * i_{XB}) * \rho_5 - \rho_8$
S _{ALK} (i=13)	$r_{13} = -\frac{i_{XB}}{14} * \rho_1 + \left(\frac{1-Y_H}{14*2.86*Y_H} - \frac{i_{XB}}{14}\right) * \rho_2 - \left(\frac{i_{XB}}{14} + \frac{1}{7Y_H}\right) * \rho_3 + \frac{1}{14} * \rho_6$

Table 3.2. Expressions for reaction rate for each process component.

Where Y_H is heterotrophic yield, Y_A is autotrophic yield, f_p is fraction of biomass yielding particulate products, i_{XB} is Mass N/Mass COD in biomass, i_{XP} is Mass N/Mass COD in products from biomass, COD is chemical oxygen demand, and finally, ρ_k represent biological processes, where k is a number between one and eight, then each number is a different process. The values of these stoichiometric parameters are listed in Table 3.3.

Parameter	Unit	Value
Y_A g cell COD formed / g Nitrogen oxidized		0.24
Y_H g cell COD formed / g Nitrogen oxidized		0.67
f_p	dimensionless	0.08
i_{XB} g N / g COD in biomass		0.08
i_{XP}	g N $/$ g COD in particulate product	0.06

Table 3.3. Values of stoichiometric parameters [3].

The representation of biological processes are also constitutive equations. In this processes there exist eight representative biological process listed in Table 3.4.

Biological process	Expression
Aerobic growth of het-	$\rho_1 = \mu_H * \frac{S_S}{K_S + S_S} * \frac{S_O}{K_{O,H} + S_O} * X_{BH}$
erotrophs	
Anoxic growth of het-	$\rho_2 = \mu_H * \frac{S_S}{K_S + S_S} * \frac{S_O}{K_{O,H} + S_O} * \frac{S_{NO}}{K_{NO} + S_{NO}} * \eta_g * X_{BH}$
erotrophs	
Aerobic growth of au-	$\rho_3 = \mu_A * \frac{S_{NH}}{K_{NH} + S_{NH}} * \frac{S_O}{K_{O,A} + S_O} * X_{BA}$
totrophs	
Decay of heterotrophs	$\rho_4 = b_H * X_{BH}$
Decay of autotrophs	$\rho_5 = b_A * X_{BA}$
Ammonification of solu-	$\rho_6 = k_a * S_{ND} * X_{BH}$
ble organic nitrogen	
Hydrolysis of entrapped	$\rho_7 = k_h * \frac{X_S / X_{BH}}{K_T + (X_S / X_{BH})} * \left(\frac{S_O}{K_{OH} + S_O} + \eta_h * \frac{K_{OH}}{K_{OH} + S_O} * \frac{S_{NO}}{K_{NO} + S_{NO}}\right) *$
organics	X_{BH}
Hydrolysis of entrapped	$\rho_8 = k_h * \frac{X_S / X_{BH}}{K_x + (X_S / X_{BH})} * \left(\frac{S_O}{K_{OH} + S_O} + \eta_h * \frac{K_{OH}}{K_{OH} + S_O} * \frac{S_{NO}}{K_{NO} + S_{NO}}\right) *$
organic nitrogen	$X_{BH} * (X_{ND}/X_S)$

Table 3.4. Expressions of biological processes.

Where μ_H , K_S , $K_{O,H}$, K_{NO} and b_H are parameters of growth and decay of heterotrophic, μ_A , K_{NH} , $K_{O,A}$ and b_A are parameters of growth and decay of autotrophic, η_g is correction factor for anoxic growth of heterotrophs, k_a is kinetic parameter of ammonification, k_h and K_X are kinetics parameters of hydrolysis and finally η_h is correction factor for anoxic hydrolysis. The values of kinetics parameters are showed in Table 3.5.

Parameter	ter Unit	
μ_H	d^{-1}	4.0
K_S	g COD $/~m^3$	10.0
$K_{O,H}$	${\sf g}({\sf -COD})/m^3$	0.2
K_{NO}	g NO_3 -N / m^3	0.5
b_H	d^{-1}	0.3
η_g	dimensionless	0.8
η_h	dimensionless	0.8
k_h	g slowly biodegradable COD $/$ g cell COD * d	3.0
K_X	g slowly biodegradable COD $/$ g cell COD	0.1
μ_A	d^{-1}	0.5
K_{NH}	g NO_3 -N $/~m^3$	1.0
b_A	d^{-1}	0.05
$K_{O,A}$	${\sf g}({\sf -COD})/m^3$	0.4
k_a	m^3 $/$ g COD * d	0.05

Table 3.5. Values of kinetic parameters [3].

Plant performance is evaluated according to some parameters that must be maintained under the law limit Table 3.6 [28], [3].

Variable	Value
N_{tot} (total nitrogen)	$< 18gN.m^{-3}$
COD_t	(chemical oxygen demand) $< 100 g COD.m^{-3}$
$S_{NH} \left(NH_4^+ + NH_3 ext{ nitrogen} ight)$	$< 4gN.m^{-3}$
TSS (total suspended solid)	$< 30 gSS.m^{-3}$
BOD_5 (biochemical oxygen demand)	$< 18 gBOD.m^{-3}$

Table 3.6. Effluent quality limits.

In this benchmark the mass transfer is not strictly modeled, because it is no relevant in order to represent the global process. In this case, the mass transfer is represented by volumetric mass transfer coefficient $(k_L a)$, but this parameter is calculated only in accordance to the temperature and some empirical parameters and it is a constitutive equation of model structure. Actually, the mass transfer process is represented by the Equation 3.16 in BSM1.

$$k_L a = k_L a * \alpha * F * \theta^{T-15} \tag{3.16}$$

Where α , F and θ are empirical parameters and T is temperature in the system.

Evidently, the $k_L a$ from the Equation 3.16 does not represent the real process because this parameter is global and it does not take into account other physical phenomena that have great influence in the mass transfer, for example the bubble size and quantity or gas hold up [29] [30]. Additionally, in real processes is not possible to manipulate the $k_L a$ directly because is not a physically manipulated variable. It is necessary to highlight that the volumetric mass transfer coefficient is the product between the liquid phase mass transfer coefficient (k_L) and the specific area or specific interfacial area (a). If these parameters are separated it is possible to understand the gas - liquid mass transfer mechanism because these parameters are affected by manipulated variables in a different way. For this reason, it is important to know the relation between them. In this sense, this work proposes a model in order to represent it and it is explained in the next section.

3.2. Mass transfer coefficient model

As mentioned previously, the volumetric mass transfer coefficient $(k_L a)$ is computed considering the liquid phase mass transfer coefficient (k_L) and specific area (a). These parameters define the relation between the manipulated variables (in real processes) and controllable variables. A model that represents the mass transfer phenomena associated with the oxygen dynamics in the activated sludge process is presented here and it is validated in the BSM1.

The bubble formation is an equilibrium between superficial tension (that trying to shut the bubble) and fluid pressure (that trying to expand the bubble). According to [31], the bubble formation takes place on two stages, the first is the expansion stage and the second is detachment stage. It is necessary to highlight that the equilibrium not only depend on materials physico-chemical properties, depends on mechanical energy applied to stirred fluid [32]. The bubble formation is important since the size and quantity of bubbles determine the
oxygen transfer in the aerobic zone. The bubble diameter is described by Equation 3.17.

