Efficient Energy Reduction in a Closed-Loop Uncertain Water-Treatment Aeration Sequencing Batch Reactor

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Abstract

Sequential batch reactors are increasingly used in the purification and waste water treatment since it is one of the main innovative alternatives with great flexibility operation and low investment costs. The uncertainty is present in most practical and real cases. The effect of the uncertainty in the model parameters could be determined through a parametric sensitivity analysis. In this work we present the formulation of the Non Linear Model Predictive Control (NMPC) to optimal aeration policies on closed-loop using the SBR technology under conditions of uncertainty, using two approaches: stochastic and robust (NMPC) such that the target specified determined are achieved within the operation time.

Keywords: Uncertainty, Stochastic, Optimization, Predictive control

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1 Introduction

Water biological treatment processes can be classified depending on the metabolic functions of microorganisms as follows [20]: (a) aerobic processes, in which oxygen is the primary electron acceptor, (b) anoxic processes which is carried out in presence of low concentrations of molecular oxygen, and (c) anaerobic processes, carried out in the absence of oxygen. Depending on the form of association of microorganisms, they can be classified as of fixed growth or in suspension. In processes with biomass, the microorganisms grow adhered to an inert material whereas in the suspended biomass processes, the flocks are kept in suspension due to mixing. The aerobic process with suspended biomass is commonly referred to as activated sludge [14]. In a typical biological wastewater treatment process the degradation of organic matter by microorganisms occurs first followed by the separation of the treated water from the microorganisms. In a continuous process these stages are carried out in two tanks. In the first tank, also referred to as the biological reactor, the set of biochemical reactions are carried out allowing mineralization of pollutant organic material; in the second tank, a sedimenter is deployed and separates the microorganisms of the treated effluent. In batch systems both treatment processes are performed in the same tank, i.e. biochemical reactions followed by a phase of sedimentation and the subsequent draining of the reactor.

The use of sequencing batch reactors (SBR), is one of the main innovative alternatives that has been used for the treatment of water effluents as shown in Figure 1. The SBR system operates as a dynamic system through a series of stages, i.e. (1) Filling, (2) Reaction, (3) Sedimentation, (4) Decantation and (5) Idle. In the filling phase the substrate (waste water) is added to the reactor. In the reaction step, the microorganisms decompose the organic matter using the oxygen provided from aeration. In the sedimentation phase, the separation of solids to achieve a supernatant, clarified as effluent, takes place. In the decantation phase, the separation of solids is carried out without disturbing the settled sludge. In the idle stage the wastage of sludge is pumped to a digester anaerobic to reduce the volume of sludge to be scrapped. The SBR water treatment process offers the following benefits with respect to continuous processes: flexibility in the operation and reduced investment costs, since a single tank is employed as both reactor and settler.

Mathematical models are widely used at the process design stage to specify the optimal set of operating conditions that meet the design goals at minimum cost. Typically, these decisions assume perfect knowledge of the process model parameters, and that those values may not be changing significantly during process operation.However, in practice the model parameters may change thus making the operation dynamically infeasible, i.e. the system may not meet the product specifications. While feedback control systems can be implemented to account for model parameter uncertainty, it is often difficult to state explicitly the amount of uncertainty that a feedback controller can tolerate before the system becomes infeasible, (unless uncertainty is part of the design of the feedback mechanism). Another approach used to account for model uncertainty has to do with the deployment of stochastic and robust optimization approaches [8], [1], [37], [9]. In the stochastic and robust schemes, uncertainty is incorporated in the optimal design formulation as a probability distribution function or as upper and lower bounds on the uncertain parameters, respectively [38], [35], [6].

In a previous work [2] we have proposed a deterministic optimization approach for the calcu-

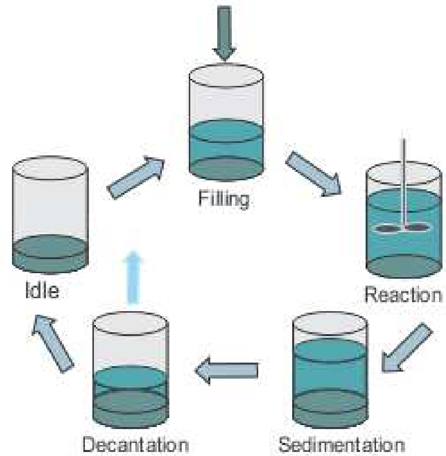


Figure 1: Operation stages in a sequencing batch reactor.

lation of open-loop optimal control policies of SBR water treatment systems. In that work, it has been shown that fractional values of the aeration control actions resulted in more attractive solutions rather than using the traditional on/off control policies typically implemented in SBR systems. Accordingly, a non-linear programming formulation suffices for proper optimal control purposes and that a more challenging and intensive mixed-integer non-linear programming approach is not needed. In the present study, we extended that previous work to include the impact of model uncertainty on the performance of the optimal control policies. Hence, we propose robust and stochastic non-linear model predictive control schemes to deal with model parameter uncertainty. A sensitivity analysis was carried out to gain insight on the model parameters featuring the strongest influence on model response. For the stochastic formulation, the uncertain parameters were assumed to follow a user-defined probability distribution function and power series expansions where used to propagate the uncertainty effects into the process outputs. In the robust formulation, the uncertainty was modeled as lower and upper bounds on selected model parameters and a multi-scenario optimization approach was then used for its discretization.

2 Problem definition

The removal of pollutants from wastewater streams is a public health problem which demands technically efficient and cost competitive strategies. Some of the proposed wastewater treatment processes involves chemical reaction systems from which pollutants are transformed into nontoxic compounds. The set of reactions are carried out in chemical reactors whose proper design and operation are crucial for achieving efficient pollutant removal at minimum capital and operating costs. Amongst the approaches proposed for wastewater treatment, sequencing batch reactors (SBR) have shown great operating flexibility and profitability. Although there have been many published works addressing the design and operation of SBR's, very few works have addressed the impact of process uncertainty on the performance of such reactors. The importance of taking into account uncertainty during the operation of SBR's turns out to be critical because otherwise the operation of these reactors can be infeasible and/or unprofitable.

The problem under consideration can be formulated as follows:

Given,

- A dynamic model that describes the transient behavior of a wastewater treatment deploying microorganisms,
- A set of nominal parameter values,
- A set of uncertain process parameters with either a probability-based (stochastic scheme) or bound-based (robust scheme) description, and
- Target values of those variables influencing water quality.

Then, the problem consists in computing closed-loop optimal control policies of the aeration profiles under model uncertainty such that the target values determining water quality are reached in minimum operating time deploying a robust and stochastic nonlinear model predictive control approach.

Mathematical model

One of the most common mathematical models used for wastewater treatment is the ASM1 model [19], [18]; an extension of the model presented in [26], [23] is used in the present work. The activated sludge model 3 (ASM3) takes into account the energy storage to describe the biodegradable substrate and oxygen consumption. As shown in 2.1-2.8, the dynamic model used in this work consists of 8 states. The present model assumes that the organic matter and nitrogen are the main pollutants that must be removed from a domestic wastewater stream.

$$\frac{dS_s}{dt} = \left(-\frac{r_{aae}}{Y_{Haer}} - \frac{(r_{aNO3} + r_{aNO2})}{Y_{Hanox}}\right)(1 + S_{t_s}) \tag{2.1}$$

$$\frac{dX_H}{dt} = r_{aae} + r_{aNO3} + r_{aNO2} \tag{2.2}$$

$$\frac{dX_{Ns}}{dt} = r_{aaNs} \tag{2.3}$$

$$\frac{dX_{Nb}}{dt} = r_{aaNb} \tag{2.4}$$

$$\frac{dS_O}{dt} = u(t) \cdot K_{La}(S_0'' - S_0) - \frac{(1 - Y_{Haer})}{Y_{Haer}} r_{aee} - \left(\frac{3.43}{Y_{A1}} - 1\right) r_{aaNs} - \left(\frac{1.14}{Y_{A2}} - 1\right) r_{aaNb} \tag{2.5}$$

$$\begin{aligned} \frac{dS_{NH4}}{dt} = &- \left(-\frac{i_{NSS}}{Y_{Haer}} + i_{NB}\right) r_{aae} - \left(-\frac{1}{Y_{A1}} + i_{NB}\right) r_{aaNs} - i_{NB} r_{aaNb} - \left(-\frac{i_{NSS}}{Y_{Hanox}} + i_{NB}\right) r_{aNO3} \\ &- \left(-\frac{i_{NSS}}{Y_{Hanox}} + i_{NB}\right) r_{aNO2} \end{aligned} \tag{2.6}$$

$$\frac{dS_{NO2}}{dt} = \frac{r_{aaNs}}{Y_{A1}} - \frac{r_{aaNb}}{Y_{A2}} + \frac{(1 - Y_{Hanox})}{1.14 Y_{Hanox}}(r_{aNO3} - r_{aNO2}) \tag{2.7}$$

$$\frac{dS_{NO3}}{dt} = \frac{r_{aaNb}}{Y_{A3}} - \frac{(1 - Y_{Hanox})}{1.14 Y_{Hanox}} r_{aNO3} \tag{2.8}$$

