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# **ASM3 extended for two-step nitrification-denitrification: a model reduction for Sequencing Batch Reactors**

The ASM3 extended for two step nitrification-denitrification is reduced in order to match the specific conditions of Sequencing Batch Reactor systems with Shortcut Biological nitrogen Removal

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## **Abstract**

BACKGROUND: The ASM3 extended for two-step nitrification-denitrification represents the most accurate model for the description of the Activated Sludge Process with Nitrate Bypass Nitrification-Denitrification. This model includes 20 reaction rates, 15 state variables, and more than 35 parameters, which make its calculation costly and difficult to estimate. The lack of a fast and accurate model, able to predict both, concentration of nitrite and nitrate over time, is the principal obstacle for efficient model-based optimization and model-based control.

RESULTS: In this work, a fast and accurate model for the activated sludge process in a Sequencing Batch Reactor is proposed. For this purpose, the ASM3 extended for two step nitrification-denitrification is reduced in order to match the specific conditions of Sequencing Batch Reactor systems with Shortcut Biological nitrogen Removal. The proposed model considers a two-step nitrification-denitrification process and can thus describe the bypass of nitrate. Different approaches for model reduction together with an exhaustive analysis of the extended ASM3 model as well as the process are discussed.

CONCLUSIONS: The resulting model with only five differential equations reduces the calculation time up to one order of magnitude while maintaining a high description accuracy, which states the advantages of model reduction.

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**Keywords:** model reduction, activated sludge, ASM3, two-step nitrification-denitrification, nitrate bypass, nitrification-denitrification, invariant reaction, time scale analysis

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## 1. Introduction

Modeling of the Activated Sludge Process (ASP) for wastewater treatment represents a mayor bioengineering challenge. A wide consortium of microorganisms consumes carbonaceous matter producing energy and new products in a complex symbiotic process. Biological nitrogen removal through nitrification/denitrification is currently widely practiced in order to produce a clarified effluent to be discharged to sensitive receiving water bodies, preventing eutrophication. Furthermore, the description of the nitrification-denitrification process as a reaction with at least two steps is gaining importance for the simulation of optimal ASPs. It has been suggested that the Nitrate Bypass Nitrification-Denitrification (NBND), also known as shortcut Biological Nitrogen Removal (SBNR), process shows important advantages over conventional nitrification-denitrification<sup>1</sup>. It is evident that nitrate bypassing process can only

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1 be represented by a model which considers nitrate production and consumption during  
2 nitrification-denitrification.

3 Although an exact description of the multiple biochemical reactions taking place in the  
4 process is impossible, some models achieve to describe the general behavior of the system  
5 and have been widely implemented in practice. The ASM3 extended for two-step  
6 nitrification-denitrification (referred in this work as extended ASM3 <sup>2</sup>) represents the most  
7 accurate model for the description of the ASP with NBND, other similar works can be found  
8 in literature <sup>3</sup>. This model includes 20 reaction rates, 15 state variables, and more than 35  
9 parameters, which make its calculation costly and the model highly unidentifiable. The lack of  
10 a fast and accurate model, able to predict both concentration of nitrite and nitrate, is the  
11 principal obstacle for an efficient model based optimization and model-based control strategy  
12 considering NBND.

13 Many efforts have been made to create simple models for Waste Water Treatment (WWT)  
14 processes, in particular for the Activated Sludge Process (ASP) <sup>4</sup>. Some examples represent  
15 the boundary relocation <sup>5</sup>, neural networks <sup>6</sup>, and model reduction for steady state model  
16 based control <sup>7</sup>. Nevertheless, a systematic model reduction of an Activated Sludge Model  
17 (ASM) able to describe the bypass nitrate nitrification-denitrification while maintaining the  
18 important dynamics of the mechanistic model has to our best knowledge never been reported.

Aim of this work is to create a model for an efficient simulation of the SBR process under NBND. To achieve this goal, the extended ASM3 is reduced to match the specific conditions of SBR systems under NBND conditions.

## 2. Background

### 2.1. Activated Sludge

The most applied method for biological treatment of waste water is the ASP<sup>8</sup>. The family of Activated Sludge Models (ASM) represents the state-of-the-art model framework for ASP simulation<sup>6</sup>. ASM1 is the most widely used in practice<sup>9</sup>, ASM2<sup>10</sup> is applied to simulate processes that include biological phosphorus removal<sup>11</sup> and the latest version, ASM3<sup>12</sup>, includes the quantification of energy storage in order to describe ready biodegradable substrate and oxygen uptake with higher accuracy. Finally, a newer version of ASM3, referred to in this contribution as extended ASM3, where nitrification and denitrification are considered as two-step processes, taking into account nitrite as an intermediate, has recently been presented<sup>2</sup>.

In order to extend the ASM3, 7 process equations were included, resulting in a stoichiometric matrix with dimension 15x20. In addition to a low parameter identifiability, the extended ASM3 demands significant computation time. These drawbacks represent the main obstacle for efficient optimization and model-based control. On the other hand, the extended ASM3 describes many states, which can be neglected for the specific case of SBR process<sup>13, 14</sup>.

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## 2.2. Sequencing Batch Reactor

Small and medium size WWT plants are strongly affected by changing concentrations of contaminants in the wastewater<sup>15</sup>. Sequencing Batch Reactors (SBR), because of its high flexibility and operation range, offer an adept solution for such cases. Furthermore, an SBR is able to treat different kinds of effluents such as municipal, domestic, hypersaline, tannery, brewery, dairy wastewaters, and landfill leachates among others<sup>16</sup>. The SBR has gained great popularity in recent years. Advances in process measurement, as well as automation and control, increase the process efficiency, reducing operation costs, while fulfilling the strict environmental regulations<sup>17, 18</sup>.

In SBRs, the retention time, the duration of the aeration and anoxic phases, the settling time, and other conditions can be fitted to a changing quality of load as well as effluent requirements. SBRs can also be considered to be a process which operates with variation in time, whereas a continuous process operates with variations in space<sup>19</sup>. A complete cycle of the sequencing batch process consists of five steps; 1) Idle, 2) Fill, 3) React, 4) Settle and 5) Draw (see Figure 1).

Nowadays, SBR technology has become important in particular for small and medium-sized Waste Water Treatment Plants (WWTP). When properly designed and operated, an SBR also offers a process with important advantages over continuous processes, not only because of its efficiency and economical aspects<sup>20-22</sup>, but also because of its small footprint<sup>19</sup>.

### 2.3. Nitrate Bypass Generation

In the ASP, nitrogen is removed from wastewater by the nitrification/denitrification process.

Most of the nitrogen contained in wastewater is converted into ammonia. Ammonia is then converted into molecular nitrogen by a two-step biological processes, namely nitrification followed by denitrification (Figure 2).

In the first stage, *Nitrosomonas* and other ammonia oxidizers convert ammonia and ammonium to nitrite, whereas in a second stage, *Nitrobacter* and other nitrite oxidizers finish the conversion of nitrite to nitrate.

Turc and Mavinic<sup>1</sup> proposed the Nitrate Bypass Nitrification-Denitrification (NBND) process, which can be achieved by inhibiting the production of nitrate and proposed various methods for bringing about this effect.

The NBND has the following advantages over conventional nitrification-denitrification:

- 40% reduction of COD demand during denitrification

- 63% higher rate of denitrification

- 300% lower biomass yield during anaerobic growth

- no apparent nitrite toxicity effects for the microorganisms in the reactor

The group of Professor Lyberatos<sup>23</sup> showed that a frequent enough change between aerobic and anoxic conditions suppresses nitrate formation. Ammonia is converted to nitrite in the

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1 presence of oxygen (nitrification), which is then converted into nitrogen under anoxic  
2 conditions before the second oxidation producing nitrate (nitrification) can take place. It was  
3 also proved that this is caused by the inability of nitrite oxidizers to adapt to aerobic  
4 conditions following an anoxic phase. Intermittent aeration is the less costly means of  
5 securing nitrate bypass.

### 6 **3. Solution approach**

#### 7 *3.1. Basic approaches to Model Reduction*

8 The reduction of a particular model maintaining the model characteristics is a common task in  
9 all fields of engineering. Representative examples are Lumping<sup>24,25</sup>, Sensitivity Analysis<sup>26</sup>,  
10 The Quasi Steady State Assumption (QSSA)<sup>27</sup>, and Time-Scale Analysis<sup>28-30</sup>. We refer to  
11 Okino and Mavrovouniotis for a further elaborated review of these methods<sup>31</sup>.

