



Control of an alternating aerobic–anoxic activated sludge system — Part 1: development of a linearization-based modeling approach

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Abstract

A two-phase model (linear in each phase) is developed for an alternating aerobic–anoxic completely mixed activated sludge process for the removal of carbonaceous substrates, nitrification, and denitrification. The linearized model is adapted from the activated sludge model No. 1 (ASM1) originally developed by the International Association on Water Pollution Research and Control. The modified dynamic model captures the essential process features of ASM1 while dramatically reducing demand on computational resources. Simulations may be conducted in such short times that the simplified model is suitable for inclusion in on-line optimization-based process control schemes. Calibrated model parameters are within the ranges specified in ASM1. Comparison of model predictions with experimental measurements from two different sets of bench-scale alternating aerobic–anoxic reactors indicates reasonable prediction accuracy of the model; further compensation for inaccuracy is achievable by introducing a feedback loop. © 2000 Elsevier Science Ltd. All rights reserved.

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1. Introduction

Activated sludge processes for nutrient removal are versatile systems which, with proper design and operation, can meet effluent requirements of total nitrogen and total phosphorus concentrations of less than 8 and 1 mg/l, respectively. However, process control and optimization in the wastewater treatment field is in its infancy. A few plants have implemented sensors and computers to monitor dissolved oxygen (e.g., oxygen uptake rate for control of anaerobic duration in a sequencing batch system, Larose, Perrier & Comeau, 1997), but optimization is mostly used in simulations (e.g., Potter, Koopman & Svoronos, 1996) and seldom implemented in actual plant operations. One of the contributing factors for the relative inactivity in wastewater process optimization is the lack of suitable and easily implemented models to represent the process dynamics. While some models adequately describe the behavior of

activated sludge systems, they are often too complicated or unwieldy (e.g., high-dimensional or stiff) to be of practical use in ordinary control operations.

It is true that modeling biological phenomena in wastewater treatment plants has recently received considerable attention. A good model not only encapsulates a better understanding of the complicated biological process fundamentals but is also essential for process design (Oles & Wilderer, 1991; Daigger & Nolasco, 1995), start-up (Finsson, 1993), dynamics predictions (Marsili-Libelli & Giovannini, 1997), performance prediction (Stokes, Takacs, Watson & Watts, 1993), control (Coen, Vanderhaegen, Boonen, Vanrolleghem & van Meenen, 1997) and optimization (Lesouef, Payraudeau, Rogalla & Kleiber, 1992; Potter et al., 1996; Lukasse, Keesman, Klapwijk & van Straten, 1998). To date the most successful model and the industrial standard is the activated sludge model No. 1 (ASM1) developed in 1986 (Henze, Grady, Gujer, Marais & Matsuo, 1986) by the Task Group of the International Association on Water Pollution Research and Control (now IAWQ, the International Association on Water Quality). Widespread use of ASM1 to describe carbonaceous biological oxygen demand (BOD) removal, nitrification, and denitrification in

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many applications has validated its capability to predict process performance. In 1995, an updated version (ASM2) was introduced to incorporate biological phosphorus removal (Gujer, Henze, Mino, Matsuo, Wentzel & Marais, 1995), and in 1998 further revisions were presented (Henze, Gujer, Mino, Matsuo, Wentzel, Marais & van Loosdrechi, 1998). Another version of ASM1 (called ASM3) has also been introduced which corrects a number of known defects present in the original model (Gujer, Henze, Mino & van Loosdrechi, 1998).

A common trait among the versions of these models is that each is high-dimensional and possesses a large number of kinetic and stoichiometric parameters. For example, ASM3 comprises 12 process rate equations involving seven dissolved and six particulate components, 21 kinetic parameters, and 13 stoichiometric and composition parameters. Though this level of model complexity is necessary to describe and relate dynamics over a wide range of operating conditions, it can present a significant computational encumbrance for performing simulations and analysis. Some applications do not require “universal” model validity (i.e., reliability over *all* possible operating conditions), and in these cases it may be advantageous to implement a simpler model form which performs well over a more limited operating region.