where the terms for the chemical reactions are as follows:

$$
\begin{aligned}
r_{aae} &= \mu_H \left(\frac{S_s}{S_s+K_s}\right)\left(\frac{S_O}{S_O+K_{O1}}\right)\left(\frac{S_{NH4}}{S_{NH4}+K_{NH}}\right) X_H && (2.9)\\
r_{aNO3} &= \mu_{H1} \left(\frac{S_s}{S_s+K_s}\right)\left(\frac{S_{NO3}}{S_{NO3}+K_{NO3}}\right)\left(\frac{K_{O21}}{K_{O21}+S_O}\right)\left(\frac{S_{NH4}}{S_{NH4}+K_{NH}}\right) X_H && (2.10)\\
r_{aNO2} &= \mu_{H2} \left(\frac{S_s}{S_s+K_s}\right)\left(\frac{S_{NO2}}{S_{NO2}+K_{NO2}}\right)\left(\frac{K_{O22}}{K_{O22}+S_O}\right)\left(\frac{S_{NH4}}{S_{NH4}+K_{NH}}\right) X_H && (2.11)\\
r_{aaNs} &= \mu_{A1} \left(\frac{S_O}{S_O+K_O}\right)\left(\frac{S_{NH4}}{S_{NH4}+K_{NH}}\right) X_{Ns} && (2.12)\\
r_{aaNb} &= \mu_{A2} \left(\frac{S_{NO2}}{S_{NO2}+K_{NO21}}\right)\left(\frac{S_O}{S_O+K_O}\right)\left(\frac{S_{NH4}}{S_{NH4}+K_{NH}}\right) X_{Nb} && (2.13)
\end{aligned}
$$

The description of the main states and the initial values of the states are shown in Table 1; Table 2 lists the nominal values of the model parameters.

Table 1: States initial values

	State	Description	Value	Units
(1)	S_S	Carbonaceous substrate	1000	$gCOD/m^3$
(2)	X_H	Heterotrophic bacteria	500	
(3)	X_{N_s}	Ammonia oxiders	100	
(4)	X_{N_b}	Nitrite oxiders	100	
(5)	S_O	Dissolved oxygen	0	gO_2/m^3
(6)	S_{NH4}	Ammonia	50	gN/m^3
(7)	S_{NO2}	Nitrite	2	gN/m^3
(8)	S_{NO3}	Nitrate	5	gN/m^3

3 Robust non-linear dynamic optimization formulation

It has been widely demonstrated that model uncertainty affects process operation and may lead to a loss in performance and process economics. In this section we consider the deployment of a model predictive control (MPC) strategy that specifies suitable control policies while considering the influence of model uncertainty on process performance in closed-loop. Although feedback control systems have embedded robustness properties [25] they do not guarantee feasibility in the presence of plant-model mismatch since uncertainty is not explicitly considered in the control algorithm.

In this work only time-invariant model uncertainty has been considered for both MPC schemes. That is, the true value of the uncertain parameters is not known with certainty; however, its value is assumed to remain constant during operation and lie between certain (user-defined) bounds or follow a (user-defined) probability distribution function. Therefore, there are at least two ways to approach the solution of optimization problems when it comes to consider the presence of model uncertainty, i.e. Stochastic and Robust optimization. In the stochastic optimization framework [8],

Table 2: Nominal parameter values

Parameter	Value	Units
K_{La}	1000	day^{-1}
i_{NB}	0.086	gN/gCOD
Y_{Haer}	0.1302	
Y_{A1}	0.1327	gCOD/gN
Y_{A2}	0.0985	gCOD/gN
Y_{A3}	0.0331	gCOD/gN
i_{NSS}	0.01	
Y_{Hanox}	0.0632	day^{-1}
S_{t_s}	1.6	
K_s	1	mgCOD/L
μ_H	0.6021	day^{-1}
μ_{H1}	0.0511	day^{-1}
μ_{H2}	0.0362	day^{-1}
μ_{A1}	1.4	day^{-1}
μ_{A2}	0.3	day^{-1}
K_{O1}	0.2	mgO_2/L
K_{NH}	0.1	mg/L
K_O	0.8	mg/L
K_{NO2}	0.25	mgN/L
K_{NO3}	0.5	mgN/L
K_{O21}	0.2	mgO_2/L
K_{O22}	0.2	mgO_2/L
K_{NO21}	0.5	mg/L
S_0''	7	mgO_2/L

[4] model uncertainty is represented as probabilistic distribution functions, whereas in the Robust optimization approach [1] ,[12] model uncertainty is represented as member of an uncertain set. The decision about which approach is more convenient for handling uncertainty depends on the available information and the goals to attain by the designer. If enough uncertainty measurements are available, so a probabilistic distribution function can be established, then the stochastic approach can be a feasible approach for optimization under uncertainty. On the other hand, when only very few or no measurements are available, or the value of a given design parameter is unknown, but it can be described within a given set, then robust optimization is preferred. In this work, we will deploy both the robust and stochastic optimization approaches for handling uncertainty.

There are several ways of representing uncertainty in robust optimization [9], [39]; in any case, the uncertain parameters are assumed to belong to some of the following uncertain sets: (1) Finite, (2) Interval-based, (3) Polytopic, (4) Norm-based, (5) Ellipsoidal and (6) Constrain-wise uncertainty. The selection as to how to describe model uncertainty totally depends upon the way uncertainty emerges in the problem under consideration. The first approach (Finite uncertainty) is one of the fundamental approaches to deal with uncertainty in robust optimization and it consists of assuming that the true value of the uncertain parameter is located within an uncertain set whose realizations are given in terms of lower and upper bounds. This is the representation that has been used in this work to model uncertainty.

After process uncertainty has been addressed the following step in the robust optimization approach consists in formulating the Robust Optimization Counterpart which consists in the approximation of the original uncertain optimization problem by a numerically tractable optimization formulation. There are several examples of how to deal with this approximation for linear or convex optimization problems for several types of uncertain sets [9]. However, for nonlinear programming problems such approximation can be difficult or impossible to establish. In these cases, the approach based on the deployment of *scenarios* [15], [34], [3] is a feasible way to take into account the effect of model uncertainty on optimization. Therefore, as shown in Figure 2, the approach consists in discretizing the $[X^U - X^L]$ uncertain interval into a number of *scenarios* (the total number of scenarios is denoted as N_s); within each scenario the value of the uncertain parameter remains constant. Hence, instead of solving a single optimization problem, as each process constraint is explicitly defined in terms of the scenarios considered for the uncertain parameters, i.e. a single constraint will be represented in the robust formulation with N_s constraints, each evaluated at a particular realization in the uncertain parameter set. In the deterministic case, the solution of N_s optimization problem is sought assuming that uncertainty is present in only one model parameter. It should be stressed that deploying this approach for handling model uncertainty, the original uncertain optimization problem is transformed into a larger deterministic optimization problem (with the size depending on the number of scenarios).

While easier to implement, there are at least two disadvantages associated to the robust approach for handling model uncertainty. The first one is related to the fact that *conservative* solutions can be obtained from this approach since the optimized values in the decision variables have to meet system constraints for every realization considered in the uncertain parameter set. This is normally achieved at the expense of sacrificing performance. The second disadvantage was already highlighted and has

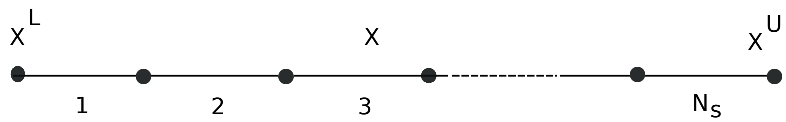


Figure 2: Multi-scenario approach to represent model uncertainty in an optimization framework.

to do with the fact that the robust multiscenario approach tend to produce larger optimization problems as the number of scenarios increases, which may become computationally intractable. One way to deal with this problem consists in solving the resulting deterministic large scale problem using an optimization decomposition approach [16], [17]. In addition, the traditional or conventional robust optimization approach only handles "here and now" decisions meaning that all decision variables are calculated before uncertainty realization is known. However, improved optimal solutions can be obtained by also considering the calculation of "wait and see" decision variables [28]. Attempts have been reported [36], [5] to extend the robust optimization approach for dealing with two-stage uncertain problems in the way is performed in stochastic optimization [8]. A recent review on the effect of uncertainty on optimization can be found elsewhere [13]. Moreover, some interesting connections between robust optimization and flexibility problems [21] in Process System Engineering have been recently reported [29].

An alternative option that can reduce the conservatism in the results is to treat the uncertain variables as random variables. That is, in the robust scheme, the uncertain parameters are discretized to a specific set of scenarios, each with an equal (uniform) probability of occurrence. In the stochastic approach, the uncertain parameters are treated as time-invariant random variables that are assumed to follow a probability distribution function, which is used to weight the realizations in the uncertain parameters. Thus, stochastic descriptions may reduce the conservatism in the solution at the expense of allowing violations to the process constraints. Nevertheless, the user can assign different levels of satisfaction to each constraint based on their level of importance (i.e. risk). Both the robust and stochastic approaches are presented here in the context of MPC, which is discussed next.