Bubble diameter is computed using the expression 3.17 [33]. Where d_0 is orifice diameter of diffuser membrane (m), σ is surface tension (N/m), $\Delta\rho$ is the density difference between liquid and gas (kg/m^3) and g is gravitational constant.

$$d_b = \sqrt[3]{\frac{6*d_0*\sigma}{\Delta\rho*g}} \tag{3.17}$$

 $\Delta \rho$ is calculated according to:

$$\Delta \rho = \rho_L - \rho_G \tag{3.18}$$

Where ρ_L the liquid density, that can be considered the density water pure and ρ_G the gas density, calculated using ideal gas equation with internal pressure of the bubble P_{int} . It should be noted that internal pressure is the pressure inside of bubble and it is necessary to take into account the liquid pressure and the drop pressure in the diffuser orifice, like is expressed in the Equation 3.2.

$$\rho_G = \frac{P_{int} * Wm}{R * T_G} \tag{3.19}$$

Where Wm the gas molecular weight, R the ideal gas constant, and T_G the gas temperature. The bubble internal pressure is calculated as:

$$P_{int} = P_{iny} - \Delta P_{or} \tag{3.20}$$

Where P_{iny} is the injection pressure (Pa) and ΔP_{or} the drop pressure at orifice(Pa), calculated according to [34]:

$$\Delta P_{or} = \left(\frac{Q_{air}}{k_0}\right)^2 \tag{3.21}$$

Where Q_{air} is instantaneous gas flow rate through the diffuser orifice and k_0 the orifice constant $(m^3/Pa^{0.5}s)$, that is a function of gas flow rate, gas density (ρ_g) , gas viscosity (μ_g) , orifice diameter and orifice plate thickness (L). The orifice constant is evaluated with:

$$k_0 = \sqrt{\frac{2}{\rho_g * C_g}} * \left(\frac{\pi * d_0^2}{4}\right)$$
(3.22)

Where C_g is the constant dimensionless calculated as:

$$C_g = 1.5 + 4f_F \frac{L}{d_0} \tag{3.23}$$

Where f_F the Fanning friction factor and assumming that the gas flow through the orifice is laminar. The friction factor is calculated according to:

$$f_F = \frac{16}{Re_0} = \frac{4 * \pi * \mu_g * d_0}{\rho_g * Q_{air}}$$
(3.24)

The volumetric mass transfer coefficient $k_L a$ is calculated considering the effect of liquid-phase mass transfer coefficient k_L and the gas-liquid interfacial area a independently. However, it is important to highlight that the mass transfer coefficient quantifies how quickly the species are moving across an interphase [35]. The mass transfer rate is estimated according to the mass transfer coefficient and the coefficient strongly depends on the presence of contaminants [36] [35]. Besides, the liquid phase mass transfer coefficient considers the effects the liquid flow that surrounds the rising gas bubbles and the specific area reflects the system bubble behaviour [37]. In [29] are proposed some empirical correlations in order to calculate k_L , but their use depends on the operation conditions and the relation between the compounds, see Table 3.7.

Correlation	Mathematical expression	Observations
name		
Perry	$k_L = \frac{D_L (Re * Sc)^{(1/3)}}{d_b}$ $k_L = \frac{1.13 * D_L (Re * Sc)^{(1/2)}}{d_b}$	This expressions are applied when are considered spherical bubbles. The first one is a the- oretical expression used when $d_b \leq 0.1cm$ and the second one is applied when $d_b \geq 0.5cm$ [38].
Nedelchev	$k_L = \sqrt{\frac{4D_L}{\pi t_c}}$	This expression is valid when the bubble Peclet number is higher than 100 and bubble Reynold number is much higher than 400 and when the Schmidt number is higher than the unity [37]. t_c is gas-liquid contact time.
Calderbank	$k_L = \frac{0.42(\frac{\mu_L * g}{\rho_L})}{Sc^{0.5}}$	This correlation was corrobo- rated in [29] and it proposed in [39] for large bubbles. It should be noted that it is considered a large bubble when $d_b \ge 0.25cm$
Kawase	$k_L = \sqrt{\frac{D_L}{\pi} * \sqrt{\frac{U_G * g}{\mu}}}$	This correlation is based on Higbie's penetration theory and it is studied experimentally in [29] and [40]. This equation is based on phenomenological model and depends on bubble size [29] and [40].

Table 3.7. Correlation tested for liquid phase mass transfer coefficient.

Kawase correlation has been selected to compute k_L in this work, because it is used in conditions similar to the BSM1, and additionally this correlation complies whit the necessary range operation for the mass transfer in BSM1 [29]:

$$k_L = \sqrt{\frac{D_L}{\pi} * \sqrt{\frac{U_G * g}{\mu}}}$$
(3.25)

Where D_L the diffusivity of the gas in liquid (m^2/s) , g the gravity constant (m/s^2) , μ the liquid viscosity (Pas), and U_G the superficial gas velocity (m/s). This superficial gas velocity is calculated according to volumetric gas flow rate (Q_{air}) and empty spaces or active cross

area of diffuser. It should be noted that superficial velocity is defined as volumetric flow rate that goes through the cross sectional area. This area is the empty spaces of diffuser (membrane) or active area, calculated according to the membrane porosity. The diffusers are membrane type according to waste water treatment plant *El Marin* in Salamanca [41], the information about this diffusers is related to active area. In this sense, the gas flows through the area calculated in the denominator of Equation 3.2.

$$U_G = \frac{Q_{air}}{A_{active} * DiffuserNumbers}$$
(3.26)

In the other hand, the specific area is the interfacial area per unit of volume. The interfacial area is the area of transfer between the gas and fluid [42]. The specific area is calculated according to Equation 3.2 [43], because the bubbles are considered spherical [40]. This expression considers the gas gold-up and the bubble diameter.

$$a = \frac{6 * \epsilon_G}{d_b} \tag{3.27}$$

In the Equation 3.2 ϵ_G is gas hold-up (*dimensionless fraction*). This parameter is interpreted as the gas retention in the fluid. Essentially, ϵ_G is affected by the diameter of gas inlet orifice or diffuser orifice, superficial gas velocity, liquid density, surface tension and gravity[44]. There exist many expressions in order to calculate ϵ_G , the majority are from experimentation, i.e. empirical expression. The expression is determined using different systems and fluids. This parameter has been extensively studied because it affects the mass transfer directly [45]. In [29] are proposed many expressions in order to calculate ϵ_G . The physical conditions are the same, i.e. it was used a column in order to represent a vertical slide of an activated sludge tank, but according to the region of mass transfer or operation conditions the expression 3.2 is chosen.

$$\epsilon_G = \frac{0.91 * U_G^{1.19}}{\sqrt{g * d_b}} \tag{3.28}$$

3.3. Remarks

In this chapter, the process model was explained. The model is compound by two parts: the first one is BSM1. This model describes nitrification and denitrification processes. The second one describes mass transfer in aerobic section, considering the k_L and a effects. In this sense, it is important to highlight that:

 The phenomenological based model about full process is essential in the control strategy proposed in this thesis because it supplies information to the control strategy. BSM1 and the mass transfer model represent the behaviour of real plant. Moreover, biological processes are considered in order to represent the full process.

• The mass transfer model is used in order to implement control loops with the specific area and liquid phase mass transfer coefficient because the volumetric mass transfer coefficient is a global parameter that is not directly manipulated. In this way, the k_L and a effects are considered in the model.