The use of simplified process models (SPMs) to facilitate process control has been demonstrated by several investigators (e.g., Kabouris & Georgakakos, 1990; Zhao, Isaacs, Seberg & Kummel, 1994a,b, 1995) for improving nitrogen removal in wastewater treatment systems. Jeppsson and Olsson (1993) combined filtering and model reduction techniques to simplify ASM1 and identify parameters for modeling wastewater treatment plant operation. A simplified model may exhibit poor accuracy due to model simplification and approximation. Zhao, Isaacs, Seberg and Kummel (1994c) compensated for the inaccuracy of a simplified model of a wastewater treatment process by introducing a feedback loop comparing on-line process measurements with the predicted values and using the differences to offset future model-predicted values.

Hybrid modeling techniques offer one possible avenue for creating a simplified representation of complicated systems. One approach is to exploit empirical components (such as neural networks) to substitute for terms or expressions in the full model which are either not well described by the existing understanding of the process physics or are too complicated to be directly incorporated. The empirical portions are combined with first-principles knowledge to allow prediction of the overall process behavior. Another approach is parallel use of both SPM and neural networks, in which the outputs of the trained networks compensate for the output errors of the SPM. The final hybrid model predictions are then obtained by summing the outputs from both the SPM and neural networks. Hybrid modeling has been applied

in the chemical engineering field (Psichogios & Ungar, 1992; Su, McAvoy & Werbos, 1992; Su, Bhat, Minderman & McAvoy, 1992; Thompson & Kramer, 1994) and have potential applications in wastewater process modeling. Indeed, a few results have been published which demonstrate that hybrid models can adequately model process dynamics in nitrification, denitrification, and biological phosphorus removal (Zhao & McAvoy, 1996; Zhao, Hao, McAvoy & Chang, 1997; Zhao, Hao & McAvoy, 1999; Birdi, Hao & Zhao, 1998).

The objective of the present paper is to describe an alternative modeling strategy for the simplification of ASM1, which yields a computationally efficient model with reasonable prediction capabilities. The approach is based upon linearizing the full ASM1 model for each of the operating phases (in our case, “air-on” and “air-off” phases) of a bench-scale alternating aerobic–anoxic (AAA) activated sludge system. Results are presented comparing the predicted dynamics versus experimental measurements obtained. The companion paper then describes the implementation of the “linearized” model in a control setting for process optimization of the AAA system to minimize energy expenditure while maintaining the effluent discharge permit of ammonia.

2. Model development

The “linear system” developed is specific for the AAA system, which performs organic removal and nitrification (biological oxidation of inorganic ammonia to nitrates) during the aerobic (“air-on”) cycle and denitrification (biological nitrate reduction to nitrogen) in the subsequent anoxic (“air-off”) cycle. Because the AAA system is forced by regularly switching air on and off, its dynamics do not normally asymptote to a steady state, even under constant influent composition. Therefore, the linearization of ASM1 is not approached here by the traditional means of partial differentiation of the model equations about a steady state. Instead, linear approximations for nonlinear terms are substituted in the dynamic equations of ASM1. The final overall model implementation involves alternating between each linear phase model.

Eight different chemical reactions (ρ_j) are described in the ASM1 model; their rate expressions are:

- Aerobic growth of heterotrophs:

$$\rho_1 = \mu_H \left(\frac{S_S}{K_S + S_S} \right) \left(\frac{S_O}{K_{OH} + S_O} \right) X_{BH}. \quad (1)$$

- Anoxic growth of heterotrophs:

$$\rho_2 = \mu_H \left(\frac{S_S}{K_S + S_S} \right) \left(\frac{K_{OH}}{K_{OH} + S_O} \right) \left(\frac{S_{NO}}{K_{NO} + S_{NO}} \right) \eta_G X_{BH}. \quad (2)$$

- Aerobic growth of autotrophs:

$$\rho_3 = \mu_A \left(\frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left(\frac{S_O}{K_{OA} + S_O} \right) \times \left(\frac{S_{ALK}}{K_{ALK} + S_{ALK}} \right) X_{BA}. \quad (3)$$