Model predictive control is the one of the most powerful strategies to perform control for chemical systems due to its ability to handle explicit constraints and nonlinearities embedded in mathematical models as well as dead time and multivariable systems [24], [10], [31], [11]. Moreover, in this work we consider the presence of uncertainty in some model parameters on the closed-loop performance. This control strategy is known as uncertain non-linear model predictive control. Figure 3 shows the typical behavior of a closed loop model predictive control system. At every k sampling time m control actions are computed in advance deploying a prediction horizon composed of m sampling times; the corresponding control actions are denoted by u_{k+m}. Although several control actions are computed, only the first control action is implemented ignoring the remaining control actions. When the new measurements are available, the nonlinear MPC (NMPC) algorithm is updated and a new calculation of the control action is performed.

The multi-scenario uncertain NMPC reads as follows:

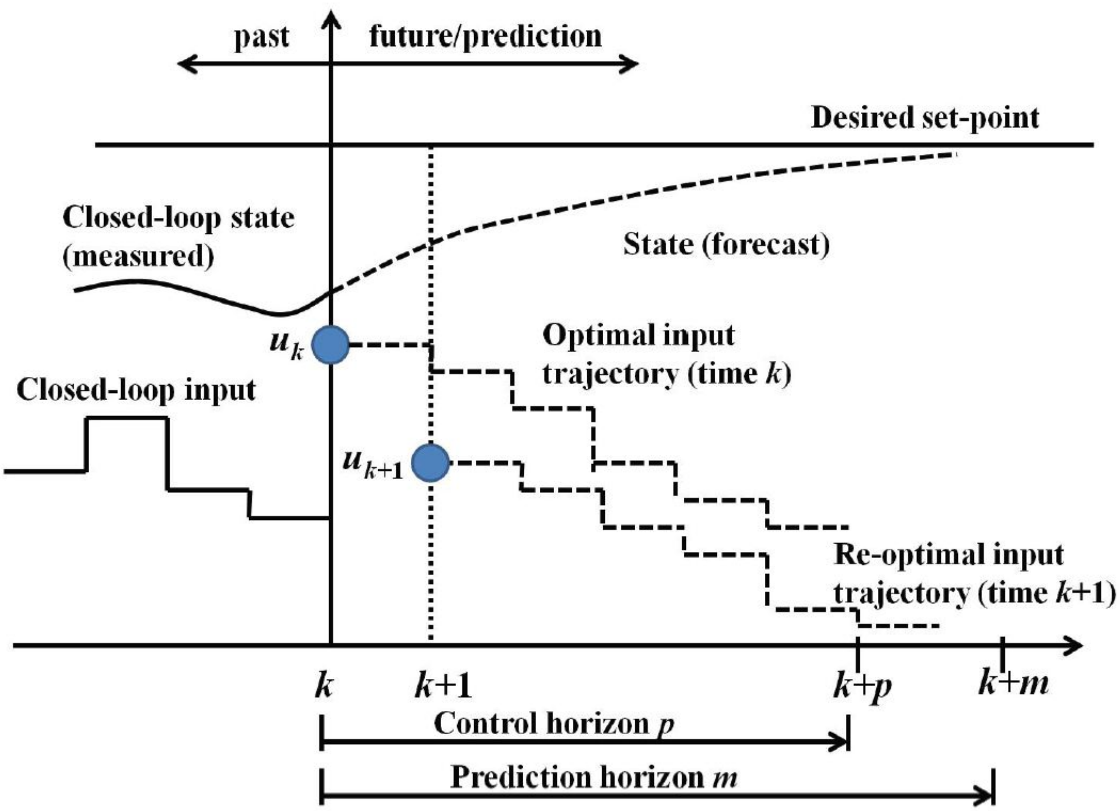


Figure 3: MPC Approach

$$\text{Minimize } \Omega_{\mathbf{x}_i,\mathbf{u}} = \sum_{i}^{N_s} \omega_i J_i(\mathbf{x_i}, \mathbf{u}, \hat{\theta}) \quad (3.14)$$

$$\text{Subject to :}$$

$$\frac{dx_i}{dt} = f_i(\mathbf{x}_i, \mathbf{u}, \Theta_i), i = 1, ..., N_s \quad (3.15)$$

$$h_i(\mathbf{x}_i, \mathbf{u}, \Theta_i) \leq 0, \qquad i = 1, ..., N_s \quad (3.16)$$

$$x^L \leq \mathbf{x}_i \leq x^U \quad (3.17)$$

$$u^L \leq \mathbf{u} \leq u^U \quad (3.18)$$

where J is the objective function, $\mathbf{x} \in \Re^n$ is the state vector, $\mathbf{u} \in \Re^m$ is the vector of manipulated variables, $\Theta \in \Re^{N_p}$ is the set of parameters with uncertainty, w is a weighting function, f is the map representing the dynamic process behavior and h is the set of system constraints. In this work, L represent the lower bound, U is an upper bound and t is the processing time and the subscript i denotes a given scenario and N_s is the total number of scenarios. To meet the water quality requirements we have deployed the following form of objective function:

$$J_i = \int_0^{t_f} \left\{ (S_s(t) - S_s^t)^2 + (S_{NH_4}(t) - S_{NH_4}^t)^2 + (S_{NO_3}(t) - S_{NO_3}^t)^2 + ((S_{NO_2}(t) + S_{NO_3}(t)) - S_{NO_{23}}^t)^2 \right\} dt \quad (3.19)$$

where the superscript t stands for target values so that treated water complies with demanded purity requirements. In the previous optimization formulation control actions are independent of the scenarios. This means that the same value of control actions must comply with all restrictions of the process in all the scenarios and be optimal with respect to the objective function.

Similarly, the corresponding stochastic NMPC formulation is as follows:

$$\text{Minimize } \phi_{\mathbf{x_i},\mathbf{u}} = \int_{t=0}^{T-1} J_t\left(\mathbf{x_i}, \mathbf{u}, \hat{\theta}\right) + \int_{t=T-1}^{T} J'_t\left(\mathbf{x_i}, \mathbf{u}, \hat{\theta}\right) \quad (3.20)$$

$$\text{Subject to :}$$

$$J_t = \left(S^t{}_S - S_S(t)\right)^2 + \left(S^t{}_{NH_4} - S_{NH_4}(t)\right)^2 + \left(S^t{}_{NO_3} - S_{NO_3}(t)\right)^2 + \left(S^t{}_{NO_2} + S^t{}_{NO_3} - (S_{NO_2}(t) + S_{NO_3}(t))\right)^2 \quad (3.21)$$

$$J'_t = \left(S^t{}_S - S_S(t) - K_S\right)^2 + \left(S^t{}_{NH_4} - S_{NH_4}(t) - K_{NH_4}\right)^2 + \left(S^t{}_{NO_3} - S_{NO_3}(t) - K_{NO_3}\right)^2 + \left(S^t{}_{NO_2} + S^t{}_{NO_3} - (S_{NO_2}(t) + S_{NO_3}(t) + K_{NO_2} + K_{NO_3})\right)^2 \quad (3.22)$$

$$K_d = \sum_{p=1}^{Np} \eta_{d,p} \frac{\partial x_d}{\partial \theta_p}\Big|_{t=T}$$

$$d \in \{S, NH_4, NO_2, NO_3\} \quad (3.23)$$

$$t = 0, \Delta t, ..., T-1, T \quad (3.24)$$

$$T - 1 = (N-1)\Delta t \quad (3.25)$$

$$T = N\Delta t \quad (3.26)$$

where $\phi_(\mathbf{x_i}, \mathbf{u})$ is the stochastic NMPC objective function whereas $\hat{\theta} \in R^N p$ is the set of uncertain parameters, which are fixed in the stochastic NMPC framework to its nominal (expected) values; T is the final time, i.e. $(t_f = T = N\Delta t)$. Moreover, K_d represents a penalty (back-off) term added to each organic matter that accounts for the variability in the uncertain parameters Θ. The penalty term K_d is defined as the product of a user-defined weight factor $(\eta \in R^{dxNp})$ and the sensitivity of the organic matter with respect to uncertain parameters at the final time T. That is, the present approach performs a first order power series expansion to estimate output variability due to model uncertainty. The weight factor $\eta_{d,p}$ is a user-defined weight that is used to account to the spread (variability) in the distribution of the d^{th} organic matter due to uncertainty in the p^{th} uncertain parameter whereas the sensitivity terms can be obtained from a sensitivity analysis (see Parametric sensitivity analysis section). Setting $\eta_{d,p}$ to large values imposes stringent restrictions on the concentrations of the d^{th} organic matter whereas lower values reduces the impact of variability of that specie in the stochastic NMPC calculations. The present approach is only an approximation since process variability is represented here as a first-order power series expansion that accounts for the sensitivity of the output variables with respect to the uncertainty parameters, at the final time T. Note that this approach has been successfully used in the literature, see e.g.[30],[27].