12 In model reduction for continuous processes based on time scale analysis, the fast modes are  
13 neglected. Only the slow modes, which determine the path to reach the equilibrium point, are  
14 maintained<sup>32</sup>. On the contrary, when a system is far from equilibrium (as is usually the case  
15 in dynamic processes) the fast modes are of major importance and the very slow modes can  
16 be considered constant (quasi-steady state). In addition, these new constants may give rise to  
17 new reaction invariants, which should be considered because of their model reduction  
18 potential.

#### 19 *3.2. Mathematical model for a batch biochemical reactor*

7



The biochemical reactions by mixed microbial cultures involve numerous chemical species consumed (substrates) and produced (intermediate or final metabolic products) and microbial groups mainly grown. Chemical species produced by a microbial group are often the substrate for the growth of other microbial groups, making the whole process a sequence of individual process steps in a scheme, where the preceding steps may be independent of those that follow.

Assuming that biochemical reactions, generally described through



take place in a batch biochemical reactor, the following differential equations can be derived:

$$\begin{aligned} \dot{S}_i &= \sum_{k=1}^n c_{i,k} * r_k(S_1, \dots, S_l, X_1, \dots, X_m), \quad i = 1, \dots, l \\ \dot{X}_j &= \sum_{k=1}^n Y_{j,k} * r_k(S_1, \dots, S_l, X_1, \dots, X_m), \quad j = 1, \dots, m \end{aligned} \quad (2)$$

where:

$S_i, i = 1, \dots, l$  are the concentrations of the chemical species (substrates and/or products) in

the reactor,  $X_j, j = 1, \dots, m$  are the concentrations of the microbial masses in the reactor,

$r_k(S_1, \dots, S_l, X_1, \dots, X_m), k = 1, \dots, n$  are the reaction rates,  $C_{i,k}$  and  $Y_{j,k}$  are the stoichiometric coefficients for substrate consumption and microbial growth, respectively.

It should be noted that the consumption of a substrate (e.g. particulate matter) may not be associated with biomass growth. Moreover, a single microbial group may grow on more than one substrate and vice versa. Therefore, in the general case, the number of the substrates involved in a bioreaction scheme will not be equal to the number of microbial masses grown, i.e.  $l \neq m$ .

Introducing vector notation for the concentrations and the rates

$$\underline{S} = \begin{bmatrix} S_1 \\ \vdots \\ S_l \end{bmatrix}, \underline{X} = \begin{bmatrix} X_1 \\ \vdots \\ X_m \end{bmatrix}, \underline{r}(\underline{S}, \underline{X}) = \begin{bmatrix} r_1(S_1, \dots, S_l, X_1, \dots, X_m) \\ \vdots \\ r_n(S_1, \dots, S_l, X_1, \dots, X_m) \end{bmatrix}$$

and denoting by  $\underline{C}$  and  $\underline{Y}$  the  $l \times n$  and  $m \times n$  matrices of the stoichiometric coefficients, model

(2) takes a more compact form:

$$\begin{aligned} \dot{\underline{S}} &= \underline{C} \cdot \underline{r}(\underline{S}, \underline{X}) \\ \dot{\underline{X}} &= \underline{Y} \cdot \underline{r}(\underline{S}, \underline{X}) \end{aligned} \tag{3}$$

### 3.3. Reaction invariants

The theory of reaction invariants has long been known and applied to chemical engineering<sup>33</sup>.

In the general model of equations (2) or (3), there are  $(l + m)$  differential equations that are affected by  $n$  reaction rates. As long as  $l + m > n$  and the differential equations are independent of each other, there will be  $l + m - n$  linear combinations of the concentrations that are completely unaffected by the reaction rates and therefore completely unaffected by the progress of the chemical reactions. In the literature, these are referred to as reaction invariants; they capture the reaction stoichiometry relations, which are unaffected by the reaction rates.

The reaction invariants can be easily calculated from the general model of (3).

Assuming  $l + m > n$  and

$$\text{Rank} \begin{bmatrix} \underline{C} \\ \underline{Y} \end{bmatrix} = n,$$

one can find  $(l + m - n)$  linearly independent row vectors  $\alpha_v, v = 1, \dots, (l + m - n)$  of length  $(l + m)$  such that

$$\alpha_v \begin{bmatrix} \underline{C} \\ \underline{Y} \end{bmatrix} = 0 \quad v = 1, \dots, (l + m - n)$$

This means that the  $(l + m - n) \times (l + m)$  matrix

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$$\underline{A} = \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_v \end{bmatrix}$$

has rank  $(l + m - n)$  and satisfies

$$\underline{A} \begin{bmatrix} \underline{C} \\ \underline{Y} \end{bmatrix} = 0 \tag{4}$$

It can then be easily verified, as a result of (2) and (3), that the quantity

$$\underline{z} = \underline{A} \begin{bmatrix} \underline{S} \\ \underline{X} \end{bmatrix} \tag{5}$$

remains constant throughout the entire batch:

$$\underline{\dot{z}} = 0 \tag{6}$$

and so

$$\underline{A} \begin{bmatrix} \underline{S}(t) \\ \underline{X}(t) \end{bmatrix} = \underline{A} \begin{bmatrix} \underline{S}(0) \\ \underline{X}(0) \end{bmatrix} \quad \forall t > 0 \tag{7}$$

3.4. Illustrative Example

1 Consider the following reaction in a closed vessel:

2 Now let us assume that the reaction can be described by the following ODE system:

$$\begin{aligned}\frac{dC_d}{dt} &= -k_1 * C_D * C_E + k_2 * C_F \\ \frac{dC_E}{dt} &= -k_1 * C_D * C_E + k_2 * C_F \\ \frac{dC_F}{dt} &= k_1 * C_D * C_E - k_2 * C_F\end{aligned}\tag{8}$$

3 and can also be represented as

$$\underline{\dot{C}} = \underline{Y} * r\tag{9}$$

4 with:

$$size(\underline{\dot{C}}) = 3 \times 1$$

where:

$$r = k_1 * C_D * C_E - k_2 * C_F\tag{10}$$

1 and

2

$$\underline{Y} = \begin{bmatrix} -1 \\ -1 \\ 1 \end{bmatrix}$$

3 with:  $\text{rank}(\underline{Y}) = n = 1$ . The system has then  $m - n = 3 - 1 = 2$  reaction invariants.

4 Finally, solving the equation:

5

$$\underline{A} * \underline{Y} = 0 \tag{11}$$

6 we obtain :

7

$$A = \begin{bmatrix} 1 & -1 & 0 \\ 1 & 0 & 1 \end{bmatrix}$$

8 Equation (7) states that  $A * C = A * C^0$  thus the original system can be also represented by:

9

$$\begin{aligned} \frac{dC_D}{dt} &= -k_1 * C_D * C_E + k_2 * C_F \\ C_E &= C_E^0 - C_D^0 + C_D \\ C_F &= C_F^0 + C_D^0 - C_D \end{aligned} \tag{12}$$

10 This illustrative example shows how the reaction system can be described by a system with  
11 only one differential equation without any loss of information.

12 *3.5. Switching functions and the reaction invariant*

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Switching functions (SF) are widely applied in biological systems. Its most common form corresponds to the simplified Michaelis-Menten equation (13).

$$v = v_m \frac{[S]}{K_s + [S]} \quad (13)$$

where  $v$ ,  $v_m$ ,  $K_s$ ,  $[S]$  are the reaction rate, the maximum reaction rate, the inverse of enzyme affinity and the substrate concentration, respectively.

Switching functions enable activation or deactivation of reaction paths depending on the concentration of certain species. The objective is to create a continuous and smooth function, which equals 1, when the concentration of the limiting component is high, and 0 when its concentration is 0. Inhibition functions present the opposite behavior.

Referring to equation (13),  $v$  will have the value  $v_m$  when the concentration of substrate is high and 0 when the concentration of substrate is near 0. The behavior of switching functions can be characterized in three phases (see Figure 4).

active and constant (species concentration is significantly higher than the limiting

constant  $> 100$ )

transition phase (when the ratio species/constant is between 100 and  $1 \cdot 10^{-2}$ )

inactive and constant (species concentration is significantly lower than the limiting

constant  $< 1 \cdot 10^{-2}$ )

1 This particular characteristic of the switching functions opens interesting possibilities for  
2 model reduction. The presence of switching functions in a mathematical model may engender  
3 temporal reaction invariants during specific time intervals in a process. To be more precise,  
4 the process presents different reaction invariants under limitation of different species.

5 To visualize this idea, considering the simplified Michaelis-Menten equation in (13), it can be  
6 seen that if  $[S] > 100 \forall t > 0$ , then  $\mu \approx \mu_m = \text{constant}$ . Therefore, it is possible to create  
7 reduced versions of the original model, which behave exactly as the original model under  
8 specific conditions. This can be very useful when applying general mathematical models to  
9 defined conditions. When a model describes a wide range of process conditions all species  
10 limitations, which may or may not occur during the process, have to be considered. However,  
11 once the conditions of the process are well defined, some limitations can be neglected and  
12 new reaction invariants can be found.