- Decay of heterotrophs:

$$\rho_4 = b_H X_{BH}. \quad (4)$$

- Decay of autotrophs:

$$\rho_5 = b_A X_{BA}. \quad (5)$$

- Ammonification of soluble organic nitrogen:

$$\rho_6 = k_a S_{ND} X_{BH}. \quad (6)$$

- Hydrolysis of entrapped organics:

$$\rho_7 = k_h \frac{X_S}{K_X + (X_S/X_{BH})} \left[\left(\frac{S_O}{K_{OH} + S_O} \right) + \eta_H \left(\frac{K_{OH}}{K_{OH} + S_O} \right) \left(\frac{S_{NO}}{K_{NO} + S_{NO}} \right) \right], \quad (7)$$

- Hydrolysis of entrapped organic nitrogen:

$$\rho_8 = k_h \frac{X_{ND}}{K_X + (X_S/X_{BH})} \left[\left(\frac{S_O}{K_{OH} + S_O} \right) + \eta_H \left(\frac{K_{OH}}{K_{OH} + S_O} \right) \left(\frac{S_{NO}}{K_{NO} + S_{NO}} \right) \right]. \quad (8)$$

The symbols $\mu_H, \mu_A, K_S, K_{OH}, K_{NO}, K_{NH}, \eta_G, \eta_H, K_{OA}, K_X, k_s, b_H, b_A, k_a$ and k_h are defined in Table 1. The switching functions in the large round brackets activate or deactivate different kinetic terms, depending on the presence or absence of a particular chemical species. The various kinetic parameters of ASM1 are calibrated to best reflect the experimentally observed dynamics of a bench-scale AAA system, and these are also provided in Table 1. Air-on and air-off phases are, respectively, implemented by toggling k_{La} between $k_{La} = 225$ and $k_{La} = 0$.

For simplification of ASM1, first-order expressions are used which best approximate each reaction rate expression in both the “air-on” and the “air-off” phases. The dissolved oxygen concentration (S_O) during the aeration period is assumed to be high enough that biological reactions are not limited. The alkalinity (S_{ALK}) term has been removed since denitrification can partially recover some alkalinity consumed through nitrification. The oxygen behavior is controlled and does not need to be modeled. Actually, “Monod terms” for S_O and S_{ALK} in the models are negligible, if dissolved oxygen and alkalinity levels are maintained at high level, since the known kinetic parameters for those variables, K_{OA}, K_{OH} , and K_{ALK} , are small (Table 1). X_P is a product that does not interact with the other species and has also been omitted

from the dynamic model (though the remaining equations still reflect the correct stoichiometry). These approximations do not affect growth rate equations. The following eight equations are used from ASM1; note that flow terms have been introduced in the continuous-flow completely mixed system evaluated:

$$\dot{S}_S = \frac{S_{S,INF} - S_S}{\theta} - \frac{1}{Y_H} (\rho_1 + \rho_2) + \rho_7, \quad (9)$$

$$\dot{X}_S = \frac{X_{S,INF}}{\theta} - \frac{X_S}{\tau} + (1 - f_P) (\rho_4 + \rho_5) - \rho_7, \quad (10)$$

$$\dot{X}_{BH} = \frac{X_{BH}}{\tau} + \rho_1 + \rho_2 - \rho_4, \quad (11)$$

$$\dot{X}_{BA} = \frac{X_{BA}}{\tau} + \rho_3 - \rho_5, \quad (12)$$

$$\dot{S}_{NH} = \frac{S_{NH,INF} - S_{NH}}{\theta} - i_{XB} (\rho_1 + \rho_2) - \left(i_{XB} + \frac{1}{Y_A} \right) \rho_3 + \rho_6, \quad (13)$$

$$\dot{S}_{NO} = \frac{S_{NO,INF} - S_{NO}}{\theta} - \frac{1 - Y_H}{2.86 Y_H} \rho_2 + \frac{\rho_3}{Y_A}, \quad (14)$$

