NATIONAL TECHNICAL UNIVERSITY OF ATHENS
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Master Thesis

TITLE

Development of an identification and predictive control framework for wastewater treatment plants using a reduced-order model

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Abstract

Wastewater treatment plants are a major part of local communities, since they are responsible of purifying the contaminated water coming from the urban area and of safely returning it back to the water cycle. Their inherent nonlinear dynamic behavior is influenced by numerous factors including the large fluctuations of the wastewater entering the facility and the highly complex biological and biochemical phenomena occurring as the wastewater is being processed by the reactive units of the plant. Consequently, WWTPs are forced to operate for long periods of time under the influence of uncertain disturbances, leading to potential unacceptable violations of the environmental regulations regarding the effluent quality. In order to deal with the aforementioned factors, the energy demands in WWTPs are significantly escalated, thus leading to increased operational costs. Therefore, advanced closed-loop control methodologies have to be developed, capable of considering the numerous parameters affecting the optimal operation of WWTPs, aimed to optimize their performance regarding the effluent quality, energy consumption and total operational costs.

Developing automatic control schemes for such complex plants, though, is a challenging procedure, due to the fact that the mathematical models describing their dynamic behavior are complex and consequently, cannot be used for control design purposes. As a result, the complexity of these models necessitates the need of deriving reduced-order models that are capable of simulating the dynamic behavior of the plant precisely, while also being simple enough for integration in closed-loop control configurations. To this end, in this work a complete modelling and control framework for WWTPs is proposed. A model of lower complexity compared to those proposed in the literature is derived, followed by the formulation of an identification scheme for estimating the values of the numerous coefficients included in its differential equations. The identified reduced-order model is then integrated in predictive control schemes aimed to optimize the performance of WWTPs during full-scale operation. In particular, a nonlinear tracking model predictive control configuration is, firstly, developed for the purpose of maintaining the plant at a specific steady state operating point. However, to achieve this goal, the controller may resort to unnecessary high energy demands since it seeks to drive specific states of the system to predetermined setpoints, regardless of the magnitude of the disturbances affecting the plant operation. To deal with this situation, an economic-oriented nonlinear model predictive control scheme is proposed aimed to optimize the energy efficiency and total operational costs of the plant. In contrast to the tracking formulation, the latter approach seeks to maintain the operating region of the plant within specified limits, hence leading to reduced energy demands. Finally, to validate the superiority of employing the presented modelling and control framework, comparison results against alternative control methodologies are presented.

To Alex, my fellow life traveler,
who has always been there.

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Contents

List of Figures

List of Tables

1 Introduction

1.1 Motivation

Wastewater treatment facilities are considered as one of the major industries, which exist in most of the countries around the world. They play a crucial role in the functionality of the local communities, based on where they are constructed, since they are responsible of handling the large volumes of polluted water that is being produced by the homes, restaurants, businesses and industries placed around its area of affection. The polluted water entering a wastewater treatment facility is subject to a wide range of complex chemical processes while flowing through the plant, with the purpose of being converted to an effluent which can be safely returned to nearby water elements, such as rivers, lakes or even the sea. However, the effluent stream of a wastewater treatment facility has to satisfy specific strict environmental criteria so that it can be reused by the local community. Satisfaction of these stringent regulations, though, is a challenging aspect since the optimal operation of wastewater treatment plants (WWTPs) is influenced by numerous reasons. For instance, large fluctuations of the influent stream entering a WWTP is one of the most important factors, which affect the overall performance and consequently, the treatment facility needs to be capable of dealing with these disturbances in an appropriate manner.

Optimization of the performance and functionality of these large-scale plants considering the time-varying conditions under which they operate, is a really difficult task and advanced process control techniques have to applied. In the procedure of designing automatic control schemes, the most critical part is the existence of a mathematical model capable of accurately capturing the highly nonlinear nature of these complex plants. Moreover, the mathematical models aimed to be used in control systems design, except from accurate, need also to be simple enough in order to be suitable for integration in the development of advanced closed-loop control configurations. For instance, the implementation of predictive control schemes requires the incorporation of a mathematical model capable of predicting the future dynamic behavior of the plant. As a consequence, a simple, yet accurate, model would lead to the controller complexity being lower, and thus to a more computationally efficient control algorithm. However, deriving models for WWTPs that are simple enough, while simultaneously being able to capture the highly nonlinear system dynamics is a demanding procedure and advanced modelling techniques have to employed.

Many attempts have been made to model the operation of WWTPs by utilizing data-driven technologies such as artificial neural networks [1]–[5], which seem to be capable of accurately simulating the dynamic behavior of WWTPs. On the other hand, though, the procedure for training neural network models requires large volumes of quality data to be collected from the actual WWTP; a task that is difficult for a variety of reasons:

1. The number of sensors that can installed in WWTPs is limited. Not all chemical elements of the wastewater can be measured reliably, or even measured at all.

2. The installed sensors of a WWTP face a number of failures such as discontinuities or missing values. Furthermore, specific sensors being used in WWTPs require costly

reagents to obtain the measurements. This situation leads to the usage of large sampling times, leading to collected data, which are inappropriate to be used for training machine learning models.

3. Exciting the WWTP by imposing specific inputs during its full-scale operation in order to be able to collect data with sufficient information is not always possible. WWTPs operate for the most of the time at steady state, rendering the collection of quality data a difficult, or even sometimes impossible.

Except from the aforementioned difficulties in terms of the data collection, the employment of machine learning models to simulate the dynamic behavior of WWTPS may lead to poor performance when considering different operating regions of the plant. These models may be capable of really accurately predicting the behavior of the plant under specific operating conditions, but may fail when considering operating conditions, which are far from those used for their training. To overcome the aforementioned situations, first-principles models of WWTPs have been proposed, the most widely known being the Benchmark Simulation Model No. 1 (BSM1) [6], developed in 2008. BSM1 models WWTPs, the operation of which is based on the concept of nitrification with denitrification aiming to achieve full biological removal for processed wastewater. The same task group also proposed the Benchmark Simulation Model No. 2 (BSM2) [7], which includes the biological treatment undertaken by BSM1 but also incorporates a number of additional units (primary clarifier, thickener for the wasted sludge etc.) to model different parts of the treatment process.

These first-principles models can simulate the dynamic behavior of WWTPs with high accuracy since they also integrate a precise model for describing the activated sludge process (ASP) of the biological reactive units, namely the Activated Sludge Model No. 1 (ASM1) [8]. Despite the fact that the aforementioned first-principles models are capable of precisely capturing the highly nonlinear dynamics of WWTPs, their utilization in developing automatic control schemes is prohibitive due to their increased complexity. For instance, BSM1, which is the simplest between the two, consists of 145 state variables, rendering its incorporation in closed-loop control configurations inappropriate. To this end, and also by considering the need for designing advanced control loops for optimizing the performance of WWTPs, the derivation of reduced-order models that are capable of representing the dynamic behavior of WWTPs accurately and at the same time can be efficiently handled in the design of automatic control systems, is necessary.

1.2 Thesis Objectives

Research in the area of WWTPs has been for many years concerned with a wide range of subjects, some of the being outlined below:

- Description of the activated sludge process of the reactive units by attempting to model the numerous biological and biochemical phenomena taking place.

- Derivation of reduced-order models that can be efficiently handled and therefore, are suitable for utilization in the development of model-based online control strategies.

- Development of system identification techniques for estimating a number of parameters that exist in the mathematical models describing the behavior of WWTPs. The proper adaptation of these models to specific WWTPs requires a precise estimation of the values of their coefficients (kinetic and stoichiometric), since these parameters are significantly influenced by the conditions under which the WWTP operates (e.g., pH of the wastewater entering the facility, environmental conditions such as the average local temperature, weather conditions etc.).

- Development of advanced process control methodologies, aimed to be applied in WWTPs for optimizing their performance, energy consumption and operational costs.

This thesis is based on the current state-of-the-art aspects on modelling the chemical processes occurring in a WWTP and investigates the aspect of deriving an appropriate reduced-order model and its integration in advanced predictive control schemes.

The main contribution of this thesis is the development of an economic-oriented nonlinear model predictive control scheme ((E)MPC), aimed to optimize the energy efficiency and total operational costs of WWTPs during full-scale operation. The formulated (E)MPC configuration utilizes an objective function including the plant aeration and pumping energy and seeks to minimize it by properly selecting the manipulated input values. In addition, in order to achieve compliance with the strict environmental regulations in terms of the effluent quality, constraints are imposed on specific state variables of the plant guaranteeing their satisfaction. The objective of the proposed closed-loop controller is to maintain the operating region of the plant within acceptable limits by considering the magnitude of the disturbances affecting its operation, while simultaneously limiting the energy demands. Except from the aforementioned economic-oriented predictive control scheme, in this thesis, two distinct formulations of a tracking nonlinear model predictive control (NMPC) scheme are presented. In contrast to the (E)MPC formulation, this approach seeks to maintain the plant at a specific operating point regardless the disturbance magnitude influencing its dynamic behavior. Consequently, this control configuration may lead to unnecessary energy requirements in cases where the environmental criteria can be met by consuming less amount of electrical power. To prove the superiority of the proposed (E)MPC and NMPC schemes, comparison results against alternative control methodologies proposed in the literature are presented.

The aforementioned predictive control formulations require the integration of a mathematical model capable of predicting the future dynamic behavior of the controlled plant. In this thesis, a reduced-order model of BSM1 is derived and incorporated in the proposed predictive control schemes. The obtained reduced-order model is of significant lower complexity compared to the original one, yet proves to be capable of accurately simulating its dynamic behavior. The procedure of model reduction is firstly based on selecting the ASM1 state variables that are important to model the chemical reactions and moreover, that can be reliably collected from sensors installed in actual WWTPs. The selection of the important state variables is also driven by considering those that can be used as the controlled variables in the control methodologies to be developed, such as the dissolved oxygen or the ammonia nitrogen concentration. In addition to this, a complete reduced-order BSM1 configuration requires a way of modelling the secondary clarifier, yet without incorporating the highly complex models that have been proposed [9]. In this thesis, a simple procedure of replacing the secondary settler model with a time-varying parameter based on measurements of the WWTP’s influent flow rate, suggested in [10], is adopted. Consequently, a complete structure of a reduced-order BSM1 model that can be used in the design of automatic control schemes is presented.

The derivation of a reduced-order model that can be utilized in designing automatic control schemes should be accompanied with a proper estimation of its coefficients, for the purpose of adapting it to the operating conditions of specific WWTPs. As already stated, the mathematical models used to describe the dynamic behavior of WWTPs include a large number of parameters, influenced by numerous factors specific to the investigated WWTP, necessitating the need of developing system identification techniques for approximating their values. The contribution of this thesis regarding the aforementioned procedure is the introduction of a system identification scheme for estimating these values that is based on solving a nonlinear optimization problem. To deal with the fact that the formulated optimization problem consists of a high number of design variables, a customized cooperative particle swarm optimization (CPSO) method for solving it, is introduced. The proposed approach takes advantage of the correlations that inherently exist between the design variables of the optimization problem, i.e., the parameters of the derived reduced-order model, and manages to successfully estimate their values. Moreover, the formulation of the system identification scheme is based on measuring specific chemical compounds of the WWTPs biological tanks, which can be directly and reliably collected by commonly installed sensors.

1.3 Thesis Outline

This thesis consists of seven chapters including the introduction. More specifically, the work is organized as follows:

- In chapter 2, a general introduction of the importance of WWTPs in societies is given along with a brief description of the components that form the BSM1 model. The kinetic and stoichiometric coefficients included in this generic model are presented and their typical values under different environmental conditions are provided. In the last section of this chapter, the number of differential equations that describe the activated sludge process, the secondary clarifier and the hydraulic delays, formulating the complete model, are briefly presented.

- Chapter 3 deals with the aspect of deriving a reduced-order model of BSM1. A detailed literature review on different approaches that have been proposed is firstly presented. Then, the detailed procedure of selecting the important state variables of ASM1, forming the reduced-order model for the activated sludge process of the reactors is introduced. The reduction technique in terms of the settling process is presented and the differential equations of the model, accompanied by the chemical reactions considered in it, are stated.

- The identification scheme applied for estimating the values of the kinetic and stoichiometric coefficients of the reduced-order model is extensively discussed in chapter 4. The formulation of the nonlinear optimization problem is presented in conjunction with the necessary compounds that need to be directly collected from a WWTP in order to perform the identification process. Validation of the derived model is performed by employing the original BSM1 as the reference model and results are presented proving the successful identification of the aforementioned coefficients.

- In chapter 5, the default control strategy of BSM1 as provided in [6] is described. Evaluation metrics by performing simulations under dynamic influent profiles, i.e., active disturbances influencing the operation of the plant, are presented and the reasons, for which the implementation of advanced control methodologies is necessary are briefly addressed.

- The development of advanced optimal control strategies, namely model predictive control schemes, is presented in chapter 6. Two distinct formulations of a nonlinear tracking model predictive control scheme are outlined, aiming to keep the plant at a predetermined fixed steady-state operating point. In addition, as the main contribution of this thesis, an economic-oriented nonlinear model predictive control configuration aimed to optimize the energy efficiency of the plant, is presented. The proposed approach, in contrast to the aforementioned one, seeks to maintain the operating region of the plant within specified limits. The developed closed-loop configurations utilize the reduced-order model, presented in this thesis, and are tested using the original BSM1 model as the controlled plant. Simulations have been conducted by applying all the dynamic influent profiles provided in [6], indicating the robustness of the proposed schemes in dealing with large fluctuations of the disturbances. Finally, comparison results against existing control formulations found in the literature, validate the superiority of the developed methodologies.

- In chapter 7, the concluding remarks of this thesis and an overall overview of the developed framework for optimizing the performance of WWTPs are summarized. Future research plans are also shortly stated.

2 Benchmark Simulation Model No. 1

In this chapter, a general introduction to the aspect of Wastewater Treatment Plants (WWTP) is given, accompanied with the presentation of one of the most widely known mathematical models used to simulate the dynamic behavior of WWTPs, namely the Benchmark Simulation Model No. 1 (BSM1). The set of differential equations used to describe the Activated Sludge Process (ASP) in the reactors is presented as well as the modeling of the settling procedure. A number of parameters affecting the ASP process are particularly discussed and the complete model structure is finally presented. Detailed information regarding the BSM1 model can be found in [6].

2.1 Wastewater Treatment Plants

One of the major issues that concerns societies, nowadays, is the adaptation to circular economy models, where the recycling and reusing of materials and products is the highest priority in order to extend their life cycles for as long as possible. In the design and implementation of the aforementioned economical models, though, one of the most essential materials is water since, among others, the means of production, the industry, the agriculture and, of course, life itself are almost entirely dependent on it. As a result, in order for a circular economy model to be efficient and profitable, the recycling and reusing of the polluted water should be examined carefully considering also the fact that the available water resources are being continuously diminished.

Today, in the modern urban environments, the development and integration of vast drainage systems able to transport the total amount of wastewaters from homes, businesses and industries to wastewater treatment facilities is necessary and enforced by the law. Once the wastewaters have been transported to the appropriate facilities, they are exposed to a number of processes aimed to purify it as much as possible and, then, safely return it to the water cycle in order to be reused.

As it is obvious, wastewater treatment plants play a crucial role in the implementation of a circular economy model due to their ability of accepting large volumes of contaminated water as influent and convert it to an effluent that can be reused by local communities without any harm. However, the task of accomplishing this difficult procedure includes a series of highly complex biological and biochemical phenomena that are taking place during the processing of the wastewater in the plant, in order to ensure that the effluent stream satisfies the strict local environmental regulations and can, therefore, be safely returned to the water cycle. As a result, optimizing the operation of these complex plants is a really challenging task not only due to the complexity of the chemical procedures involved but also because other factors, like the energy consumption and the quality of the effluent, have to be taken under consideration.

Optimizing the operation of such plants, though, requires accurate mathematical models that can be either used to design and test various automatic control methodologies or that can be incorporated in advanced control configurations, like Model Predictive Control schemes, and also that can be adapted to specific wastewater treatment plants by appropriately formulating the structural layout and by estimating the values of the parameters affecting the complete process as well. One of the most widely known first-principles models being used to simulate the dynamic behavior of WWTPs is the Benchmark Simulation Model No. 1 (BSM1) [6].

2.2 BSM1 Overview

The BSM1 model consists of five reactive units placed in sequential order, the first two of them constituting the anoxic zone, where the denitrification procedure takes place and the remaining three form the aerobic section of the plant, where the nitrification process is performed. Following the anoxic and aerobic tanks is the secondary clarifier from which part of the effluent is returned to the first anoxic unit, a portion of it is being returned to the water cycle and the remaining amount of the effluent stream is being disposed as wastage. In **Error! Reference source not found.** the complete layout of the model is depicted.

The model combines the nitrification with denitrification processes in a configuration that is commonly being used in actual WWTPs in order to achieve full-scale biological removal. The wastewater enters the plant at a flow rate Q_o and concentration Z_o, where Z represents the concentration of the chemical elements found in the wastewater, and goes through the anoxic and aerobic tanks until it reaches the last aerated unit, namely unit number 5. Part of the stream exiting unit 5 is recycled to the first anoxic tank (unit 1) at a flow rate Q_a and concentration Z_a, while the rest of the stream is fed to the secondary settler, which is modelled as a non-reactive ten-layer unit. The part of the stream that exits the settler from the upper layer is the one that is being returned to the water cycle at a flow rate Q_e and concentration Z_e and the part of the stream that exits the settler from the bottom layer, namely the underflow stream, is divided into two distinct flows. The first flow, i.e., the external recirculation flow, at a rate Q_r and concentration Z_r is recycled to the first anoxic unit while the second flow at a rate Q_w and concentration Z_w is disposed as wastage. In Table 2.1 the values of the model parameters are listed as given by [6].

The BSM1 model serves a reference model on which modelling and control techniques can be applied and tested since it provides analytical information regarding the quality of the effluent stream that exits the plant, the energy consumption and the total operational cost of

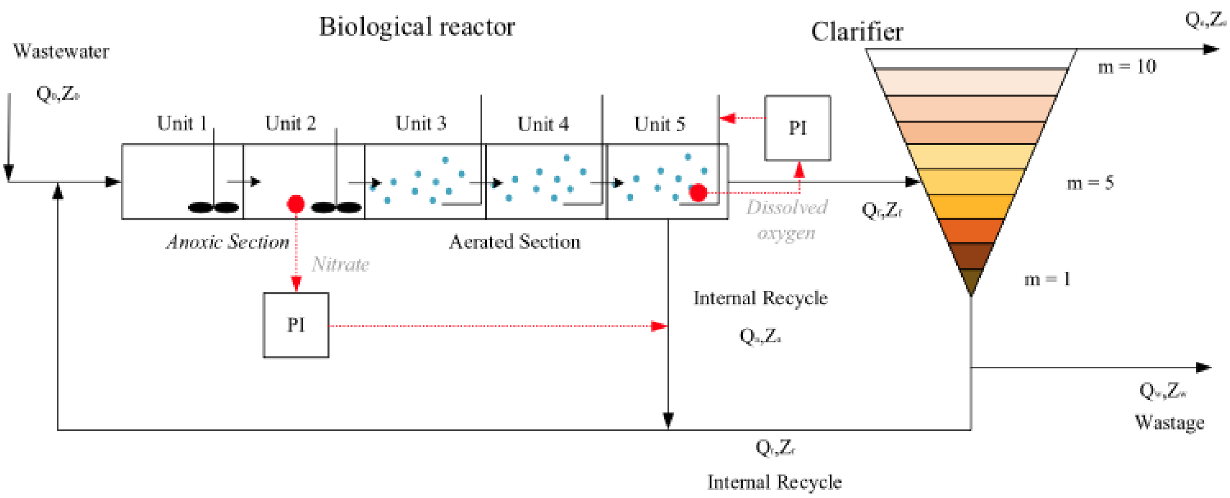


Figure 2.1 Overview of the BSM1 model

the plant. In addition to these, BSM1 is implemented in Simulink environment, which renders it easy to be modified and adapted to a specific WWTP.

2.3 Activated Sludge Process Model

The most important processing of the wastewater during the various phases, once it has entered the treatment facility, takes place inside the anoxic and aerobic tanks. Therefore, a mathematical model capable of accurately and quantitatively describing the complex procedure occurring in the reactors is necessary, i.e., a set of differential equations representing the activated sludge process of each reactor. In the BSM1 model, the aforementioned process is modeled by utilizing the Activated Sludge Model no. 1 (ASM1) [8].

2.3.1 State Variables and Dynamic Processes

ASM1 is a detailed mathematical model consisting of 13 state variables; Table 2. depicts the symbols and definitions for the state variables. ASM1 was firstly presented in 1987 and despite the fact that extensions and modifications have been proposed [11]–[13] throughout the years, it is still the most widely used mathematical model for describing the processes of a WWTP when the biological phosphorus removal is not considered.

By incorporating the state variables listed in the aforementioned table, ASM1 thoroughly describes a number of dynamic processes that are taking place while the wastewater is being processed in the biological reactor. More specifically, 8 dynamic processes are considered, each one of them closely related to certain chemical compounds that exist in the wastewater. A list of these processes along with the state variables that are associated with them is given in Table 2.. Detailed information regarding the state variables and the dynamic processes can be found in [8], [10].

Table 2.1 BSM1 model parameters

Parameter	Value
Anoxic tank volume $(\mathbf{V_i})$ $\mathbf{i} = \mathbf{1}, \mathbf{2}$	$1000\ \mathrm{m}^3$
Aerobic tank Volume $(\mathbf{V_i})$ $\mathbf{i} = \mathbf{3}, \mathbf{4}, \mathbf{5}$	$1333\ \mathrm{m}^3$
Settler volume	$6000\ \mathrm{m}^3$
Area of settler	$1500\ \mathrm{m}^3$
Height of each layer	$0.4\ \mathrm{m}$
Wastage flow $\mathbf{Q_w}$	$385\ \mathrm{m}^3\ \mathrm{d}^{-1}$
External recycle flow $\mathbf{Q_r}$	$18446\ \mathrm{m}^3\ \mathrm{d}^{-1}$

Table 2.2 ASM1 state variables

Definition	Symbol
Soluble inert organic matter	S_I
Readily biodegradable substrate	S_S
Particulate inert organic matter	X_I
Slowly biodegradable substrate	X_S
Active heterotrophic biomass	$X_{B,H}$
Active autotrophic biomass	$X_{B,A}$
Particulate products arising from biomass decay	X_P
Dissolved oxygen	S_O
Nitrate and nitrite nitrogen	S_{NO}
NH_4^+ + NH_3 nitrogen	S_{NH}
Soluble biodegradable organic nitrogen	S_{ND}
Particulate biodegradable organic nitrogen	X_{ND}
Alkalinity	S_{ALK}

Table 2.3 ASM1 dynamic processes

Process	State Variables
Aerobic growth of heterotrophs	$S_S, S_O, X_{B,H}$
Anoxic growth of heterotrophs	$S_S, S_O, S_{NO}, X_{B,H}$
Aerobic growth of autotrophs	$S_{NH}, S_O, X_{B,A}$
Decay of heterotrophs	$X_{B,H}$
Decay of autotrophs	$X_{B,A}$
Ammonification of soluble organic nitrogen	$S_{ND}, X_{B,H}$
Hydrolysis of entrapped organics	$X_S, X_{B,H}, S_O, S_{NO}$
Hydrolysis of entrapped organic nitrogen	$X_S, X_{B,H}, S_O, S_{NO}, X_{ND}$

2.3.2 Model Parameters

The mathematical model described in the previous section incorporates a number of critical parameters affecting the processing of the wastewater in the biological reactor. More specifically, in the ASM1 model there exist 14 kinetic and 5 stoichiometric parameters, the values of which have to be determined in order for the model to accurately describe the chemical procedures occurring in the anoxic and aerobic tanks of the WWTP. Table 2.4 depicts the definitions and symbols of these parameters.