#### 13 **4. Model reduction of the extended ASM3**

##### 14 *4.1. A proposed 9state model*

15 The model proposed in this section is named 9state, according to the number of state variables  
16 contained in the equation system. Thus there are nine differential equations which describe  
17 the basic variables (concentrations), namely: 1.- carbonaceous substrate, 2.- heterotrophic  
18 bacteria, 3.- ammonia oxidizers, 4.- nitrite oxidizers, 5.- dissolved oxygen, 6.- ammonia, 7.-  
19 nitrite, 8.- nitrate and 9.- stored substrate.



## 4.2. Storage

The implementation of energy storage represents the principal improvement of ASM3 in comparison to older versions. Neglecting this equation would impede a proper process description and would result in an incorrect model reduction. Consequently, energy storage and its effects on substrate and oxygen concentration cannot be ignored. For this reason, the proposed 9state model includes some adaptations to carbonaceous substrate and oxygen uptake equations. The new set of equations is presented in such a way, that both carbonaceous substrate uptake and oxygen uptake increments caused by the storage are now included in the original ready biodegradable substrate and oxygen differential equations.

By these means, the relation between both, carbonaceous substrate consumption rate and oxygen consumption rates, to energy storage are linear, which is accurate as long as the carbonaceous substrate concentration is above zero. This could appear to be an inconsistent assumption, though it is almost certain that the process continues after carbonaceous substrate elimination in order to achieve further ammonia degradation. Nevertheless, previous model versions (ASM1 and ASM2) fit the data although they lack a storage variable. In other words, the 9state model responds to the carbonaceous substrate limitation similarly to ASM1, but describes carbonaceous substrate and oxygen uptake as well as energy storage as precisely as the extended ASM3.

ASM3 considers that bacteria utilize part of carbonaceous substrate for energy storage for its later use under substrate limiting conditions. This storage is not only responsible for lower

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1 biomass growth under equal carbonaceous substrate consumption, but also for the bacterial  
2 growth when no carbonaceous substrate is present in the medium. In the case of an SBR  
3 process, it is considered that energy storage does not limit bacterial growth. The assumption is  
4 based on the fact that in a process with optimal aeration strategy, bacteria never exhaust their  
5 stored energy for two reasons:

6 In order to minimize process time and costs, the environmental regulations should be  
7 fulfilled as soon as carbonaceous substrate is consumed.

8 Excepting the idle phase, bacteria are always in a medium rich in carbonaceous  
9 substrate. Therefore, the value of the stored energy should be high at any moment  
10 during the process and never limit bacterial growth.

11 If these assumptions are valid, the relation between the carbonaceous substrate used for  
12 energy storage and ready biodegradable substrate used for growth is valid as well. In the  
13 extended ASM3, the relation between carbonaceous substrate and biomass growth is  
14 described by a second order differential equation. However, as long as the concentration of  
15 the stored energy is high, this second-order differential equation can be accurately  
16 approximated with a first order differential equation. A graphical interpretation is presented in  
17 Figure 5.

18 *4.3. Reduction of the extended ASM3 model to a 9state model*

In this work, the 15 ordinary differential equations of the extended ASM3 include only the process rate variables without their explicit equation. The process rate equations are shown in Table 1 and have been numbered in the same order as previously presented in <sup>2</sup>:

First, three state equations of the extended ASM3 directly involved in the energy storage are analyzed.

Readily biodegradable substrate:

$$\frac{dS_r}{dt} = -r_2 - r_3 - r_4 + (1 - f_{sl}) * r_1 \quad (14)$$

where the term  $(1 - f_{sl}) * r_1$  represents the conversion of slow biodegradable substrate into readily biodegradable substrate. A closer look to the dynamics of both, readily biodegradable and particulate substrate, confirms that the mode of conversion of particulate to readily biodegradable (hydrolysis) is considerably faster. For this reason, all organic matter is considered to be readily biodegradable in this process.

Energy Storage:

$$\frac{dX_{STO}}{dt} = Y_{STO_{aer}} * r_2 + Y_{STO_{NO3}} * r_3 + Y_{STO_{NO2}} * r_4 - \frac{1}{Y_{H_{aer}}} * r_5 - \frac{1}{Y_{H_{NO3}}} * r_6 - \frac{1}{Y_{H_{NO2}}} * r_7 - r_{11} - r_{12} - r_{13} \quad (15)$$

where the terms -  $r_{11}$  -  $r_{12}$  -  $r_{13}$  represent the respiration reactions. Respiration reactions are neglected in the 9state model based on their low sensitivity.

Heterotrophic Biomass:

$$\frac{dX_H}{dt} = r_5 + r_6 + r_7 - r_8 - r_9 - r_{10} \quad (16)$$

where the terms -  $r_8$  -  $r_9$  -  $r_{10}$  denote the death rates of the heterotrophic bacteria. These are substituted by death constants.

A closer look at the rate equations (14) - (16) shows that all of them are dependent on  $X_H$ .

Hence, considering that the switching functions have a constant value, i. e. the concentrations are large enough in comparison to the switching constant, there is a linear relation  $k_{sto}/\mu_H$  between (17) - (19) and (20) - (22):

$$r_2 = k_{sto} * \frac{S_O}{S_O + K_{H,O2}} * \frac{S_S}{S_S + K_S} * X_H \quad (17)$$

$$r_3 = k_{sto} * \eta_{H,NO3} * \frac{K_{H,O2inh}}{K_{H,O2inh} + S_O} * \frac{S_S}{S_S + K_S} \frac{S_{NO3}}{S_{NO3} + K_{H,NO3}} * X_H \quad (18)$$

$$r_4 = k_{sto} * \eta_{H,NO2} * \frac{K_{H,O2inh}}{K_{H,O2inh} + S_O} * \frac{S_S}{S_S + K_S} \frac{S_{NO2}}{S_{NO2} + K_{H,NO2}} * X_H \quad (19)$$

$$r_5 = \mu_H * \frac{S_{Alk}}{S_{Alk} + K_{Alk}} * \frac{S_O}{S_O + K_{O1}} * \frac{S_{NH4}}{S_{NH4} + K_{NH}} * \frac{X_{STO}/X_H}{K_{H,STO} + X_{STO}/X_H} * X_H \quad (20)$$

$$r_6 = \mu_H * \eta_{H,NO3} * \frac{K_{H,O2inh}}{K_{H,O2inh} + S_O} * \frac{S_{Alk}}{S_{Alk} + K_{Alk}} * \frac{S_{NO3}}{S_{NO3} + K_{H,NO3}} * \frac{X_{STO}/X_H}{K_{H,STO} + X_{STO}/X_H} * X_H \quad (21)$$

$$r_7 = \mu_H * \eta_{H,NO2} * \frac{K_{H,O2inh}}{K_{H,O2inh} + S_O} * \frac{S_S}{S_S + K_S} * \frac{S_{NO2}}{S_{NO2} + K_{H,NO2}} * \frac{X_{STO}/X_H}{K_{H,STO} + X_{STO}/X_H} * X_H \quad (22)$$

- 1 We now bound our process conditions such that ammonia, alkalinity, carbonaceous substrate  
2 and storage are not limiting to the process to obtain equation (23):

$$k * \frac{S_S}{S_S + K_S} = \frac{S_{Alk}}{S_{Alk} + K_{Alk}} * \frac{S_{NH4}}{S_{NH4} + K_{NH}} * \frac{X_{STO}/X_H}{K_{H,STO} + X_{STO}/X_H} \quad (23)$$

- 3 where k represents an arbitrary constant.