$$\dot{S}_{ND} = \frac{S_{ND,INF} - S_{ND}}{\theta} - \rho_6 + \rho_8, \quad (15)$$

$$\dot{X}_{ND} = \frac{X_{ND,INF}}{\theta} - \frac{X_{ND}}{\tau} + (i_{XB} - f_P i_{XE}) (\rho_4 + \rho_5) - \rho_8, \quad (16)$$

where θ is the hydraulic detention time and τ the mean cell residence time. Kinetic parameters have the same values as listed in Table 1 and constants with the subscript INF are the influent concentrations also listed in Table 1. The rate expressions for ρ_1 through ρ_8 are adapted to different forms than used in ASM1; first-order expressions are used in the linear-phase models, and these are presented in matrix form in Table 2. The last column in Table 2 also lists rate expressions for the two separate phases. The components in the model and the transformation processes are characterized with the indices i and j , respectively. The coefficients in the matrix (v_{ji}) represent the stoichiometric relationships between state variables and the process rate equations which form a vector ρ_j . The blanks in the matrix represent 0's. Therefore, the change of a component i according to time (e.g., soluble organic nitrogen (S_{ND}) in column 7) can be read by multiplying all the stoichiometric coefficients (i.e., v_{j7}) in the vertical column of the component to the corresponding kinetic rate equations, ρ_j and the resultant kinetic equation for the component is given by the summation of these products (i.e., $r_i = \sum v_{ji} \rho_j$). In this

Table 1
State variables and parameters used in the ASM1 and linearized model

Parameter	Definition and units	Values used	
		ASMI ^a	Linearized model ^b
Influent composition for the AAA system			
$S_{S,INF}$	Readily biodegradable substrate, mg COD/l	182	210
$X_{S,INF}$	Slowly biodegradable substrate, mg COD/l	69	95
$S_{NH,INF}$	Ammonia nitrogen, mg N/l	24.1	14.7
$S_{NO,INF}$	Nitrate and nitrite nitrogen, mg N/l	0.0	0.0
$S_{ND,INF}$	Soluble biodegradable organic nitrogen, mg N/l	6.9	5.5
$X_{ND,INF}$	Particulate biodegradable organic nitrogen, mg/l	8.8	6.2
$S_{ALK,INF}$	Alkalinity, mmol/l	4.3	3.4
$S_{O,INF}$	Dissolved oxygen, mg COD/l	5.4	5.0
Stoichiometric coefficients			
Y_H	Heterotrophic yield, mg COD/mg COD removed	0.67	0.4
Y_A	Autotrophic yield, mg COD/mg N oxidized	0.24	0.24
f_P	Fraction of biomass yielding decay products	0.08	0.08
i_{XB}	Fraction of nitrogen in biomass, mg N/mg COD	0.086	0.086
i_{XP}	Fraction of nitrogen in decay products, mg N/mg COD	0.06	0.06
Kinetic coefficients			
μ_H	Maximum specific growth rate for heterotrophs, d ⁻¹	6.0	6.0
μ_A	Maximum specific growth rate for autotrophs, d ⁻¹	0.65	0.65
b_H	Decay rate for heterotrophs, d ⁻¹	0.62	0.62
b_A	Decay rate for autotrophs, d ⁻¹	0.12	0.12
η_θ	Correction factor for anoxic growth, dimensionless	0.8	0.8
η_h	Correction factor for hydrolysis. Dimensionless	0.7	0.62
k_a	Ammonification rate for soluble organic nitrogen, d ⁻¹	5.0	0.16
k_h	Particulate organic hydrolysis rate, d ⁻¹	0.1	3.0
Monod half-saturation coefficients			
K_S	S_S , mg COD/l	0.16	
K_{OH}	S_O for heterotrophs, mg COD/l	0.1	
K_{NO}	S_{NO} , mg N/l	0.2	
K_{NH}	S_{NH} , mg N/l	0.2	
K_{OA}	S_O for autotrophs, mg COD/l	1.0	
K_X	X_S , mg COD/mg COD	0.15	
K_{ALK}	ALK , mmol/l	0.1	
Reactor condition			
θ	Hydraulic retention time, hr	12	12
τ	Mean cell residence time, day	15	12

^aParameters except Monod half-saturation coefficients are incorporated into the linearized model for Huang's data.