CHAPTER 4 Strategy for Collaborative Control Including the Controllable Parameters

Traditionally, the controlled variables in control loops are states considered as outputs (with fully measured state). In this work it is presented the situation where it is possible to take as controlled "variable" a process parameter, calling this parameter as a controllable parameter. In this sense, some processes can be strongly affected by parameters but usually it is not evident, even when measuring this parameter can be easy. Taking into account the controllable parameters it is possible to increase the degrees of freedom of a control structure with the possibility to add more control loops.

In this chapter the methodology of collaborative control including the controllable parameters is exposed, based on the proposal of [2] explained in the Section 2.3. The methodology proposed here is validate in a wastewater treatment plant benchmark, the BSM1 [3], see Section 3.1. The importance of including the controllable parameter in the control strategy studied is explained here. The next section explains the controllable parameters concept and the difference with other parameters. Different controllable parameters that it is possible to find in processes are mentioned below. The detailed methodology is exposed in order to use controllable parameters in collaborative control strategy.

4.1. Controllable parameters in the collaborative control strategy

The basic structure of a phenomenological based semi-physical model (PBSM) is obtained from applying the conservation principle. Constitutive equations are part of the extended model structure. The full model is comprises by variables, constants and parameters [25], assembled into total model structure. The variables only can be determined solving the model. Variables commonly are process outputs. On the other hand, the parameters do not arise from balance equations. They appear on the right-hand side of balance equations or into constitutive model equations. Therefore, the parameters are not provided by the model solution. They must be determined before solving the model. Finally, the constants do not need to be calculated, because are fixed, input or disturbances [46]. In this sense, the mathematical model of a process can have different types of parameters like it is shown in Figure 4.1.



Figure 4.1. Parameters classification.

As it shown in Figure 4.1, the parameters can be grouped in process parameters and control parameters. Within the first group are design, transport and physico-chemical properties parameters, which are related to the process operation and used materials. The controller parameters are the controller tuning parameters. Into the first group, there are some parameters which are manipulable, but there are other impossible to manipulate. More specifically, the design parameters are not on-line manipulable, for example, it is impossible to modify reactor volumes. On the other hand, transport and physico-chemical parameters can be manipulated and it is possible to generate extra degrees of freedom in order to have additional control actions. The parameters with this characteristic, in this work are named **controllable parameters**. The controller tuning parameters are not considered here as on-line manipulable in spite of adaptive controller availability. It is important to clarify that in a process normally it is not possible to do a direct control action using all manipulated variables. Some of them are left as constant during process design and operation. In this sense, now is defined controllable parameters concept.

Definition 4.1. Controllable Parameters. This is a kind of process parameter that can be directly manipulated using one or more available control actions. When a controllable parameter has its control loop, it gives an extra degree of freedom through the additional control actions.

In chemical and biological processes the controllable parameters are frequent, because global transfer parameters appear in each transfer operation and reaction. These parameters can be can be broken down into other parameters that provide more information about the real process and to generate extra degrees of freedom in the control structure. A first example, is the continuous stirred tank reactor (CSTR) shown in Figure 4.2, where the reaction: $A \rightarrow B$ takes place and the temperature control is one of the control tasks. The Figure 4.2 shows the typical control loop, where the controlled variable is the reactive mass temperature and the manipulated variable is the refrigerant flow into the jacket. The Equation 4.1 is the energy balance describing the behavior of reactive mass temperature.



Figure 4.2. Process flow diagram of a Continuous Stirred Tank Reactor (CSTR).

$$\frac{dT_r}{dt} = \frac{F_{in}}{V_r} (T_{in} - T_r) - \frac{\Delta H k_0}{\rho C p} C_{A,r} e^{-Ea/RT_r} - \frac{U * As}{V_r \rho C p} (T_r - T_j)$$
(4.1)

where T_r is the temperature inside the reactor, F_{in} is the feed flow rate, V_r is the reactor volume, T_{in} the feed temperature, ΔH is the heat of reaction, k_0 is the frequency factor, ρ is the density of the reactive mass, Cp is the heat capacity, $C_{A,r}$ is the A reactive concentration in the reactor, Ea is the activation energy, R is the universal gas constant, U * As is the product of the overall heat transfer coefficient and the jacket - reactor heat transfer area and T_j is the temperature inside the jacket.

In this process it is possible that the response of reactor temperature is not right, because the stirred system is not manipulated and its current velocity is not the best, in spite of being a more appropriate control action. Then, with the control strategy proposed in the Figure 4.2 it is not possible modify the agitation automatically. k_0 is the parameter directly related to the agitation. In this sense, this parameter generates a new control action and it is necessary to determine the set point for this parameter. Also, the overall heat transfer coefficient (U) can be broken down and identify the local heat transfer coefficients or some parameter that more affects to U and to create the control action for this parameter (local heat transfer coefficients for each side of the exchanger). In this sense, k_0 can be manipulated with power unit velocity and U with fluid flow or some variable related mathematically with the parameter. Then, these parameters are controllable parameters. It is necessary to highlight that As will be a parameter relevant in the reactor temperature, but this parameter is difficult to manipulate on-line, because it is a design parameter and there is not a control action for it, except when the jacket can operate partially full.

Another example of process where controllable parameters can be used is an aerobic reactor. The process flow diagram is shown in the Figure 4.3. In this reactor a nitrification process is taken place conducting to an operation in aerated environment. In this sense, mass transfer is an important phenomenon in this reactor. The control objective is to keep the oxygen concentration in its reference. The oxygen concentration state is directly related to the current applied aeration. Obviously, the intermediate step between the oxygen concentration

and the aeration is the mass transfer, described by the volumetric mass transfer coefficient. The equation that describes the oxygen concentration is the Equation 4.2.



Figure 4.3. Process flow diagram of an aerobic reactor.

$$\frac{dS_O}{dt} = S_O * \dot{m_{in}} + r_O * V_2 + K_L a * V * (S_O^* - S_O) - S_O * \dot{m_{out}}$$
(4.2)

where S_O is the oxygen concentration, $\dot{m_{in}}$ and $\dot{m_{out}}$ are the input and output liquid flows, V is the reactive mass volume, S_O^* is oxygen saturation concentration and $k_L a$ is the volumentric mass transfer coefficient.

As it was mentioned previously and it is shown in Equation 4.2, the mass transfer is very important in the dynamic of oxygen concentration. Additionally, this phenomenon was described in the Section 3.2 where it was explained the separation of k_L and a like two independent parameters. It should be noted that these two parameters are controllable parameters because it can be to keep in their set points by manipulating injection pressure or air flow, i.e. they can be controllable in the process. Eventually, when the air flow or injection pressure are modified, the oxygen concentration changes due to the chained relationship with mass transfer, like it was shown in the model developed in the Section 3.2. However, the control action is more direct or faster when the control loop is done with k_L and a independently. Moreover, one degree of freedom is gained because it is added a control loop. It is important to note that commonly a single control loop manipulating directly the $k_L a$ is reported in the literature, as it is shown in the Figure 4.3 but this direct manipulation is not physically possible. Taking into account these situations, next section explains the collaborative control strategy including the controllable parameters and the consideration to be considered in order to implement this strategy.

4.2. Collaborative control strategy methodology including controllable parameters

This section explains in detail the methodology of collaborative control proposed in this thesis, including the use of controllable parameters to increase the degrees of freedom of the plantwide control structure. In this sense, the methodology summary is shown in the Figure 4.4.