- 4 Equation (24) can now be implemented:

$$k * Y_{STO_{aer}} * \frac{r_i}{\mu_H} = \frac{1}{Y_{H_{aer}}} * r_{i+4} = a_i \text{ for } i = 2, 3, 4 \quad (24)$$

1 Substitution in the three state equations (14) - (16) results in:

$$\frac{dS_s}{dt} = \left( \frac{1}{Y_{STO_{aer}}} * a_2 + \frac{1}{Y_{STONO3}} * a_3 + \frac{1}{Y_{STONO2}} * a_4 \right) * \frac{k_{STO}}{k * \mu_H} + \frac{1}{Y} \quad (25)$$

$$\begin{aligned} \frac{dX_{STO}}{dt} &= (a_2 + a_3 + a_4) * \frac{k_{STO}}{k * \mu_H} - a_2 - a_3 - a_4 \\ &= (a_2 + a_3 + a_4) * \left( \frac{k_{STO}}{k * \mu_H} - 1 \right) \end{aligned} \quad (26)$$

$$\frac{dX_H}{dt} = Y_{H_{aer}} * a_2 + Y_{HNO3} * a_3 + Y_{HNO2} * a_4 \quad (27)$$

2 If we define a new constant  $St_s = \frac{k_{STO}}{k * \mu_H} - 1$  while considering that:

3  $Y_{H_{aer}} = Y_{STO_{aer}}$  and  $Y_{H_{aer}} = Y_{STONO3} = Y_{STONO2} = Y_{HNO3} = Y_{HNO2}$  (which is true for the  
4 values shown in <sup>2</sup>) and replace them in the simplified state equations (12) – (14), we obtain:

$$\frac{dS_s}{dt} = \left( -\frac{1}{Y_{H_{aer}}} * a_2 - \frac{1}{Y_{H_{aer}}} * (a_3 + a_4) \right) * (1 + St_s) \quad (28)$$

$$\frac{dX_{STO}}{dt} = (a_2 + a_3 + a_4) * (St_S) \quad (29)$$

$$\frac{dX_H}{dt} = Y_{HAsr} * a_2 + Y_{HNO3} * a_3 + Y_{HNO2} * a_4 \quad (30)$$

1 The most important characteristic of this new set of equations is given in equation (31)

$$\frac{dS_S}{dX_{STO}} = \frac{dX_H}{dX_{STO}} = 0 \quad (31)$$

2 Finally, a rearrangement of the equations, so as to substitute  $a_i$ 's with new rate constants in  
 3 the equations (15) – (17) results in a model with 9 state equations. The mathematical  
 4 representation of the 9state model is given in the following section.

## 5. Mathematical representation of the 9state model

### 5.1. Ordinary differential equations

7 The 9 ordinary differential equations are shown in equations (32) - (40). Their corresponding  
 8 rate equations are described in (41) - (45). The 9state version in MATLAB2008b® code is  
 9 presented. The model was created automatically with the modeling tool MOSAIC<sup>34</sup>.

10 This model was chosen to enable the use of any ODE solver for its integration. In addition,  
 11 the model calculates the integrals of oxygen and nitrate concentrations. These state variables  
 12 can be used as objective functions by the optimizer.

$$\frac{dS_s}{dt} = \left( -\frac{1}{Y_{Haeer}} * r_{aas} - \frac{1}{Y_{Hanox}} * (r_{aNO3} + r_{aNO2}) \right) * (1 + St_s) \tag{32}$$

$$\frac{dX_H}{dt} = r_{aas} + r_{aNO3} + r_{aNO2} \tag{33}$$

$$\frac{dX_{Ns}}{dt} = r_{aasNs} \tag{34}$$

$$\frac{dX_{Nh}}{dt} = r_{aasNb} \tag{35}$$

$$\frac{dS_O}{dt} = K_{La}(S_O^* - S_O) - \frac{1 - Y_{Haeer}}{Y_{Haeer}} r_{aas} - \left( \frac{3.43}{Y_{A1}} - 1 \right) r_{aasNs} - \left( \frac{1.14}{Y_{A2}} - 1 \right) r_{aasNb} \tag{36}$$

$$\frac{dS_{NH4}}{dt} = - \left( -\frac{l_{NSS}}{Y_{Haeer}} + i_{NB} \right) r_{aas} - \left( \frac{1}{Y_{A1}} + i_{NB} \right) r_{aasNs} - i_{NB} r_{aasNb} - \left( -\frac{l_{NSS}}{Y_{Hanox}} + i_{NB} \right) r_{aNO3} - \left( \frac{l_{NSS}}{Y_{Hanox}} + i_{NB} \right) r_{aNO2} \tag{37}$$

$$\frac{dS_{NO2}}{dt} = \frac{1}{Y_{A1}} r_{aasNs} - \frac{1}{Y_{A2}} r_{aasNb} + \frac{1 - Y_{Hanox}}{1.14 Y_{Hanox}} (r_{aNO3} - r_{aNO2}) \tag{38}$$

$$\frac{dS_{NO3}}{dt} = \frac{1}{Y_{A3}} r_{aasNb} - \frac{1 - Y_{Hanox}}{1.14 Y_{Hanox}} r_{aNO3} \tag{39}$$

$$\frac{dX_{Sto}}{dt} = \left( -\frac{1}{Y_{Haeer}} * r_{aas} - \frac{1}{Y_{Hanox}} * (r_{aNO3} + r_{aNO2}) \right) * (-St_s) \tag{40}$$

1            5.2. Reaction rates



$$r_{acs} = \mu_H * \frac{S_S}{S_S + K_S} * \frac{S_O}{S_O + K_{O1}} * \frac{S_{NH4}}{S_{NH4} + K_{NH}} * X_H \quad (41)$$

$$r_{acNs} = \mu_{A1} * \frac{S_O}{S_O + K_O} * \frac{S_{NH4}}{S_{NH4} + K_{NH}} * X_{Ns} \quad (42)$$

$$r_{acNb} = \mu_{A2} * \frac{S_{NO2}}{S_{NO2} + K_{NO21}} * \frac{S_O}{S_O + K_O} * \frac{S_{NH4}}{S_{NH4} + K_{NH}} * X_{Nb} \quad (43)$$

$$r_{aNO3} = \mu_{H1} * \frac{S_S}{S_S + K_S} * \frac{S_{NO3}}{S_{NO3} + K_{NO3}} * \frac{K_{O21}}{K_{O21} + S_O} * \frac{S_{NH4}}{S_{NH4} + K_{NH}} * X_H \quad (44)$$

$$r_{aNO2} = \mu_{H2} * \frac{S_S}{S_S + K_S} * \frac{S_{NO2}}{S_{NO2} + K_{NO2}} * \frac{K_{O22}}{K_{O22} + S_O} * \frac{S_{NH4}}{S_{NH4} + K_{NH}} * X_H \quad (45)$$

### 5.3. Stoichiometric matrix

The stoichiometric matrix of the 9state model is presented in Table 2. This matrix represents the  $(l + m - n)$  matrix of equation (3). In other words, the analysis of the stoichiometric matrix gives us the information about the number of reaction invariants hidden in the 9state model.

### 5.4. Saturation constants:

The saturation constants define the dynamics of the model near limitations. In order to maintain this information, the reduced models have the same values as the extended ASM3.

1 All the constants  $K_x$  have the same value as published in the extended version of ASM3<sup>2</sup>.

2 The values used for the saturation constants are shown in Table 3.

3 *5.5. Limitations of the reduced models*

4 It should be noted that the proposed 9state model is not valid for the whole range of  
5 conditions as the extended ASM3 is. Some limitations are to put up with in order to reduce  
6 the model and speed up the simulation in the region of interest. Moreover, because of the new  
7 energy storage equation, the bacteria can store energy, but cannot use it when no more  
8 carbonaceous substrate is available. For this reason, the prediction accuracy of the reduced  
9 models depends on the carbonaceous substrate concentration in the medium.

10 In the extended ASM3, the ammonia concentration does not limit the energy storage. This  
11 results in a consumption of carbonaceous substrate even under ammonia limitation. Once  
12 again, because of the coupled equations, the 9state model predicts carbonaceous substrate  
13 consumption only as long as ammonia is present in the medium. Finally, the growth of  
14 heterotrophic biomass can be mathematically described as a second order differential  
15 equation. For this reason, if the energy stored by the bacteria is low, a time delay can be seen  
16 in the growth curve. This time delay is not predicted by the 9state model. Taken into  
17 consideration that the storage has a value at least larger than 100 gCOD/m<sup>3</sup>, both growth  
18 curves match.

19 *5.6. A proposed 6state model*

The 9state model involves 9 differential equations, with only one of them depending on the process input (oxygen supply). The reaction invariant theory can then be applied to the 8 differential equations, which are not affected by the oxygen input, i.e. to (32) - (35) and (37) - (40).