The values of the aforementioned parameters play a really important role to accurately modelling a specific WWTP. A number of environmental factors influence their values, three of them being the most important; specific factors in the wastewater, pH and temperature. It is obvious that in order to derive the best possible model for a certain WWTP under investigation, the values of these parameters have to be calculated based on data that are specifically related to the local environmental conditions under which the WWTP is operating. For example, measurements obtained from sensors installed in the WWTP can be used to formulate system identification schemes, the goal of which would be to accurately estimate the values of the kinetic and stoichiometric parameters of the ASM1 model. In Table 2.5 typical values of these parameters at neural pH and temperatures of $20\ ^0\mathrm{C}$ and $10\ ^0\mathrm{C}$ as given in [8] are listed. The values of these parameters used in the BSM1 model correspond to a temperature of $15\ ^0\mathrm{C}$ and can be found in [6].

Table 2.2 ASM1 kinetic & stoichiometric parameters

Definition	**Symbol**
Stoichiometric Parameters	
Yield for autotrophic biomass	$\mathrm{Y_A}$
Yield for heterotrophic biomass	$\mathrm{Y_H}$
Fraction of biomass leading to particulate products	$\mathrm{f_P}$
Mass of nitrogen per mass of COD in biomass	$\mathrm{i_{XB}}$
Mass of nitrogen per mass of COD in products from biomass	$\mathrm{i_{XP}}$
Kinetic Parameters	
Maximum specific growth rate for heterotrophic biomass	$\mathrm{\mu_H}$
Half-saturation coefficient for heterotrophic biomass	$\mathrm{K_S}$
Oxygen half-saturation coefficient for heterotrophic biomass	$\mathrm{K_{O,H}}$
Nitrate half-saturation coefficient for denitrifying heterotrophic biomass	$\mathrm{K_{NO}}$
Decay coefficient for heterotrophic biomass	$\mathrm{b_H}$
Correction factor for $\boldsymbol{\mu_H}$ under anoxic conditions	$\mathrm{n_g}$
Correction factor for hydrolysis under anoxic conditions	$\mathrm{n_h}$
Maximum specific hydrolysis rate	$\mathrm{k_h}$
Half-saturation coefficient for hydrolysis of slowly biodegradable substrate	$\mathrm{K_X}$
Maximum specific growth rate for autotrophic biomass	$\mathrm{\mu_A}$
Ammonia half-saturation coefficient for autotrophic biomass	$\mathrm{K_{NH}}$
Decay coefficient for autotrophic biomass	$\mathrm{b_A}$
Oxygen half-saturation coefficient for autotrophic biomass	$\mathrm{K_{O,A}}$
Ammonification rate	$\mathrm{k_a}$

2.3.3 ASM No. 1 Differential Equations

The complete set of the ordinary differential equations (ODEs) that form the ASM1 model by combining the state variables, dynamic processes and coefficients that have been presented in the previous sections is quite complex and their detailed formulation and derivation can be found in [6], [8], [10].

2.4 Settling Process Model

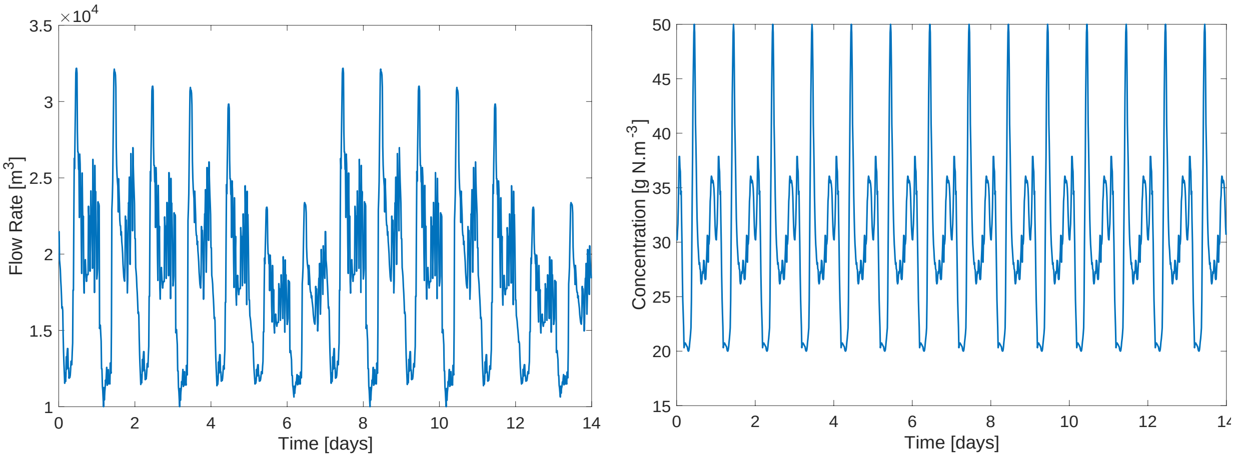
As already stated, part of the wastewater exiting the last aerobic tank (unit 5) is recycled to the first anoxic tank (unit 1) at a flow rate Q_a and concentration Z_a and the rest of it is fed to the secondary settler at a flow rate Q_f and concentration Z_f, as depicted in **Error! Reference source not found.**. Thus, except from the mathematical model describing the ASP process of the aerobic and anoxic tanks, a mathematical model capable of accurately describing the settling process is necessary as well. In BSM1, this process is modelled by utilizing a model comprising 80 ordinary differential equations, detailed information about which can be found in [6], [14].

Table 2.3 Typical parameter values

Symbol	Unit	20 ^{0}C	10 ^{0}C
$\mathbf{Y_A}$	$\text{g cell COD formed.}(\text{g N oxidized})^{-1}$	0.24	0.24
$\mathbf{Y_H}$	$\text{g cell COD formed.}(\text{g COD oxidized})^{-1}$	0.67	0.67
$\mathbf{f_P}$	dimensionless	0.08	0.08
$\mathbf{i_{XB}}$	$\text{g N.}(\text{g COD})^{-1}\text{in biomass}$	0.086	0.086
$\mathbf{i_{XP}}$	$\text{g N.}(\text{g COD})^{-1}\text{in pariculate products}$	0.06	0.06
$\boldsymbol{\mu_H}$	d^{-1}	6	3
$\mathbf{K_S}$	g COD.m^{-3}	20	20
$\mathbf{K_{O,H}}$	$\text{g}(-\text{COD}).\text{m}^{-3}$	0.2	0.2
$\mathbf{K_{NO}}$	$\text{g NO}_3-\text{N.m}^{-3}$	0.5	0.5
$\mathbf{b_H}$	d^{-1}	0.62	0.2
$\mathbf{n_g}$	dimensionless	0.8	0.24
$\mathbf{n_h}$	dimensionless	0.4	0.4
$\mathbf{k_h}$	$\text{g slowly biodegradable COD.}(\text{g cell COD.d})^{-1}$	3	1
$\mathbf{K_X}$	$\text{g slowly biodegradable COD.}(\text{g cell COD})^{-1}$	0.03	0.01
$\boldsymbol{\mu_A}$	d^{-1}	0.8	0.3
$\mathbf{K_{NH}}$	$\text{g NH}_3-\text{N.m}^{-3}$	1	1
$\mathbf{b_A}$	d^{-1}	0.05	0.05
$\mathbf{K_{O,A}}$	$\text{g }(-\text{COD}).\text{m}^{-3}$	0.4	0.4
$\mathbf{k_a}$	$\text{m}^3\ (\text{g COD.d})^{-1}$	0.08	0.04

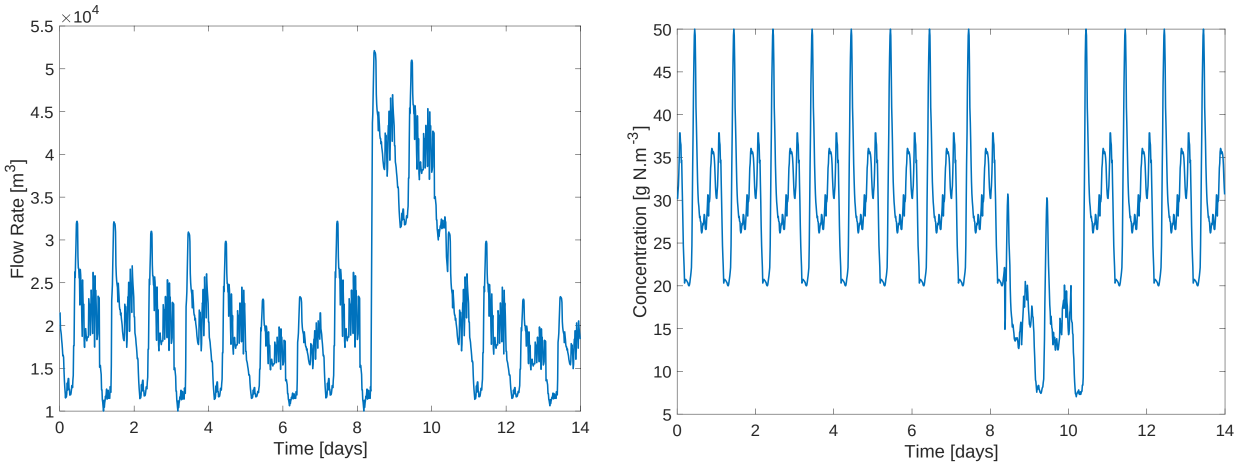
2.5 BSM1 Influent Compounds

In order to apply and test different modelling and control methodologies by simulating the BSM1 model, three influent files are provided, each one of them corresponding to different weather conditions. More specifically, the first file represents dry weather conditions, the second one rainy weather conditions while the third one corresponds to a stormy weather profile. The chemical compounds that constitute these files are those that have been defined in Table 2. with the addition of the flow rate Q_{in} measured in m^3. In Figures 2.2 – 2.4 the influent flow rate and the ammonia concentration of the three influent files are indicatively presented. It is worth noticing that an increase in the flow rate of the wastewater is equivalent to a decrease in the ammonia concentration, and vice versa.



(a) (b)

Figure 2.2 Dry weather influent profile: (a) Flow Rate - (b) Ammonia Concentration



(a) (b)

Figure 2.3 Rainy weather influent profile: (a) Flow Rate - (b) Ammonia Concentration

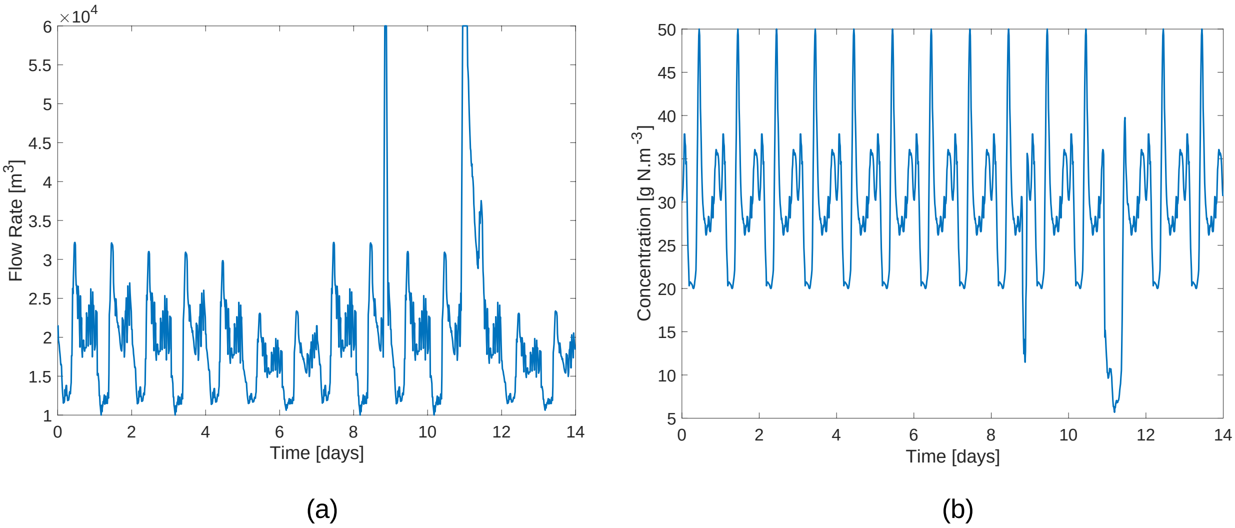


Figure 2.4 Stormy weather influent profile: (a) Flow Rate - (b) Ammonia Concentration

2.6 Complete Model Structure

In addition to the aforementioned ODEs that model the ASP and settling processes of the BSM1 model, there exist 15 additional first order differential equations [6] that represent the hydraulic delays affecting the wastewater processing. Therefore, the complete model structure consists of the following distinct parts combined in the configuration depicted in **Error! Reference source not found.**, forming the BSM1 model:

1. 15 ODEs modelling the hydraulic delays
2. 65 ODEs modelling the ASP processes of the 2 anoxic and 3 aerobic tanks
3. 80 ODEs modelling the settling process

In conclusion, the complete BSM1 model consists of 160 ODEs, thus forming a rather complex yet accurate benchmark model capable of simulating the dynamic behavior of WWTPs with high accuracy. However, the design and implementation of automatic control schemes based on this large-scale model is a really difficult task and the necessity of deriving reduced-order models that are capable of capturing the highly nonlinear dynamics of WWTPs, while simultaneously being simple enough to be used in the design and implementation of advanced closed-loop control formulations, is urgent.

3 Reduced-Order Model

In this chapter the development of a reduced-order model of BSM1 is presented. The procedure of selecting the important state variables of the ASM1 model is thoroughly described followed by the complete set of the ODEs that formulate the derived model. Moreover, the model reduction procedure of the settling process is also presented and finally, the complete reduced-order model structure is provided.

3.1 Literature Review

The derivation of a reduced model for BSM1 consists of two distinct stages; firstly, a reduced model for the ASM1 model describing the reactions taking place inside the anoxic and aerobic units has to be obtained and afterwards a model reduction of the settling process is essential since the secondary clarifier of BSM1 includes 80 states. In [15], a reduced model of ASM1 is proposed consisting of 9 state variables, which is further reduced to 5 by combining X_S and S_S into one state and X_{ND}, S_{ND}, S_{NH} into another state. The dissolved oxygen concentration is not considered as a state variable, which may prove to be an important drawback since S_o can be directly and reliably measured, thus it is easy to be integrated in automatic control schemes. Moreover, as it is clearly stated in the article, the secondary settler has not been modified, meaning that the 80 states model has been preserved. The simplifications proposed would lead to a 90-state reduced model, since the anoxic and aerobic zones are each replaced by a single reactor. The derived is still too complex to be used in control design and therefore further simplifications have to be made.

Two very similar reduced-models for the activated sludge process have been proposed in [16]–[18], including 3 or 4 state variables, respectively. Despite the fact that the derived models are significantly reduced compared to the generic ASM1 model, some important variables have been neglected, such as the dissolved oxygen concentration and more importantly the two unique states describing the microorganisms, i.e., active heterotrophic and autotrophic biomass (X_{BH}, X_{BA}). Its integration in a reduced-order BSM1 model for describing the activated sludge process of each reactor would lead to poor performance. In [19], two reduced models consisting of 7 and 5 state variables have been proposed, yet their formulation also lacks the description of the microorganisms, a fact which would lead to a low performance when considering the full BSM1 model. Furthermore, the suggested models include the soluble inert organic inert matter (S_I) component as a state variable, which does not have any effect on the wastewater entering a WWTP [10], and consequently there is not any apparent reason to consider it in the order reduction procedure. Moreover, in [10], a reduced-order model of the activated sludge process is presented consisting of 5 states. However, the proposed model neglects the dissolved oxygen (DO) concentration, assuming it is being controlled and therefore the respective growth expressions would be independent from it. In order to control the DO concentration, though, a model is needed and thus, including it in a reduced-order model of the activated sludge process would not increase its complexity compared to the architecture presented in [10].

In the following sections of this chapter, the entire procedure of deriving a reduced-order BSM1 model is described. The goal of the reduced-order model is to be capable to accurately predict the dynamic behavior of the generic BSM1 model, while being of lower computational complexity compared against it.

3.2 Model Formulation

3.2.1 State Variables

As already stated in the second chapter of this thesis, the ASM1 model consists of 13 state variables and its incorporation in the BSM1 model in order to describe the activated sludge process of the 2 anoxic and 3 aerobic tanks, leads to a highly complex model consisting of 65 state variables. Therefore, utilization of this model in order to design and implement advanced closed-loop control configurations aimed to optimize the performance and operation of the WWTPs, is really difficult and may lead to control formulations that are extremely complex. Obviously, deriving reduced-order models that are of lower complexity, while also being capable of simulating the dynamic behavior of the plant with high accuracy is necessary for the purpose of efficiently developing advanced methodologies for the on-line control of WWTPs. The procedure of model reduction consists of a number of assumptions based on the biological perspective of the chemical elements included in the ASM1 model and on their dynamic response rate. In the following paragraphs, the steps which lead to the final structure of the reduced-order model are described in detail.

The first difference with the original ASM1 model is regarding the description of the organic matter, which is modelled by 5 state variables, i.e., five fractions of organic matter exist in ASM1 [8]. In particular, it is combined by the following five components:

1. Soluble inert organic matter (S_{I})
2. Particulate inert organic matter $(\mathrm{X_I})$
3. Particulate products arising from biomass decay $(\mathrm{X_P})$
4. Readily biodegradable substrate (S_{S})
5. Slowly biodegradable substrate $(\mathrm{X_S})$

As described in [10], the inert fractions included in the representation of the organic matter are not important from a biological perspective. Specifically, the soluble inert organic matter passes through the biological reactors of a WWTP without having any effect on the modification of the wastewater. In addition, the particulate fractions $(\mathrm{X_I}, \mathrm{X_P})$ are used for predicting the sludge production in a WWTP, the variations of which consist a really slow process, and therefore including them in a reduced-order model aimed for control design, is not appropriate. Consequently, the remaining two fractions of the organic matter, namely the readily and slowly biodegradable substrates are maintained in order to model the organic matter concentration of the wastewater as it flows through the WWTP facility. In contrast to the reduced-order model presented in [10], in the model developed in this thesis these two chemical compounds are not replaced by a single variable and are kept separated. It should be noted that the biodegradable substrate is difficult to be measured during the full-scale operation of a WWTP, i.e., online, however a respirometer can be used, capable of measuring the short-term COD of the wastewater, which includes both of the biodegradable substrates.

The next step in developing the reduced-order model involves investigating the total nitrogen that exists in the wastewater. In ASM1, four different compounds are used to describe its concentration and these are the following:

1. Nitrate and nitrite nitrogen (S_{NO})
2. Ammonia nitrogen (S_{NH})
3. Soluble biodegradable organic nitrogen (S_{ND})
4. Particulate biodegradable organic nitrogen (X_{ND})

Measurements of both nitrate and nitrite nitrogen and ammonia concentration are assumed to be available by measuring them online; a fact which is very common in actual WWTPs. Furthermore, due to the fact that the soluble and particulate biodegradable organic nitrogen compounds mainly describe the formation mechanism of the ammonia nitrogen [10], which is assumed to be directly available from the WWTP, their inclusion in the developed reduced-order model is not necessary. Therefore, only the nitrite and nitrate nitrogen and ammonia concentration are included in the reduced-order model to represent the total nitrogen existing in the wastewater.

Another important difference with the reduced-order model developed in [10] is the inclusion of the dissolved oxygen concentration (S_O) as a state variable. Online measurement of the dissolved oxygen concentration in the aerobic reactors of WWTPs is the most common case and also considered to be the most reliable, so its incorporation as a controlled variable in the designed closed-loop control configurations can greatly improve the performance of the applied control laws. For example, in chapter 5 of this thesis, the default control strategy of the BSM1 model is presented, at which the dissolved oxygen concentration of the last aerobic tank is one of the two controlled variables. Furthermore, a predictive control formulation developed in this thesis, which is presented in chapter 6, incorporates the dissolved oxygen concentration as an imposed state constraint. Moreover, including the S_O concentration in the reduced-order model is not considered to increase the complexity of the model at an unacceptable level.

Finally, the last two chemical compounds of the wastewater, which are included as state variables in the reduced model are the active heterotrophic and autotrophic biomasses (X_{BH}, X_{BA}), i.e., the two kinds of microorganisms included in the ASM1 model.

3.2.2 The Reduced-Order Model

The assumptions and simplifications presented in the previous subsection have led to a reduced-order model that consists of 7 state variables compared to the 13 included in the original ASM1 model. It should be noted that even though the developed model consists of 2 additional states compared to the one presented in [10], the reasons for this choice have been clearly described. As already stated, a respirometer can be used to measure the short-term COD and there are not any proofs that this compound is solely equal to S_S, meaning that by using this measurement, the values of both S_S and X_S can be obtained. Moreover, in [10], it is assumed that the dissolved oxygen of the last aerobic tank of BSM1 is controlled by a separate control layer in a hierarchical closed-loop control scheme, meaning that S_O is a controlled variable and as a result a model describing its evolution is necessary. In addition to this, the online measurement of the S_O concentration is one of the most reliable and its incorporation in the designed control formulations will lead to enhanced overall control performance.

To sum up, the reduced-order model developed in this thesis is first of all clearly of lower order compared to the original ASM1, which is used to model the activated sludge process of the anoxic and aerobic reactors of BSM1. Furthermore, the produced model may contain 2 additional states compared to the one introduced in [10], but there are solidly specified reasons for this choice and the slight increase of the complexity is clearly justified, as it will lead to a reduced-order model of increased accuracy. The processes used to describe the states included in the developed model, provided in [6], [8], are given below:

- **Aerobic growth of heterotrophs**

$$\rho_1 = \mu_H \cdot \left(\frac{S_S}{K_S + S_S}\right) \cdot \left(\frac{S_O}{K_{OH} + S_O}\right) \cdot X_{BH}$$

- **Anoxic growth of heterotrophs**

$$\rho_2 = \mu_H \cdot \left(\frac{S_S}{K_S + S_S}\right) \cdot \left(\frac{K_{OH}}{K_{OH} + S_O}\right) \cdot \left(\frac{S_{NO}}{K_{NO} + S_{NO}}\right) \cdot n_g \cdot X_{BH}$$

- **Aerobic growth of autotrophs**

$$\rho_3 = \mu_A \cdot \left(\frac{S_{NH}}{K_{NH} + S_{NH}}\right) \cdot \left(\frac{S_O}{K_{OA} + S_O}\right) \cdot X_{BA}$$

- **Decay of heterotrophs**

$$\rho_4 = b_H \cdot X_{BH}$$

- **Decay of autotrophs**

$$\rho_5 = b_A \cdot X_{BA}$$

- **Ammonification of soluble organic nitrogen**

$$\rho_6 = \alpha_3 \cdot X_{BH}$$

- **Hydrolysis of entrapped organic nitrogen**

$$\rho_7 = k_h \cdot \left(\frac{X_S/X_{BH}}{K_X + (X_S/X_{BH})}\right) \cdot \left(\left(\frac{S_O}{K_{OH} + S_O}\right) + n_h \cdot \left(\frac{K_{OH}}{K_{OH} + S_O}\right) \cdot \left(\frac{S_{NO}}{K_{NO} + S_{NO}}\right)\right) \cdot X_{BH}$$

Finally, the conversion rates of the chemical compounds considered for the derived reduced-order model are the following:

$$\dot{S}_s = -\frac{1}{Y_H} \cdot \rho_1 - \frac{1}{Y_H} \cdot \rho_2 + \rho_7$$

$$\dot{X}_s = (1 - f_P) \cdot \rho_4 + (1 - f_P) \cdot \rho_5 - \rho_7$$

$$\dot{X}_{BH} = \rho_1 + \rho_2 - \rho_4$$

$$\dot{X}_{BA} = \rho_3 - \rho_5$$

$$\dot{S}_O = -\left(\frac{1 - Y_H}{Y_H}\right) \cdot \rho_1 - \left(\frac{4.57 - Y_A}{Y_A}\right) \cdot \rho_3$$

$$\dot{S}_{NO} = -\left(\frac{1 - Y_H}{2.86 \cdot Y_H}\right) \cdot \rho_2 + \left(\frac{1}{Y_A}\right) \cdot \rho_3$$

$$\dot{S}_{NH} = -i_{XB} \cdot \rho_1 - i_{XB} \cdot \rho_2 - \left(i_{XB} + \frac{1}{Y_A}\right) \cdot \rho_3 + \rho_6$$

The parameters that exist in the reduced-order model are the ones presented in Table 2.4, except from k_a and i_{XP}, which affect biological processes that have been neglected. Moreover, a new coefficient is introduced, namely α_3, describing the ammonification of soluble organic nitrogen. It should be clearly stated that the inclusion of this parameter is not contradictory to the fact that the soluble organic nitrogen (S_{ND}) is removed in order to derive the reduced-order model. As shown by the mathematical formulation of the particular process, the ammonification procedure is considered constant and influenced only by the evolution of the active heterotrophic biomass, an element that has been maintained in the reduced-order model.