^bParameters used for the current AAA system.

case, the rate of S_{ND} change during aerobic cycle can be represented by

$$r_7 = \dot{S}_{ND} = -1 \times k_a J_4 + 1 \times k_h J_6 X_{ND}. \quad (17)$$

For the nominal operating conditions of ASM1, it was observed that a number of the state variables, such as the amount of heterotrophic biomass, remained approximately constant throughout each cycle; this allowed substitution of constant values in place of such variables for simplification of the higher-order rate expressions. In some process equations such as ρ_1 , ρ_2 , ρ_3 , ρ_7 , and ρ_8 , an appropriate constant factor (J_i , $i = 1, 2, \dots, 6$) was used to replace a nonlinearity of switching factors (hyperbolic

term of Monod expression, $S/(K + S)$). The values used for these correction factors, which can be tuned to minimize prediction error, are provided in Table 3. To achieve further computational speedup, these linear models describing the air-on and air-off phase dynamics were discretized, treating the influent terms as constant inputs. All coding was performed in MATLAB.

2.1. Model calibration and testing

The numerous unknown parameters of the full ASM1 equations were hand-tuned to provide qualitative agreement with experimental data obtained on a bench-scale

Table 2
Process kinetics and stoichiometry in the linearized model

Component, $i \rightarrow$	1	2	3	4	5	6	7	8	Process Rate, ρ_j [$\text{ML}^{-3} \text{T}^{-1}$]
S_S		X_S	$X_{B,H}$	$X_{B,A}$	S_{NH}	S_{NO}	S_{ND}	X_{ND}	Aerobic cycle
S_S									Anoxic cycle
1 Aerobic growth of heterotrophs	$-\frac{1}{Y_H}$		1		$-i_{XB}$				$\mu_H J_1 S_S$ 0
2 Anoxic growth of heterotrophs	$-\frac{1}{Y_H}$		1		$-i_{XB}$	$-\frac{1 - Y_H}{2.86 Y_H}$			0 $\mu_H \eta_g J_2 S_S$
3 Aerobic growth of autotrophs				1					0
4 Decay of heterotrophs		$1 - f_p$	-1		$-i_{XB} - \frac{1}{Y_A}$	$\frac{1}{Y_A}$		$i_{XB} - f_p i_{XP}$	$\mu_A J_3 S_{NH}$ $b_H X_{B,H}$
5 Decay of autotrophs		$1 - f_p$		-1				$i_{XB} - f_p i_{XP}$	$b_H X_{B,H}$ $b_A X_{B,A}$
6 Ammonification of soluble organic nitrogen					1		-1		$k_d J_4 S_{ND}$
7 Hydrolysis of entrapped organic nitrogen	1						1	-1	$k_H \eta_p J_5 X_S$ $k_H \eta_p J_5 S_{ND}$
8 Observed Conversion Rate [$\text{ML}^{-3} \text{T}^{-1}$]									

$$r_j = \sum_i v_{ij} \rho_j$$

Table 3
Correction factors used in the linearized model

Symbol	J_1	J_2	J_3	J_4	J_5	J_6
Huang's data	184	180	45	1100	2.9	9.0
Current study	180	250	100	1100	3	6.7