These equations are of the form of equation (2) with  $n = 5, l + m = 8$ . Therefore, it is possible in this case, to find  $(l + m) - n = 3$  linearly independent reaction invariants. For example (46) - (48),

$$S_{NH4} + l_{NSS} * \frac{S_S}{1 + St_S} + l_{NB} * (X_H + X_{NS} + X_{NB}) + \frac{X_{NS}}{Y_{A1}} \quad (46)$$

$$S_{NO2} + 2 * S_{NO3} + \frac{1 - Y_{Hanox}}{1.14} * \frac{Y_{Haer}}{Y_{Hanox} - Y_{Haer}} * \left( \frac{S_S}{1 + St_S} + \frac{X_H}{Y_{Haer}} \right) - \frac{X_{NS}}{Y_{A1}} - \frac{2 * Y_{A2} - Y_{A3}}{Y_{A2} * Y_{A3} * X_{NB}} \quad (47)$$

$$\frac{S_S}{1 + St_S} + \frac{St_O}{St_S} \quad (48)$$

The above quantities remain constant throughout the entire batch. Therefore, it is possible to substitute three differential equations (37), (38) and (40) for three algebraic (49) - (51).

$$S_{NH4} = c_{NH4} - \left( l_{NSS} * \frac{S_S}{1 + St_S} + l_{NB} * (X_H + X_{NS} + X_{NB}) + \frac{X_{NS}}{Y_{A1}} \right) \quad (49)$$

$$S_{NO2} = c_{NO2} - 2 * S_{NO3} - \frac{1}{1.14} * \frac{Y_{Hanox}}{Y_{Hanox} - Y_{Hacr}} * \left( \frac{S_S}{1 + St_S} + \frac{X_H}{Y_{Hacr}} \right) + \frac{X_{NS}}{Y_{A1}} - \frac{2 * Y_{A2} - Y_{A3}}{Y_{A2} * Y_{A3} * X_{NB}} \quad (50)$$

$$X_{Sto} = c_{XSto} - \frac{S_S * St_S}{1 + St_S} \quad (51)$$

were  $c_{NH4}$ ,  $c_{NO2}$  and  $c_{XSto}$  are constants obtained after solving equations (46) - (48) for the initial conditions. Based on the method of reaction invariants, we find three equations which are linearly dependent. Therefore, the 6state model represents the 9state model exactly.

### 5.7. A proposed 5state model

Taking a closer look at the growth of the biological matter during one SBR in short cycles, we can see that the overall change in biomass does not exceed 10%. Based on this observation a further reduction of the mode is possible for the special case of a batch process. We can eliminate these three differential equations (33) - (35) from our 9state model and consider a constant biomass concentration throughout each cycle of the SBR so as to obtain a model with 6 differential equations. Again it can be shown that this system has one reaction invariant which is the same as indicated for the case of the 9state (51). As a result we obtain a model with only 5 state equations. This 5state model is almost as accurate as the 6state model. However, it can only be applied for batch processes where the change of biomass can be neglected.

### 5.8. Dissolved oxygen

Finally for any of the cases proposed above, the calculated oxygen concentration can be substituted by online measurements. By these means, a further reduction of the model is possible. Nevertheless, the substitution of the equation for the calculation of the dissolved oxygen concentration is straightforward and will not be discussed in this work. Furthermore, the integration of the aeration curve for optimization purposes is only possible if the oxygen concentration curve is calculated.

## 6. Results

### 6.1. Simulations

The 9state, 6state, and 5state models were set to various conditions so as to confirm their stability and accuracy. The most representative results of the comparison between extended ASM3 and the 5state model are presented in Figure 6-Figure 9.

The simulation represents a batch tank ideally mixed and the only control variable is the aeration of the tank. The initial value of energy storage is set to 400 gCOD/m<sup>3</sup> assuming bacteria have stored energy on previous cycles.

The system of Differential Algebraic Equations (DAE) is solved with two different integrators:

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1            sDACL: An in house tool for the combined step-wise state and sensitivity integration  
2            tailored to the Orthogonal Collocation in Finite Elements (OCFE) integration method  
3            <sup>35</sup>.  
4            ODE15s: An integrator based on Numerical Differentiation Formulas (NDFs) <sup>36</sup>.  
5            The main purpose is to set both models to drastic changes and various limitations. The  
6            aeration is turned on and off intermittently to produce a strongly dynamic process. As a result,  
7            a process with constantly changing conditions is obtained, which makes it very difficult to be  
8            described identically by two models with different characteristics. The results show that the  
9            5state model describes accurately the limitations of dissolved O<sub>2</sub>, NO<sub>2</sub><sup>-</sup> and NO<sub>3</sub><sup>-</sup>.  
10           Figure 6 shows the results for ready biodegradable substrate and energy storage. The initial  
11           value of energy storage was set to 400 gCOD/m<sup>3</sup> as explained in 4.2. All reduced versions  
12           describe perfectly the behavior of energy storage even though it is calculated by an algebraic  
13           equation. This proves that the substitution of the differential equation for energy storage by an  
14           algebraic equation does not affect the dynamics of the model.  
15           As seen in Figure 7, considering constant biomass values throughout the process does not  
16           affect the results of the other state variables. Growth rate is a crucial parameter of the process.  
17           Nevertheless, changes on biomass concentration in short batch cycles can be neglected.

Concentration of  $\text{NO}_2$  and  $\text{NO}_3$  are lower than 20 mgN/L during the whole cycle. The control variable is the aeration of the tank. Figure 8 shows how precise the reduced model describes the curves of nitrite and nitrate even in these extreme conditions.

Finally, the results for oxygen and ammonia calculations can be seen in Figure 9.

## 6.2. Simulations Results

The most representative results of the comparison of both models are presented in Table 4 and Table 5.

As we can see in Table 4, the reduced models are up to one order of magnitude faster. This reduction in the computation cost is not only caused by the reduction of the number of state variables calculated, but also because the stiffness of the system has been reduced. The evaluation of the jacobian matrixes is one of the most expensive calculations during model integration. Table 5 shows the difference of calculation time between the three models.

## 7. Conclusions

The resulting 6state and 5state models mimic properly the behavior of the extended ASM3 for the case of SBR process while being faster to calculate, less stiff and having a higher identifiability. Different approaches to model reduction have been applied to develop reduced versions of the extended ASM3 maintaining its characteristic dynamics. Furthermore, it could

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1 be shown, how an elaborated model can be simplified for specific operating conditions while  
2 keeping its prediction accuracy.

3 The results obtained suggest that the 5state model can in fact be applied for the simulation of  
4 the nitrate bypass reaction in SBR processes, and thus, for model-based control and online  
5 optimization. Moreover, the extended ASM3 was successfully simplified by reducing its  
6 computational load up to one order of magnitude. In addition, the accuracy obtained with the  
7 reduced models is remarkable good in comparison to the extended ASM3.

8  
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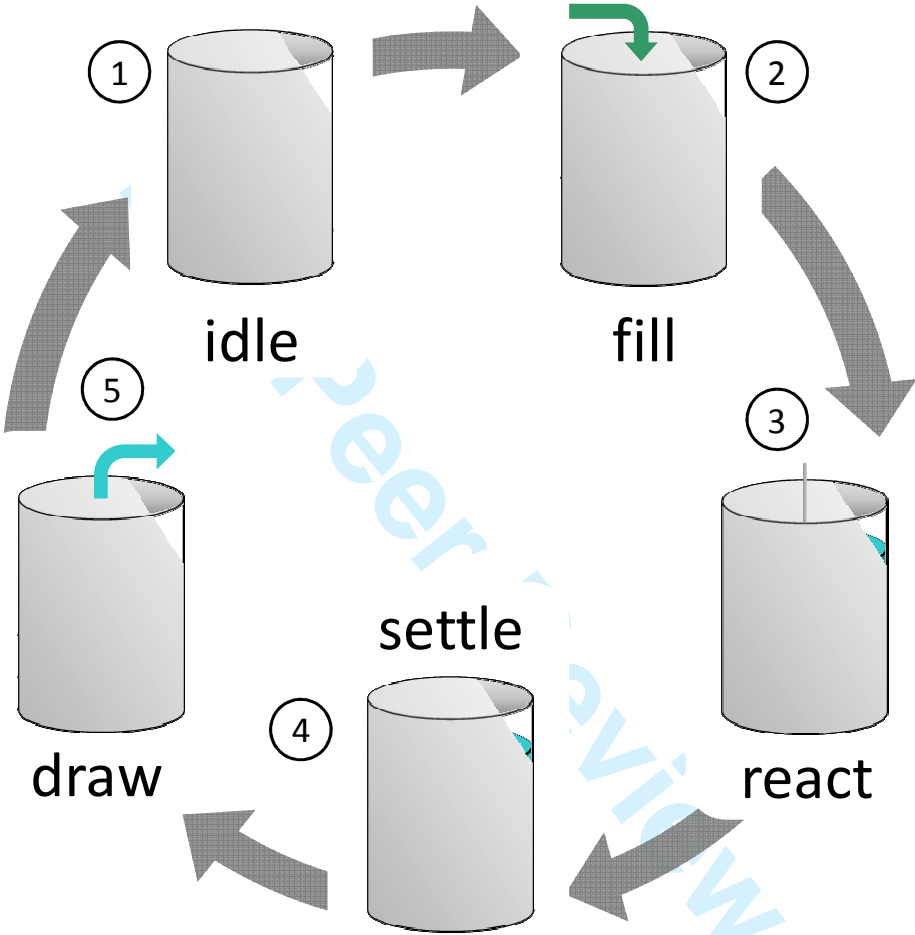
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Figures

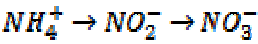


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Figure 1. SBR cycle

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Figure 2. Nitrification-denitrification process described as a two -step reaction.