Obviously, in order for the derived reduced model to simulate the dynamic behavior of the original model accurately, the values of these parameters have to be estimated. So, for the purpose of approximating these numerous coefficients, improved system identification techniques have to be applied, a fact addressed in chapter 4.

3.3 Settler Model

The settling process, which is carried out as soon as the wastewater exits the last aerobic tank of BSM1, is modelled by a 10-layer settler, the behavior of which is described by a set of 80 state variables, i.e., 80 first-order differential equations [6]. Obviously, this way of modelling the secondary clarifier significantly increases the complexity of the model and therefore, a reduction procedure has to be applied. However, the inclusion of a settler model is necessary and undoubtedly, it cannot be entirely removed from the reduced-order model, since it also affects the dynamic behavior of 3 compounds included in the reduced-order model.

Due to the fact that the reduced-order model will be used for control development purposes, it is not essential to be capable of predicting the concentrations of the chemical compounds that form the effluent stream. Consequently, the settling process is modelled by using a single time-varying parameter, as described in [10], which depends on the plant's influent flow rate at each time instant k. This coefficient is defined as the compaction ratio γ and is computed by using the below mathematical expression:

$$\gamma = \frac{Q_{in}(k) + Q_r - \left(\frac{V}{\theta_X}\right)}{Q_r}$$

where:

$Q_{in} \rightarrow$ influent flow rate
$Q_r \rightarrow$ sludge recycle flow rate from the settler
$\theta_X \rightarrow$ sludge retention time
$V \rightarrow$ total bioreactor volume

The parameters involved in computing the compaction ratio constant are directly available from the WWTP except from the influent flow rate Q_{in}. However, measurements of the influent flow rate can be easily available online, i.e., during full-scale operation of the plant, and as a result, the aforementioned coefficient can be directly computed at each discrete time-step of the closed-loop operation. Thus, the 80 state variables simulating the secondary settling procedure in the generic BSM1 model are entirely removed and replaced by a single constant, remarkably reducing model complexity.

3.4 Complete Model Structure

By applying the techniques and assumptions stated in the previous subsections of this chapter, the complete structure of the reduced-order model is obtained. The numbers of first-order differential equations utilized in the reduced-order BSM1 are given below:

1. 8 ODEs modelling the hydraulic delays

2. 35 ODEs in total modelling the ASP processes of the 2 anoxic and 3 aerobic tanks

The ODEs modelling the hydraulic delays are reduced since only 7 chemical compounds of the wastewater are considered in the reactor activated sludge process, and the sole remaining ODE is related to the delay of the wastewater flow rate. In conclusion, the reduced-order BSM1 model consists of a total of 43 first-order differential equations, and thus is obviously of significantly lower complexity compared to the original BSM1 model.

In order for the obtained model of the activated sludge process to be integrated in a reduced-order BSM1 formation, the chemical processes occurring in the interior of the reactors should be described by the appropriate mass-balance equations [10]. The dynamic behavior of a single component of each reactor's influent stream is represented by the following expression:

$$\mathbf{accumulation} = \mathbf{input} - \mathbf{output} + \mathbf{reaction}$$

The mathematical formulation of the aforementioned expression is given below:

$$\frac{dZ_i}{dt} = \frac{Q}{V} \cdot [Z_{in} - Z_i + (r_Z \cdot V)]$$

where $Z_i, i = 1, \dots, 7$ represents the chemical element considered, i.e., the states of the reduced-order model. Z_{in} denotes the value of the identical compound of the reactor's influent stream, Q is the volumetric flow rate of the reactor's influent, V corresponds to the volume of the reactor and r_Z is the conversion rate of each element as described in subsection 3.2.2. However, for the purpose of applying automatic control techniques to the WWTP, external inputs need to be introduced that can be manipulated by the implemented control formulation. One of these manipulated inputs is the internal recirculation flow rate Q_a, described in section 2.2 and shown in Figure 2.1. Except from this input, another aspect that can be affected during the operation of a WWTP is the aeration of the aerobic units [6]. For the purpose of doing so, a manipulative input is introduced for each one of the aerobic reactors, which is called the oxygen transfer coefficient (KL_a). This specific input to each aerobic unit directly affects the dissolved oxygen concentration of the particular reactor and consequently, a corresponding term describing this influence has to be added in the respective mass-balance equation:

$$\frac{\mathrm{dS_O}}{\mathrm{dt}} = \frac{\mathrm{Q}}{\mathrm{V}} \cdot \left[\mathrm{S_{O,in}} - \mathrm{S_O} + \left(\mathrm{r_{S_O}} \cdot \mathrm{V}\right) + \mathrm{KL_a} \cdot \mathrm{V} \cdot (\mathrm{S_O^*} - \mathrm{S_O})\right]$$

where S_O^* denotes the saturation concentration of the oxygen and is considered to be:

$$\mathrm{S_O^*} = 8\ \mathrm{g.m^{-3}}$$

By employing the aforementioned mass-balance equations, the complete structure of the reduced-order BSM1 model is obtained. The sequential order of the reactors follows the identical formulation of the original BSM1, which is depicted in Figure 2.1. In the following chapter, the system identification procedure applied in order to estimate the values of the coefficients that exist in the derived reduced-order model is presented.

4 Reduced-Order Model Identification

In this chapter, the identification procedure for estimating the values of the parameters that exist in the reduced-order model analyzed in chapter 3 is presented. The formulation of the system identification scheme is firstly described followed by an introduction to the particle swarm optimization (PSO) algorithm for solving complex optimization problems. Then, a customized cooperative particle swarm optimization (CPSO) approach is introduced along with the results from its application for estimating the values of the reduced-order model parameters. Finally, validation results of the obtained model are shown based on the guidelines for model evaluation, which are specifically defined in [6].

4.1 System Identification Scheme

The reduced-order model that was developed and analyzed in chapter 3 of this thesis includes 17 parameters, whose values significantly affect its dynamic behavior. Obviously, in order for the reduced-order model to simulate the original BSM1 model with high accuracy, the values of these coefficients have to be estimated. In this thesis, for the purpose of approximating these values, a system identification scheme is formulated. In particular, the objective of the proposed identification scheme is to be capable of accurately estimating the aforementioned parameters by using only data that can be directly collected from actual WWTPs, i.e., data that can be reliably measured by installed sensors. More specifically, the identification scheme in terms of the plant state variables, requires only measurements of the nitrate and nitrite nitrogen, dissolved oxygen and ammonia concentration of the plant's specific reactive units. In real WWTPs, these chemical compounds are almost certainly being measured and the corresponding sensors are considered to be reliable. Moreover, in order to increase the robustness and accuracy of the reduced-order model, measurements of the disturbances, which influence the dynamic behavior of the plant are also integrated in the identification scheme. To be more specific, measurements of the influent flow rate and its ammonia concentration are fed to the identification process, significantly increasing the dynamical range at which the reduced-order model captures the highly nonlinear dynamics of the original BSM1. It should be also noted that in actual WWTPs, it is a very common situation to measure these influent characteristics.

In this thesis, BSM1 plays the role of the actual plant and consequently, the real data at which the reduced-order model has to be fitted, are generated by dynamically simulating it. The procedure of data generation has been conducted in a way that could be directly applied to an actual WWTP. Specifically, the influent stream used is a modified rainy weather profile based on the one that is provided in [6]. In Figure 4.1, the flow rate and the ammonia concentration of the aforementioned modified influent profile are depicted. Furthermore, the inputs of the plant, namely the oxygen transfer coefficients of the three aerobic tanks $(\mathrm{KLa}_3, \mathrm{KLa}_4, \mathrm{KLa}_5)$ and the internal recirculation flow rate $(\mathrm{Q_a})$, are excited by imposing a sequence of random step tests every 10 days and with a difference of 2 hours between the step change of each variable. In Figure 4.2, their dynamic profiles are shown..

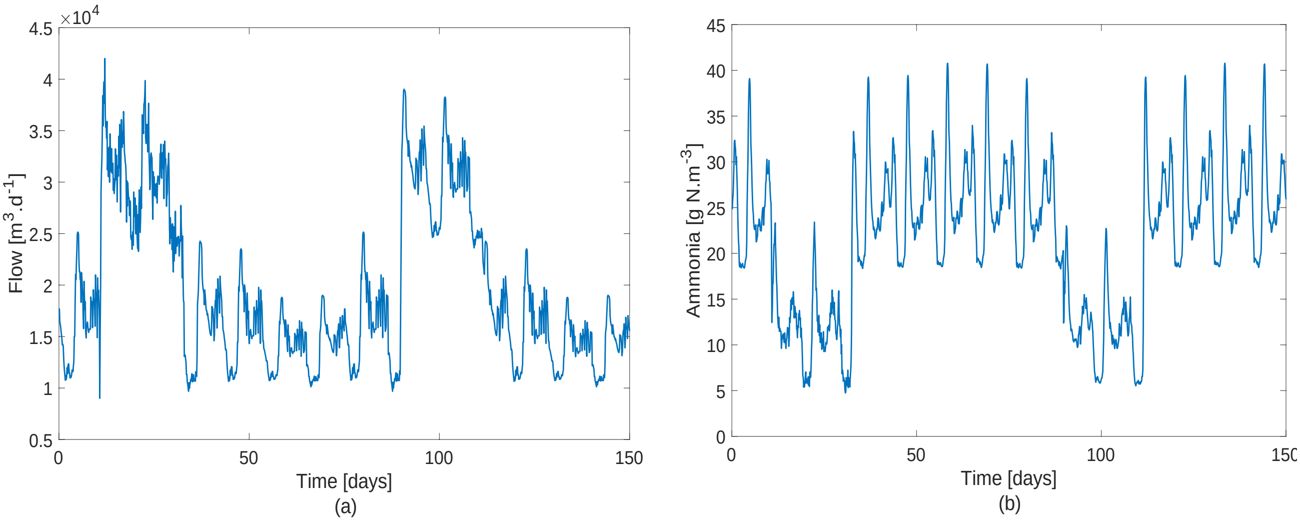


Figure 4.1 Modified rainy influent profile: (a) Flow Rate – (b) Ammonia Concentration

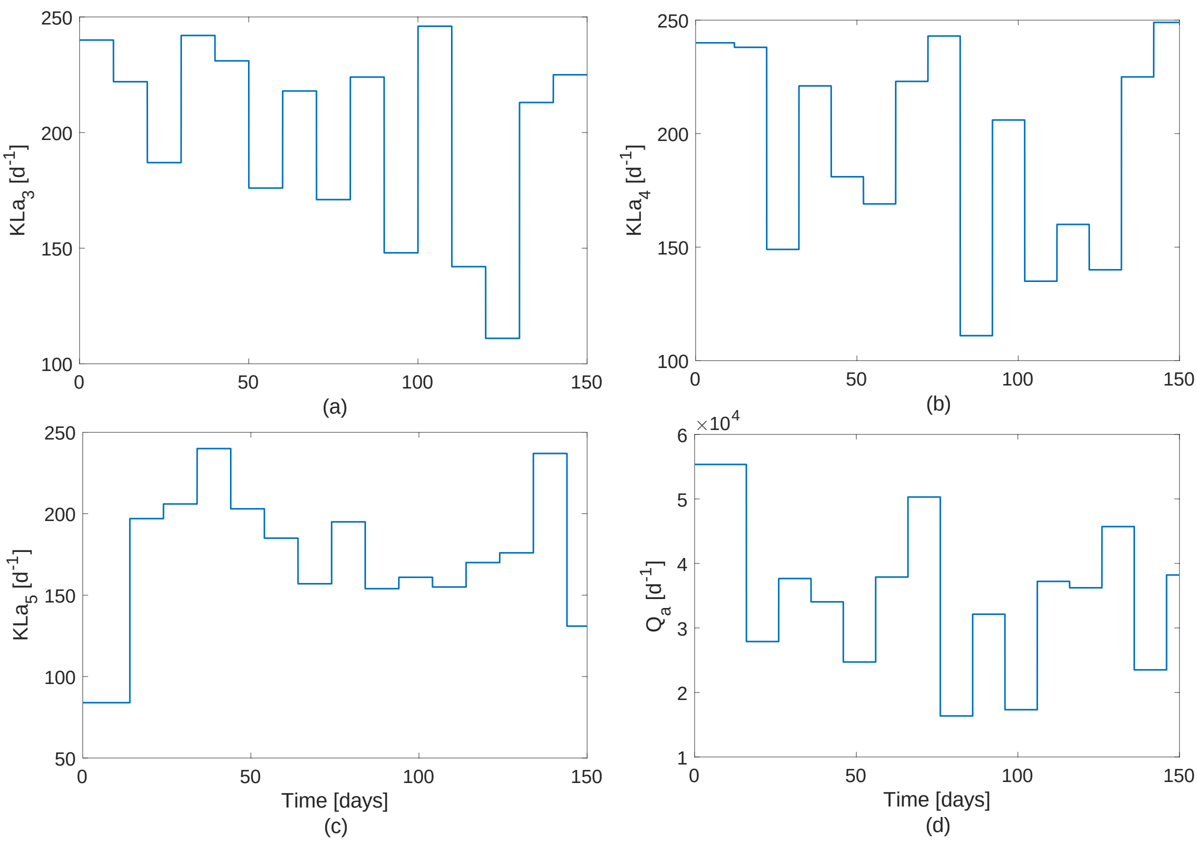


Figure 4.2 System inputs profiles

By applying the excitation described in the previous paragraph of this section, the responses of the state variables of BSM1 are obtained. The states used in this work for carrying out the identification procedure are the nitrate and nitrite nitrogen concentration of the second anoxic tank ($S_{NO,2}$), the dissolved oxygen concentration of all three aerobic tanks ($S_{O,3}, S_{O,4}, S_{O,5}$) and the nitrate and nitrite nitrogen and ammonia concentration of the last aerobic tank ($S_{NO,5}, S_{NH,5}$). This selection of variables leads to a total of 6 chemical compounds needed to perform the proposed identification scheme, with all of them capable of being directly and reliably measured in real WWTPs. It should be also noted that the sampling time considered for data collection is 15 minutes, as suggested in [6], allowing the required time interval for the sensors to operate properly.

As soon as the data collection process has been carried out, the identification procedure takes place. In this work, the formulation of the identification scheme is based on solving a nonlinear optimization problem, the purpose of which is to minimize an appropriately defined objective function. This cost function is chosen to be the mean squared error (MSE) between the real data collected and the simulated data produced by the reduced-order model. The applied optimization solver seeks to minimize this objective function by properly selecting the values of the kinetic and stoichiometric parameters that exist in the reduced-order model. The formulation of the employed objective function is given below:

$$J = \frac{1}{N} \cdot \sum_{k=1}^{N} \left(y_r(k) - \hat{y}(k)\right)^2$$

where y_r is the matrix containing the real data, $\hat{y}$ is the matrix containing the simulated data and N is the number of samples considered.

The formulated system identification scheme aims to accurately estimate the values of the coefficients that exist in the reduced-order model. However, the large number of these coefficients, in conjunction with the correlations that inherently exist between them, lead to a complex optimization problem characterized by a number of unwelcome properties such as high-dimensionality and multimodality. These properties render the classical optimization techniques inefficient for approaching a satisfactory solution and advanced methodologies have to be employed; the particle swarm optimization (PSO) algorithm, described in detail in the following section, appears as a promising solution.

4.2 Particle Swarm Optimization

Particle swarm optimization (PSO) [20], [21] is a metaheuristic search method for solving complex, high-dimensional optimization problems that is based on a population of potential solutions, called particles. The design variables of the optimization problem form one group, which is called swarm and a matrix containing possible solutions of the problem is created. Each row of the matrix represents one particle and its length is equal to the number of the design variables (N_d) of the formulated optimization problem. Each column of the matrix contains the possible values of each design variable, which are updated during the optimization procedure, and its length is equal to the number of particles (N_p) that has been selected, i.e., the number of potential solutions. The quantity of the potential solutions is a tuning parameter of the algorithm and theoretically, increasing this number may lead to a better overall solution. The particles of the created swarm “fly” into the search space trying to approach the best possible solution and at each iteration their position and velocity are updated according to the following equation:

$$\mathrm{v_{ij}(t+1) = v_{ij}(t) + c_1 r_{1j} \cdot \left[y_{ij}(t) - x_{ij}(t)\right]} + \cdots$$

$$\cdots + \mathrm{c_2 r_{2j}(t) \cdot \left[\hat{y}_{ij}(t) - x_{ij}(t)\right]}$$

$$\mathrm{x_{ij}(t+1) = x_{ij}(t) + v_{ij}(t+1)},\ i = 1, \dots, N_p, j = 1, \dots, N_d$$

where v_{ij} is the velocity of particle i in $j-th$ dimension, c_1, c_2 are the local and global adjustment weights, r_{1j}, r_{2j} are uniformly distributed random numbers, $\hat{y}$ corresponds to the position of the best particle, y_{ij} represents the best position of particle i in dimension j and x_{ij} denotes the position of particle i in the j dimension.

In each iteration of the algorithm, the values of each particle of the swarm, i.e., the values of the design variables of the optimization problem, are combined and the value of the objective function is calculated. The particle, the position of which corresponds to the smaller value of the cost function, is assigned as the global best particle. As shown in the above equation, the velocity of each particle is updated by considering the distance of each particle from its own best position multiplied by the local adjustment weight and the distance of each particle from the position of the global best particle multiplied by the social adjustment weight. Consequently, the selection of the values of the local and social weights denotes whether each particle should be more trustful to its personal trajectory in the search space, and the best position it has achieved, or if it should be more trustful to the trajectory of the global best particle inside the search space. As also suggested in [20], a common strategy is to keep these values equal. The termination criteria of the PSO algorithm are the common ones used when solving optimization problems, such as the objective limit, meaning that the procedure is terminated if the value of the objective function is below a defined threshold. Another termination criterion considers the relative change in the objective function. If the relative change is smaller than a specified constant for a number of continuous iterations, the procedure is stopped since the algorithm is stuck to a minimum and there is not any improvement in terms of the cost function value. A detailed description of the PSO algorithm and its different parameters can be found in [20].

The PSO algorithm groups all the design variables of the optimization problem into one unique swarm and therefore seeks to estimate their optimal values simultaneously. This fact leads to a situation that is called two steps forward – one step back problem, which means that the algorithm may come up with a better estimation for a specific design variable of the problem but at the same time, other variables may be drawn away from their best positions and therefore, the value of the objective function will not improve. This situation will lead to a rejection of the improved approximation found for the specific design variable and the iterations will continue. Moreover, by grouping the design variables into one unique swarm, the correlations that may exist between some of them are not taken into consideration. For example, the values of two design variables of the optimization problem may change in a specific pattern independently from the remaining, yet no advantage of this property is taken since the algorithm tries to optimize them concurrently. The aforementioned disadvantages of the PSO algorithm in conjunction with the fact that the formulated optimization problem, presented in section 4.1 of this chapter, consists of a large number of design variables, render the utilization of the PSO approach inappropriate for approaching a satisfactory solution. To remedy this situation, a cooperative PSO solver is introduced and in the following subsection, a detailed explanation of its functionality and advantages are presented.

4.3 Cooperative Particle Swarm Optimization

4.3.1 Overview

As already stated in the previous section, one of the most important drawbacks of the standard PSO algorithm is the fact that it cannot take advantage of the correlations that may exist between the design variables of the optimization problem. To cope with this situation, in this work, a customized cooperative PSO [22]–[24] approach is employed for solving the highly complex formulated nonlinear optimization problem. In this cooperative solver, the design variables of the optimization problem are not grouped into one unique swarm, but they are separated and form several distinct swarms.

The formation of the distinct swarms is the most crucial part of this algorithm. The selection of the design variables that will be grouped into one swarm has to be based upon the characteristics of the system that is represented by the model under investigation and on how these parameters affect its physical and dynamic behavior. In order to estimate the values of the parameters included in the reduced-order model of BSM1 developed in the previous chapter of this thesis, the distinction of the swarms is the following:

1. **First swarm** → 8 parameters related to heterotrophic phenomena $(\mathrm{Y_H}, \mathrm{K_{O,H}}, \mathrm{K_{NO}}, \mathrm{K_S}, \mathrm{b_H}, \mathrm{\mu_H}, \mathrm{n_g})$
2. **Second swarm** → 5 parameters linked with the autotrophic phenomena $(\mathrm{K_{NH}}, \mathrm{K_{O,A}}, \mathrm{Y_A}, \mathrm{b_A}, \mathrm{\mu_A})$
3. **Third swarm** → 3 parameters affecting the hydrolysis procedure $(\mathrm{n_h}, \mathrm{k_h}, \mathrm{K_X})$
4. **Fourth swarm** → 2 parameters related to the COD in biomass and in products from the biomass $(\mathrm{i_{XB}}, \mathrm{f_P})$
5. **Fifth swarm** → 1 parameter related to the ammonification process (α_3)

By separating the design variables of the problem into distinct groups, each swarm contains only part of the design vector, in contrast with the standard PSO algorithm, where the unique swarm includes all the information regarding the design variables. Consequently, in each iteration of the algorithm, in order to calculate the value of the cost function, a context vector is created. This vector associates the particles of each swarm with the global best particles of the other swarms and the value of the objective function is obtained. The positions and velocities of the particles of each swarm are updated according to the following equations:

$$P_k v_{ij}(t+1) = w \cdot P_k v_{ij(t)} + c_1 \cdot r_{1j}(t) \cdot [P_k y_{ij}(t) - P_k x_{ij}(t)] + \cdots$$
$$+ c_2 \cdot r_{2i}(t) \cdot [P_k\, \hat{y}_j(t) - P_k x_{ij}(t)$$
$$P_k x_{ij}(t+1) = P_k x_{ij}(t) + P_k v_{ij}(t+1)$$

where $P_k x_{ij}(t)$ is the position of $i-\mathrm{th}$ particle in $j-\mathrm{th}$ dimension of the $k-\mathrm{th}$ swarm and $P_k v_{ij}(t)$ is the corresponding velocity. $P_k y_{ij}(t)$ denotes the position of each swarm's best particle and $P_k\, \hat{y}_j((t)$ is the position of the global best particle. The remaining coefficients play the same role as described in the mathematical expressions of the standard PSO algorithm.

During the algorithm iterations, each swarm explores the search space independently, seeking to approach its own best position, while simultaneously sharing information with the other swarms. This property of the proposed CPSO approach, significantly improves the diversity of the final solution that is returned. Furthermore, the fact that the design variables of the optimization problem are separated into distinct swarms based on the correlations that exist between them, leads to the avoidance of the two steps forward-one step back problem, which appears in the standard PSO methodology.

4.3.2 Identification Results

The identification procedure for estimating the values of the parameters that exist in the reduced-order model developed in chapter 3 of this thesis, has been carried out by employing the CPSO approach described in the previous subsection. Before feeding them to optimization solver, the data generated by the original BSM1 model using the nominal values of the parameters given in Table 2.5, have been corrupted with Gaussian noise $\sim N(0, \sigma)$, where σ is set to 5.5% of the average value of each measured variable. This corrupted set of data is then provided to the CPSO solver and the optimization process occurs.