In this work the discretization of the dynamic mathematical model is carried out using the method of collocation orthogonal on finite elements [7]. Thus, the time trajectory is divided in a finite number of finite elements, inside each finite element the dynamic behavior is approximate using internal collocation points. Accordingly, the process model equation shown in 3.15 is represented as follows:

$$x_{f,c,i} = x^o_{f,i} + th_f \Sigma_k \Lambda_{k,c} \dot{x}_{f,k,i}, \qquad f = 1, ..., N_{fe}; c = 1, ..., N_c \tag{3.27}$$

$$x^o_{f,i} = x^o_{f-1,i} + th_{f-1} \Sigma_c \Lambda_{c,Nc} \dot{x}_{f-1,c,i}, \qquad f = 2, ..., N_{fe} \tag{3.28}$$

$$\dot{x}_{f,c,i} = f(x_{f,c,i} u_{f,c}, \Theta_i), \qquad f = 1, ..., N_{fe}; c = 1, ..., N_c \tag{3.29}$$

$$x^o_{f,i} = x^{init}_f, \qquad f = 1 \tag{3.30}$$

where N_{fe} is the number of finite elements, N_e is the number of internal collocation points, h_f is the length of each finite element, t is the dimensionless time, Λ is the collocation matrix and theta is the uncertain parameter vector. $x^n_{f,c,i}$ represents the value of the n^{th} system state at each one of the discretized points c of finite element f in the scenario s, $xo^n_{f,i}$ represents the value of the n^{th} system state at the beginning of each finite element, $\dot{x}^n_{f,c,i}$ is the first-order derivative of the n-th state. The superscripts indicate the values of initial states and state values in each of the finite elements.

4 Parametric sensitivity analysis

In the practice, most of the mathematical models intended to approximate the behavior of a given system are prone to plant-model mismatch. In order to identify the parameters that may critically affect the operation of this process, a local sensitivity analysis was performed to make an assessment about which of the parameters have deeper impact on the performance of the system under consideration. Typically, the parametric sensitivity analysis is performed as a local linear analysis procedure meaning that their results are only strictly valid around the linearization region. Using this approach, the parametric sensitivity analysis can allow identification of those parameters featuring the strongest influence on system behavior.

To compute the sensitivity coefficients we proceed as follows. Assuming that a dynamic mathematical model is available:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t, \mathbf{p}) \tag{4.31}$$

where $\mathbf{x}$ stands for the state vector and $\mathbf{p}$ is the vector of system parameters. The equations describing the way a state depends upon a given parameters reads as follows:

$$\frac{d\mathbf{S}}{dt} = \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)\mathbf{S} + \left(\frac{\partial \mathbf{f}}{\partial \mathbf{p}}\right) \tag{4.32}$$

where $\mathbf{S} = [S_{ij}]$ and $S_{ij} = \frac{\partial x_i}{\partial p_j}$. Moreover, S_{ij} are named the sensitivity coefficients. Recognizing that the magnitudes of the sensitivity coefficients can be different by several orders of magnitude, normally a kind of scaling procedure is deployed so to compare the magnitudes of S_{ij} on a similar basis. In this work we have used the following scaling procedure:

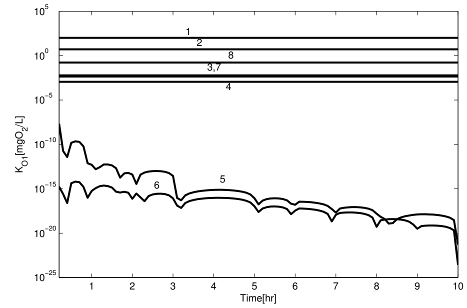
$$S_{ij} = \left(\frac{\partial x_i}{\partial p_j}\right)\left(\frac{p_j}{x_i}\right) \tag{4.33}$$

5 Results and discussion

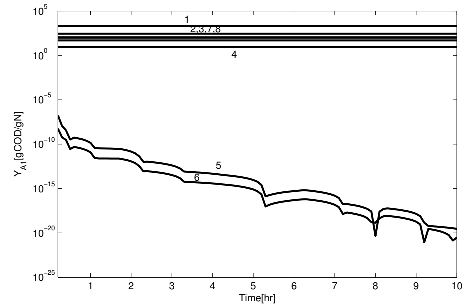
After testing all the parameters described in Table 2 we arrived to the conclusion that only the following model parameters have significative influence on the dynamic response of the SBR system: $K_{01}, Y_{Haer}, Y_{a1}, Y_{a2}$ and Y_{a3}. The dynamic sensitivity plots are shown in Figure 4. These results helped us to establish that only that set of parameters should be examined to test their potential influence on system's performance in closed-loop.

Table 3: Lower and upper bounds on the nominal value of uncertain parameters. The asterisk symbol stand for the nominal values, ω represents a weighting factor stressing the importance of each uncertain value and Δ are the minimum and maximum deviation (as percentage) of each parameter with respect to the nominal values.

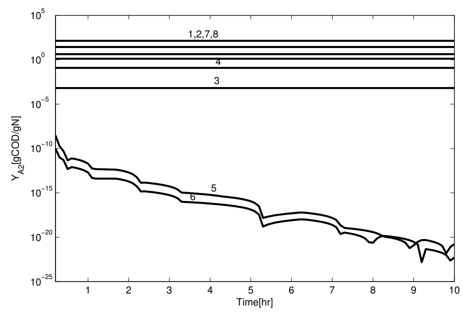
ω	K_{01}	Y_{Haer}	Y_{a1}	Y_{a2}	Y_{a3}
0.2	0.18	0.06	0.06	0.03	0.01
0.2	0.2*	0.08	0.08	0.06	0.02
0.2	0.25	0.1302*	0.1327*	0.0985*	0.0331*
0.2	0.3	0.16	0.16	0.11	0.04
0.2	0.35	0.18	0.18	0.13	0.05
Δ	(10,75)	(54, 38)	(54, 35)	(70, 32)	(70,51)



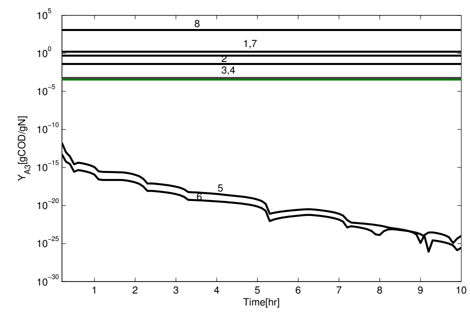
(a) K_{01}



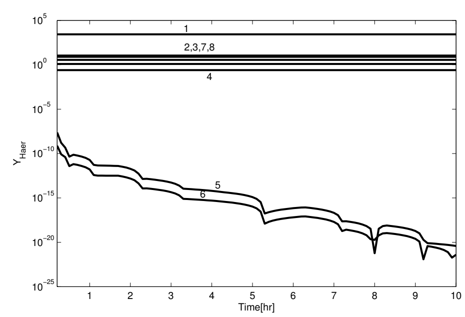
(b) Y_{a1}



(c) Y_{a2}



(d) Y_{a3}



(e) Y_{Haer}

Figure 4: Sensitivity plots displaying the influence of system parameters on the response of the SBR system.

Based on the above, robust NMPC was considered first in the analysis. Accordingly, bounds on the uncertain parameters around their nominal values were considered as shown in Table 3. To address the impact of parameter uncertainty on closed-loop optimal control, the uncertain parameter set was discretized to five realizations or scenarios. Each scenarios was assumed to have the same probability weight reflected trough the ω term. As shown in Table 3, the percentage of uncertainty was considerable and in some cases this percentage was chosen as the last parameter value which returned a feasible solution. The results discussed in this section are local optimal solutions obtained deploying the nonlinear programming CONOPT solver available in GAMS [33]. For the discretization of the SBR dynamic model 20 finite elements and 3 internal collocation points were used. In the robust NMPC framework, 5 prediction horizon intervals and 30 min sampling time were considered.

In a previous work [2] we have deployed the same SBR dynamic model for performing open-loop optimal control calculations. In that study we demonstrated that a well structured nonlinear programming formulation is only needed to compute open-loop dynamic profiles and allowing fractional values of the feed stream oxygen control valve (instead of on/off behavior) would help to obtain improved control profiles. In addition to those features, in the present work we have considered the presence of model uncertainty and deployed a robust nonlinear model predictive control approach to accommodate model uncertainty such that the impact of uncertainty does not deteriorate the control performance behavior. Then, the effect of model uncertainty is addressed by a combination of feedback control action and a proper robust optimization formulation. Following, the results of these two combined mechanisms are discussed.

In Figures 5-9 the closed-loop optimal control results are shown for uncertainty in the K_{01}, Y_{A1}, Y_{A2}, Y_{A3} and Y_{Haer} parameters, respectively. As it can be observed, in most of these cases the difference in the performance of the control actions between the deterministic and the uncertain cases is not significant. Moreover, all the water quality requirements are fully met. These results are interesting especially when recalling that the magnitude of the uncertainty in each one of the parameters is large as shown in Table 3. Moreover, the robust non-linear model predictive control scheme is able to cope with such large parameter uncertainty values. From the same set of plots we can observe that although the processing time (around 9.7 hr) was slightly larger than the one found in our previous work (8.5 hr) this is due to the fact that in the present work a different objective function was deployed. However, the presence of model uncertainty did not demand longer processing times for meeting purity specifications.