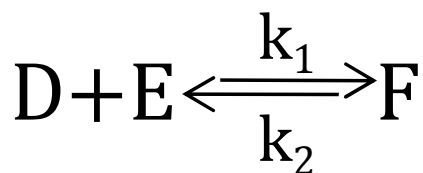


Figure 3. Chemical reaction

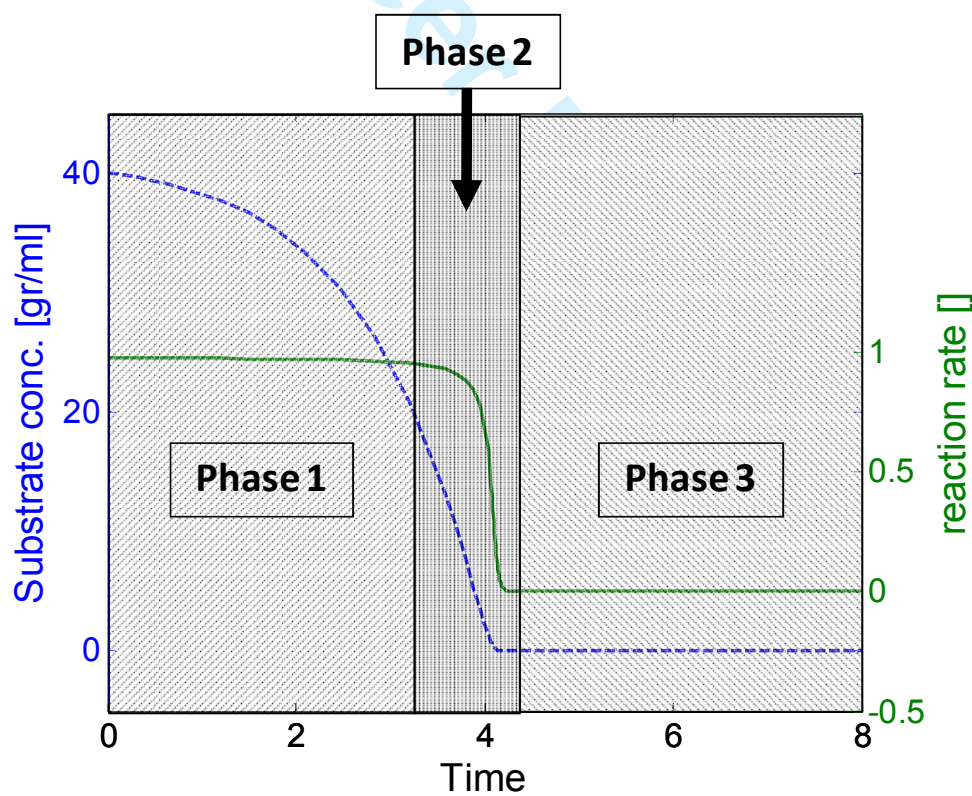


Figure 4. Behavior of a switching function in dependence of the limiting species.

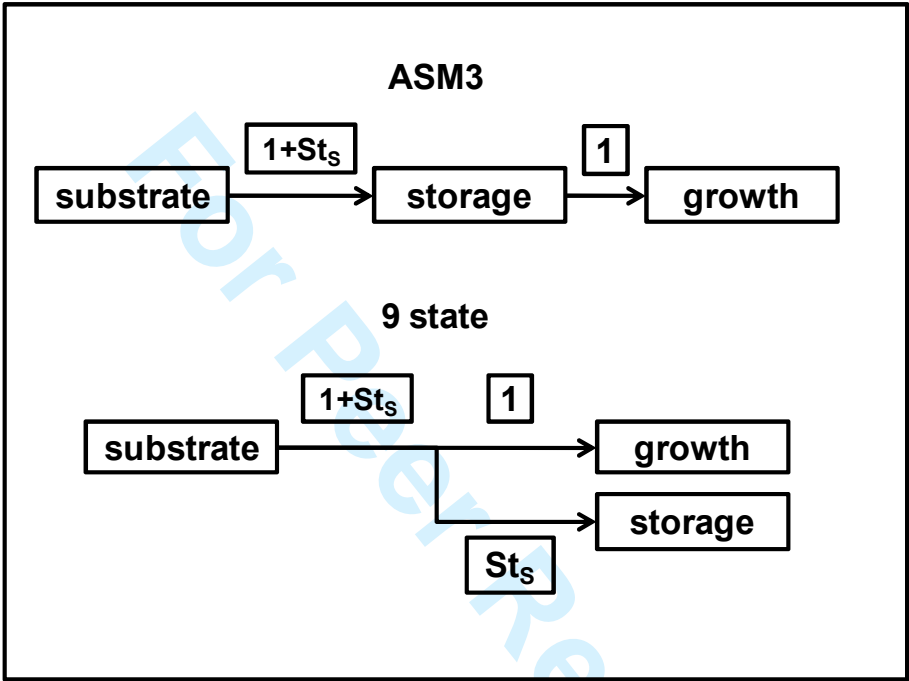


Figure 5. Substitution of the storage equation

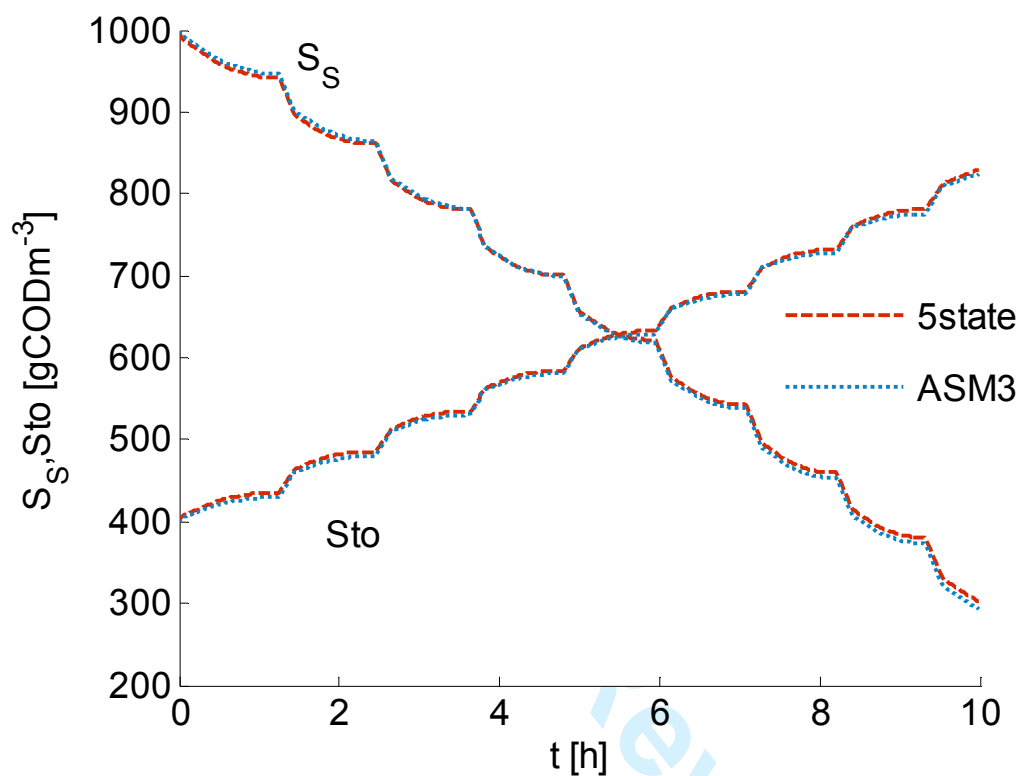


Figure 6. Ready biodegradable substrate concentration  $S_s$  and stored energy  $S_{to}$  against time.