As it is depicted in Figure 4.3, the distinct swarms formed, evolve independently while the algorithm is executing, searching for the best possible solution regarding the values of their design variables. While the iterations continue, the swarms converge to their best positions, achieving a value for the fitness function, i.e., the mean squared error between the real data and the simulated data, equal to 0.01208. Figure 4.4 presents the dynamic responses of the

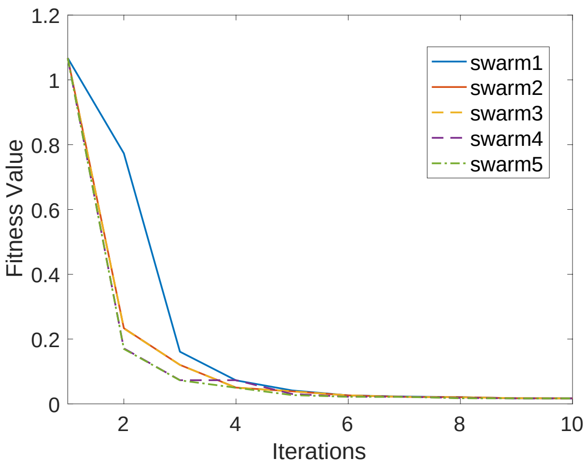


Figure 4.3 Swarm evolution

state variables used in the identification procedure, where it is shown that the reduced-order model is capable capturing the generic model dynamics with high accuracy. Finally, **Error! Reference source not found.** presents the mean squared errors of each state variable, proving that the process has been successfully completed. It should be noted that the calculations have been performed without normalizing the data. [6]

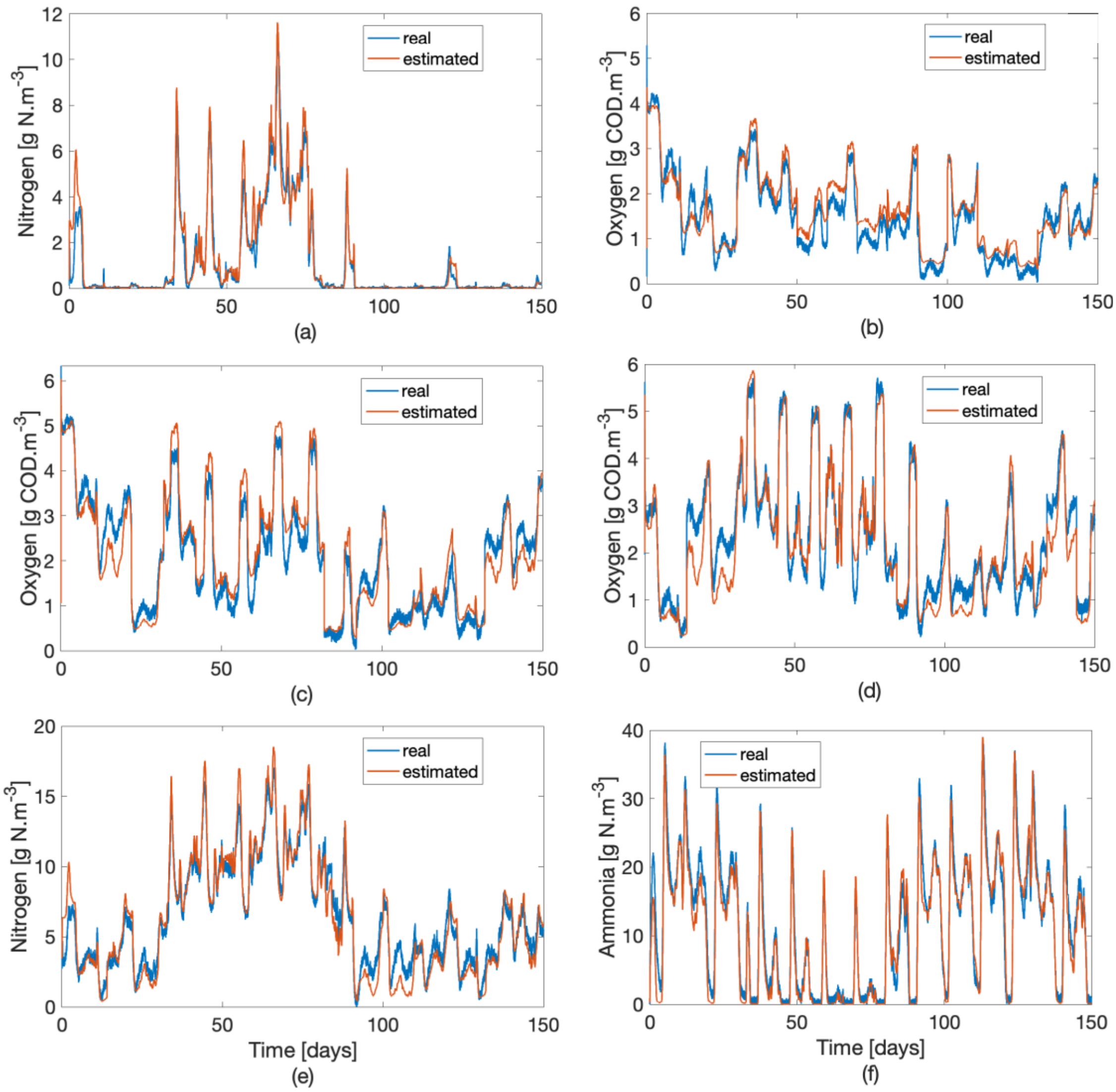


Figure 4.4 Concentrations: (a) Reactor 2 nitrate and nitrite nitrogen - (b) Reactor 3 dissolved oxygen - (c) Reactor 4 dissolved oxygen - (d) Reactor 5 dissolved oxygen - (e) Reactor 5 nitrate and nitrite nitrogen - (f) Reactor 5 ammonia

4.4 Model Evaluation

In order to evaluate the model obtained from the identification procedure, the guidelines specifically defined in [6] have been followed. In particular, firstly the original BSM1 model is stabilized by simulating it for 100 days under constant influent conditions. Then, the three dynamic influent profiles, as described in chapter 2 of this thesis, have been used and the plant is simulated for 14 days, while a sequence of random steps is imposed on its inputs. The values of the nitrate and nitrite concentration of the second anoxic tank, the dissolved oxygen concentration of all three aerobic tanks and the ammonia concentration of the last aerobic tank have been stored with a sampling time of 15 minutes. As specifically stated in [6], only the second week of the dynamic influent files, i.e., the last 7 days of simulation, are kept and used for evaluation. Finally, the same procedure is implemented on the identified reduced-order model as well, i.e., identical inputs applied and state variables stored, and in the following subsections the results of the validation procedure are presented. It should be noted that the values of the metrics shown have been calculated by using unnormalized data. In addition, the data used in the model's validation process, have not been used in the identification process and are generated anew from the original BSM1 model.

4.4.1 DRYINFLUENT Profile

In this subsection, the validation results of the identified reduced-order model using the DRYINFLUENT dynamic profile are shown. The dynamic responses of the states used to conduct the identification procedure are shown in Figure 4.5. **Error! Reference source not found.** shows the statistic results for the evaluation of the obtained model performance. Specifically, the coefficient of determination R^2, the mean squared error (MSE) and the mean absolute root error (MARE) are shown. It is obvious that the reduced-order model is capable of estimating the dynamic behavior of the original model with high accuracy.

Table 4.1 DRYINFLUENT statistical metrics

State Variable	$\mathbf{R^2}$	MSE	MARE
$\mathbf{S_{NO,2}}$	0.63	0.71	0.73
$\mathbf{S_{O,3}}$	0.59	0.13	0.44
$\mathbf{S_{O,4}}$	0.80	0.08	0.39
$\mathbf{S_{O,5}}$	0.90	0.09	0.32
$\mathbf{S_{NO,5}}$	0.83	1.37	0.26
$\mathbf{S_{NH,5}}$	0.81	7.87	0.29

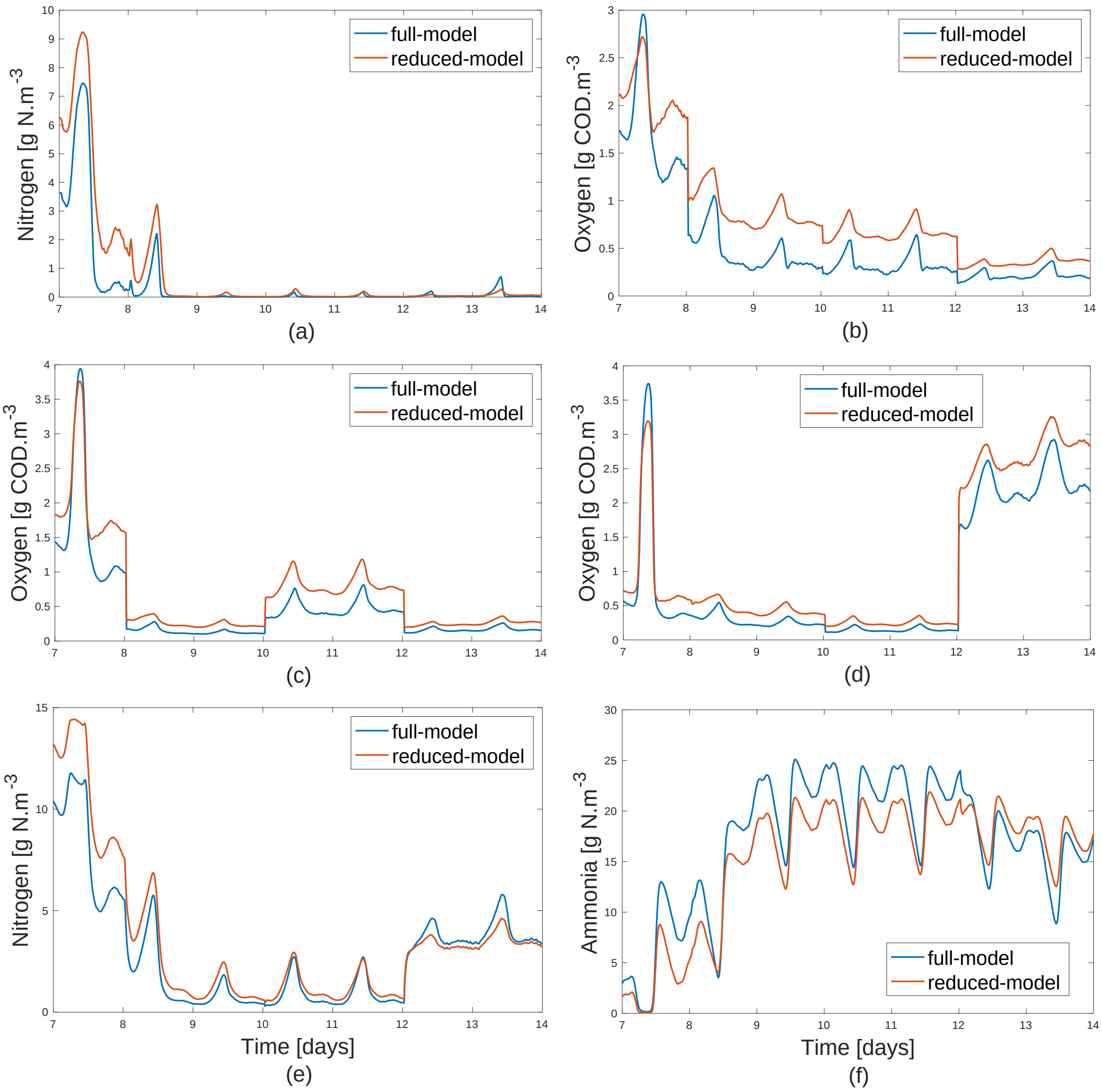


Figure 4.5 DRYINFLUENT Validation results

4.4.2 RAININFLUENT Profile

In this subsection, the validation results of the identified reduced-order model using the RAININFLUENT dynamic profile are shown. **Error! Reference source not found.** presents the dynamic responses of the states used to conduct the identification procedure are shown, followed by Table 4.3, where statistic results are shown evaluating the obtained model's performance. Specifically, the coefficient of determination R^2, the mean squared error (MSE) and the mean absolute root error (MARE) are shown.

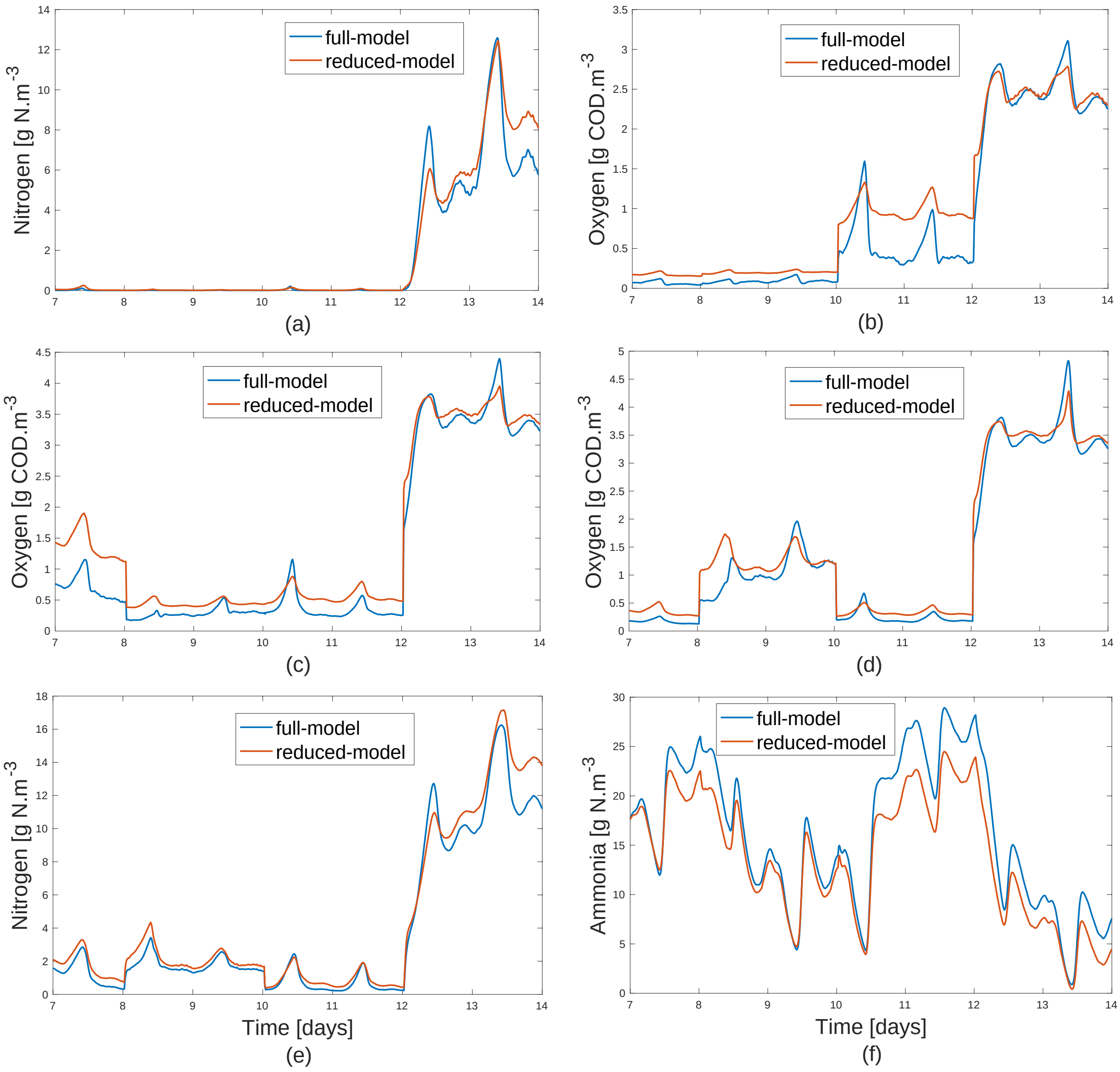


Figure 4.6 RAININFLUENT Validation Results

Table 4.2 RAININFLUENT statistical metrics

State Variable	R^2	MSE	MARE
$S_{NO,2}$	0.94	0.51	0.61
$S_{O,3}$	0.92	0.08	0.40
$S_{O,4}$	0.94	0.10	0.30
$S_{O,5}$	0.97	0.06	0.24
$S_{NO,5}$	0.96	0.76	0.23
$S_{NH,5}$	0.85	8.01	0.21

4.4.3 STORMINFLUENT Profile

In this subsection, the validation results of the identified reduced-order model using the STORMINFLUENT dynamic influent profile are shown. The dynamic responses of the state variables used to conduct the identification procedure are shown **Error! Reference source not found.**, followed by Table 4.4, where statistic results are shown evaluating the obtained

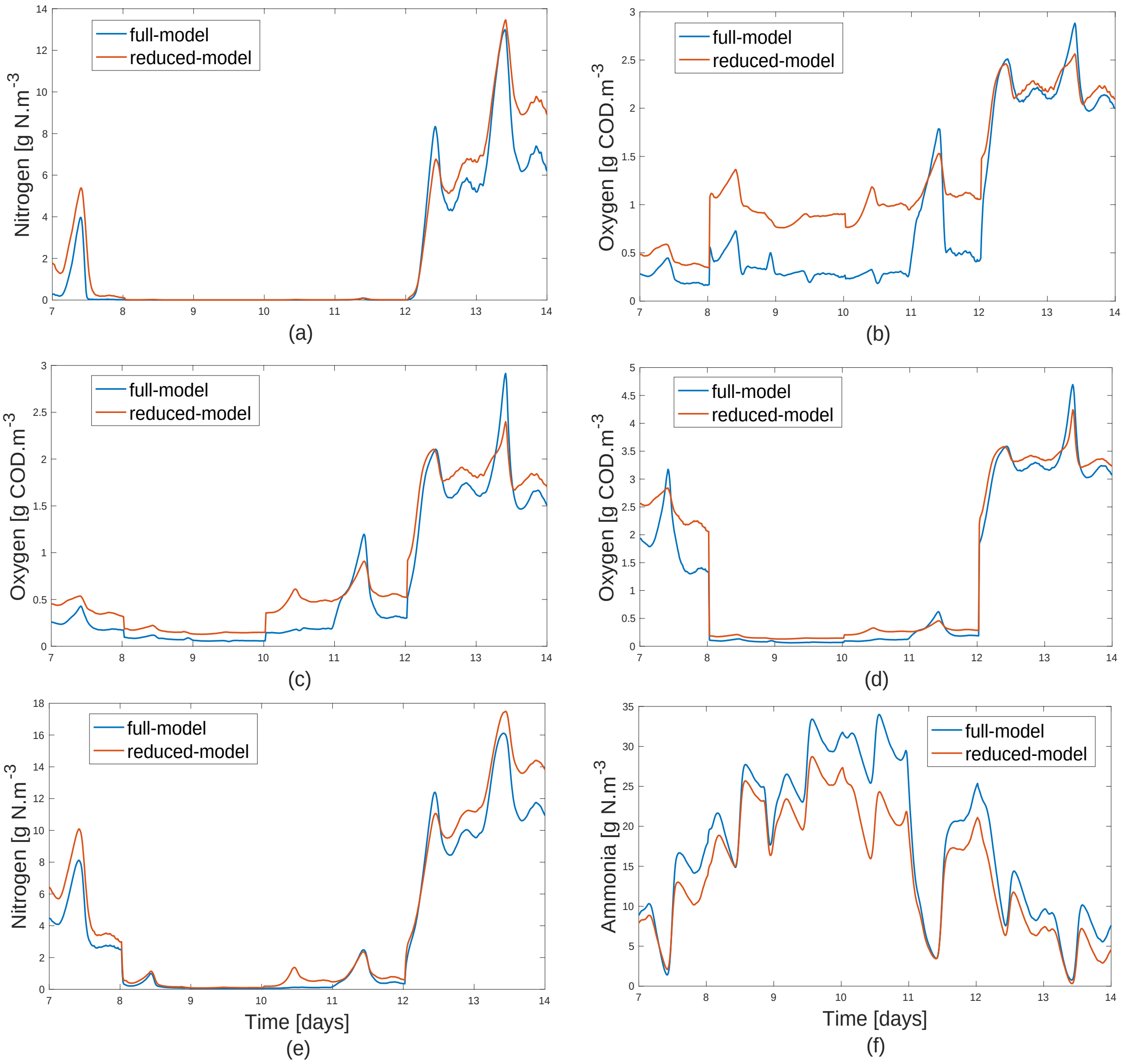


Figure 4.7 STORMINFLUENT Validation Results

model performance. Specifically, the R^2, the mean squared error (MSE) and the mean absolute root error (MARE) are shown. It is obvious that in this case as well the reduced-order model is capable of estimating the dynamic behavior of the original model with high accuracy.

4.5 Discussion

As shown by the presented results, the obtained reduced-order model is capable of accurately simulating the dynamic behavior of the original BSM1 model. However, as it is depicted in the above figures, the dynamic responses of the state variables of the reduced model exhibit an offset compared to the corresponding ones obtained by simulating the original BSM1. This situation is completely expected since the order of the reduced model is 117 times lower than the order of the generic BSM1, as clearly analyzed in chapter 3 of this thesis. Despite the existence of the aforementioned offset, the reduced-order model seems to be capable of capturing the dynamic response trend of the original model, a fact of crucial importance for integrating it in closed-loop control formulation. The closed-loop control schemes that will be implemented for optimizing the operation of WWTPs should be robust enough to account for this mismatch between the derived reduced-order model and the original one and in the following chapters of this thesis, it is shown that the closed-loop controllers are capable of handling this issue successfully. Finally, comparison results, which will be presented in the following chapters, between existing control configurations for WWTPs in the literature, validate the superiority of using the obtained reduced-order model in advanced predictive control schemes aimed to optimize the performance, energy efficiency and total operational costs of WWTPs.

Table 4.3 STORMINFLUENT statistical metrics

State Variable	R^2	MSE	MARE
$S_{NO,2}$	0.91	0.87	0.64
$S_{O,3}$	0.70	0.21	0.41
$S_{O,4}$	0.93	0.04	0.38
$S_{O,5}$	0.95	0.09	0.30
$S_{NO,5}$	0.95	1.20	0.34
$S_{NH,5}$	0.80	16.92	0.26

5 Control of Wastewater Treatment Plants

In this chapter an introduction to automatic control schemes aimed to improve the operation of wastewater treatment plants is presented. The objectives of the closed-loop control configurations in terms of the effluent quality and the operational costs of the WWTPs are specifically given. Moreover, an overview of the default control strategy implemented in the BSM1 model is described along with the guidelines specifically defined in [6], based on which the performance evaluation of the designed control schemes has to be carried out. Finally, the simulation results of the application of the default control strategy on BSM1 are presented along with the corresponding evaluation metrics.

5.1 Control Objectives and Evaluation

As it has been already stated, during the operation of WWTPs large quantities of contaminated and polluted water are fed to the plant as its influent stream. By a series of complex biological and biochemical phenomena that occur in the interior of the plant and particularly in the interior of the anoxic and aerobic tanks, the influent stream is converted to an effluent, which is recycled back to the water cycle, as it is safe enough to be re-used by the local communities. However, one of the most important issues is the fact that the quality of the effluent stream has to meet specific criteria, in order to comply with the stringent environmental regulations imposed by the laws. In particular, the limits regarding certain chemical compounds that exist in the effluent stream and which are defined [6], are given in Table 5.1.

Due to the fact that WWTPs are complex, large-scale plants and also because the procedure of converting the polluted influent into a reusable effluent stream is really difficult, these plants require a great amount of electrical power in order to carry out the aforementioned processes, satisfy the environmental limits and operate properly. Nowadays, the aspects of energy consumption and operational cost reduction of these plants are crucial and have to be taken under consideration when designing modern closed-loop controllers aimed to be applied on WWTPs. In addition, the difficulty in carrying out the process of influent conversion is increased since the disturbances affecting the operation of WWTPs, i.e. the influent flow rate and its ammonia concentration, exhibit large fluctuations depending on the weather conditions and the current season (e.g. during the summer, which is a touristic season, WWTPs have to cope with an increased volume of influent flow), thus leading to increased energy demands; a fact the applied control configurations have to be able to cope with by handling the disturbances, while also maintaining the energy requirements in the lowest possible levels.