The situation is different when considering simultaneous uncertainty in all the model parameters. As shown in Figure 10 this time the performance difference of the deterministic and robust control actions is larger with respect to the cases in which uncertainty in a single parameter was considered. In fact, in Figure 10(f) we observe that the robust aeration control action oscillates around the deterministic control action. Note that even for this extreme case no additional processing time was required to meet water quality requirements. This result is important since it means that water quality specifications can be met for any of the values of the uncertain parameters without evident degradation of the control performance.

The performance of the SBR plant when the stochastic NMPC formulation presented in equation 3.21 is employed in the calculations of the optimal control actions is presented next. A typical assumption in engineering is to consider that the uncertain parameters follow a normal probability distribution with specific means and standard deviations [32]. As shown above, a parametric sensitivity analysis was carried out for the SBR plant. That analysis showed that the model parameters K_{01} and Y_{Haer} affect the performance of the activated sludge process significantly, as shown in Figures 4 a) and e), respectively. This information can therefore be used in the stochastic NMPC formulation to account for the variability in the organic matter due to uncertainty in K_{01} and Y_{Haer}. Hence, these parameters were assumed to be the uncertain parameters in the present stochastic NMPC formulation, i.e. $\Theta = K_{01}, Y_{Haer}$. To simplify the analysis, K_{01} and Y_{Haer} were assumed to be normally distributed uncertain parameters with expected (nominal) values and covariance matrix defined as follows:

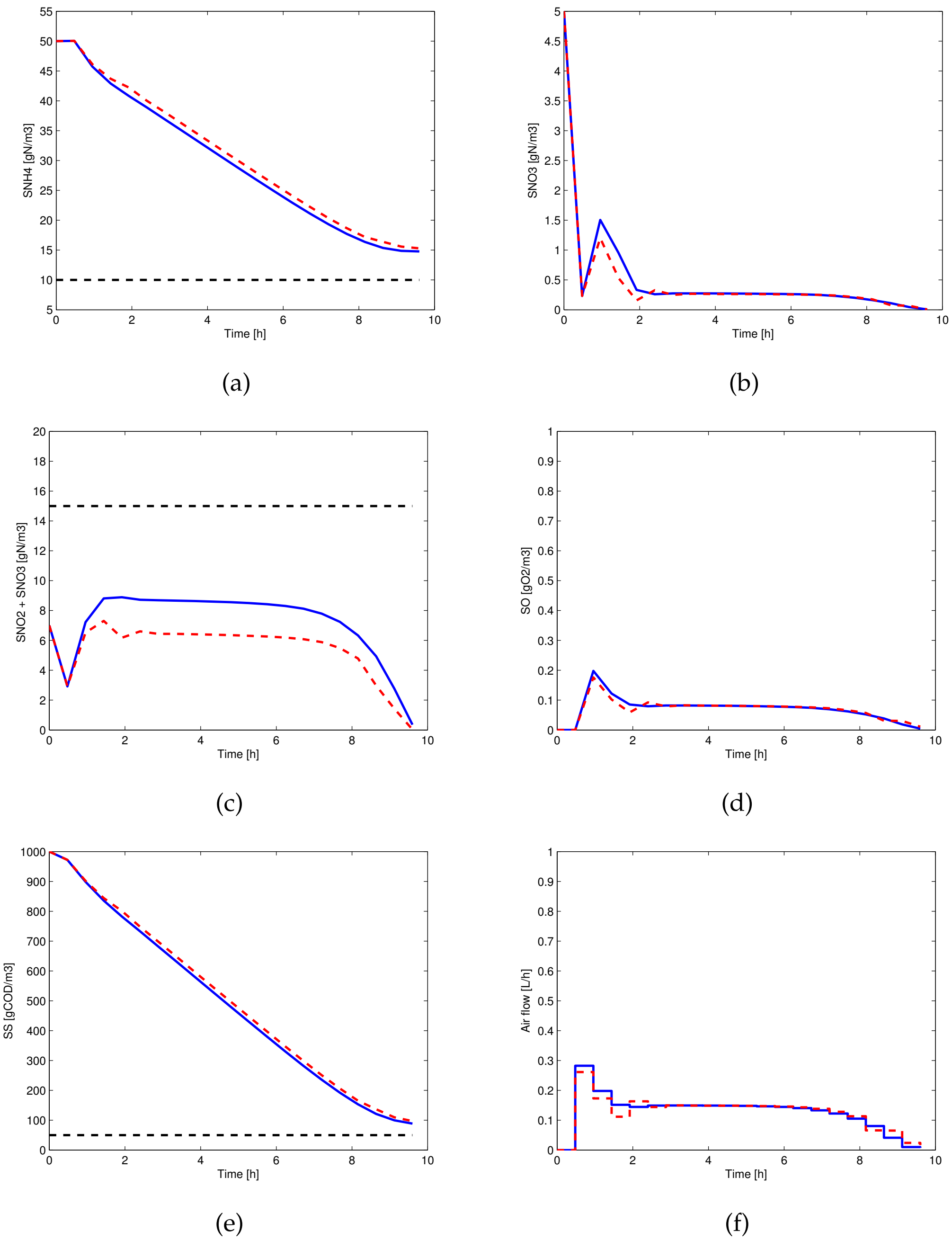


Figure 5: Dynamic local optimization results considering uncertainty in the K_{01} parameter: Continuous line refers to the deterministic case, while dashed line refers to robust optimization results. (a)-(e) composition profiles and (f) aeration control action.

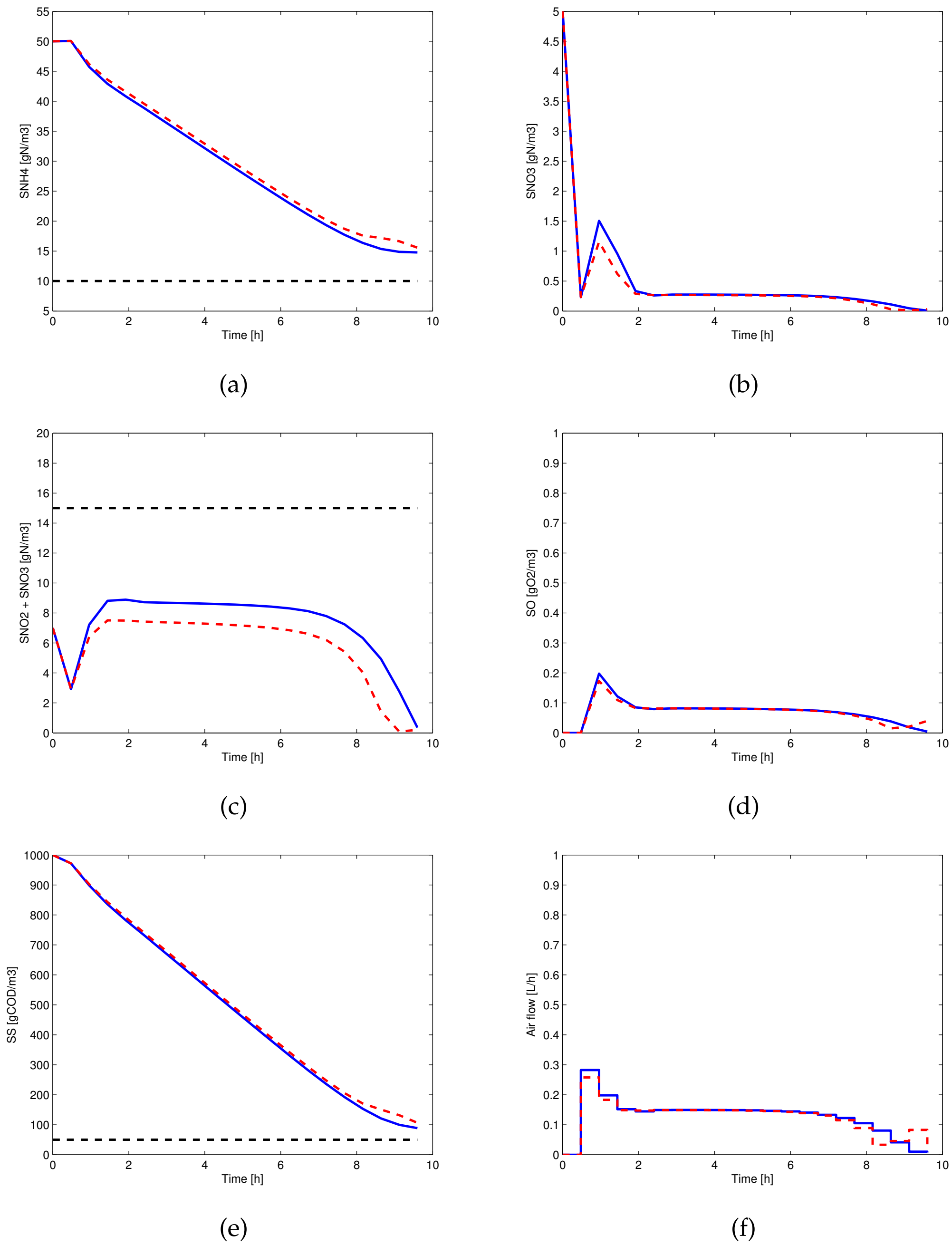


Figure 6: Dynamic local optimization results considering uncertainty in the Y_{A1} parameter: Continuous line refers to the deterministic case, while dashed line refers to robust optimization results. (a)-(e) composition profiles and (f) aeration control action.