Figure 4.4. Design methodology of collaborative control strategy.

The methodology is divided into three stages. The first one consist of the process analysis to know the process in detail and its mathematical description. This stage allows determining the process characteristics by means of a set of preliminary calculations. The second stage is the design of regulatory layer. In this stage PID controllers are distributed over the full plant. These controllers act over secondary dynamics or controllable parameters as tracking controllers, and over the main dynamic as the only regulatory PID. Finally, the third stage is the supervisory layer design. In this stage the optimization problem is stated including information about main and secondary dynamic and controllable parameters. The structure of this strategy is shown in the Figure 4.5, repeated here for text completeness. The control structure is formed by supervisory layer, regulatory layer and plant. In the following the mentioned three stages are described in detail. In the next section the three stages are described in detail.



Figure 4.5. Centralized hierarchical control architecture [2].

4.2.1. Process analysis

It is very important to know the process to be controlled. This knowledge is important for an efficient control strategy design. To fulfill with this stage, the methodology proposed here states next steps, which results basic for the proposed collaborative control strategy.

Step 1: Development of a process phenomenological based semi-physical model (**PBSM**). The development of a PBSM of the process is necessary for the development of the collaborative control strategy. It is important to highlight that if a phenomenological based process model is not available, the model can be structured in accordance to the methodology proposed by [25] because the implementation is easy and it is not necessary to have expertise in process modeling. The modeling methodology proposed by [25] is development in ten steps. The steps are summarized like this:

- 1. Develop a verbal description of process functioning and process flow diagram.
- 2. Propose the modelling hypothesis according the level of detail for the model depending on the objectives proposed. For example macroscopic or microscopic levels.
- 3. Define process systems and plot a block diagram for the relation among these process systems.
- 4. Obtain the dynamic balance equations using the principle of conservation (mass, energy, etc.) for each process system.
- 5. Select the dynamic balance equations with most significant information.
- 6. Recognize variables, parameters and constants of the model. It should be noted that, this information is relevant for the steps two and three of the proposed collaborative control methodology.

- 7. Find constitutive equations for calculating the parameters of the model.
- 8. Verify the degrees of freedom of the model. Obviously, it must be zero for a solvable model.
- 9. Build a computer program in order to simulate the model.
- 10. Validate the model response.

Step 2: Determination of available manipulated variables, states and parameters. This information provides a prospect of possible control loops or control structures. In this sense, it can take each unit and look for availability of this information. It should be noted that in model simulation any variable or parameter can be considered as measured, but it is important to distinguish in the real process which information is available in accordance to installed instruments.

Step 3: Determinate if there exist controllable parameters. In this step the controllable parameter are chosen, i.e. those parameters that can be controlled and fulfill the characteristics explained in Section 4.1. These parameters can be used to implement the collaborative control strategy.

Step 4: Definition of the operating point and span of states and input variables. This step is related with the real operation of the process, i.e. the operation conditions and stationary state are chosen because they will be the references in the global control structure.

Step 5: Determination of dynamic hierarchy. This is the last step from process analysis, fundamental for collaborative control strategy because according to the result obtained here the supervisory layer is designed. Even [14], [47] and [48] propose different criteria for obtaining this layer, in this work the decision criterion is the main dynamic of the process. That main dynamic is found using the state impactability index (SII_{yk}) calculated with the Hankel Matrix, as it was explained in Section 2.3.

4.2.2. Regulatory layer design

This stage is related to the individual closed loops to be implemented on the plant. These control loops include controllers originally operating in regulatory mode. However, collaborative control strategy commutes secondary dynamic controllers to tracking mode because they must track the reference given by the coordinator controller. This level can be composed of MPC controllers but here PID controllers are used because they are easy to implemented and understand. In addition, PID stability properties are well known and easy to guarantee. On the contrary, MPC controllers are more complex, take more time for execution and their stability requirements are more difficult to fulfill.

Step 6: Identification of control objective. This step is essential for any control strategy. In this case, it is important to define the global control objective and the control objective for each process unit. According to the control objectives it will be necessary additional control

loops.

Step 7: Selection of input-output paring for control loop at each process unit, based on steps 3 to 5. In accordance to control objectives and determined the main dynamic, the control loops that will be present in the regulatory layer are stated. It is important to take into account the process main dynamic and all the relationships between secondary dynamic and controllable parameters.

Step 8: Preliminary control tuning. The last task to finish the regulatory layer design is to tune each proposed controller. This can be done with any available tuning method. However, the performance of these controllers should be evaluated before designing the supervisory layer.

4.2.3. Supervisory layer design

This is the last stage of the methodology, including the main dynamic, the secondary dynamics and the controllable parameters. The structure of regulatory layer and its individuals control loops is located the coordinator controller, which function is to decide the set points for each individual controller, except the main dynamic controller. Those set points values try to achieve the control objective minimizing the error of main dynamic, the only one with regulatory control loop.

Step 9: Formulation of the optimization problem. In this point, the regulatory level has a good performance acting with fixed setpoints but this performance is not enough for plantwide control objectives. The supervisory layer is directly linked to the main dynamic and the optimization problem, where it is evident the collaboration with the secondary dynamics to satisfy the plantwide objectives. In this sense, the optimization problem is stated as:

$$\min_{x_{1,sp},\dots,x_{j,sp},\theta_{1,sp},\dots\theta_{k,sp}} J = \alpha(x_{ss}^* - x_{sp}^*) + \sum_{i=1}^{n-1} \beta_i \frac{1}{S_i} + \sum_{k=1}^k \gamma_k \frac{1}{Ss_k}$$
(4.3)
S. t. $x_{i,sp_{min}} \leq x_i \leq x_{i,sp_{max}}$

$$\begin{array}{l} \Delta x_{i,sp_{min}} \leq \Delta x_i \leq \Delta x_{i,sp_{max}} \\ \theta_{k,sp_{min}} \leq \theta_k \leq \theta_{k,sp_{max}} \\ \Delta \theta_{k,sp_{min}} \leq \Delta \theta_k \leq \Delta \theta_{k,sp_{max}} \end{array}$$

Where $x_{j,sp}$ and θ_k are controllable variables and parameters, respectively. α , β_i and γ_k are weights acting as tuning factors, x_{sp}^* is the set point of the main dynamic (x^*) , x_{ss}^* is the x^* steady-state value that would be achieved if the system reached steady-state with the $x_{j,sp}$ values determined during the optimization and the rest of states at the current value. S_i is the sensitivity of main dynamic to changes on i - th secondary dynamic at the current values of the process state, Ss_k correspond to the sensitivity of main dynamic to changes on k-th controllable parameter at the current values of the process state. $x_{i,sp_{min}}$, $x_{i,sp_{max}}$, $\theta_{k,sp_{min}}$ and $\theta_{k,sp_{max}}$ are the limit values for secondary dynamics and controllable parameters set points guaranteeing process stability, $\Delta x_{j,sp_{min}}$, $\Delta x_{j,sp_{max}}$, $\Delta \theta_{k,sp_{min}}$ and $\Delta \theta_{k,sp_{max}}$

are the maximum and minimum changes possible in the set points of secondary dynamics and controllable parameters. These values are related directly to the effect of manipulated variables over parameters.