Table 5.1 Effluent chemical compounds limits

Variable	Definition	Upper Limits
$\mathbf{N_{tot}}$	Total Nitrogen Concentration	$18\ \mathrm{g\ N.m^{-3}}$
$\mathbf{COD_{eff}}$	Chemical Oxygen Demand	$100\ \mathrm{g\ COD.m^{-3}}$
$\mathbf{S_{NH,eff}}$	Ammonia Concentration	$4\ \mathrm{g\ N.m^{-3}}$
$\mathbf{TSS_{eff}}$	Total Suspended Solids	$30\ \mathrm{g\ SS.m^{-3}}$
$\mathbf{BOD_{eff}}$	Biochemical Oxygen Demand	$10\ \mathrm{g\ BOD.m^{-3}}$

The evaluation of the control frameworks applied on BSM1 in the current thesis has been carried out by following the detailed guidelines defined in [6]. In particular, the plant is firstly stabilized to a steady state operating point under constant influent conditions, i.e. no active disturbances influencing its behavior, by simulating it for a period of 150 days. Afterwards, the influent profiles representing different weather conditions, which have been introduced in chapter 2 of the current thesis, are applied. Finally, in order to calculate the essential metrics regarding the controller performance, the results of the second week of simulating the plant under the dynamic influent profiles are kept. It should be also noted that all closed-loop simulations have been conducted by including the actuator and sensor dynamics as they are provided in [6]. The performance metrics that have been used in this thesis for controller evaluation are the total number of days at which the total nitrogen ($\mathrm{N_{tot}}$) and ammonia concentration ($\bar{\mathrm{S}}_{\mathrm{NH,eff}}$) of the effluent violate their limits, the average values of the effluent nitrate and nitrite ($\bar{\mathrm{S}}_{\mathrm{NO,eff}}$) and ammonia concentration ($\bar{\mathrm{S}}_{\mathrm{NH,eff}}$), the aeration energy (AE) being consumed by the manipulation of the oxygen transfer coefficient of the last aerobic tank (KLa_5), the pumping energy (PE) consumed by manipulating the internal recirculation flow rate (Q_a), the cost index (CI) which is computed as the summation of AE and PE and finally and the total effluent quality (EQ). The mathematical expressions for computing these metrics are the following:

$$\mathrm{AE} = \frac{\mathrm{S_O^{sat}} \cdot \mathrm{V_5}}{\mathrm{t_{obs}} \cdot 1.8 \cdot 1000} \sum_{\mathrm{t=7\ days}}^{\mathrm{t=14\ days}} \mathrm{KLa_5(t)}\ \ (\mathrm{kWh\ d^{-1}})$$

$$\mathrm{PE} = \frac{0.004}{\mathrm{t_{obs}}} \cdot \sum_{\mathrm{t=7\ days}}^{\mathrm{t=14\ days}} \mathrm{Q_a(t)}\ \ (\mathrm{kWh\ d^{-1}})$$

$$\mathrm{CI} = \mathrm{AE} + \mathrm{PE}\ (\mathrm{kWh\ d^{-1}})$$

$$\mathrm{EQ} = \frac{1}{\mathrm{t_{obs}} \cdot 1000} \cdot \sum_{\mathrm{t=7\ day}}^{\mathrm{t=14\ days}} \begin{matrix} [\mathrm{B_{TSS}} \cdot \mathrm{TSS_{eff}(t)} + \mathrm{B_{COD}} \cdot \mathrm{COD_{eff}(t)} \\ +\mathrm{B_{NKj}} \cdot \mathrm{S_{NKj}(t)} + \mathrm{B_{NO}} \cdot \mathrm{S_{NO,eff(t)}} + \mathrm{B_{BOD5}} \cdot \mathrm{BOD_{eff}(t)}] \end{matrix} (\mathrm{kg\ d^{-1}})$$

where $\mathrm{S_O^{sat}}$ is the saturation concentration of the dissolved oxygen, $\mathrm{V_5}$ is the volume of the last aerobic reactor as given in Table 2.1 and $\mathrm{t_{obs}}$ is the period of observations considered to compute the evaluation metrics, i.e., the second week of the simulations under dynamic influent profiles. The coefficients $\mathrm{B_i}$, which appear in the expression for the effluent quality calculation are called weighting factors and are given in [6] and in Table 5.2. $\mathrm{S_{NKj}}$ is the Kjeldahl nitrogen concentration, as defined in [6]. In the following section, the default control strategy implemented in BSM1 along with the results of its application under the dynamic influent profiles are presented.

Table 5.2 Weighing factors for EQ calculation

Factor	$\mathbf{B_{TSS}}$	$\mathbf{B_{COD}}$	$\mathbf{B_{NKj}}$	$\mathbf{B_{NO}}$	$\mathbf{B_{BOD5}}$
Value ($\mathbf{g\ pollution\ unit.g^{-1}}$)	2	1	30	10	2

5.2 BSM1 Default Control Strategy

5.2.1 Overview

The default control strategy of BSM1 consist of two simple proportional-integral controllers (PI) responsible for maintaining specific state variables of the plant to a predetermined fixed setpoint. More specifically, the first controller aims to keep the nitrate and nitrite nitrogen concentration of the second anoxic tank ($S_{NO,2}$) to the fixed value of $1\ \mathrm{g\ N.m^{-3}}$ by manipulating the internal recirculation flow rate Q_a. The goal of the second PI controller is to maintain the value of the dissolved oxygen concentration of the last aerobic tank ($S_{O,5}$) at the level of $2\ \mathrm{g\ COD.m^{-3}}$ by manipulating the oxygen transfer coefficient KLa_5. The parameters of the two controllers are given in Table 5.3.

5.2.2 Simulation Results

In this section, the simulation results by applying the default control strategy on BSM1 are presented. In **Error! Reference source not found.**, **Error! Reference source not found.** and **Error! Reference source not found.** the manipulated variables $(\mathrm{KLa_5}, \mathrm{Q_a})$ and the total nitrogen $(\mathrm{N_{tot,eff}})$ and ammonia concentration $(\mathrm{S_{NH,eff}})$ of the effluent stream for the three different influent profile cases, i.e. DRYINFLUENT, RAININFLUENT and STORMINFLUENT respectively, are depicted. In Table 5.4, the performance metrics are shown, as they are defined in the previous section. It should be noted that there are no limit violations regarding the $\mathrm{COD_{eff}}$, $\mathrm{TSS_{eff}}$ and $\mathrm{BOD_{eff}}$ of the effluent and therefore their responses and characteristics are, omitted, with the exception of 0.021 days at which the limit regarding the total suspended solids $(\mathrm{TSS_{eff}})$ is violated under the STORMINFLUENT profile.

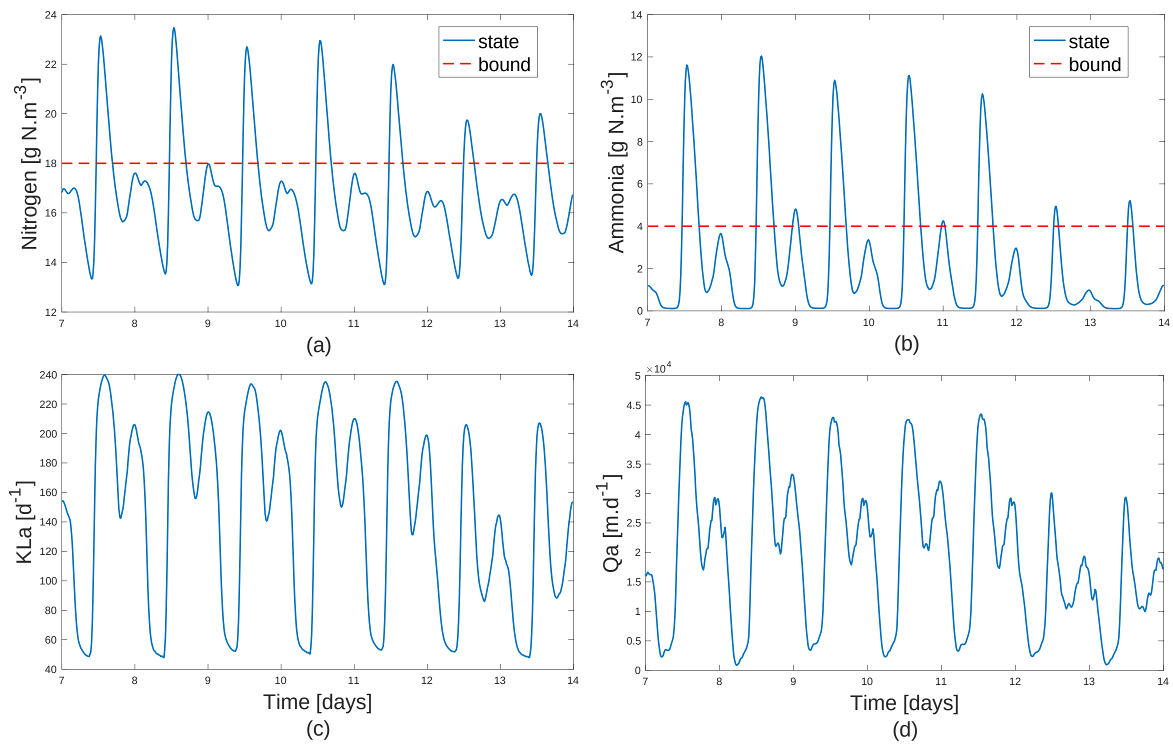


Figure 5.1 DRYINFLUENT profile: (a) Nitrogen Concentration - (b) Ammonia Concentration - (c) Oxygen Transfer Coefficient - (d) Internal Recirculation

Table 5.3 Default PI control strategy parameters

Variable	K	T_t	T_i
$S_{NO,2}$	$10000\ m^3 d^{-1}\ (g\ N.m^{-3})^{-1}$	0.015 d	0.025 d
$S_{O,5}$	$25\ d^{-1}(g(-COD)m^{-3})^{-1}$	0.001 d	0.002 d

Table 5.4 Performance metrics under dynamic influent profiles

Influent Profile	$N_{tot,eff}$ (days)	$S_{NH,eff}$ (days)	AE ($kWh\ d^{-1}$)	PE ($kWh\ d^{-1}$)	CI ($kWh\ d^{-1}$)	EQ ($kg\ d^{-1}$)
DRYINFLUENT	1.35	1.40	853.71	157.05	1010.76	6260.93
RAININFLUENT	1.06	2.05	823.63	204.94	1028.57	8367.31
STORMINFLUENT	1.26	1.91	872.82	184.87	1057.68	7404.69

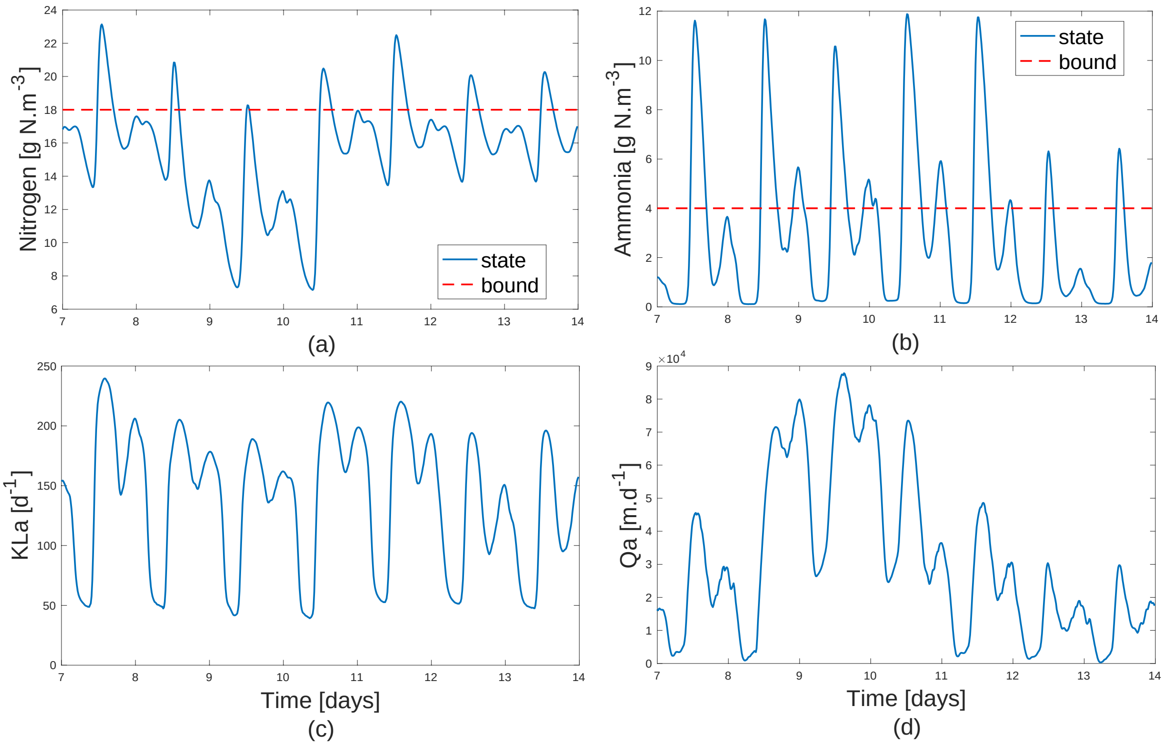


Figure 5.2 RAININFLUENT profile: (a) Nitrogen Concentration - (b) Ammonia Concentration - (c) Oxygen Transfer Coefficient - (d) Internal Recirculation

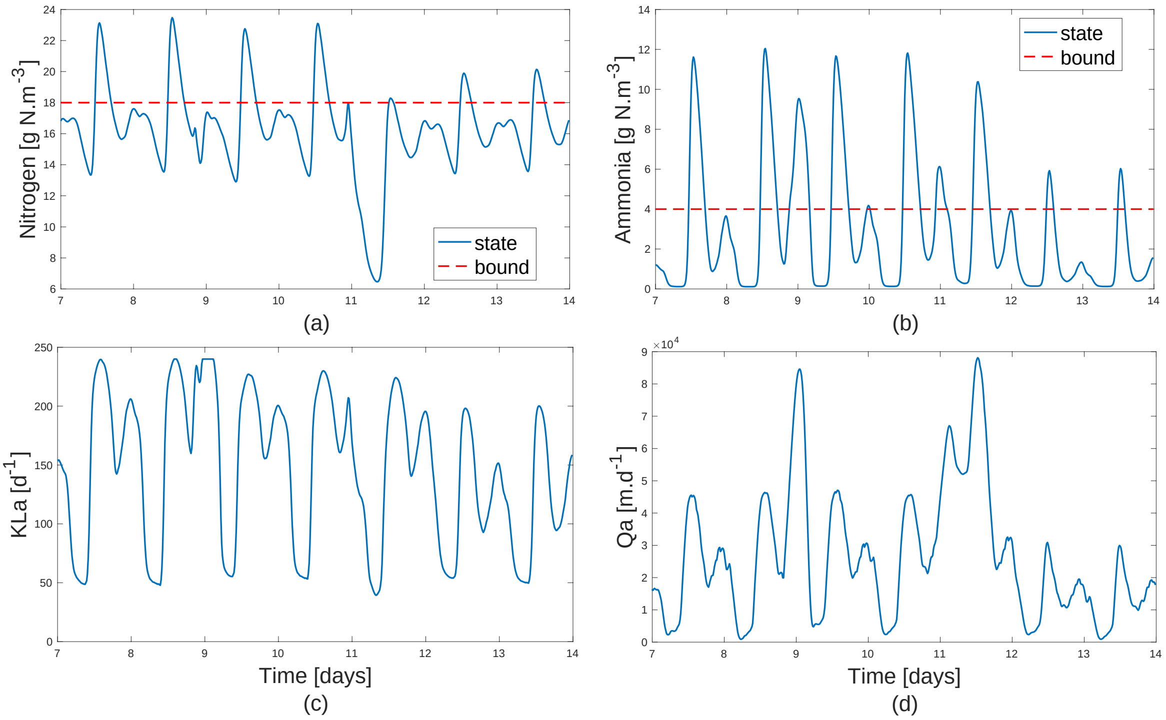


Figure 5.3 STORMINFLUENT profile: (a) Nitrogen Concentration - (b) Ammonia Concentration - (c) Oxygen Transfer Coefficient - (d) Internal Recirculation

5.3 Discussion

Different PI control approaches have been proposed in the literature for controlling the operation of WWTPs [25], [26]. However, these simplistic control formulations are not capable of handling all the different and important factors that influence the performance of these complex plants. For example, constraints regarding the range of the manipulated variables and their deviations between successive time-steps or constraints that need to be imposed on specific state variables in order to maintain compliance with the environmental regulations, cannot be taken under consideration. Moreover, the PI controllers will almost certainly lead to unnecessary high energy demands due to the fact that their objective is to maintain the plant at a fixed operating point but without considering energy consumption and operational costs.

As a result, the need of designing and applying advanced control methodologies aimed to optimize the overall performance of WWTPs by considering the numerous parameters, which affect its operation, is urgent. Model predictive control (MPC) appears as a promising approach for optimizing the operation of these large-scale plants and comparison results that show the superiority of the MPC control approach against the standard PI methodologies can be found in [27], [28]. In the following chapter, this advanced control formulation is introduced and two different formulations designed and applied on the BSM1 model are presented.

6 Model Predictive Control (MPC)

In this chapter, the model predictive control (MPC) methodology is introduced. An overview of the method is initially presented followed by a literature review on the existing proposed approaches for controlling WWTPs. Moreover, the closed-loop control schemes designed and implemented in this thesis aimed to optimize the operation and performance of WWTPs are described. Finally, the simulation results from the application of the control configurations on the generic BSM1 model under the dynamic influent profiles along with comparison cases against alternative MPC control configurations are presented.

6.1 MPC Overview

Model predictive control (MPC) was firstly introduced in late ‘70s [29]**.** MPC is an optimal control methodology that is based on a dynamical model of the process under control, which is used to predict the future dynamic behavior of the plant. Based on these predictions, an optimization problem is formulated at each discrete time-step of the closed-loop operation, the goal of which is to minimize an appropriately defined objective function, by properly selecting the values of the manipulated variables of the plant. As soon as the optimization problem has been solved, the first control actions included in the optimal trajectory of the manipulated variables are applied to the plant and the horizon is moved one-step towards, thus forming a receding horizon strategy [30].

Model predictive control does not correspond to a specific control method but includes a number of control strategies, which utilize a dynamical model of the controlled process to predict the dynamic response of the plant. For example, dynamic matrix control (DMC) [31] is one of the most widespread methodologies among the model predictive control family, which is being widely used in the process industry, and incorporates step or impulse response models to obtain the future states of the plant. Another predictive control approach that is based on a truncated impulse or step response of the controlled process is model algorithmic control (MAC). The MAC methodology has been also used in the process industry, yet its drawback is the fact that since it is based on a truncated response of the process, it can only be employed to control open-loop stable processes [30]. Except from the aforementioned approaches, many more predictive control formulations have been proposed, such as predictive functional control [32] for fast processes and generalized predictive control (GPC) [33], which has been also successfully implemented in industrial processes [34].

The aforementioned predictive control configurations along with many others, exhibit a number of differences, yet their closed-loop operation is based on the exact same strategy. Firstly, the future outputs of the plant for a defined horizon N_p, i.e., the prediction horizon of the controller, are obtained by making use of the explicit process model that has been integrated. These predictions $\left(\hat{y}(t+1), \hat{y}(t+2), \dots, \hat{y}\left(t+N_p\right)\right)$ are based on the past values of the system outputs that have been measured and on the future control actions $\left(u(t), u(t+1), \dots, u\left(t+(N_p-1)\right)\right)$, aimed to be applied in the controlled process. A usual concept in terms of the future control actions to be determined is to select a horizon N_c, i.e. the control horizon of the controller, that is smaller (or equal) than the prediction horizon and keep the remaining values equal to that of the last control horizon step, meaning $\left(u(t+N_c+1), \dots, u\left(t+N_p-1\right) = u(t+N_c)\right)$. The future control actions are calculated as the solution of an optimization problem, the purpose of which is to minimize an objective function comprising the error terms, calculated as deviation of the process from a reference trajectory. The objective function is usually formulated in such a way to be quadratic and a common strategy is to include also a penalization term regarding the control effort of the plant. Finally, the control action $u(t)$ is sent to the plant and the remaining actions of the optimal control trajectory, returned as the solution of the optimization problem, are either discarded or given as the initial conditions of the optimization problem that will be formulated in the successive discrete time-step. The number of the design variables of the optimization problem that needs to be solved at each discrete time-step is equal to the value of the selected control horizon. A basic structure of the closed-loop MPC schemes is shown in Figure 6.1.

6.2 MPC for Wastewater Treatment Plants

In the last decades, model predictive control configurations are increasingly being adopted in a wide range of applications [35]–[37] and especially in the process industry [38], [39]. MPC is really well-suited for process control mainly because of the large sampling times under which these complex large-scale plants, like WWTPs, operate. This long time-interval between the successive sensor measurements, ensure first of all that the properly defined optimization problem will be solved and also that the actuators will reach the commanded values before the following samples are collected. However, the necessary time for solving the optimization problem greatly depends on the number of its design variables and on the complexity of the predictive model that has been integrated in the MPC formulation. Consequently, a simple, yet accurate, predictive model along with an optimization problem consisting of a few design variables would form the ideal closed-loop MPC configuration.

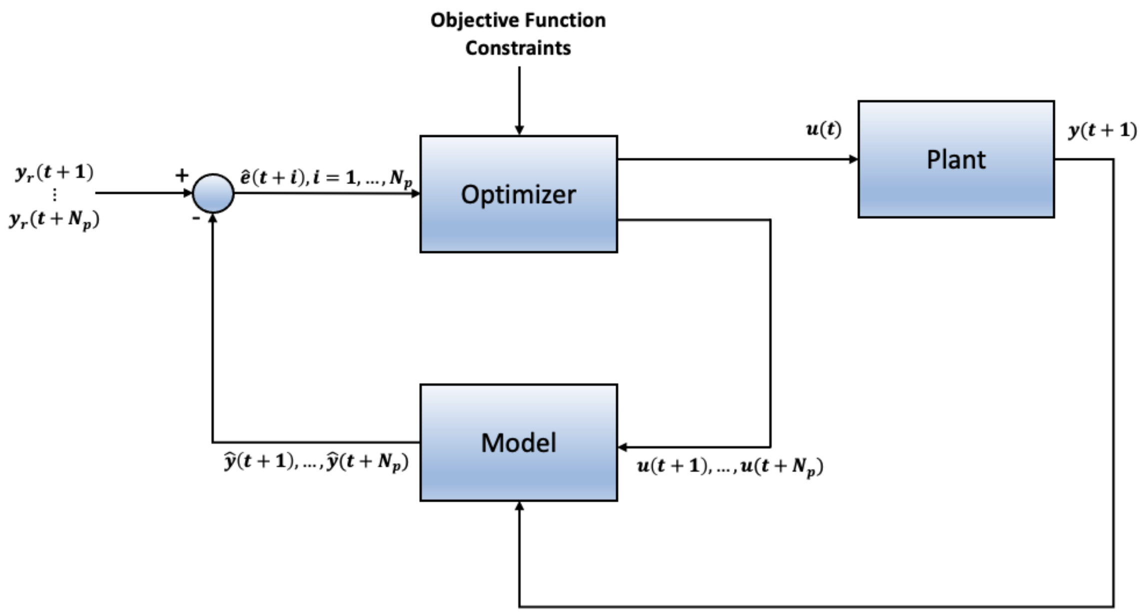


Figure 6.1 Closed-loop MPC block diagram

Many different approaches have been proposed in the literature for implementing MPC schemes to optimize the operation of WWTPs. In [40], an MPC configuration that needs to be tuned by solving a separate mixed sensitivity optimization problem is proposed. The model used to obtain the future predictions of the plant is a linear discrete time model obtained by linearizing the ASM1 model and by replacing the two anoxic reactors by one, the volume of which is equal to the summation of the volumes of the separate ones. The same technique has been applied to the three aerobic reactors, leading to a predictive model incorporating 26 states for the reactive units and 5 states for the secondary settler, which is modelled as a one-layer clarifier. While the utilized predictive model is really simple compared to the actual process, the tuning procedure involves solving a distinct optimization problem, leading to increased complexity. Moreover, there is no investigation regarding the robustness of the model under extreme disturbances (rainy weather, stormy weather) since only the dry weather influent has been applied. In addition, in order to achieve the results presented, the pumping energy needed is really high and also no information regarding the demanded aeration energy is provided despite the fact that the aeration energy is responsible for $45\% - 75\%$ of the total energy consumed in a WWTP [41].

In [42], an MPC approach with feedforward compensation is presented. Step-response predictive models are integrated in the MPC scheme for predicting the future dynamic behavior of the plant and an optimization problem with control horizon equal to 45, i.e. 180 design variables for the 4 inputs of the system, is formulated and solved at each discrete time-step. The step-response models do not exhibit a highly accurate representation of the controlled process and in order to derive them in real-life situations, the plant needs to operate at steady state and impose a step test on each manipulated variable in a sequential order. This means that in order to impose a step change in the next manipulated variable, the plant has to return to its previous steady state operating condition, a fact that is not easily implementable during full scale operation of the WWTP under disturbances. Moreover, the aeration and pumping energy needed to achieve the presented performance are really high. Finally, the robustness of the proposed control scheme is not investigated since there are no results regarding the rain and storm weather profiles.