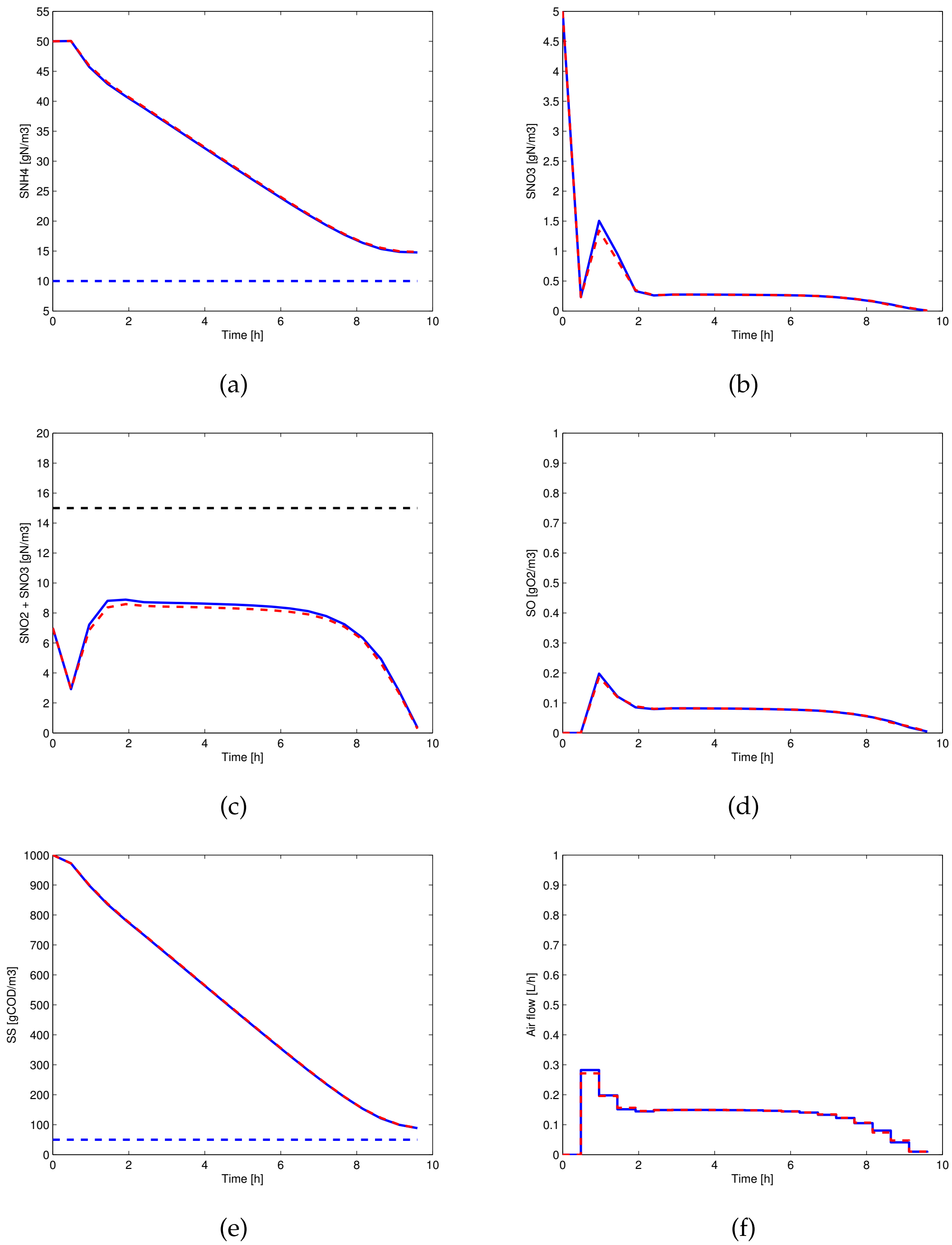


Figure 7: Dynamic local optimization results considering uncertainty in the Y_{A2} parameter: Continuous line refers to the deterministic case, while dashed line refers to robust optimization results. (a)-(e) composition profiles and (f) aeration control action.

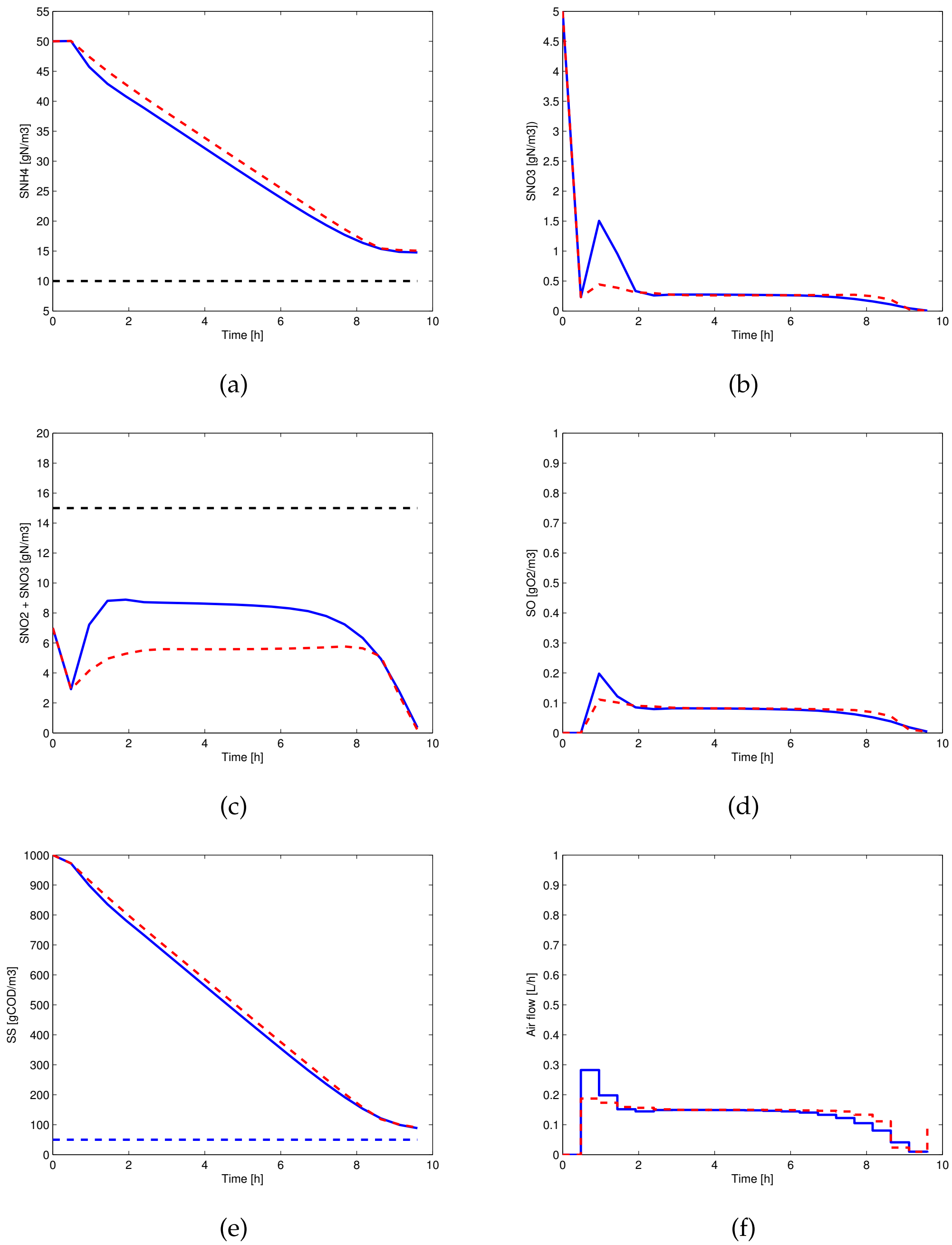


Figure 8: Dynamic local optimization results considering uncertainty in the Y_{A3} parameter: Continuous line refers to the deterministic case, while dashed line refers to robust optimization results. (a)-(e) composition profiles and (f) aeration control action.