The term S_i is calculated according to the Equation 4.4, where x_i corresponds to the *i*-th secondary dynamic, explained in the Section 2.3.

$$S_i(\mathbf{x}(t), \mathbf{u}(t)) = \left. \frac{\partial x^*}{\partial x_i} \right|_{x_i \neq i}$$
(4.4)

Additionally, the new sensitivity included in the original cost function proposed in [2], regarding main dynamic and controllable parameters, is described by the Equation 4.5.

$$Ss_k(x(t), u(t)) = \frac{\partial x^*}{\partial \theta_k}$$
(4.5)

It should be noted that the plantwide stability is assumed as guaranteed if all the local controllers are stable. In this sense, local controller design should be stable and the changes in set point should be restricted by operation conditions, physical and chemistry properties, transport parameters or control final element capabilities, to guarantee that all local controller movements are in the stable region of the plant as a whole. The major advantage in the collaborative proposal treated here is the use of PID controllers as local controllers, because a lot of techniques to design stable PID controllers are available today.

Step 10: Establishment of triggers for each optimization. This is the last step of methodology and it is related to optimization execution, because if main dynamic is very close to its set point, a collaborative effort is not required. In this case, all control effort is applied from the main dynamic control loop itself. Trigger criteria determine when optimization is executed. Examples of triggers are a maximum deviation of main dynamic regarding its set point or a maximum deviation in cost function values during two or more past time steps.

4.3. Illustrative example

In this section the previous stated collaborative control strategy is applied to an aerobic reactor. This reactor was explained in the Section 4.1. The compounds considered on this process are: soluble inert organic matter, readily biodegradable substrate, particulate inert organic matter, slowly biodegradable substrate, active heterotrophic biomass, active autotrophic biomass, particulate products arising from biomass decay, Oxygen, nitrate and nitrite nitrogen, $NH_4^+ + NH_3$ nitrogen, soluble biodegradable organic nitrogen, particulate biodegradable organic nitrogen, and alkalinity. However, it should be noted that the control objective is to control the oxygen concentration. Calculating the state impactability index SII_{yk} from a singular value decompositon of Hankel matrix of the process model, the oxygen concentration have the highest index. Therefore, this variable is the main dynamic of the process and the concentration of the rest of compounds are secondary dynamics. As it was explained in Section 4.1, the system has two controllable parameters, k_L and a. In this sense,

the coordinator controller in the supervisory layer has the oxygen concentration as the fixed objective and the regulatory level with two control loops collaborates to reach this objective. In this case, the control loops on regulatory layer are associated to controllable parameters k_L and a. The first control loop manipulates the air flow to control k_L . The second loop manipulate the air injection pressure to control a. The Figure 4.6 shows the collaborative control strategy proposed for this system.



Figure 4.6. Collaborative control strategy applied to an aerobic reactor.

As it is possible to see in the Figure 4.6, the coordinator controller sends information about set points to control loops located in the regulatory layer. The regulatory layer comprises for two PID controllers. It must be pointed out that no real feedback there exist for this two controllable parameters. The only measured variable in this structure is the oxygen concentration in the liquid phase in order to compare with its set point and make decisions about next action, i.e. it decides if the set points of controllable parameter would have been changed.

Regarding to the main dynamic of this process, the oxygen concentration, Equation 4.2 represents the dynamic behavior of this variable. Secondary dynamics are not considered here because the effects over the process are not important in accordance to the control objective and therefore the term of secondary dynamic sensitivity is removed from objective function. However k_L and a are controllable parameters and they make up the regulatory level. For that reason, the objective function for the coordinator controller is represented by the Equation 4.6.

$$\min_{k_{L,sp}, a_{sp}} J = \alpha (S_{O_{ss}}^* - S_{O_{sp}}^*) + \beta_{k_L} \frac{1}{S_{k_L}} + \beta_a \frac{1}{S_a}$$
(4.6)
S. t. $0.1 \le k_L \le 10$
 $0 \le a \le 50$

It should be noted that $S_{O_{ss}}^*$ is the stationary state of oxygen concentration if the system achieve the k_L and a values calculated in the optimization, with the rest of the states keep at

their current values achieves.

Using this optimization procedure the set points for k_L and a in the regulatory control level are calculated. These two PID manipulate the injection pressure and the air flow in response to their set points changes. It should be noted that S_{k_L} and S_a are calculated according to Equations 4.7 and 4.8 respectively.

$$S_{k_L} = \frac{\partial S_O^*}{\partial k_L} = -a(S_O - S_O^*) \tag{4.7}$$

$$S_a = \frac{\partial S_O^*}{\partial a} = -k_L (S_O - S_O^*) \tag{4.8}$$

The tuning parameters are shown in the Table 4.1, where α , β_{k_L} and β_a are the parameters from Equation 4.6 and P, t_i and t_D are PID parameters.

Supervisory layer parameters				
$\alpha = 1$	$\beta_{k_L} = 1$	$\beta_a = 0.1$		
Regula	Regulatory layer parameters			
	k_L control loop			
$P_{k_L} = 0.01$ $t_i = 0.005$ $t_D = 0.001$				
a control loop				
$P_{k_a} = 100$	$t_i = 0.0009$	$t_D = 0.0001$		

Table 4.1. Parameters of collaborative control structure shown in Figure 4.6.

In order to validate the case study, different simulations have been performed, including the application of disturbances to the process. In Table 4.3 shows the time, kind and magnitude of the disturbances and set point changes applied to the system in order to evaluate the behaviour of oxygen concentration. Fourteen days were simulated for the aerobic reactor with constant conditions of plant influent. Two set point changes are applied to oxygen concentration at the begining of the test.

Time [day]	Disturbance	Magnitude
0.5	Set point change	From 0.5 to 2.2 g/m^3
1.5	Set point change	From 2.2 to 2 g/m^3
3	Temperature change	From 15 to 10° C
4.5	Temperature change	From 10 to $15^{\circ}C$
6	Temperature change	From 15 to 20° C
8	Temperature change	From 20 to 15° C
9.5	Plant input flow change	From nominal value to 30% of nominal value
11.5	Plant input flow change	From 30% of nominal value to 130% of nominal value

The Figure 4.7 shows the behaviour of oxygen concentration. It is clear the tracking and disturbance rejection capabilities of collaborative control structure. Even thought some overshoot exist after applied changes on oxygen set point and inputs, the oxygen concentration quickly return to reference value. These overshoots are caused by respective overshoots in the set points provided for k_L and a calculated by the coordinator controller as it is shown in

Figures 4.9a and 4.9b. The dashed line represents the set points calculated at the supervisory level. It is shown an overshoot in the set point, but the process value has a softer behaviour. The controllable parameters have this performance because control actions at the regulatory level are slower.



Figure 4.7. Oxygen concentration in aerobic reactor.

The Figure 4.8 represents the mass transfer coefficient. On this research, this parameter is separated for two controllable parameters. In many works, $k_L a$ is a manipulated variable, but in the real process it is no possible a direct manipulation. However, the range is reasonable according to the proposed by [3].



Figure 4.8. Volumetric mass transfer coefficient in aerobic reactor.



The control actions of PID controllers at regulatory layers are the air flow and the injection pressure, which are shown in Figure 4.10. The changes on this variables is smooth due to their inherent slow behaviour.



The methodology studied in this Chapter can be used in large scale processes. Therefore, it is a plantwide control strategy if the plant is partitioned in macro-processes with clear distinguisable process product objectives. The next Chapter shows the results of this methodology applied to a waste water treatment plant. Additionally, this control strategy will be compared to MPC control.