Other approaches have been also proposed in the literature using neural networks as the predictive models in the MPC scheme [43], yet these formulations are quite complex either because large volumes of data are needed to train the neural networks offline – collecting large volumes of quality data from actual WWTPs is a difficult procedure - or because the neural networks are being trained online during the operation of the WWTP, thus increasing the computational burden of the closed-loop controller. Furthermore, [43] presents a model-free adaptive predictive control formulation based on linearizing the complete model of the process at each operating point, while also utilizing a hybrid optimization problem based on particle swarm optimization and genetic algorithms combined with multi-parameter sensitivity analysis, leading to a quite complex configuration.

Except from the standard MPC schemes that have been proposed, in the last years extensive research is being conducted oriented towards designing controllers aimed to optimize the energy performance and total operational costs of WWTPs, while also satisfying the environmental criteria. For example, in [44], an economic MPC configuration is proposed, where it is assumed that there exists a perfect fit between the controlled plant and the predictive model incorporated in the MPC scheme. However, this situation does not correspond to real-life applications since a number of different factors affect the process (sensor noise, unexpected disturbances, not all states of the system are measured), meaning that there will always be mismatches between the predictive model and the actual process. In [45], a number of different economic oriented MPC approaches are presented, which make use of a reduced order model introduced in [46]. However, as shown in the Appendix of [45], the utilized predictive model is not capable of simulating the dynamic behavior of the plant with high accuracy. An economic oriented DMC (EDMC) approach along with standard DMC formulations for optimizing the performance, energy consumption and total operational costs of WWTPs are presented in [47]. Step-response predictive models are used to obtain the future dynamic responses of the state variables of the plant by considering horizons equal to 48 (EDMC_48) and 96 (EDMC_96) regarding two alternative cases, in order to calculate the necessary coefficients for the models. As already stated, the step-response predictive models are not capable of highly accurately simulating the dynamic behavior of the plant and require large prediction horizons to achieve satisfactory responses. Specifically, the control horizon of the EDMC formulations is set to 48 and 96, thus leading to complex optimization problems consisting of 96 and 192 design variables, respectively; the objective of these problems is to calculate the values of the internal recirculation flow rate (Q_a) and oxygen transfer coefficient of the last aerobic tank ($KL_{a,5}$).

6.3 Nonlinear Tracking MPC

6.3.1 A Classical Formulation

In this subsection, a classical nonlinear tracking MPC (NMPC) formulation for optimizing the performance of WWTPs is presented. The goal of the implemented closed-loop control configuration is to maintain the plant, i.e. the original BSM1 model, at a specific steady state operating point by controlling the nitrate and nitrite nitrogen concentration of the second anoxic tank ($S_{NO,2}$) and the nitrate and nitrite nitrogen and ammonia concentration of the last aerobic tank ($S_{NO,5}, S_{NH,5}$) to predetermined fixed setpoint values, given in **Error! Reference source not found.** [6]. The structure of the MPC scheme is similar to the basic one depicted in Figure 6.1.

The model that is integrated in the closed-loop controller for obtaining the future predictions of the controlled variables, is the identified reduced-order model that has been derived by applying the methodologies described in chapters 3 and 4 of this thesis. Moreover, the objective function defined for this particular control approach consists of five terms. The first three of them correspond to the deviations of the controlled variables from their desired setpoint values and the remaining two are penalization terms that correspond to the deviations of the manipulated variables between successive discrete time-steps, so as to account for the control effort as well. As already stated, at each discrete time-step of the closed-loop operation

Table 6.1 Controlled variables setpoints

Variable	$\mathbf{S_{NO,2}}$	$\mathbf{S_{NO,5}}$	$\mathbf{S_{NH,5}}$
Setpoint	$3.66\ \mathrm{g\,N.m^{-3}}$	$10.42\ \mathrm{g\,N.m^{-3}}$	$1.73\ \mathrm{g\,N.m^{-3}}$

an optimization problem is formulated, the goal of which is to minimize the aforementioned objective function by properly selecting the values of the manipulated variables, i.e. the internal recirculation flow rate (Q_a) and the oxygen transfer coefficient of the last aerobic tank $(KL_{a,5})$. Furthermore, a number of constraints are imposed on the inputs of the plant and on specific state variables in order to comply with the environmental regulations, as it has been described in chapter 5. The formulation of the nonlinear optimization problem is given below:

$$\min_{\substack{\Delta KLa(k),\Delta KLa(k+1),\dots,\Delta KLa(k+Nc)\\ \Delta Q_a(k),\Delta Q_a(k+1),\dots,\Delta Q_a(k+N_c)}} \begin{aligned} &\left(e_1^T \cdot Q_1 \cdot e_1\right) + \left(e_2^T \cdot Q_2 \cdot e_2\right) + \left(e_3^T \cdot Q_3 \cdot e_3\right) + \cdots \\ &\cdots + \left(\Delta KLa^T \cdot R_1 \cdot \Delta KLa\right) + \left(\Delta Q_a^T \cdot R_2 \cdot \Delta Q_a\right) + \cdots \\ &\cdots + w_{slack} \cdot \left[\sum_{i=1}^{N_P}\sum_{j=1}^{3} \epsilon_{max,j}(k+i) + \sum_{i=1}^{N_P}\sum_{j=1}^{3} \epsilon_{min,j}(k+i)\right] \end{aligned}$$

$$\begin{aligned}
\text{s.t.}\quad & e_1 = \left[\left(y_{sp,1} - \hat{y}_1(k+1)\right)\cdots\left(y_{sp,1} - \hat{y}_1(k+N_P)\right)\right]^T \\
& e_2 = \left[\left(y_{sp,2} - \hat{y}_2(k+1)\right)\cdots\left(y_{sp,2} - \hat{y}_2(k+N_P)\right)\right]^T \\
& e_3 = \left[\left(y_{sp,3} - \hat{y}_3(k+1)\right)\cdots\left(y_{sp,3} - \hat{y}_3(k+N_P)\right)\right]^T \\
& 0 \le \epsilon_{min,j}(k+i) \le \bar{\epsilon}_{min}, i = 1,\dots,N_P, j = 1,2,3 \\
& \epsilon_{max,j}(k+i) \le \infty, i = 1,\dots,N_P, j = 1,2,3 \\
& \underline{Q_a} \le Q_a(k+i) \le \overline{Q_a}, i = 1,2,\dots,N_c \\
& \underline{KLa} \le KLa(k+i) \le \overline{KLa}, i = 1,2,\dots,N_c \\
& \underline{\Delta Q_a} \le \Delta Q_a(k+i) \le \overline{\Delta Q_a}, i = 1,2,\dots,N_c \\
& \underline{\Delta KLa} \le \Delta KLa(k+i) \le \overline{\Delta KLa}, i = 1,2,\dots,N_c \\
& \Delta KLa(k+i), \Delta Q_a(k+i) = 0, i = N_c+1,\dots,N_p \\
& \left(\underline{S_{NO,2}} - e_{min,1}(k+i)\right) \le S_{NO,2}(k+i) \le \left(\overline{S_{NO,2}} + e_{max,1}(k+i)\right), i = 1,2,\dots,N_p \\
& S_{NH,5}(k+i) \le \left(\overline{S_{NH,5}} + e_{max,2}(k+i)\right), i = 1,2,\dots,N_p \\
& S_{NO,5}(k+i) \le \left(\overline{S_{NO,5}} + e_{max,3}(k+i)\right), i = 1,2,\dots,N_p \\
& e_1(k+N_P) = e_2(k+N_P) = e_3(k+N_P) = 0
\end{aligned}$$

where e_1, e_2, e_3 are the errors of the three controlled variables ($S_{NO,2}, S_{NO,5}, S_{NH,5}$), respectively, $y_{sp,1}, y_{sp,2}, y_{sp,3}$ are their corresponding setpoints and $\hat{y}_1, \hat{y}_2, \hat{y}_3$ are the predictions of the three controlled variables obtained from simulating the utilized predictive model. N_p and N_c are the prediction and control horizons respectively, $\Delta KLa, \Delta Q_a$ represent the deviations of the manipulated variables between successive time-steps, $\underline{Q_a}, \underline{KLa}, \underline{\Delta Q_a}, \underline{\Delta KLa}$ are the lower bounds of the manipulated variables and their deviations that need to be selected and $\overline{Q_a}, \overline{KLa}, \overline{\Delta Q_a}, \overline{\Delta KLa}$ are the corresponding upper bounds. Q_1, Q_2, Q_3, R_1 and R_2 are positive definite diagonal matrices that penalize the respective terms and $\underline{S_{NO,2}}, \overline{S_{NO,2}}, \overline{S_{NH,5}}, \overline{S_{NO,5}}$ are the lower and upper bounds imposed on the specific state variables of the plant. The last constraint presented in the formulation of the optimization problem is the terminal constraint, which is imposed in order to guarantee the stability of the closed-loop configuration [48].

In order to ensure the feasibility of the open-loop control problem (needed also to satisfy the stability properties) formulated at each discrete time-step, slack variables are introduced to relax the imposed state constraints. In particular, $\epsilon_{\text{min,j}}$ and $\epsilon_{\text{max,j}}, j = 1, 2, 3$ correspond to the slack variables in terms of the lower and upper bounds for the nitrate and nitrite nitrogen of the second anoxic tank $\left(S_{\text{NO},2}\right)$, the ammonium nitrogen $\left(S_{\text{NH},5}\right)$ and the nitrate and nitrite nitrogen $\left(S_{\text{NO},5}\right)$ of the last aerobic tank. $\bar{\epsilon}_{min,1}$ is the slack variable corresponding to the lower bound of $S_{\text{NO},2}$ and should be selected so that it guarantees that the state variable remains positive. In the case of the presented formulation, there are not any lower bounds imposed on $S_{\text{NO},5}$ and $S_{\text{NH},5}$ and consequently $\epsilon_{min,2}(k + i) = \epsilon_{min,3}(k + i) = 0$. The slack variables are free variables that are determined by the applied optimization solver that guarantee the feasibility and the satisfaction of the constraints within acceptable "relaxed" sets. The slack weight w_{slack} is chosen to penalize this relaxation, i.e., for large values the solver tries to minimize the values of the slack variables as much as possible, leading to a stricter satisfaction of the imposed constraints. The value of this penalization term is often chosen to be really big in order to force the optimization solver to satisfy the constraints in the most optimal way.

The selection of these parameter values has been made by a trial-and-error procedure in conjunction with suggestions found in existing literature [6], [47]. The values of the prediction and control horizon (N_P, N_C) are both set equal to 8, meaning that the dynamic behavior of the plant is predicted for the following 2 hours, since the sampling time is kept at 15 minutes, as recommended in [6]. The values of the remaining parameters of the controller are given below:

The designed controller has been applied on the original BSM1 model using all the weather influent profile (DRYINFLUENT, RAININFLUENT, STORMINFLUENT). The tuning of the controller parameters is kept the same at all cases in order to properly investigate its robustness. The obtained results are presented in subsection 6.3.3 along with the results of the error-correcting formulation described below.

6.3.2 An Error-Correcting Formulation

The NMPC formulation presented in the previous subsection requires all the states that appear in the reduced-order model to be measured. This situation, however, is quite difficult to be implemented in actual WWTPs, even though many of the essential sensors exist and can be installed in real plants, as described in chapter 3 of this thesis and in [10]. To cope with this situation, an error-correcting nonlinear tracking MPC (EC-NMPC) formulation is presented, at which only the values of the controlled variables need to be measured at each discrete time-step of the closed-loop operation. Consequently, in the formulated control approach only 3 variables, i.e., the nitrate and nitrite concentration of the second anoxic tank and the nitrate and nitrite and ammonia concentration of the last aerobic tank, need to be directly available from the plant at each time-step. The block diagram of the controller is depicted in Figure 6.2.

As it is shown in the aforementioned figure, the control action calculated by the MPC controller at each time instant k is fed to the plant, i.e., the original BSM1 model, and also to an instance of the identified reduced-order model that plays the role of a parallel plant, which would be numerically solved at a real-life application, in order to obtain its state vector $\hat{x}(k+1)$. This state vector is provided to the MPC controller as the starting point for another instance of the identified reduced-order model that is integrated in the MPC and used to acquire the future N_P predictions of the states. The predictions of the three controlled variables $(S_{NO,2}, S_{NO,5}, S_{NH,5})$ are modified by a correction term $(\hat{e})$ that is calculated as the difference between the values of these variables collected from the actual plant (BSM1) and the corresponding ones obtained from simulating the identified reduced-order model $(\hat{S}_{NO,2}, \hat{S}_{NO,5}, \hat{S}_{NH,5})$. The value of the correction term is kept the same for the duration of prediction horizon.

The formulation of the optimization problem is the same as in the case of the NMPC scheme with differences in terms of the initial conditions of the states that are provided to the predictive model at each time-step and also regarding the prediction of the controlled variables. Its detailed mathematical expression is given below:

$$\min_{\substack{\Delta KLa(k),\Delta KLa(k+1),\dots,\Delta KLa(k+Nc)\\ \Delta Q_a(k),\Delta Q_a(k+1),\dots,\Delta Q_a(k+N_c)}} \begin{aligned} &\left(e_1^T \cdot Q_1 \cdot e_1\right) + \left(e_2^T \cdot Q_2 \cdot e_2\right) + \left(e_3^T \cdot Q_3 \cdot e_3\right) + \cdots \\ &\cdots + \left(\Delta KLa^T \cdot R_1 \cdot \Delta KLa\right) + \left(\Delta Q_a^T \cdot R_2 \cdot \Delta Q_a\right) + \cdots \\ &\cdots + w_{slack} \cdot \left[\sum_{i=1}^{N_P}\sum_{j=1}^{3} \epsilon_{max,j}(k+i) + \sum_{i=1}^{N_P}\sum_{j=1}^{3} \epsilon_{min,j}(k+i)\right] \end{aligned}$$

$$\begin{aligned}
\text{s.t.}\quad e_1 &= \left[\left(y_{sp,1} - \hat{y}_1(k+1)\right) \cdots \left(y_{sp,1} - \hat{y}_1(k+N_P)\right)\right]^T \\
e_2 &= \left[\left(y_{sp,2} - \hat{y}_2(k+1)\right) \cdots \left(y_{sp,2} - \hat{y}_2(k+N_P)\right)\right]^T \\
e_3 &= \left[\left(y_{sp,3} - \hat{y}_3(k+1)\right) \cdots \left(y_{sp,3} - \hat{y}_3(k+N_P)\right)\right]^T
\end{aligned}$$

$$\hat{y}_1(k+i) = \hat{y}_{1,p}(k+i) + \hat{e}_1(k), i = 1, \dots, N_p$$

$$\hat{y}_2(k+i) = \hat{y}_{2,p}(k+i) + \hat{e}_2(k), i = 1, \dots, N_p$$

$$\hat{y}_3(k+i) = \hat{y}_{3,p}(k+i) + \hat{e}_3(k), i = 1, \dots, N_p$$

$$0 \le \epsilon_{min,j}(k+i) \le \bar{\epsilon}_{min}, i = 1, \dots, N_P, j = 1,2,3$$

$$\epsilon_{max,j}(k+i) \le \infty, i = 1, \dots, N_P, j = 1,2,3$$

$$\underline{Q_a} \le Q_a(k+i) \le \overline{Q_a},\ \ i = 1,2,\dots,N_c$$

$$\underline{KLa} \le KLa(k+i) \le \overline{KLa},\ \ i = 1,2,\dots,N_c$$

$$\underline{\Delta Q_a} \le \Delta Q_a(k+i) \le \overline{\Delta Q_a}, i = 1,2,\dots,N_c$$

$$\underline{\Delta KLa} \le \Delta KLa(k+i) \le \overline{\Delta KLa}, i = 1,2,\dots,N_c$$

$$\Delta KLa(k+i), \Delta Q_a(k+i) = 0, i = N_c + 1, \dots, N_p$$

$$\left(\underline{S_{NO,2}} - e_{min,1}(k+i)\right) \le S_{NO,2}(k+i) \le \left(\overline{S_{NO,2}} + e_{max,1}(k+i)\right), i = 1,2,\dots,N_p$$

$$S_{NH,5}(k+i) \le \left(\overline{S_{NH,5}} + e_{max,2}(k+i)\right), i = 1,2,\dots,N_p$$

$$S_{NO,5}(k+i) \le \left(\overline{S_{NO,5}} + e_{max,3}(k+i)\right), i = 1,2,\dots,N_p$$

$$e_1(k+N_P) = e_2(k+N_P) = e_3(k+N_P) = 0$$

where $\hat{y}_{1,p}, \hat{y}_{2,p}, \hat{y}_{3,p}$ are the predictions of the controlled variables $(S_{NO,2}, S_{NO,5}, S_{NH,5})$ obtained from the predictive model and $\hat{e}_1, \hat{e}_2, \hat{e}_3$ are the corresponding correction terms calculated at each time-step k.

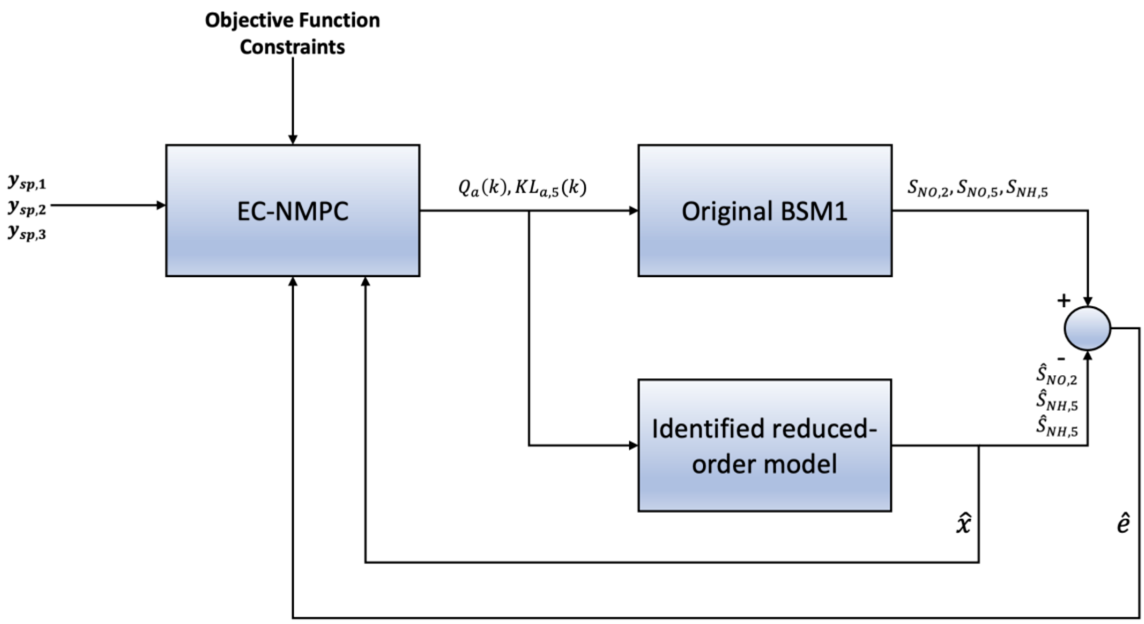


Figure 6.2 EC-NMPC block diagram

6.3.3 Simulation Results

In this subsection, the results of the two control formulations are presented and compared against the standard PI control methodology of BSM1 and against the DMC controllers designed in [47]. Simulations have been carried out by applying all the weather influent profiles and in compliance with the guidelines that are specifically defined in [6]. In particular the plant (BSM1) has been stabilized to a steady state operating point by simulating for 100 days under constant influent conditions, i.e., no active disturbances, and then dynamic influent profiles have been used and the plant is simulated for another 14 days. The sensor and actuator dynamics are included in the closed-loop simulation, as it is described in [6] and the evaluation metrics have been calculated by storing the last 7 days of the simulations, i.e., the second week of the dynamic influent profiles.

The selection of the controllers' tuning parameters was based on trial-and-error experiments and on suggestions found in the existing literature [6], [47].The prediction and control horizons for both control strategies are set equal to 8, i.e., the dynamic behavior of the plant is predicted for the upcoming 2 hours. The rest of the parameters for the NMPC approach are given below:

$$0 \le \mathrm{Q_a}(\mathrm{k}+\mathrm{i}) \le 92230, \quad \mathrm{i} = 1,2, \dots, 8$$
$$20 \le \mathrm{KLa}(\mathrm{k}+\mathrm{i}) \le 240, \quad \mathrm{i} = 1,2, \dots, 8$$
$$-3500 \le \Delta\mathrm{Q_a}(\mathrm{k}+\mathrm{i}) \le 3500, \mathrm{i} = 1,2, \dots, 8$$
$$-125 \le \Delta\mathrm{KLa}(\mathrm{k}+\mathrm{i}) \le 125, \mathrm{i} = 1,2, \dots, 8$$
$$1 \le \mathrm{S_{NO,2}}(\mathrm{k}+\mathrm{i}) \le 6, \mathrm{i} = 1,2, \dots, 8$$

$$S_{NH,5}(k+i) \leq 4, i = 1,2, \dots ,8$$

$$S_{NO,5}(k+i) \leq 12.5, i = 1,2, \dots ,8$$

$$\bar{\epsilon}_{max,1} = 1$$

$$w_{slack} = 1e^{12}$$

The penalization vectors Q_1, Q_2, Q_3, R_1, R_2 with dimensions $(N_P x N_P)$ are set as follows:

$$Q_1 = diag(1, \dots ,1)$$
$$Q_2 = diag(1, \dots ,1)$$
$$Q_3 = diag(100, \dots ,100)$$
$$R_1 = diag(1, \dots , 1)$$
$$R_2 = diag(1,6,11,16,21,26,31,36)$$

The corresponding parameters for the EC-NMPC approach are selected as follows:

$$0 \leq Q_a(k+i) \leq 92230, \quad i = 1,2, \dots ,8$$

$$20 \leq KLa(k+i) \leq 240, \quad i = 1,2, \dots ,8$$

$$-2500 \leq \Delta Q_a(k+i) \leq 2500, i = 1,2, \dots ,8$$

$$-100 \leq \Delta KLa(k+i) \leq 100, i = 1,2, \dots ,8$$

$$1 \leq S_{NO,2}(k+i) \leq 6, i = 1,2, \dots ,8$$

$$S_{NH,5}(k+i) \leq 4, i = 1,2, \dots ,8$$

$$S_{NO,5}(k+i) \leq 11, i = 1,2, \dots ,8$$

$$\bar{\epsilon}_{max,1} = 1$$

$$w_{slack} = 1e^{12}$$

The penalization vectors Q_1, Q_2, Q_3, R_1, R_2 with dimensions $(N_p x N_p)$ are set as follows:

$$Q_1 = diag(1, \dots ,1)$$
$$Q_2 = diag(1, \dots ,1)$$
$$Q_3 = diag(100, \dots ,100)$$
$$R_1 = diag(0.75, \dots , 0.75)$$
$$R_2 = diag(1,11,21,31,41,51,61,71)$$

It is worth mentioning that the predictive control schemes designed and implemented do not make use of any prediction model for the disturbances affecting the plant. The current values of the disturbances, i.e., the influent flow rate and its ammonia concentration $(Q_{in}, S_{NH,in})$, are assumed to be directly available from the plant at each time instant k, a fact that is common in real WWTPs, but future values are not known a-priori. So, the current values are kept constant for the duration of the prediction horizon in order to obtain the predictions of the state variables. The remaining elements of the influent stream, needed to obtain the predictions, i.e., the other 11 state variables of the ASM1 model, are assumed to be unknown and therefore kept to their constant values. In Table 6.2, Table 6.3, Table 6.4, the results of the closed-loop simulation and the comparison against the alternative approaches under the DRYINFLUENT, RAININFLUENT and STORMINFLUENT dynamic profiles, respectively, are presented.