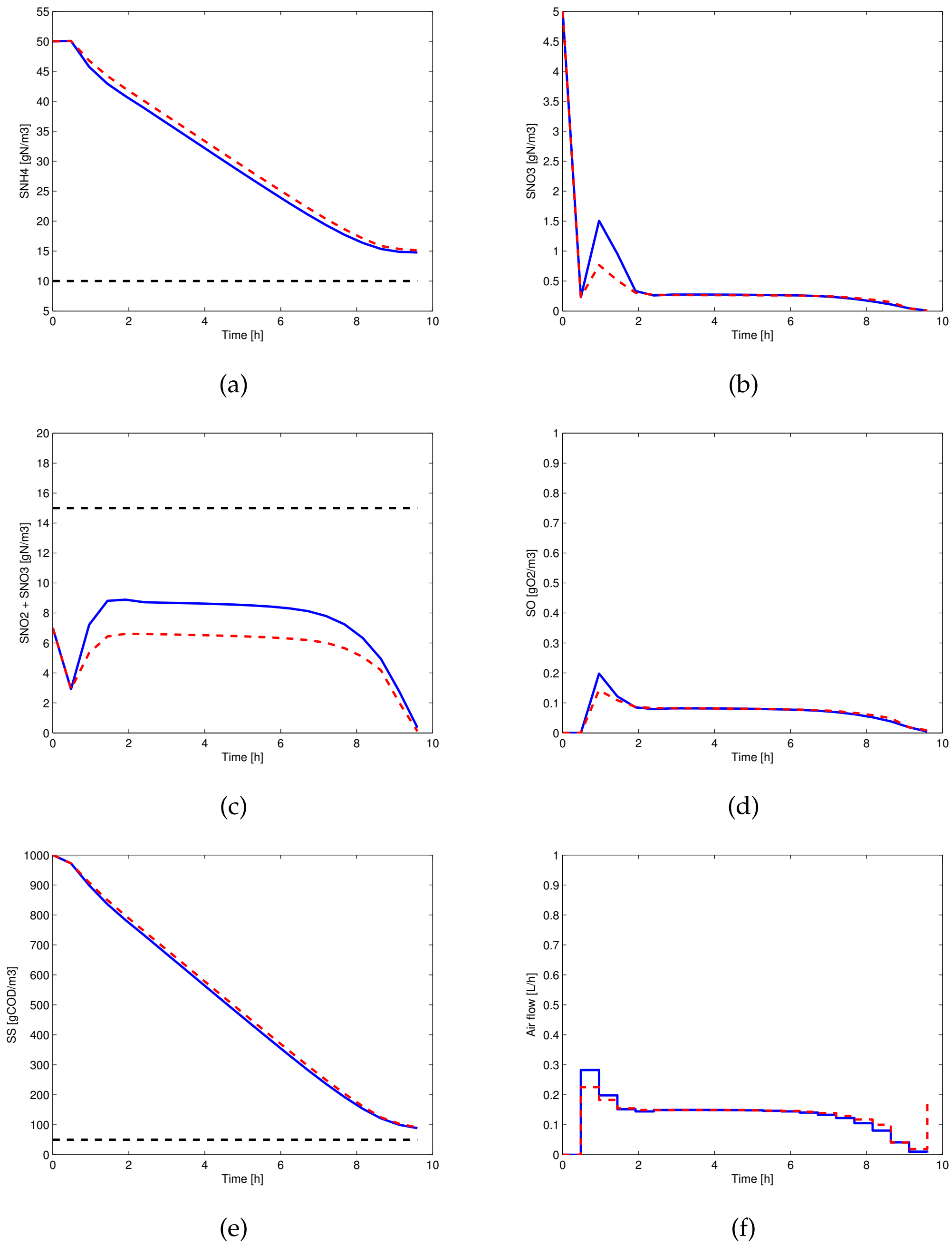


Figure 9: Dynamic local optimization results considering uncertainty in the Y_{Haer} parameter: Continuous line refers to the deterministic case, while dashed line refers to robust optimization results. (a)-(e) composition profiles and (f) aeration control action.

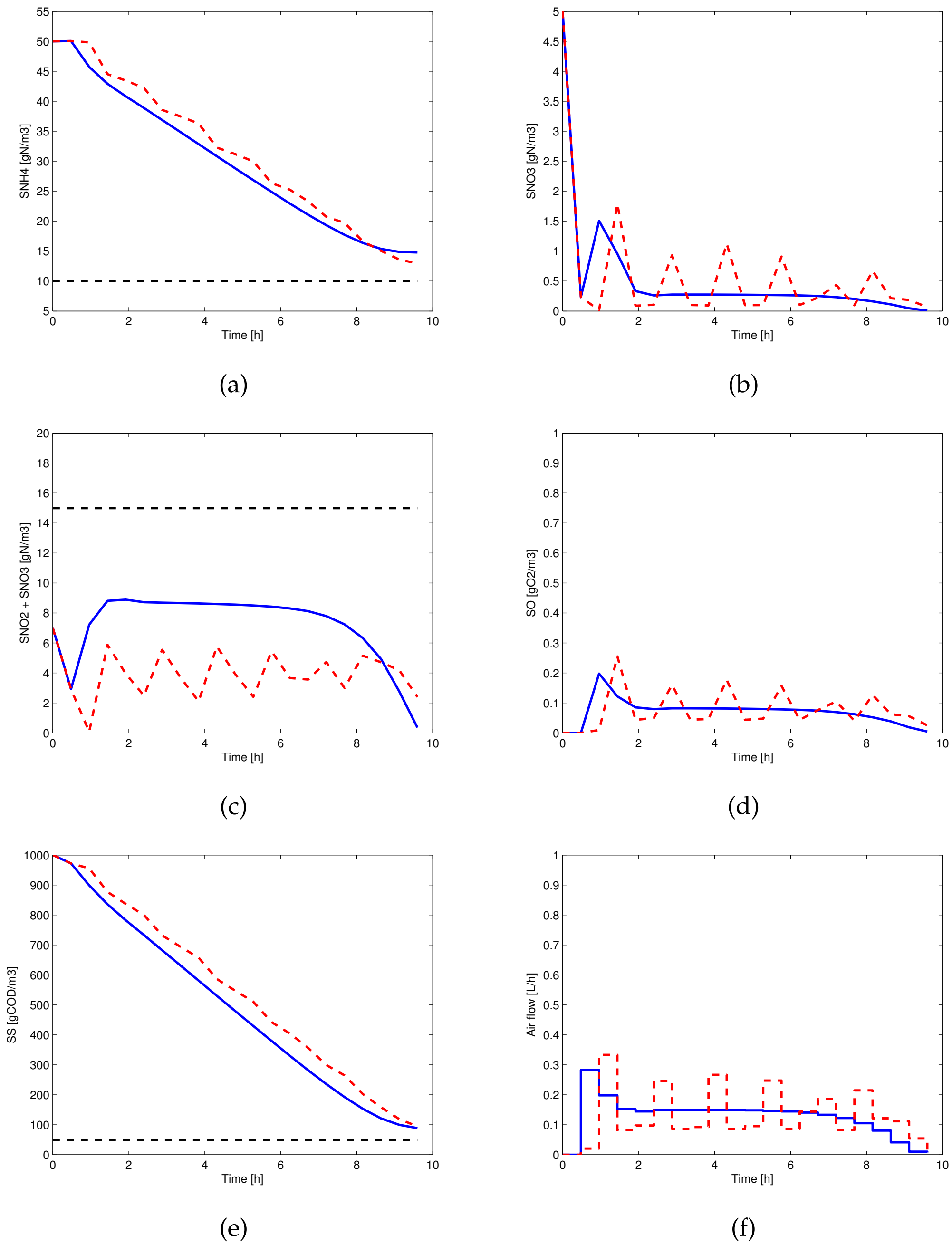


Figure 10: Dynamic local optimization results considering simultaneous uncertainty in all parameters: Continuous line refers to the deterministic case, while dashed line refers to robust optimization results. (a)-(e) composition profiles and (f) aeration control action.

$$\left[\hat{k}_{o1}, \hat{Y}_{Haer}\right] = [0.2, 0.1302] \tag{5.34}$$

$$V\left(k_{01}, Y_{Haer}\right) = \begin{bmatrix} 900\times 10^{-6} & 0 \\ 0 & 381.421\times 10^{6} \end{bmatrix} \tag{5.35}$$

Two case studies assuming $\eta = 1$ and $\eta = 2$ were considered. As in the robust NMPC, the nonlinear programming CONOPT solver available in GAMS [33] was used to generated the solutions presented in this section. To validate the results, the performance of the stochastic NMPC implementation was tested by simulating the SBR process in closed-loop using 1,000 Monte Carlo realizations in the uncertain parameters. As shown in Figure f), i), the amount of organic matter at the final time, i.e. carbonaceous substrate (S_S), ammonia (S_{NH4}), nitrites and nitrates $(S_{NO2} + S_{NO3})$, is reduced when a higher weight is used in the analysis $(\eta = 2)$ thus enabling a higher probability of satisfaction of the water quality constraints:

$$S_S\left(T\right) \leq S_S^t \tag{5.36}$$

$$S_{NH_4}\left(T\right) \leq S_{NH_4}^t \tag{5.37}$$

$$S_{NO_2}\left(T\right) + S_{NO_3}\left(T\right) \leq S_{NO_3-NO_2}^t \tag{5.38}$$

where S_S^t,$S_{NH_4}^t$,and $S_{NO_3-NO_2}^t$ are set to 50, 10 and 15, respectively [22]. When the penalty term is not considered in the analysis, i.e. $\eta = 0$, none of the water quality restrictions shown in equations 5.36-5.38 are satisfied under uncertainty. As shown 11 a) the mean concentration of S_S (85.24 g COD/m^3) is much greater than the desired concentration. On the other hand, Figures 11 (b) and (c) show that when $\eta = 1$ and $\eta = 2$, the mean S_S concentration is 44 g COD/m^3 and 40 g COD/m^3, respectively, which meet the water quality requirements for this specie at the final time T. A similar result was observed for the S_{NH_4} concentration. As shown in Figures 11 (d), (e) and (f) the mean value concentration for this specie is reduced from 14.19 g N/m^3 to 12.32 g N/m^3 and 11 g N/m^3. These results show that the use of higher weights increase the probabilities of complying with the water quality constraints at the final time.