4.4. Remarks

This chapter presented each step for applying the collaborative control strategy at any process. Additionally, the controllable parameter definition is explained and used. Moreover, the importance of mathematical model is evident in this chapter. According to this, it is important remark that:

- It is possible to control parameters, i.e. when variable pairing is done, the controllable "variable" can be a parameter. In this sense, for this kind of process the mass transfer model is essential in order to implement collaborative control strategy because it allows to use controllable parameters to improve the control behaviour and enables a more realistic representation of the process.
- The methodology is very explicit. That procedure can be adapted to many chemical and biological processes. The procedure is easy implementation when it is applied to small process, like was showed in the illustrative example. However, it can be implemented in large scale processes, like will be show in the next chapter.
- The methodology uses information from the model in order to calculate the objective function in supervisory layer, an important role of control strategy. For this reason, the semiphysical model is fundamental in the control strategy proposed. It is necessary to highlight that, the cost function has interpretable information and controllable parameters effects are explicit. Additionally, the term that predicts stationary state of main dynamic if the system achieve the values calculate in optimization (x_{ss}^*) is very important in this control strategy.

CHAPTER 5 Case of Study: BSM1

There are many studies about the control strategies applied to BSM1. For example, in [49], MPC is applied to control the dissolved oxygen in the fifth reactor of the plant and in [50] different strategies are proposed in order to control the plant. The control objective is to keep total nitrogen, COD, TSS (total suspended solids), and oxygen concentrations in the effluent below some legal environmental limits. Particularly, in this work nitrite and nitrate and oxygen concentrations are considered in the collaborative control strategy. These limit values are shown in Table 3.6. Additionally, [51] proposes a control structure using a MPC strategy and PI controllers, taking into account four reactors of the plant. Despite of the large amount of works about BSM1 control strategies, all of them consider the product of liquid phase mass transfer coefficient (k_L) and interfacial area (a), while in a real process this is not possible. In this research the novel control strategy explained in the section 4 is applied to BSM1 including the mass transfer model with separated expressions for k_L and a, as they were presented in Section 3.2.

The BSM1 provides several sets of influent disturbances depending on the weather conditionts: dry weather, rain-weather, storm-weather and dynamic influent are the typical influents option to apply to BSM1. These disturbances are considered for validating the methodology proposed. In spite of existing limit values stated by law for nitrite and nitrate nitrogen concentration, these substances are not controllable strictly, i.e. they are is not all the time under the expected limit concentration. This is evidenced in [3], [51] and [52]. For this reason, the control performance is supported by an overall behaviour in the majority of studies. The next sections show the results of applying the proposed collaborative control strategy to the fifth reactor of the plant and to the complete biological treatment section of the plant.

5.1. Collaborative control and MPC applied to the last aerobic reactor in BSM1

This section shows a comparison between two control strategies with the same control architecture, applied to the fifth reactor in the BSM1 benchmark, the last aerobic reactor in the plant. In this sense, the dynamic of the full plant is taken into account. The proposed control architecture with supervisory and regulatory levels is shown in Figure 5.1, repeated here for text completeness, where the regulatory level is formed by two PID controllers. In both cases the injection pressure and air flow effects are separated and controlled with independent control loops. This separation is for the liquid phase mass transfer coefficient (k_L) and the gas - liquid interfacial area (a). The difference between the two control strategies is in the type of main controller. For the first case it is a collaborative control and for the

second one is a model predictive control (MPC).



Figure 5.1. Hierarchical control architecture [2].

The plant layout with the control structure proposed is shown in the Figure 5.2, following the architecture of Figure 2.5. As it is possible to see, there exists a supervisory level, where the k_L and a references are calculated according to the tracking error in the oxygen concentration. The set points information is sent to the two PID controllers at regulatory level. The first PID control is for the liquid phase mass transfer coefficient, where the manipulated variable is the air flow. The second PID control is for the specific interfacial area with the manipulated variable air pressure.



Figure 5.2. Control structure for oxygen concentration in the last aerobic reactor.

Time [day]	Disturbance	Magnitude
0.5	Set point change	From 0.5 to 2.2 g/m^3
1.5	Set point change	From 2.2 to 2 g/m^3
3	Temperature change	From 15 to 10° C
4	Temperature change	From 10 to 15° C
5.5	Temperature change	From 15 to 20° C
7	Plant input flow change	From nominal value to 30% of nominal value
9	Plant input flow change	From 30% of nominal value to 130% of nominal value

To compare the collaborative control and the MPC strategies the plant is simulated during 12 days of operation. Some disturbances are applied, as described in Table 5.1 shows the time, type and magnitude of the disturbances.

Table 5.1. Disturbances applied to the system.

5.1.1. Collaborative control applied to the fifth reactor

The calculation of k_L and a set points is based on optimizing a cost function including the oxygen concentration error, which is the main dynamic of the process taken place in this reactor. Moreover, the sensitivities from main dynamic regarding controllable parameters is included in this cost functions. These two parts constitute the objective function, as explained in the section 4.2. It is important to highlight that the equations are the same because the process dose not change. However, these equations are evaluates in different operation point and considering the full plant dynamic. The tuning parameters are shown in the Table 5.2, where α , β_{k_L} and β_a are the parameters from Equation 4.6 and P, t_i and t_D are PID parameters.

Supervise	Supervisory layer parameters			
$\alpha = 1$	$\beta_{k_L} = 1$	$\beta_a = 0.1$		
Regulato	Regulatory layer parameters			
k_{I}	k_L control loop			
$P_{k_L} = 0.0008$	$P_{k_L} = 0.0008 t_i = 0.0001 t_D = 0.001$			
a	a control loop			
$P_{k_a} = 600$	$t_i = 0.0001$	$t_D = 0.006$		

Table 5.2. Parameters of collaborative control structure shown in Figure 5.2.

The obtained oxygen concentration profile is presented in Figure 5.3, showing good tracking and disturbance rejection. Even thought there exist overshoot in some cases, the oxygen concentration quickly returns to its reference value. The overshoots in the Figure 5.3 are caused by the overshoots in the set point calculated at the supervisory level, as shown in Figures 5.5a. However, the process value for the parameters never follow these overshoots.



Figure 5.3. Oxygen concentration an the last aerobic reactor for collaborative control.

The Figure 5.4 presents the volumetric mass transfer coefficient values during the 12 days of simulation. Note that, the range of $k_L a$ values produced by collaborative controller agrees with the proposed by [3]. Sudden changes in Figure 5.5 are due to set points movements dictated by the collaborative control.



Figure 5.4. Mass transfer coefficient.

The dashed line in Figures 5.5a and 5.5b represents the set point calculated on the supervisory level. In this figures it is possible to see some peaks in the set points, but the corresponding process value has a softer behaviour. The controllable parameters have this performance because the control actions (pressure and air flow) in the regulatory level do not have sudden behaviour and this avoid to follow the peak set points.



The control actions are the air flow and air pressure supply which are the manipulated variable of PID controllers, respectively (see Figure 5.6). The rate of change on these manipulate variables is not high, considering that they are applied to the real process in the lower layer of the control structure.



The environmental regulations do not permit an effluent ammonium concentration greater than $4g/m^3$. On this simulation, this limit is exceeded twice because constraints are not considered in the strategy. The Figure 5.7 shows the ammonium concentration behaviour when collaborative control is applied. However, this response is presented here for illustrating the behaviour of this variable, but this response has not direct interpretation into real plant

operation. Obviously, such a constraints can be included into the optimization process, but this is a future work.