In the columns of the tables, the evaluation metrics shown are described in chapter 5 of this thesis. It is obvious that the designed closed-loop control schemes outperform all the alternative control methodologies. More specifically, in the case of the DRYINFLUENT profile, the NMPC approach achieves 7.6%, 9.5% and 6.7% reduction of the mean value of ammonia concentration of the effluent stream compared to the DMC_48, DMC_96 and PI controllers, respectively. Moreover, despite the fact that the average value of the nitrate and nitrite nitrogen concentration of the effluent stream compared to the DMC controllers is increased by 4.4% and 5.2% - a 8.7% reduction has been achieved compared to default PI method – the effluent quality is improved by a factor of 5.2% against the PI controllers, 0.7% and 1.1% against the DMC controllers. Furthermore, the total amount of days at which the total nitrogen and the ammonia concentration of the effluent stream violates its limits have been reduced or kept at the same level. The most important aspect, though, is the fact that the aforementioned improvements have been made by reducing the total cost index of the operation of the plant by a factor of 14.8%, 2.9% and 5.1% compared to PI, DMC_48 and DMC_96 approaches. Regarding the EC-NMPC configuration, the total cost index of the operation of the plant has been reduced by a factor of 14.1%, 2.1% and 4.2% compared to the PI, DMC_48 and DMC_96 formulations. And at the same time, the quality of the effluent stream is improved by a factor of 4.6%, 0.5% and 0.8%, respectively. Consequently, the operational cost index of the plant is notably reduced; fact of significant importance, while there is also a marginally improvement of the effluent stream quality.

In the case of the RAININFLUENT weather profile, the NMPC approach manages to improve the quality of the effluent by 3.8%, and 0.4% compared to the PI and DMC_96 controllers, while reducing the total operational costs of the plant by 7.9% and 8.3% in comparison with the DMC controllers. In terms of the default PI methodology, the cost index is increased by 5%, yet the average value of the ammonia concentration of the effluent is reduced by 12.4%. Moreover, the total amount of days at which the total nitrogen and ammonia concentrations of the effluent violate their limits are reduced by 61.5% and 22%. The corresponding days regarding the DMC controllers are not given in [47]. In terms of the EC-NMPC formulation, the results are further improved. In particular, the quality of the effluent stream is improved by 4.1%, 0.4% and 0.7% against the PI and DMC controllers, while simultaneously reducing the cost index of the total operation by a factor of 7.7% and 8.1% compared to the DMC methodologies. The cost index is increased by 0.5% in comparison with the default PI controller, but the average values of the ammonia and nitrate and nitrite nitrogen concentrations of the effluent stream are reduced by 11.9% and 1.3%, respectively. In addition, the total amount of days at which violations of the effluent limits occur are improved by 62.8% and 22%.

Table 6.4 Simulation results under dry weather conditions

Controller	$\bar{S}_{NH,eff}$ $(g\,N.m^{-3})$	$\bar{S}_{NO,eff}$ $(g\,N.m^{-3})$	$N_{tot,eff}$ (days)	$S_{NH,eff}$ (days)	AE_5 $(kWh\,d^{-1})$	PE_{Qa} $(kWh\,d^{-1})$	CI $(kWh\,d^{-1})$	EQ $(kg\,d^{-1})$
Default PI	2.87	12.17	1.35	1.40	853.71	157.05	1010.76	6260.93
DMC_48	2.90	10.65	0.95	1.13	707.15	179.70	886.86	6004.73
DMC_96	2.96	10.57	0.90	1.18	734.97	171.88	906.85	6026.41
NMPC	**2.68**	**11.12**	**0.76**	**1.13**	**723.01**	**138.40**	**861.41**	**5963.83**
EC − MPC	**2.79**	**10.88**	**0.80**	**1.14**	**730.37**	**138.69**	**869.06**	**5979.01**

Table 6.3 Simulation results under rain weather conditions

Controller	$\bar{S}_{NH,eff}$ $(g\,N.m^{-3})$	$\bar{S}_{NO,eff}$ $(g\,N.m^{-3})$	$N_{tot,eff}$ (days)	$S_{NH,eff}$ (days)	AE_5 $(kWh\,d^{-1})$	PE_{Qa} $(kWh\,d^{-1})$	CI $(kWh\,d^{-1})$	EQ $(kg\,d^{-1})$
Default PI	3.55	8.94	1.06	2.05	823.63	204.94	1028.57	8367.31
DMC_48	3.20	8.72	–	–	955.88	217.40	1173.28	8055.41
DMC_96	3.24	8.70	–	–	970.55	207.99	1178.53	8082.54
NMPC	**3.11**	**8.99**	**0.43**	**1.60**	**922.16**	**158.79**	**1080.95**	**8056.46**
EC − MPC	**3.13**	**8.83**	**0.40**	**1.60**	**929.81**	**153.84**	**1083.65**	**8030.34**

Table 6.2 Simulation results under storm weather conditions

Controller	$\bar{S}_{NH,eff}$ $(g\,N.m^{-3})$	$\bar{S}_{NO,eff}$ $(g\,N.m^{-3})$	$N_{tot,eff}$ (days)	$S_{NH,eff}$ (days)	AE_5 $(kWh\,d^{-1})$	PE_{Qa} $(kWh\,d^{-1})$	CI $(kWh\,d^{-1})$	EQ $(kg\,d^{-1})$
Default PI	3.43	10.31	1.26	1.91	872.82	184.87	1057.68	7404.69
DMC_48	3.11	9.78	–	–	865.25	191.18	1056.43	7092.75
DMC_96	3.14	9.69	–	–	904.50	184.16	1088.66	7094.13
NMPC	**3.06**	**9.99**	**0.73**	**1.80**	**840.67**	**139.88**	**980.55**	**7100.59**
EC − MPC	**3.05**	**9.92**	**0.74**	**1.76**	**884.75**	**152.92**	**1037.67**	**7076.94**

In the case of the STORMINFLUENT dynamic profile, the NMPC approach reduced the total cost index of the plant by 7.3%, 7.2% and 10% in comparison with the PI and DMC configurations, while improving the effluent quality by 4.2% compared to the PI controllers. Against the DMC methods, the effluent quality is almost the same with an insignificant deterioration. The days at which violations occur are improved by 42.1% and 5.8% in terms of the total nitrogen and ammonia concentration, compared to the PI method and their average values are reduced by 3.2% and 11.8%, respectively. The corresponding days regarding the DMC configurations are not provided. The EC-NMPC approach manages to reduce the total cost index by 1.9%, 1.8% and 4.7% against the PI and DMC formulations, while improving the effluent quality by 4.5%, 0.3% and 0.3%, respectively. The number of days at which violations occur, compared to the PI strategy, are improved by 41.3% and 7.9% in terms of the total nitrogen and ammonia concentration of the effluent stream. The average values of the concentrations of these chemical compounds in the effluent stream are reduced by 11.1% and 3.8%. In Figure 6.3, Figure 6.4 and Figure 6.5, the dynamic responses of the ammonia and total nitrogen concentration of the effluent stream and the manipulated variables for the NMPC and EC-NMPC formulations under the dynamic influent profiles are shown.

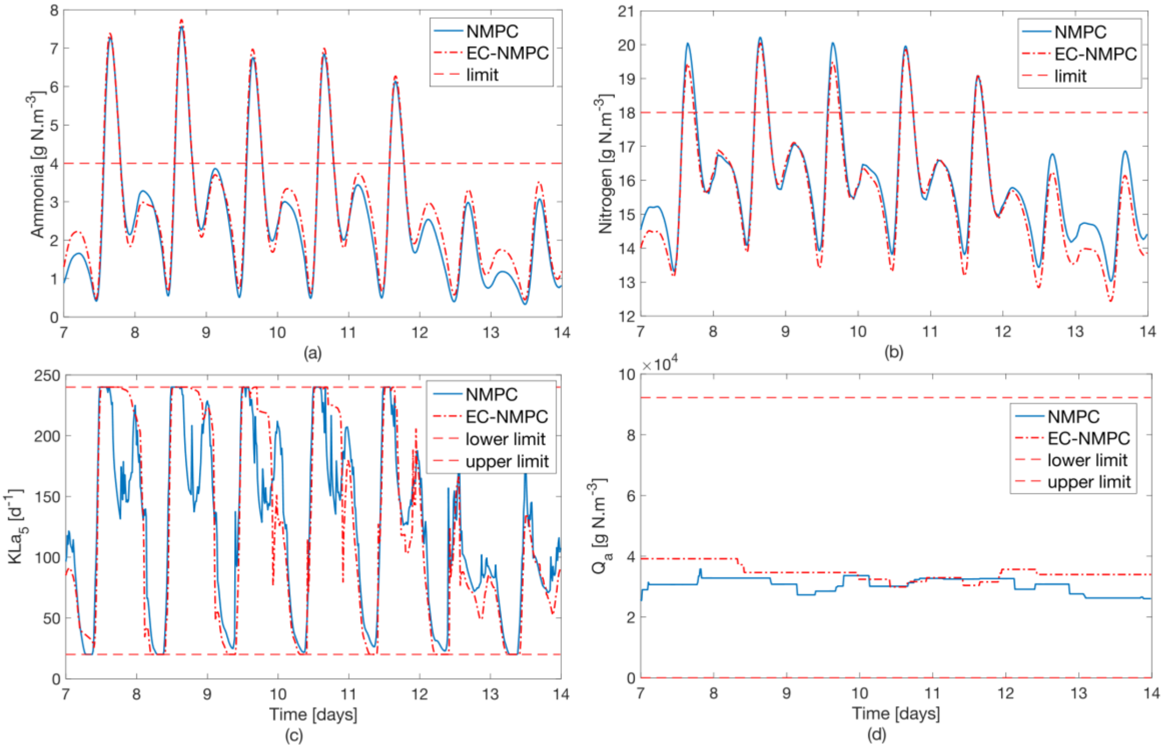


Figure 6.3 DRYINFLUENT: (a) Effluent ammonia concentration - (b) Effluent total nitrogen concentration - (c) Oxygen transfer coefficient - (d) Internal recirculation

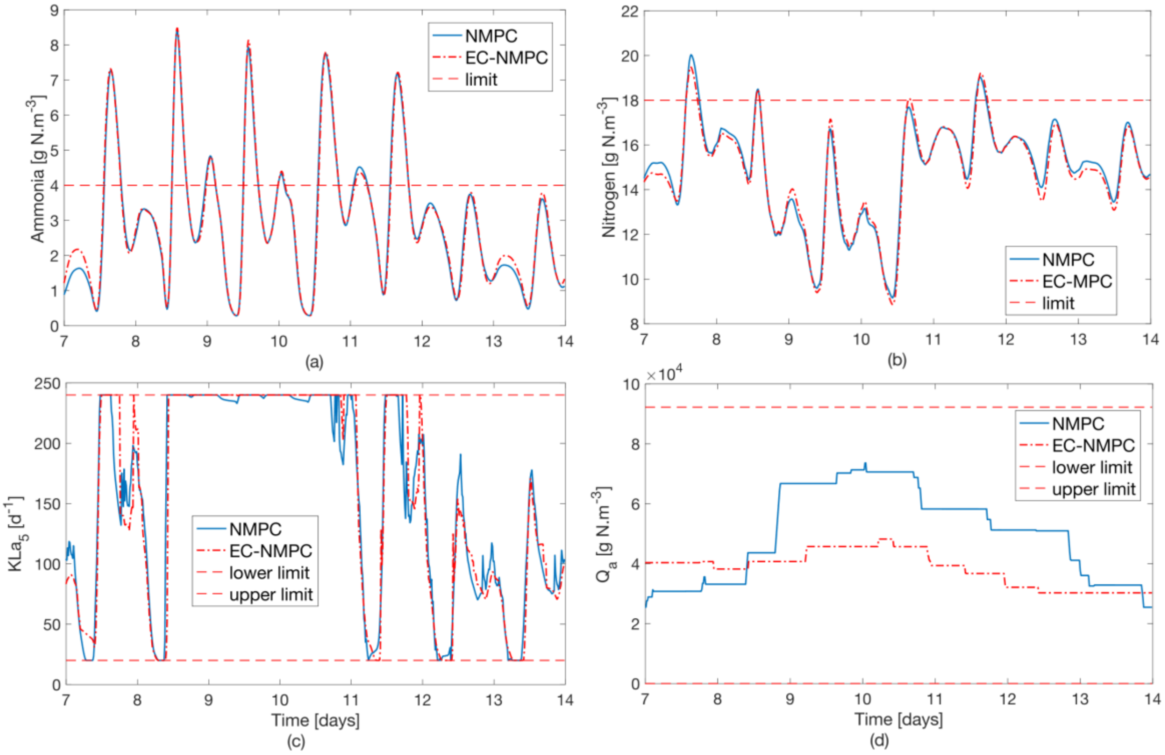


Figure 6.5 RAININFLUENT: (a) Effluent ammonia concentration - (b) Effluent total nitrogen concentration - (c) Oxygen transfer coefficient - (d) Internal recirculation

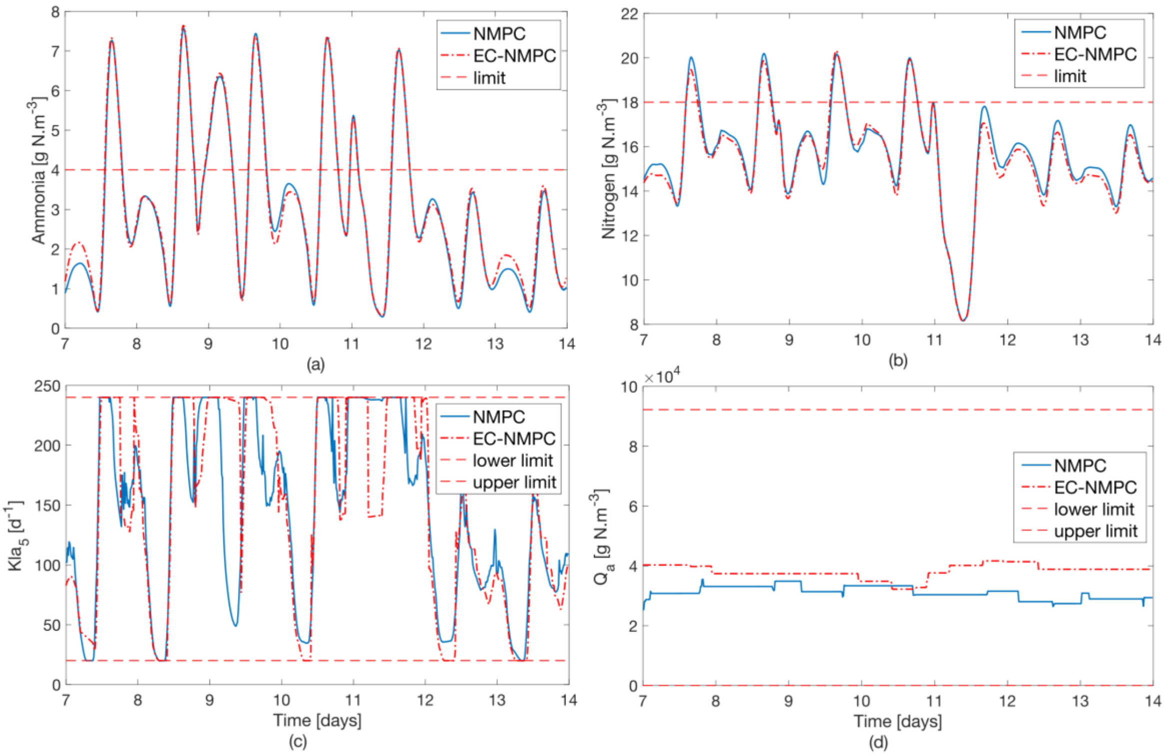


Figure 6.4 STORMINFLUENT: (a) Effluent ammonia concentration - (b) Effluent total nitrogen concentration - (c) Oxygen transfer coefficient - (d) Internal recirculation

6.4 Economic-Oriented MPC

6.4.1 Control Scheme Formulation

In this section, an economic-oriented MPC formulation is presented. As already stated, the aspects of energy consumption and total operational costs during full-scale operation of WWTPs, are of crucial importance. The predictive control approaches presented so far aim to maintain the plant at a fixed steady state operating point, in the presence of disturbances, leading in many cases to unnecessarily high energy demands in order to achieve the defined objectives. To deal with this situation, economic model predictive control (EMPC) approaches have been proposed [44], [45], [47] that aim to optimize the performance of the plant in terms of the energy efficiency, while concurrently maintaining compliance with the strict environmental regulations. In [44], an EMPC approach is proposed comprising an objective function that consists of the effluent quality and total operational cost index of the plant. To apply this control methodology full knowledge of the system's states (reactors and settlers) is required, i.e., a perfect match between the controlled process and the predictive model; a fact that is not possible when considering real-life applications. The numerous controllers designed and presented in [45] are based on predictions obtained from a model that is not capable of accurately simulating the dynamic behavior of BSM1, as already stated in section 2 of this chapter. In [47], two economic dynamic matrix control (EDMC) configurations are designed, which are based on linear step-response predictive models. However, due to their simplicity these models are not capable of predicting the future dynamic behavior of the plant with high accuracy when different operating regions are considered, thus leading to possible excessive control effort.

In this thesis, an economic oriented reformulation of the error-correcting (EC-(E)MPC) approach that was described in the previous section of this chapter, is presented. The predictions of the future dynamic responses of the states are obtained by employing the exact same methodology as the EC-NMPC configuration, but the formulation of the objective function is different. The goal of the designed control scheme is not to keep the plant at a specific steady state operating point, but to maintain it within an operating region that is predefined, while consuming the least possible amount of aeration and pumping energy. The predetermined operating region is mathematically described by specific state constraints, which are included in the optimization problem, the formulation of which is given below:

$$\min_{\substack{\Delta KLa(k),\Delta KLa(k+1),\ldots,\Delta KLa(k+Nc)\\ \Delta Q_a(k),\Delta Q_a(k+1),\ldots,\Delta Q_a(k+N_c)}} \left(AE^T \cdot R_1 \cdot AE\right) + \left(PE^T \cdot R_2 \cdot PE\right) + \cdots\cdots$$

$$\cdots + w_{slack} \cdot \left[\sum_{i=1}^{N_P}\sum_{j=1}^{3} \epsilon_{max,j}(k+i) + \sum_{i=1}^{N_P}\sum_{j=1}^{3} \epsilon_{min,j}(k+i)\right]$$

$$\text{s.t.}\quad AE = \left(\frac{8\cdot 1333}{1800}\right)\cdot [KLa(k)\ KLa(k+1)\ \ldots\ KLa(k+N_c)]^T$$

$$PE = 0.004 \cdot [Q_a(k)\ Q_a(k+1)\ \ldots\ Q_a(k+N_c)]^T$$

$$\hat{y}_1(k+i) = \hat{y}_{1,p}(k+i) + \hat{e}_1(k), i = 1,\ldots,N_p$$

$$\hat{y}_2(k+i) = \hat{y}_{2,p}(k+i) + \hat{e}_2(k), i = 1,\ldots,N_p$$

$$\hat{y}_3(\mathrm{k}+\mathrm{i}) = \hat{y}_{3,\mathrm{p}}(\mathrm{k}+\mathrm{i}) + \hat{e}_3(\mathrm{k}), \mathrm{i} = 1, \dots, \mathrm{N_p}$$
$$0 \le \epsilon_{\mathrm{min,j}}(\mathrm{k}+\mathrm{i}) \le \bar{\epsilon}_{\mathrm{min}}, \mathrm{i} = 1, \dots, \mathrm{N_P}, \mathrm{j} = 1, 2, 3$$
$$\epsilon_{\mathrm{max,j}}(\mathrm{k}+\mathrm{i}) \le \infty, \mathrm{i} = 1, \dots, \mathrm{N_P}, \mathrm{j} = 1, 2, 3$$
$$\underline{\mathrm{Q_a}} \le \mathrm{Q_a}(\mathrm{k}+\mathrm{i}) \le \overline{\mathrm{Q_a}}, \quad \mathrm{i} = 1,2, \dots, \mathrm{N_c}$$
$$\underline{\mathrm{KLa}} \le \mathrm{KLa}(\mathrm{k}+\mathrm{i}) \le \overline{\mathrm{KLa}}, \quad \mathrm{i} = 1,2, \dots, \mathrm{N_c}$$
$$\underline{\Delta\mathrm{Q_a}} \le \Delta\mathrm{Q_a}(\mathrm{k}+\mathrm{i}) \le \overline{\Delta\mathrm{Q_a}}, \mathrm{i} = 1,2, \dots, \mathrm{N_c}$$
$$\underline{\Delta\mathrm{KLa}} \le \Delta\mathrm{KLa}(\mathrm{k}+\mathrm{i}) \le \overline{\Delta\mathrm{KLa}}, \mathrm{i} = 1,2, \dots, \mathrm{N_c}$$
$$\Delta\mathrm{KLa}(\mathrm{k}+\mathrm{i}), \Delta\mathrm{Q_a}(\mathrm{k}+\mathrm{i}) = 0, \mathrm{i} = \mathrm{N_c}+1, \dots, \mathrm{N_p}$$
$$\left(\underline{\mathrm{S_{NO,2}}} - \mathrm{e_{min,1}}(\mathrm{k}+\mathrm{i})\right) \le \mathrm{S_{NO,2}}(\mathrm{k}+\mathrm{i}) \le \left(\overline{\mathrm{S_{NO,2}}} + \mathrm{e_{max,1}}(\mathrm{k}+\mathrm{i})\right), \mathrm{i} = 1,2, \dots, \mathrm{N_p}$$
$$\left(\underline{\mathrm{S_{O,5}}} - \mathrm{e_{min,2}}(\mathrm{k}+\mathrm{i})\right) \le \mathrm{S_{O,5}}(\mathrm{k}+\mathrm{i}) \le \left(\overline{\mathrm{S_{O,5}}} + \mathrm{e_{max,2}}(\mathrm{k}+\mathrm{i})\right), \mathrm{i} = 1,2, \dots, \mathrm{N_p}$$
$$\mathrm{S_{NO,5}}(\mathrm{k}+\mathrm{i}) \le \left(\overline{\mathrm{S_{NO,5}}} + \mathrm{e_{max,3}}(\mathrm{k}+\mathrm{i})\right), \mathrm{i} = 1,2, \dots, \mathrm{N_p}$$

where AE denotes the aeration energy that is being consumed in the last aerobic tank by modifying the oxygen transfer coefficient and PE is the pumping energy that is consumed by manipulating the internal recirculation flow rate. $\underline{\mathrm{S_{O,5}}}$ and $\overline{\mathrm{S_{O,5}}}$ correspond to lower and upper bounds enforced on the dissolved oxygen concentration of the last aerobic tank. The rest of the symbols are described in subsections 6.3.1 and 6.3.2. The optimization problem that is formulated at each discrete time-step based on the current values of the system's states and inputs, makes use of the identified reduced-order model, developed in this thesis, to predict the future dynamic behavior of the plant. Based on these predictions, it seeks to minimize the objective function comprising the plant's aeration and pumping energy, while simultaneously trying to satisfy the imposed constraints on specific state variables of the plant. Finally, it is worth mentioning that the proposed economic oriented predictive control scheme requires only 3 state variables to be directly collected from the actual plant and these are the nitrate and nitrite nitrogen concentration of the second anoxic tank, the dissolved oxygen and the nitrate and nitrite nitrogen concentration of the last aerobic tank. All 3 of these variables are commonly and reliably measured in real-life situations.