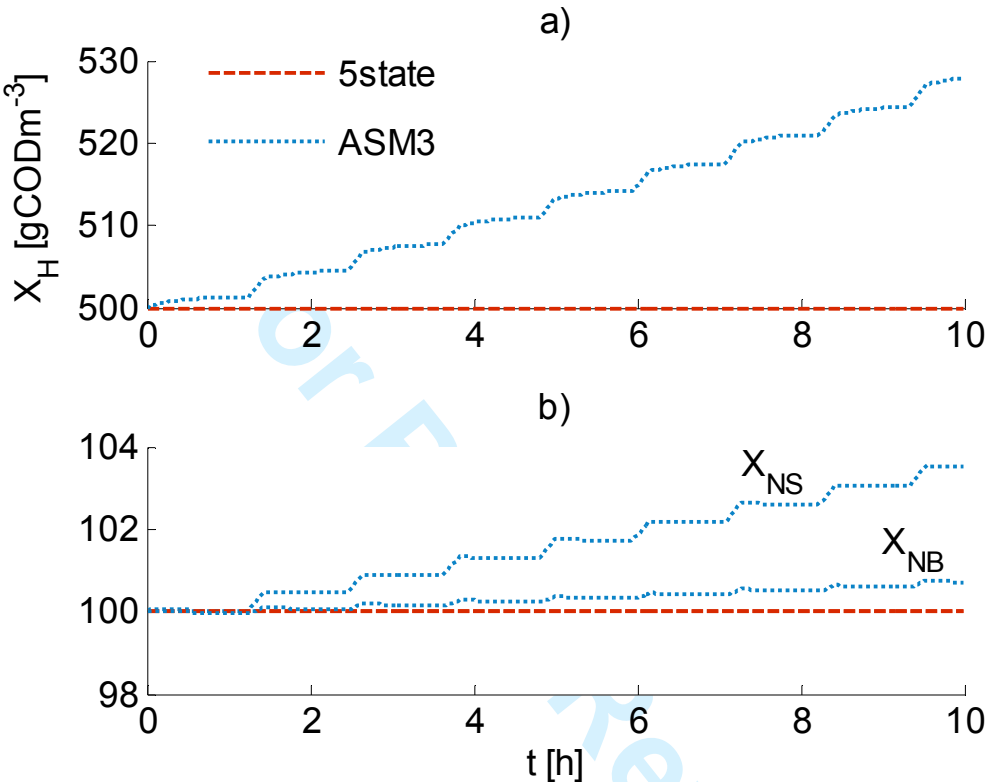


Figure 7. Biomass against time. Changes in the biomass are very small (less than 10%).



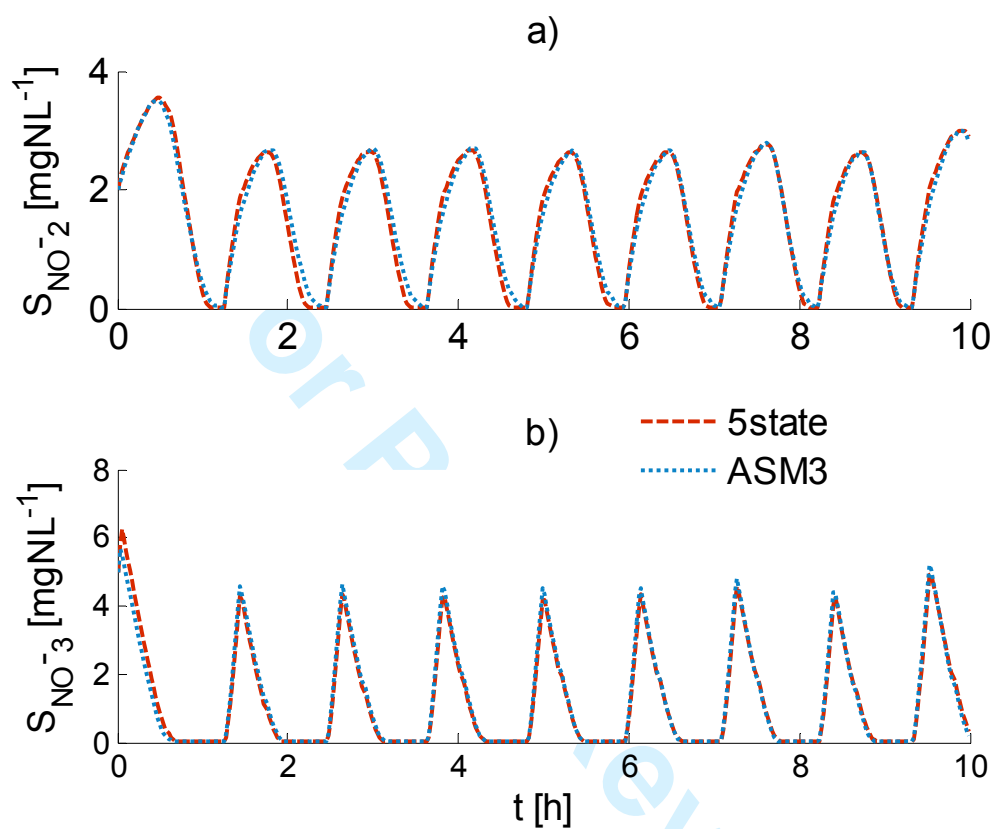


Figure 8.  $NO_x$  concentration against time.

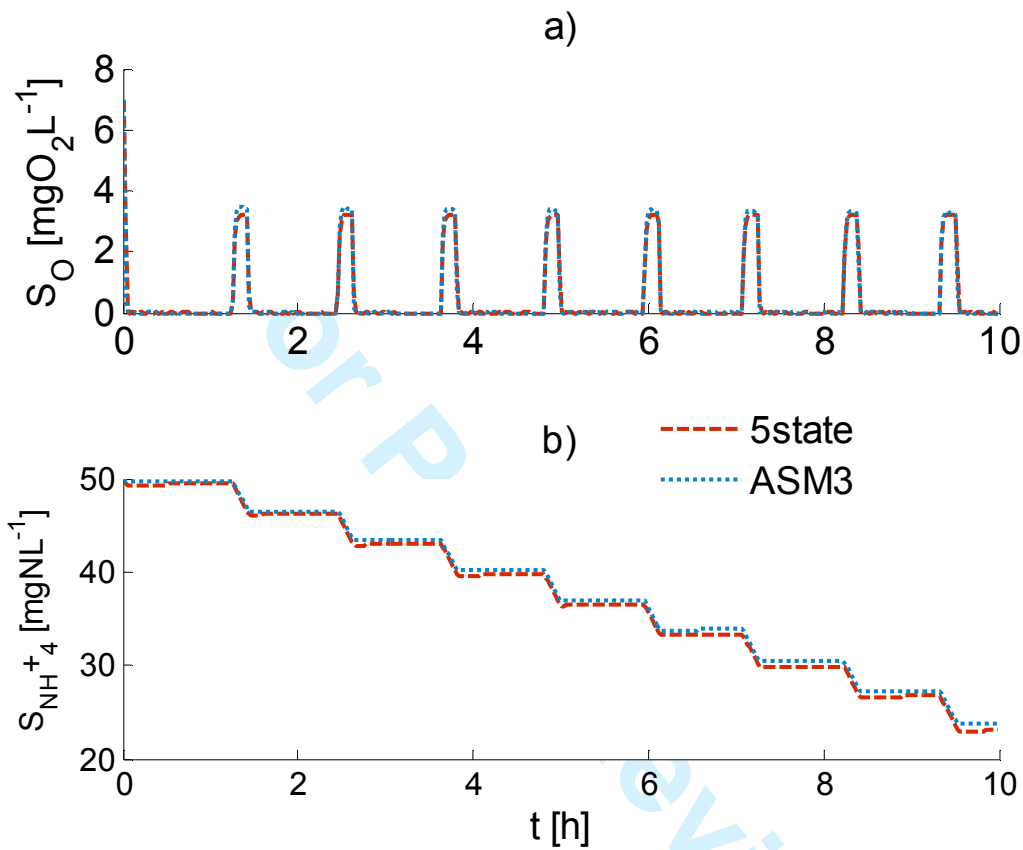


Figure 9. a) Oxygen concentration in the medium against time.

b) Ammonia concentration against time.

7.1. Tables

Table 1: reaction rates of the extended ASM3

## Heterotrophic Organisms:

- r<sub>1</sub>: Hydrolysis
- r<sub>2</sub>: Aerobic Storage
- r<sub>3</sub>: Anoxic Storage
- r<sub>4</sub>: Anoxic Storage of SS NO<sub>2</sub>-N<sub>2</sub>
- r<sub>5</sub>: Aerobic Growth of XH
- r<sub>6</sub>: Anoxic Growth NO<sub>3</sub>-NO<sub>2</sub>
- r<sub>7</sub>: Anoxic Growth NO<sub>2</sub>-N<sub>2</sub>
- r<sub>8</sub>: Aerobic Endog. Resp. of HET
- r<sub>9</sub>: Anoxic Endog. Resp. NO<sub>3</sub>-NO<sub>2</sub>
- r<sub>10</sub>: Anoxic End. Resp. NO<sub>2</sub>-N<sub>2</sub>
- r<sub>11</sub>: Aerobic Resp. of XSTO
- r<sub>12</sub>: Anoxic Resp. of SXTO NO<sub>3</sub>-NO<sub>2</sub>
- r<sub>13</sub>: Anoxic Resp. of XSTO NO<sub>2</sub>-N<sub>2</sub>

## Ammonium Oxidizing Bacteria (AOB):

- r<sub>14</sub>: Aerobic Growth, Nitritation

- r<sub>15</sub>: Aerobic End. Resp.