Figure 5.7. Effluent ammonium concentration evolution with collaborative control.

5.1.2. MPC applied to the fifth reactor

The simulation conditions and disturbances are identical to the used for previous collaborative control strategy. The supervisory layer parameters are according to the Equation 2.4. In this sense, the output weight is 1, there are two input weight, the first one is from k_L and the second from a, these weight are 0.5 and 0.1, respectively. On the other hand, the parameters of regulatory layer are the same from previous section. The Figure 5.8 shows the obtained oxygen concentration in the fifth reactor. It is possible to see that when the set point changes to 2.2 g/m^3 the system needs more time for reaching the reference than in the collaborative control. This is remarked by the red oval. It is also shown that disturbance rejection is slower than in collaborative control. These aspects are some disadvantages of MPC strategy.



Figure 5.8. Oxygen concentration using MPC strategy.

The Figure 5.9 presents the volumetric mass transfer coefficient behaviour, showing that it evolves within the limits proposed by [3].



Figure 5.9. Mass transfer coefficient for MPC supervisory control.

Figure 5.10 shows the evolution of k_L and a with an MPC controller in the supervisory layer. It shows that both set points have an oscillating behaviour in some parts, and it might worsen the behaviour of the variables. However, in this example, in the same way than for collaborative control, the real responses are softer. It should be noted that, the control

actions have not oscillations and overshoots. For this reason, the system does not present this behaviour.



The Figures 5.11a and 5.11b show the manipulates variables. Both variables have a good operation range, which is appropriated to satisfy the control objective. However, the behaviour and their variation of parameters in the process is smooth. In this sense, these control actions are not the cause of oscillation in the controllable variables (Figure 5.10). Then, the overshoots and oscillation are product of the combination of k_L and a in the mass transfer model. Because this model is highly nonlinear, it is possible that sometimes this product would result in higher values than expected by variable tendency.



Finally, the Figure 5.12 shows the ammonium concentration for BSM1 controller with the MPC. It is not different from the Figure 5.7, because in both cases the process values try to achieve the set points. Regarding dissolved oxygen control, the Figure 5.3 shows a good performance of collaborative control and the Figure 5.8 shows slow disturbance rejection for MPC.



Figure 5.12. Effluent ammonium concentration.

The ammonium concentration exceeds the limit of law concentration in both control strategies. However, it is necessary to highlight that the control strategy is concentrated in the last aerobic reactor. Then, the nitrite and nitrate concentration is not involved in the control strategy, in spite that the nitrite and nitrate concentration is considered one state in BSM1 model.

5.2. Collaborative control applied to the full plant

In this case, the methodology of collaborative control proposed is applied to the three aerobic reactors in the BSM1, see Figure 5.13. This structure has collaborative control in aerobic section (three reactors), using the same controlled and manipulated variables proposed in Figure 5.2.The control objective is oxygen concentration control in the last three reactors (aerated). Moreover, this structure has a PID control in the second anoxic reactor, where the nitrite and nitrate nitrogen concentration is the controlled variable and the internal recirculation is the manipulated variable. The set points in each reactor have been taken from [3]. These values correspond to the stationary state when the system is working in closed loop with the control structure proposed by [3], where the nitrite and nitrate nitrogen concentration in the fifth reactor are controlled in descentralized fashion with two PI controllers.

CHAPTER 5. Case of Study: BSM1



Figure 5.13. Collaborative control structure for complete plant.

Tuning parameters of supervisory layer in each reactor are the same from Table 5.2 and the tuning parameters of regulatory layer are shown in the Table 5.3. Finally, the parameters P, t_i and t_D in the reactor 2 are 30, 0.00009 and 0.006, respectively.

Regulatory layer parameters.						
	k_L control loop.			a control loop.		
	P[(1/d)/(g/m3)]	t_i [days]	t_D [days]	P[(1/d)/(g/m3)]	t_i [days]	t_D [days]
Reactor 3	0.008	0.0001	0.001	60	0.0001	0.006
Reactor 4	0.009	0.0001	0.001	5	0.00005	0.006
Reactor 5	0.0008	0.0001	0.001	600	0.0001	0.006

Table 5.3. Regulatory layer parameters of collaborative control structures shown in Figure 5.13.

The Table 5.4 shows the different disturbances applied to the system, starting in the stationary state proposed by [3].

Time [days]	Disturbance	Magnitude
1	Temperature change	From 15 to 10° C
3	Temperature change	From 10 to $15^{\circ}C$
5	Temperature change	From 15 to 20° C
7	Temperature change	From 20 to 15° C
9	Plant input flow change	From nominal value to 30% of nominal value
10.5	Plant input flow change	From 30% of nominal value to 130% of nominal value

Table 5.4. Disturbances applied to the system.

The Figure 5.14 shows the controlled variable evolution, where some short overshoots can be seen. As for the nitrite and nitrate concentration, the disturbance rejection is good, but with slower responses. Then, the overshoots can be caused by high speed response of oxygen concentration dynamic and disturbance magnitude. However, it is necessary to highlight that



the variable returns quickly to their set point in short time and the overshoots can be tolerable.

c) Oxygen concentration in third reactor. (d) Nitrite and nitrate concentration in second reactor Figure 5.14. Evolution of controlled variables.

In the collaborative control, i.e. third, fourth and fifth reactors the decision variables are the liquid phase mass transfer coefficient and specific area in each reactor. The behaviour of these controlled parameters is shown in Figure 5.15. The process values have a good behaviour reaching the new set point. Some overshoots in liquid phase mass transfer coefficient exist, but these are tolerable.



(a) Liquid phase mass transfer coefficient in fifth reactor.



(c) Liquid phase mass transfer coefficient in fourth reactor.



(b) Specific area in fifth reactor.

(d) Specific area in fourth reactor.



Figure 5.15. Controllable parameters behaviour.

The manipulated variable behaviour at each reactor is shown in Figure 5.16. Although the manipulate variables in fourth and third reactors are high, that is due to the fact that the mass transfer coefficient in reactors three and fourth are higher than in the fifth reactor. In accordance to [3], the mass transfer coefficient is 84 d^{-1} in the fifth reactor, and 240 d^{-1} in the third and fourth reactors. Therefore, the air flow and pressure in the third and fourth

reactors is three times bigger than in the fifth reactor.



Finally, ammonium concentration is shown in Figure 5.17. Although all variables are kept at their set points, the ammonium concentration is higher than the permitted limit. This indicates that with the taken oxygen set points the system can not reject all the disturbances, and it is necessary another combination of set points to keep the ammonium concentration under limit or including this constrains in the optimization problem.



Figure 5.17. Effluent ammonium concentration.

According to Figures 5.7 and 5.17, the ammonium limit is exceeded in both cases. This is happening probably because the optimization problem has not constrains or decisions about ammonium concentration. Additionally, the disturbances applied to the process are sudden steps and they are far from reality. For this reason, the next section studies the behaviour when the influent constitution is changed, i.e. the behaviour of the plant with dynamic influent.

5.3. Collaborative control strategy and MPC applied to BSM1 with dynamic influent

In this test the influent is dynamic, i.e. the inlet flow and concentrations change constantly, Figure 5.18 shows the inlet flow behaviour. This situation is presented in order to compare with others works, using more realistic operating conditions.



Figure 5.18. Inlet flow - rate.