Figure 12 shows the corresponding time-trajectory profile for S_{NH_4}. As shown in the Figure, the penalty term in the stochastic formulation ensures that the S_{NH_4} concentration constraint is met requiring twice the time when compared to the nominal case; that is, the proposed stochastic approach increases the probability of constraint satisfaction at the final time T. It can be shown that, larger values assigned to the weight η can increase constraint satisfaction of the amount of matter at the final time at the expense of producing more conservative control actions. To further validate the results, the sum of squared errors (SSE) was calculated for each of the simulations performed using the stochastic NMPC framework. The SSE was calculated as follows:

$$SSE = \frac{\sum_{i=1}^{r}\left(S_d^i\left(T\right) - S_d^t\right)^2}{r} \tag{5.39}$$

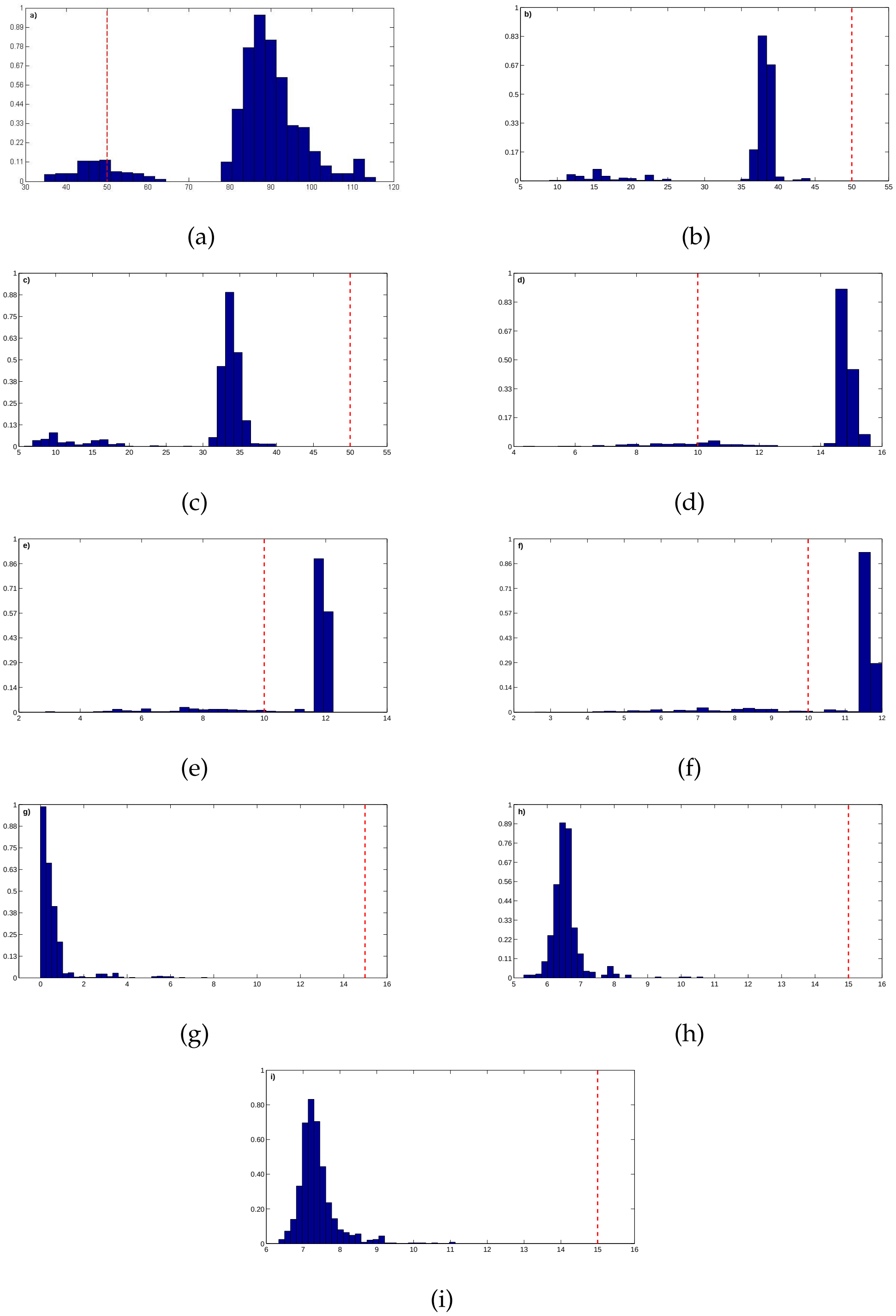
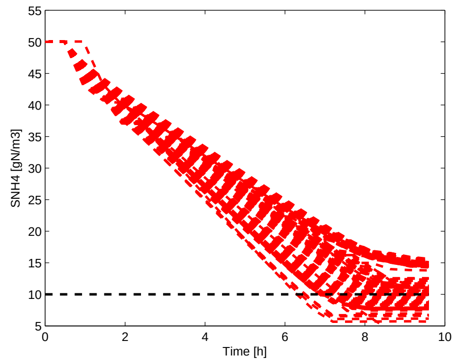
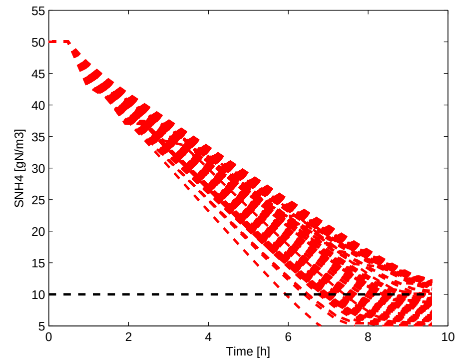


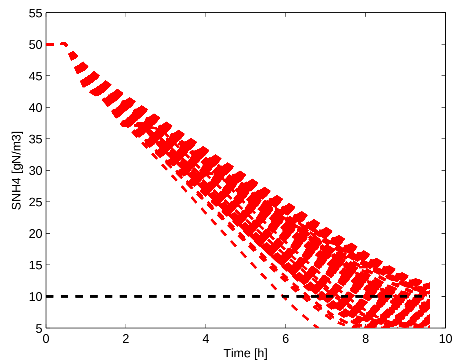
Figure 11: Histograms results for: S_S distribution in (a) nominal case, (b) stochastic case $\eta = 1$ and (c) stochastic case $\eta = 2$. S_{NH_4} distribution in (d) nominal case, (e) stochastic case $\eta = 1$ and (f) stochastic case $\eta = 2$. $S_{NO_2} + S_{NO_3}$ distribution in (g) nominal case, (h) stochastic case $\eta = 1$ and (i) stochastic case $\eta = 2$. The red dashes lines refer to the components constraints



(a) Nominal Case



(b) $(\eta = 1)$



(c) $(\eta = 2)$

Figure 12: S_{NH_4} profiles in (a) nominal case, (b) stochastic case 1 $(\eta = 1)$, (c)stochastic case 2 $(\eta = 2)$. Dashes black lines show the water constraint for S_{NH_4}

Table 4: Sum of squared errors (SSE): stochastic NMPC

SSE	S_S	S_{NH_4}	S_{NO_2} + S_{NO_3}
Nominal Case	1454.58	20.19	209.18
Stochastic case 1 $(\eta = 1)$	427.23	4.23	71.35
Stochastic case 2 $(\eta = 2)$	268.05	3.41	58.45

where r is the number of simulations, $S_d^i(T)$ the value of the i^{th} observation at the final time and S_d^t is the desired value.

As shown in Table 4, the SSE only represents 28.77% and 18.05% of the SSE obtained for the S_S specie in the nominal case. Likewise, the behavior of the S_{NH_4} component improved approximately 80% and 84% with respect to the nominal case when setting η to 1 and 2, respectively. A similar observation was made for the remaining organic matter. These results indicate the importance of implementing a penalty (back-off) term in the NMPC objective function to account for process output variability due to model uncertainty.

6 Conclusions

Nowadays, there is a concern on water resources and their relationship with energy trough the energy-water nexus. One of the facets of this nexus is related to minimum energy consumption for water treatment processes. However, there are some issues that in practice can make hard to obtain reduced energy consumption. Typically, nominal parameter values are employed to identify suitable operating conditions. However, in practice the value of some parameters can be unknown or vary meaning that the expected process performance may not be realized. In this work, we have shown that during the normal operation of SBR water treatment processes, the impact of model uncertainty on some of the more relevant parameters can be tolerated up to the point that target water purity requirements can be met even in the presence of uncertainty in the model parameters. To cope with parameter uncertainty, we deployed robust and stochastic non-linear model predictive control strategies for handling uncertainty in closed-loop for the SBR process. It is important to stress that the presence of uncertainty did not result in significant performance degradation in the control system.

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