6.4.2 Simulation Results

The prediction and control horizons for the designed control scheme are set equal to 12, i.e., the dynamic behavior of the plant is predicted for the future 3 hours. The rest of the controller's parameters are selected as follows:

$$0 \le \mathrm{Q_a}(\mathrm{k}+\mathrm{i}) \le 92230, \quad \mathrm{i} = 1,2, \dots, 6$$
$$20 \le \mathrm{KLa}(\mathrm{k}+\mathrm{i}) \le 240, \quad \mathrm{i} = 1,2, \dots, 6$$
$$-2500 \le \Delta\mathrm{Q_a}(\mathrm{k}+\mathrm{i}) \le 2500, \mathrm{i} = 1,2, \dots, 6$$
$$-75 \le \Delta\mathrm{KLa}(\mathrm{k}+\mathrm{i}) \le 75, \mathrm{i} = 1,2, \dots, 6$$
$$1 \le \mathrm{S_{NO,2}}(\mathrm{k}+\mathrm{i}) \le 6, \mathrm{i} = 1,2, \dots, 6$$
$$1.15 \le \mathrm{S_{O,5}}(\mathrm{k}+\mathrm{i}) \le 2.5, \mathrm{i} = 1,2, \dots, 6$$

$$S_{NO,5}(k+i) \leq 11.5, i = 1,2, \dots ,6$$

$$\bar{\epsilon}_{max,1} = \bar{\epsilon}_{max,2} = 1$$

$$w_{slack} = 1e^{12}$$

The penalization vectors R_1, R_2, with dimensionality $(N_c x N_c)$, are set equal to:

$$R_1 = \text{diag}(100, \dots, 100)$$

$$R_2 = \text{diag}(1,51,101,151, \dots ,551)$$

The simulations have been carried out by following the specific guidelines found in [6] and which have already been stated in subsection 6.3.3. In the presented closed-loop control scheme, the disturbances are assumed to be measured at each discrete time-step and kept constant for the duration of the prediction horizon. The rest of chemical elements of the influent stream are considered unknown and therefore kept at their constant values. Tables 6.5, 6.6 and 6.7 present the results of the control scheme application, along with three alternative strategies, namely the default BSM1 PI controllers and the two EDMC configurations found in [47]. The robustness of the proposed control scheme is investigated by applying all dynamic influent profiles (dry, rain, storm) provided by [6].

In the case of the DRYINFLUENT profile, the EC-(E)MPC scheme outperforms the default PI controllers both in terms of effluent quality and energy consumption. More specifically, the quality of the effluent stream is improved by 2.5%, while the cost index of the plant's operation is reduced by 21.5%. The average values of the ammonia and nitrate and nitrite nitrogen concentrations of the effluent are diminished by 4.2% and 4.7%. The number of days at which the total nitrogen of the effluent violates its limits are reduced by 31.4%, while the ammonia concentration violates its limits by 3.5% more days; still keeping them at acceptable levels.

Table 6.5 Simulation results under dry weather conditions

Controller	$\bar{S}_{NH,eff}$ $(g\,N.m^{-3})$	$\bar{S}_{NO,eff}$ $(g\,N.m^{-3})$	$N_{tot,eff}$ (days)	$S_{NH,eff}$ (days)	AE_5 $(kWh\,d^{-1})$	PE_{Qa} $(kWh\,d^{-1})$	CI $(kWh\,d^{-1})$	EQ $(kg\,d^{-1})$
Default PI	2.87	12.17	1.35	1.40	853.71	157.05	1010.76	6260.93
EDMC_48	3.11	12.13	2.23	1.94	693.59	64.42	758.01	6388.86
EDMC_96	3.03	10.97	0.93	1.45	737.99	94.13	832.12	6131.22
EC − (E)MPC	**2.78**	**11.60**	**0.94**	**1.45**	**698.43**	**105.91**	**804.34**	**6105.13**

Table 6.6 Simulation results under rain weather conditions

Controller	$\bar{S}_{NH,eff}$ $(g\,N.m^{-3})$	$\bar{S}_{NO,eff}$ $(g\,N.m^{-3})$	$N_{tot,eff}$ (days)	$S_{NH,eff}$ (days)	AE_5 $(kWh\,d^{-1})$	PE_{Qa} $(kWh\,d^{-1})$	CI $(kWh\,d^{-1})$	EQ $(kg\,d^{-1})$
Default PI	3.55	8.94	1.06	2.05	823.63	204.94	1028.57	8367.31
EDMC_48	3.41	9.87	–	–	915.73	77.29	993.02	8488.80
EDMC_96	3.28	8.77	–	–	940.38	123.13	1063.51	8130.62
EC − (E)MPC	**3.36**	**8.68**	**0.51**	**2.19**	**727.68**	**176.71**	**904.39**	**8162.44**

Table 6.7 Simulation results under storm weather conditions

Controller	$\bar{S}_{NH,eff}$ $(g\,N.m^{-3})$	$\bar{S}_{NO,eff}$ $(g\,N.m^{-3})$	$N_{tot,eff}$ (days)	$S_{NH,eff}$ (days)	AE_5 $(kWh\,d^{-1})$	PE_{Qa} $(kWh\,d^{-1})$	CI $(kWh\,d^{-1})$	EQ $(kg\,d^{-1})$
Default PI	3.43	10.31	1.26	1.91	872.82	184.87	1057.68	7404.69
EDMC_48	3.67	11.11	–	–	784.31	56.28	840.59	7727.24
EDMC_96	3.27	9.88	–	–	870.42	105.71	976.13	7209.32
EC − (E)MPC	**3.31**	**9.73**	**0.75**	**2.15**	**726.82**	**143.31**	**870.13**	**7204.81**

Compared to the EDMC_48 controller, the EC-(E)MPC approach is superior in terms of the effluent quality at the expense of a 6.1% increase in the required energy. However, this expense comes with the fact that the effluent quality is improved by a factor of 4.5%. Furthermore, the mean values of the ammonia and nitrate and nitrite nitrogen concentrations of the effluent stream are reduced by 11.7% and 4.4%, respectively, while the number of days at which the total nitrogen and ammonia concentrations of the effluent stream violate their limits is improved by 58.9% and 25.3%. The superiority of the proposed approach is also validated by comparing its results against the EDMC_96 controller. In particular, EC-(E)MPC outperforms the alternative control strategy by reducing the amount of energy required by 3.4%, while simultaneously improving the quality of the effluent stream by 0.5%. The average value of the effluent ammonia concentration is reduced by 8.3%, the corresponding value of the nitrate and nitrite nitrogen is increased by 6%, the number of days at which the ammonia violates its limits is the same, while the respective number for the total nitrogen concentration of the effluent stream is slightly increased by 1%. Overall, it is obvious that the proposed control approach outperforms the alternative methodologies regarding the quality of the effluent stream and the energy efficiency of the plant.

In the case of the RAININFLUENT profile, the suggested economic-oriented closed-loop controller manages to outperform all 3 of the alternative control strategies. In particular, compared to the default PI methodology, the EC-(E)MPC controller decreased the cost index by 12.1%, while simultaneously improving the quality of the effluent by 2.5%. Moreover, the average values of the ammonia and nitrate and nitrite nitrogen concentrations of the effluent are reduced by 5.4% and 3%, respectively. The number of days at which the limits in terms of the effluent are violated, is lessened by 51.9% for the total nitrogen and increased by 6.8% for the ammonia concentration. In comparison with the EDMC_48 control configuration, the EC-(E)MPC strategy manages to reduce the cost index by 9%, while the quality of effluent was raised by 3.9%. The mean value of the ammonia concentration was kept at around the same value with a slight improvement of 1.5% and the corresponding value of the nitrate and nitrite nitrogen concentration was improved by 12.1%. Compared to the EDMC_96 formulation, the proposed approach achieves a reduction of the cost index by a factor of 15%, while the effluent quality is slightly deteriorated by a factor of 0.4%. The average value of the nitrate and nitrite nitrogen concentration is lowered by 1.1% at the expense of an increase in the mean value of the ammonia by 2.4%. It is obvious that by taking all the different evaluation metrics under consideration, the formulated EC-(E)MPC scheme improves the overall performance of the controlled process.

In the case of the STORMINFLUENT profile, compared to the default PI strategy, the designed controller achieves a reduction of the cost index by 17.8%, while improving the effluent quality by 2.7%. The average values of the ammonia and nitrate and nitrite nitrogen concentrations are decreased by 3.5% and 6.7%, respectively. Furthermore, the days at which the effluent limits regarding the total nitrogen are violated, are reduced by 40.5%, while a 12.5% increase in the corresponding days for the ammonia concentration is observed. Compared to the EDMC_48 methodology, the proposed approach requires 3.5% more energy, but improves the quality of the effluent by 6.8%. Consequently, this small increase in the required energy is justified by a considerable improvement of the effluent quality. Moreover, the average values of the ammonia and nitrate and nitrite nitrogen concentration are lessened by 9.9% and 12.5%, respectively. In comparison with the EDMC_96 controller, the EC-(E)MPC formulation achieves a 10.9% reduction of the cost index while at the same maintaining the effluent quality at the same level. Finally, the mean value of the nitrate and nitrite nitrogen concentration is lowered by 1.6% and the corresponding value of the ammonia concentration is increased by 1.2%. Taking all the aforementioned under consideration, it is straightforward that the implemented closed-loop control configuration proves to be superior than the alternative control strategies. In the below figures Figure 6.6, Figure 6.7 and Figure 6.8, the dynamic responses of the ammonia and total nitrogen concentration of the effluent stream and the manipulated variables for the EC-(E)NMPC formulations under the dynamic influent profiles are shown.

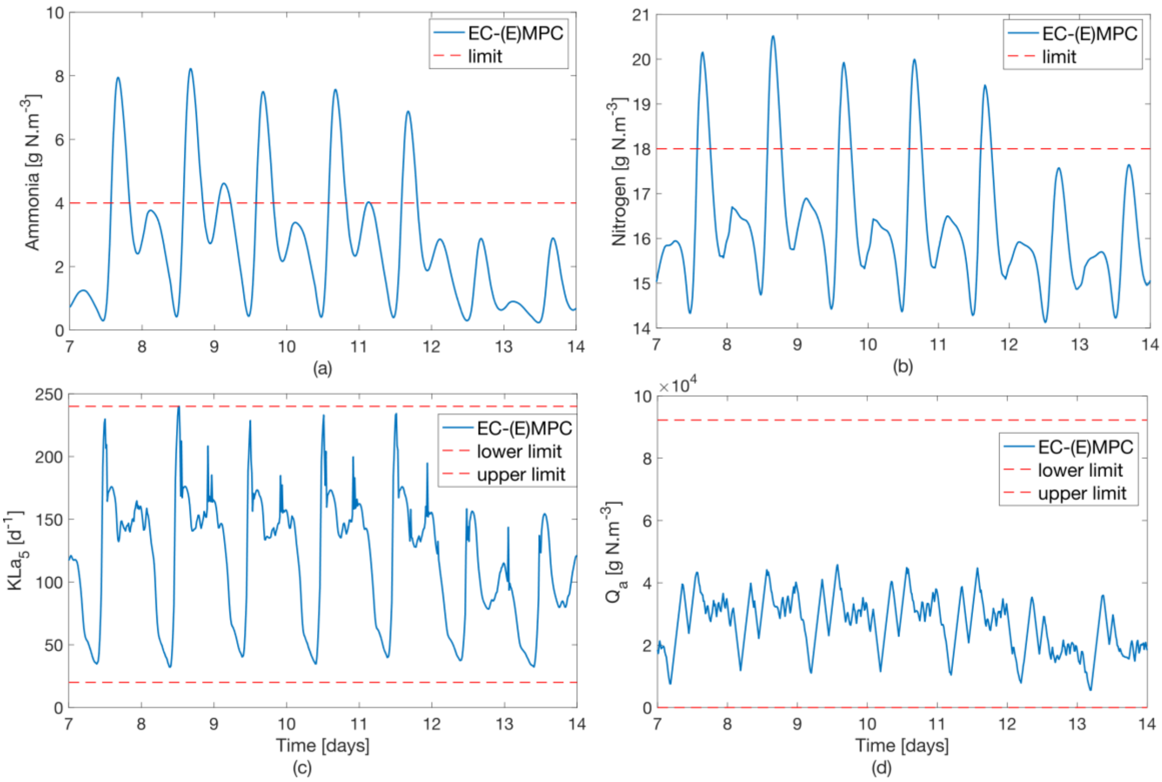


Figure 6.6 DRYINFLUENT: (a) Effluent ammonia concentration - (b) Effluent total nitrogen concentration - (c) Oxygen transfer coefficient - (d) Internal recirculation

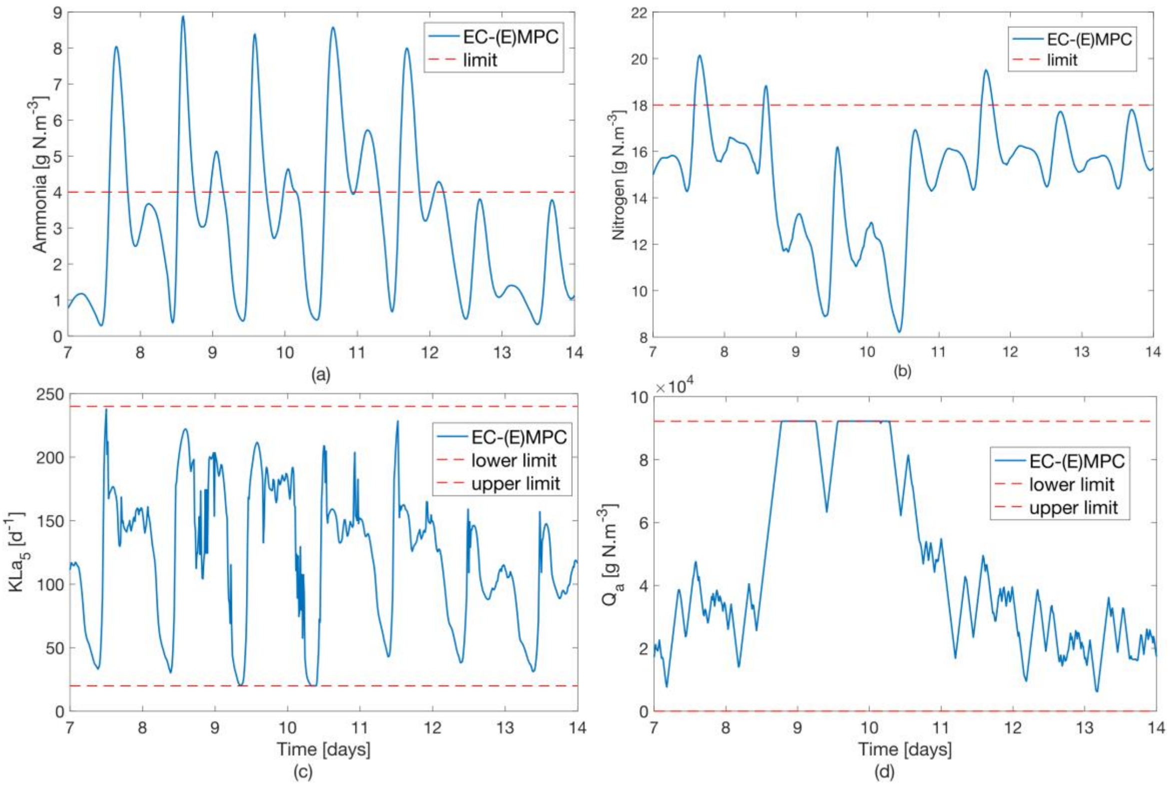


Figure 6.7 RAININFLUENT: (a) Effluent ammonia concentration - (b) Effluent total nitrogen concentration - (c) Oxygen transfer coefficient - (d) Internal recirculation

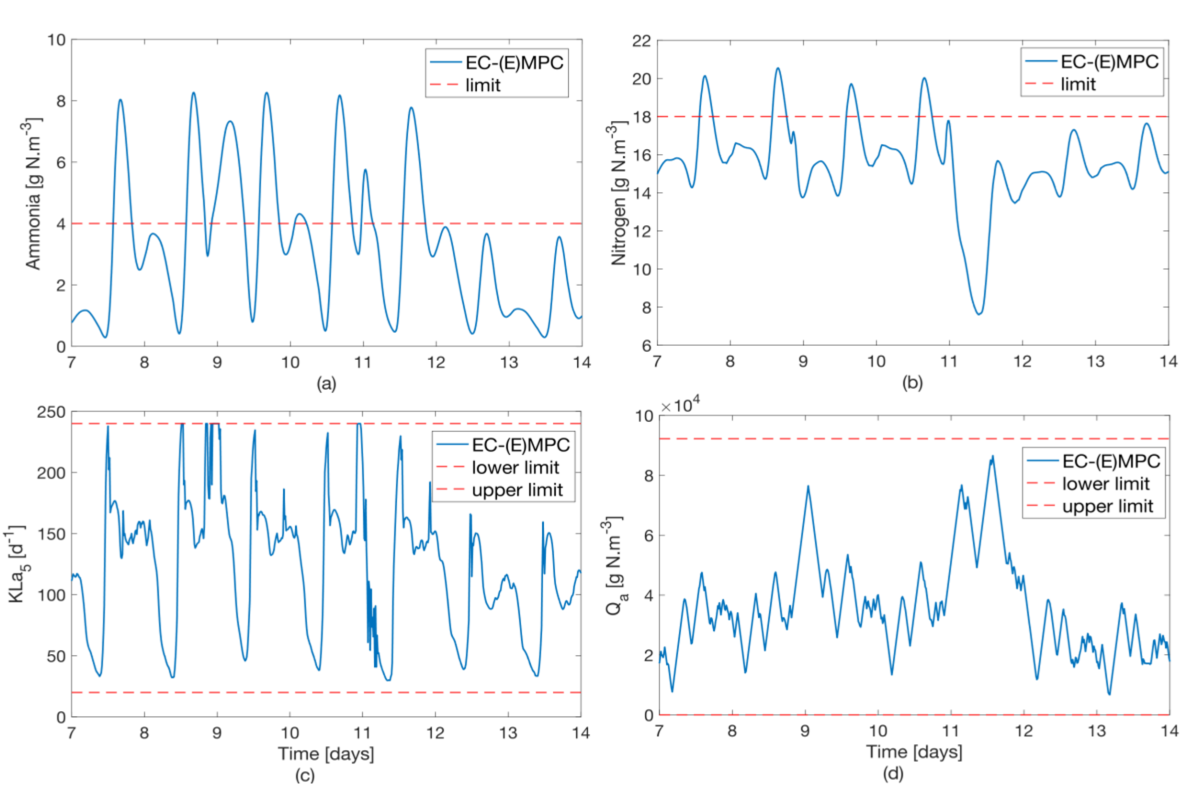


Figure 6.8 STORMINFLUENT: (a) Effluent ammonia concentration - (b) Effluent total nitrogen concentration - (c) Oxygen transfer coefficient - (d) Internal recirculation

6.5 Discussion

In this chapter, three different predictive control formulations have been presented, aiming optimize the operation of WWTPs in terms of compliance with the strict environmental regulations that have to be met and of energy efficiency. The formulated closed-loop control schemes were compared against alternative control methodologies that have been proposed in the literature and the results prove that developed schemes were able to outperform them.

In particular, the NMPC and EC-NMPC approaches proved to be superior than the DMC controllers proposed in [47] and correspondingly the EC-(E)MPC scheme outperformed the EDMC controllers designed in [47]. It should be noted that in [47], it was found that the EDMC formulations manage to outperform the economic approaches proposed in [44], [45], this being a strong indication that the economic-oriented control configuration presented in this thesis is also superior compared against those presented in [44], [45]. Furthermore, the robustness of the proposed controllers was investigated by applying the same tuned formulations on the rain and storm weather influent profiles that include large fluctuations of the active disturbances, i.e., the influent flow rate and its ammonia concentration. The results indicate that the control schemes exhibit a high level of robustness since they were able to outperform the alternative strategies without any modifications regarding their tuning parameters.

Another important advantage of the proposed predictive control formulations is their ability to achieve improved results despite the fact that the formulated optimization problems, which are being solved at each time-step, were of relative low complexity. To be more specific, in [47], the DMC and EDMC controllers need solve at each discrete time-step k optimization problems that consist of 96 and 192 design variables, since the control horizons of the schemes are set equal to 48 and 96 and the controller determines the values of two manipulated variables. In the predictive control formulations presented in this thesis, the control horizons of the NMPC and EC-NMPC approaches are set equal to 8 and of the EC-(E)MPC scheme equal to 12. Therefore, the number of design variables of the formulated optimization problems at each discrete time-step k is 16 and 24, respectively. It is obvious that although the predictive model utilized in the presented MPC controllers is more complex than the linear step-response models employed in [47], the resulting closed-loop control configurations are of lower computational complexity compared to the DMC and EDMC formulations.

7 Conclusion

7.1 Summary Results

In this thesis, a complete modelling, identification and control framework for wastewater treatment plants has been developed. At first, a reduced-order model of the widely known benchmark simulation model no. 1 has been derived by considering only the important states of the activated sludge model no. 1 and neglecting those describing the formation mechanisms of states that are commonly and reliably measured in actual WWTPs and those that are of low importance for control purposes. Moreover, the mathematical model utilized in BSM1 to describe the settling procedure consisting of 80 states was replaced by a single time-varying constant that is based on coefficients directly available from the WWTP.

The developed reduced-order model describing the activated sludge process of the anoxic and aerobic reactors of BSM1 includes 18 parameters, significantly affecting its dynamic behavior. In order for the reduced-order model to simulate the dynamic response of the original BSM1 with high accuracy, the values of these parameters have to be estimated. Due to the complexity of the process, advanced system identification techniques have to be employed, for the purpose of estimating these coefficients accurately. To this end, in this thesis a system identification scheme for estimating the values of these parameters, based on states measurements that can be reliably and directly collected from actual plants, is proposed. In particular, only measurements of nitrate and nitrite nitrogen, dissolved oxygen and ammonia concentration are needed; these chemical elements are commonly measured in actual plants.

The proposed system identification scheme is based on solving a nonlinear optimization problem, which exhibits a number of unwelcome properties such as high-dimensionality and multimodality. As classical optimization solvers would fail to approach a satisfactory solution for this type of problems, a customized cooperative particle swarm optimization approach is proposed in this work. The CPSO solver is capable of taking advantage of the correlations that exist between the design variables by separating them into distinct swarms and the presented results prove that the utilized approach manages to estimate the values of the model coefficients with high accuracy.

The identified reduced-order model is then integrated into model predictive control schemes aimed to optimize the performance, energy efficiency and total operation costs of WWTPs. Firstly, a nonlinear tracking MPC formulation is presented, which is compared against alternative predictive control schemes and the default control strategy of BSM1. The simulation results from applying all the dynamic influent profiles validate the superiority of the proposed control configuration against the other approaches. Furthermore, an error-correcting nonlinear tracking MPC configuration is introduced, which needs limited measurements to be directly collected from the plant, i.e., only the controlled variables need to be available from the actual process. This formulation is also compared against other predictive control strategies and the default controllers of BSM1, and the obtained results prove that this formulation also outperforms the alternative methodologies, in terms of effluent quality, energy efficiency and total operational costs. Moreover, an economic-oriented error-correcting nonlinear model predictive control formulation is proposed for optimizing the energy efficiency and total operational costs of the plant. The optimization problem objective function comprises the plant aeration and pumping energy and the controller tries to minimize it by properly selecting the values of the manipulated inputs. In addition, specific constraints are imposed on the controlled variables of the plant in order to guarantee compliance with the strict environmental regulations. The presented approach is compared against alternative economic-oriented predictive control schemes that have been proposed and the results validate its superiority both in terms of effluent quality and total operational costs.

It is worth mentioning that the developed modelling, identification and control framework can be applied to any wastewater treatment plant that combines nitrification and denitrification in order to achieve biological removal. The BSM1 model is implemented in the Simulink environment and therefore, it can be easily adapted to any specific WWTP by modifying the number of the process lines and of the reactive units. The data, which need to be collected in order to implement the identification procedure can directly and reliably be collected by common sensors installed in the WWTP facility. The amount of the collected data can, then, be used to identify the parameters of both the adapted BSM1 model consisting of all the states and the complete settling process [22] and of the corresponding reduced-order one by employing the system identification scheme presented in section 4.1. By using the adapted full BSM1 model as the controlled plant and the reduced-order for control design, closed-loop control configurations can be formulated and tested before being applied in the actual plant.

7.2 Future Research

The optimization of the performance and energy efficiency of WWTPs is a concept that is being widely studied, since nowadays, circular economy models are increasingly being adopted in the world and WWTPs are a major part of these economies. To this end, the orientation of future research related to the presented topics of this thesis, will be the construction of closed-loop predictive control schemes aimed to further improve the operation of WWTPs. More specifically, a major part of the future research will be oriented towards enhancing the model predictive control schemes presented by incorporating reinforcement learning techniques. The inclusion of this advanced machine learning methodology is expected to significantly improve the performance of WWTP controllers. Finally, another big part of future research will be oriented towards implementing the proposed modelling and control framework in real-world WWTPs.

Future Research

8 Bibliography

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