- r<sub>16</sub>: Anoxic End. Resp.

## Nitrite Oxidizing Bacteria (NOB):

- r<sub>17</sub>: Aerobic Growth, Nitrification

- r<sub>18</sub>: Aerobic End. Resp.

- r<sub>19</sub>: Anoxic Endog. Resp

Table 2. Stoichiometric matrix of the 9state model

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	$S_S$	$X_H$	$X_{NS}$	$X_{NB}$	$S_O$	$S_{NH4}$	$S_{NO2}$	$S_{NO3}$	$X_{Sto}$
$r_{aer}$	$-\frac{1+St_S}{Y_{Haer}}$	1	0	0	$-\frac{1-Y_{Haer}}{Y_{Haer}}$	$\frac{i_{NS}}{Y_{Haer}} - i_{NB}$	0	0	$\frac{St_S}{Y_{Haer}}$
$r_{aerNs}$	0	0	1	0	$1 - \frac{3.34}{Y_{A1}}$	$-\left(\frac{1}{Y_{A1}} + i_{NB}\right)$	$\frac{1}{Y_{A1}}$	0	0
$r_{aerNb}$	0	0	0	1	$1 - \frac{1.14}{Y_{A2}}$	$-i_{NB}$	$-\frac{1}{Y_{A2}}$	$\frac{1}{Y_{A2}}$	0
$r_{aNO2}$	$-\frac{1+St_S}{Y_{Hano2}}$	1	0	0	0	$\frac{i_{NS}}{Y_{Hano2}} - i_{NB}$	$-\frac{1-Y_{Hano2}}{1.14Y_{Hano2}}$	0	$\frac{St_S}{Y_{Hano2}}$
$r_{aNO3}$	$-\frac{1+St_S}{Y_{Hano3}}$	1	0	0	0	$\frac{i_{NS}}{Y_{Hano3}} - i_{NB}$	$\frac{1-Y_{Hano3}}{1.14Y_{Hano3}}$	$-\frac{1-Y_{Hano3}}{1.14Y_{Hano3}}$	$\frac{St_S}{Y_{Hano3}}$
	$S_S$	$X_H$	$X_{NS}$	$X_{NB}$	$S_O$	$S_{NH4}$	$S_{NO2}$	$S_{NO3}$	$X_{Sto}$
$r_{aer}$	$-\frac{1+S}{Y_{Haer}}$	1	0	0	$-\frac{1-Y_{Haer}}{Y_{Haer}}$	$\frac{i_{NS}}{Y_{Haer}} - i_{NB}$	0	0	$\frac{St_S}{Y_{Haer}}$
$r_{aerNs}$	0	0	1	0	$1 - \frac{3.34}{Y_{A1}}$	$-\left(\frac{1}{Y_{A1}} + i_{NB}\right)$	$\frac{1}{Y_{A1}}$	0	0
$r_{aerNb}$	0	0	0	1	$1 - \frac{1.14}{Y_{A2}}$	$-i_{NB}$	$-\frac{1}{Y_{A2}}$	$\frac{1}{Y_{A2}}$	0
$r_{aNO2}$	$-\frac{1+S}{Y_{Hano2}}$	1	0	0	0	$\frac{i_{NS}}{Y_{Hano2}} - i_{NB}$	$-\frac{1-Y_{Hano2}}{1.14Y_{Hano2}}$	0	$\frac{St_S}{Y_{Hano2}}$
$r_{aNO3}$	$-\frac{1+S}{Y_{Hano3}}$	1	0	0	0	$\frac{i_{NS}}{Y_{Hano3}} - i_{NB}$	$\frac{1-Y_{Hano3}}{1.14Y_{Hano3}}$	$-\frac{1-Y_{Hano3}}{1.14Y_{Hano3}}$	$\frac{St_S}{Y_{Hano3}}$

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**Table 3: 8state model constants and its values**

SOSTar =	7;	[mgO2/l]	process	K_NH2 =	0.1;	[mgCOD/l]	ASM3
K_La =	1000;	[d-1]	process	K_S =	10;	[mgCOD/l]	ASM3
i_NB =	0.086;	[gN/gCOD]	fitted	K_S1 =	0.1;	[mgCOD/l]	ASM3
mou_H =	0.6021;	[d-1]	fitted	K_S2 =	0.1;	[mgCOD/l]	ASM3
mou_A1 =	0.6552;	[d-1]	fitted	K_NHH =	0.05;	[mgN/l]	ASM3
mou_A2 =	0.3468;	[d-1]	fitted	K_O1 =	0.2;	[mgO2/l]	ASM3
Y_Haer =	0.1302;	[gCOD/gCOD]	fitted	K_NH =	0.1;	[mgN/l]	ASM3
Y_A1 =	0.1327;	[gCOD/gN]	fitted	K_O =	0.8;	[mgO2/l]	ASM3
Y_A2 =	0.0985;	[gCOD/gN]	fitted	K_NO21 =	0.5;	[mgO2/l]	ASM3
Y_A3 =	0.0331;	[gCOD/gN]	fitted	K_NO3 =	0.5;	[mgN/l]	ASM3
i_NSS =	0.01;	[gN/gCOD]	ASM3	K_O21 =	0.2;	[mgO2/l]	ASM3
Y_Hanox =	0.0632;	[gCOD/gCOD]	fitted	K_NO2 =	0.25;	[mgN/l]	ASM3
mou_H1 =	0.0511;	[d-1]	fitted	K_O22 =	0.2;	[mgO2/l]	ASM3
mou_H2 =	0.0362;	[d-1]	fitted	stS =	1.7;	[ ]	fitted
K_NH1 =	0.01;	[mgCOD/l]	ASM3	stO =	0.08;	[ ]	fitted

Table 4. Comparison of the computation time.

Models simulated with Matlab® R2008b

Number of Aer-Anox phases	ODE15s CPU time (sec)			ASM3/5State
	ASM3	9State	5State	
1	1.769	0.157	0.156	11.3
2	2.162	0.172	0.14	15.4
3	2.602	0.172	0.172	15.1
4	2.583	0.172	0.156	16.6
5	2.608	0.156	0.172	15.2

Table 5. Singular function evaluations speed

Evaluation of Jacobians	ASM3	2071.114
	8State	565.364
	5State	321.6
CPU time 100 evaluations (sec)	ASM3	2.225
Calculation of the differential eq. system	8State	0.157
	5State	0.132
	ASM3	2.225
CPU time 1000 evaluations (sec)	8State	0.157
	5State	0.132
	ASM3	2.225

	$S_S$	$X_H$	$X_{NS}$	$X_{NB}$	$S_O$	$S_{NH_4}$	$S_{NO_2}$	$S_{NO_3}$	$X_{Sto}$
$r_{aae}$	$-\frac{1 + St_S}{Y_{Haer}}$	1	0	0	$-\frac{1 - Y_{Haer}}{Y_{Haer}}$	$\frac{i_{NSS}}{Y_{Haer}} - i_{NB}$	0	0	$\frac{St_S}{Y_{Haer}}$
$r_{aans}$	0	0	1	0	$1 - \frac{3.34}{Y_{A1}}$	$-\left(\frac{1}{Y_{A1}} + i_{NB}\right)$	$\frac{1}{Y_{A1}}$	0	0
$r_{aanb}$	0	0	0	1	$1 - \frac{1.14}{Y_{A2}}$	$-i_{NB}$	$-\frac{1}{Y_{A2}}$	$\frac{1}{Y_{A3}}$	0
$r_{aNO_2}$	$-\frac{1 + St_S}{Y_{Hanox}}$	1	0	0	0	$\frac{i_{NSS}}{Y_{Hanox}} - i_{NB}$	$-\frac{1 - Y_{Hanox}}{1.14Y_{Hanox}}$	0	$\frac{St_S}{Y_{Hanox}}$
$r_{aNO_3}$	$-\frac{1 + St_S}{Y_{Hanox}}$	1	0	0	0	$\frac{i_{NSS}}{Y_{Hanox}} - i_{NB}$	$\frac{1 - Y_{Hanox}}{1.14Y_{Hanox}}$	$-\frac{1 - Y_{Hanox}}{1.14Y_{Hanox}}$	$\frac{St_S}{Y_{Hanox}}$

Table 2.  
196x93mm (96 x 96 DPI)