5.3.1. Collaborative control applied to BSM1 with dynamic influent

The control structure shown in the Figure 5.13 is implemented again. The Figure 5.19 shows the evolution of controlled variables, i.e. the main dynamics of each reactor with collaborative control strategy. The tuning parameters are the same of Section 5.2. It should be noted that this dynamics responses are trying to maintain the constant reference or law limits and plant adjustments stated in BSM1 for proper behaviour. The simulations present some periodic variations due to the also periodic variations in the influent.



The behaviour of controllable parameters following the set points provided by the supervisory layer is shown in Figure 5.20 where good tracking can be seen. Note that the regulatory layer is collaborating in order to achieve the control objective, as shown in Figure 5.18 5.19. Additionally, In 5.21 the corresponding control actions are presented, with a realistic range of operation.



(a) Liquid phase mass transfer coefficient in fifth reactor.



(c) Liquid phase mass transfer coefficient in fourth reactor.



(b) Specific area in fifth reactor.



(d) Specific area in fourth reactor.



(e) Liquid phase mass transfer coefficient in third reactor.
 (f) Specific area in third reactor.
 Figure 5.20. Controllable parameters behaviour with dynamic influent.


(g) Internal recirculation. Figure 5.21. Behaviour of manipulated variables.

Finally, the effluent ammonium concentration behaviour is shown in Figure 5.22 where can be seen some violations to the legal limit. However, it should be considered that the plant is simulated during 8 days and these moments are by short time and therefore, they are tolerable.



Figure 5.22. Effluent ammonium concentration with dynamic influent.

5.3.2. MPC applied to BSM1 with dynamic influent

The MPC presented here is only one and applied over the last reactor but maitaining the control of nitrites and nitrates in second reactor. A configuration of three MPC, one for each of the last three reactors, is not simulated here because the computational cost is high, like was evident in the section 5.1.2. In this case eight days of operation are simulated. During this time the influent is dynamic in the plant as was proved in the Section 5.3.1 but here the control strategy is a MPC. as it is shown in Figure 5.23. In this case, there are two output weight, oxygen concentration and nitrite and nitrate concentration, both weight are 1. Input weigh are 0.1 en all cases, the inputs are k_L , a and internal recirculation flow. The results obtained are shown in the Figure 5.24 for 8 days of operation, where it is possible to see the overshoots in oxygen concentration that if it is compared with the Figure 5.19a are bigger and it is further of set point value. Additionally, nitrite and nitrate concentration presents more oscillations if it is compared with 5.19d.



Figure 5.23. Control structure of MPC applied to BSM1 with dynamic influent.



Figure 5.24. Controllable variables in BSM1 with dynamic influent.

On the other hand, the Figure 5.26 presents the controllable parameters behaviour. Evidently, the PID controllers are working well because the tracking of the reference is adequate, despite the short overshoots present in the varying set point.



The Figure 5.26 shows the control actions and effluent ammonium concentration. As can be seen, the ammonium concentration satisfies the legal limit without violations, due to higher control efforts that in the collaborative control strategy. Additionally, some overshoots in Figure 5.26d match with overshoots in Figure 5.24a. This can correspond to control efforts because does not exist control loops or control communication with the rest of plant. The communication is internal, just among dynamics of processes. Even in this case the effluent ammonium concentration is good there exist control effort and this could damage equipment. Instead of that, the last subsection shows less effort and the ammonium concentration is normal because this is not considered in the optimization problem.



This separation adds a degree of freedom to control system and it is evident the additional control loop, which results closer to the real process. it should be noted that in the literature only one control loop is used to keep the oxygen concentration at its set point. With this proposal, the collaborative control strategy improves the system performance compared to MPC control strategy.

5.4. Remarks

This chapter showed the features and advantages of the proposed collaborative control strategy. Additionally, the results of the control applied over BSM1 where specified. In this way, it was showed that the control strategy can be implemented in large scale processes. According to this, it is relevant to remark that:

• Evidently, if the computational time of MPC and collaborative control are compared, MPC needs more computational time. For this reason, collaborative control is more

favorable for real control implementation.

- Collaborative control strategy proposed in this thesis can be implemented in large scale processes and the results are adequate for control objective.
- Considering controllable parameters in this control strategy allows to improve the process performance. It is important to highlight that the cost function is a simple expression and allowing decrease the computational cost and easy interpretability.

6.1. Conclusions

The methodology of collaborative control is centralized and hierarchical. It is centralized because there exist only one coordinator controller (supervisory layer), where the decisions about set points take place. Then, for that reason is a hierarchical control strategy. In this sense, the set points information is send to PID controllers (regulatory layer). To choose the control strategy and the kind of information management is very important and depends on the process and control objective.

This work presents a methodology to obtain a collaborative control strategy including controllable parameters. The control strategy is based on a process model and comprises a supervisory layer and a regulatory layer. The first layer is designed by determining the dynamics hierarchy, using states impactability indices from Hankel Matrix. Controllable parameters are involved in supervisory level in order to improve the control performance through sensitivities of main dynamic respect to these parameters.

The collaborative control strategy has been applied to BSM1 and compared with MPC strategy. The results from Chapter 5 show the advantages of proposed control strategy. In accordance to the results showed in the Section 5.1, for collaborative control the simulation takes 20.5 minutes for the 12 days of process operation and in the same conditions, for MPC the simulation takes 330 minutes, indicating worse behaviour of MPC regarding a real time implementation and higher computational cost.

Additionally, it is evident the improvement of system performance when controllable parameters are used in regulatory layer because the control system increases its performance. This is important when the k_L and a effects are determinate in the complete model. In this sense, the mass transfer model represent a fundamental part for control strategy implementation. Moreover, controllable parameters allow to guide the main dynamic to control objective.

The methodology proposed can be applied to large-scale processes, supported by the good results in this work. Particularly, the proposed control strategy may be more profitable in large-scale processes because it reduces model solving time. This reduction is given because it is not necessary to predict the model for a horizon time, like in MPC. In collaborative control strategy, the decision variables are calculated at each time step without solving the complete model at each sampling time.

The mass transfer model proposed is in accordance to real phenomenon because this model describes the liquid phase mass transfer coefficient and the specific area, taking into account variables and parameters like injection pressure, air flow, surface tension, liquid density, etc. as was explained in the Chapter 3. Then, the controllable parameters are evident in the mass transfer model. Additionally, the model shows the relationship between controllable parameters and manipulated variables. Moreover, this mass transfer model permits to add a degree of freedom to control the system as is shown in Chapter 4. The validation of this model is qualitative and it is compared with the model proposed in [3] with adequate results.

6.2. Future works

Several topics could be explored after completing this work. Some of them are:

- Implement collaborative control strategy including controllable parameter in another large-scale process in order to evaluate its performance in another process and exploring its generality. Additionally, it is necessary to implement this control strategy in real process, i.e. implementing this control strategy using for example a PLC module.
- Include in supervisory layer some constraints related to process limitations different to manipulated variables or final control elements movements. In this sense, it can be explored the inclusion of constraints on some critical concentrations of compounds or some parameters values. Additionally, it can be proposed a collaborative control strategy including the anoxic section of BSM1.
- Incorporate dynamic sensitivities of secondary dynamic and controllable parameter because in this case the first ones were considered statics. However, it is necessary to highlight that dynamic sensitivities add computational cost to the control strategy.
- Validate the mass transfer model with experimental data. Even the mass transfer model was validated qualitatively, it is important to consolidate the model and this is possible through a quantitative validation with real data.

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