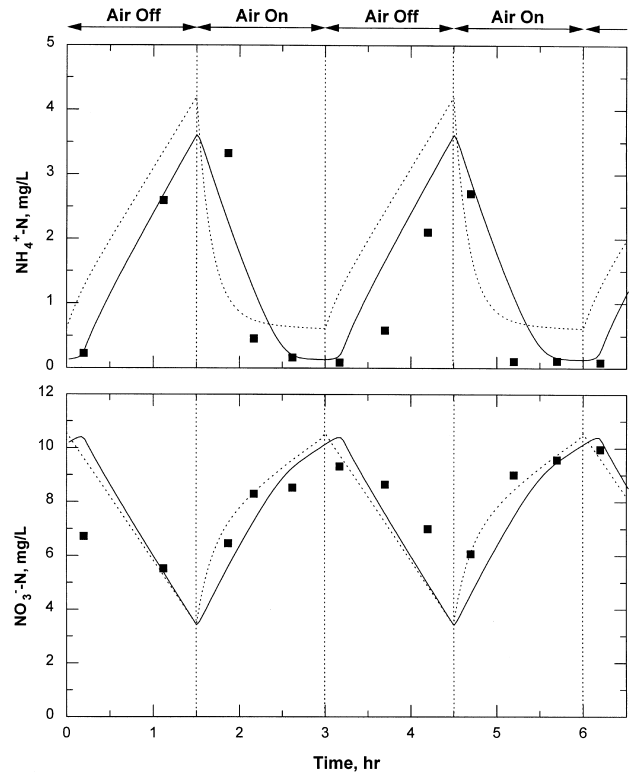


Fig. 1. Comparison of full ASM1 (solid) and linearized model (dashed) with experimental data used for calibration. $\theta = 12$ h, $\tau = 15$ days, air on/off = 1.5 h/1.5 h.

AAA wastewater treatment system (Huang, 1993). An automated approach to parameter estimation was in this case prohibitively time consuming due to the stiffness of the equations and the need to determine the limiting (long term) behavior. The linear model is based on the parameter set used for the full ASM1 model, with some further hand tuning applied to the parameters J_i . Each of the model system parameters was chosen within ranges appropriate for a typical system (Henze et al., 1986).

The long-term dynamic behavior predicted by each model is represented in Fig. 1, in which the time series of the full ASM1 model (solid lines) and the linear model (dashed lines) are plotted along with the available experimental data from Huang (rectangles). Time series for ammonia-nitrogen and nitrate-nitrogen are, respectively, presented in the upper and lower graphs. Good qualitative agreement was obtained between the two models and the actual data of the bench scale system.

Further verification of the simplified model was conducted using data from the currently operating AAA system. The slightly different operating conditions of the system (from those of Huang) necessitated a second calibration of the linearized model. The model captured the dynamics of the system rather well and was subsequently implemented in an optimization-based control system (see the companion paper, Kim, McAvoy, Anderson & Hao, 2000).

3. Materials and methods

Experimental data were obtained from a laboratory AAA reactor which had been in operation for 13 months. The reactor is made of acrylic fiber plastics and has a working volume of 5 l, with a reactor volume of 4 l and a clarifier volume of 1 l. The settled sludge in the clarifiers is recycled internally. The primary effluent taken twice a week from a local plant was used as influent feed. The typical compositions were: total chemical oxygen demand (COD) 150–300 mg/l; soluble COD 60–150 mg/l, total Kjeldahl nitrogen 23–40 mg/l, $\text{NH}_4^+\text{-N}$ 13–24 mg/l, and ortho-phosphorus 3 mg/l. The influent wastewater was supplemented with an additional carbon source including a mixture of acetate, methanol and ethanol to increase the wastewater strength (total COD \approx 300 mg/l) to provide adequate COD/N ratio. The system was also operated at $\theta = 12$ h and $\tau = 12$ days.

The results of dynamic studies in different aeration cycles (i.e., 1 or 1.5 h air-on) and total cyclic duration periods (i.e., 2 or 3 h) were used for model calibration and verification. The on/off period of the AAA reactor was controlled by a preset timer and a solenoid valve. Sample analyses for NH_4^+ , NO_3^- , and NO_2^- follow the procedures in the standard methods (Standard Methods, 1995).

4. Results and discussion

One set of the data was first used to calibrate the linearized model. The calibrated parameter values are summarized in Tables 1 and 3; parameter values are close to those used in Huang's simulation. The calibrated results are shown in Fig. 2. In general, the model predictions describe reasonably well the trend of biological nitrification during aeration and denitrification during anoxic periods. It was noted, however, that the model predicts the rapid disappearance of nitrate during air-off periods, whereas experimental results indicate a lag. This is apparently due to the oversimplification of the role of dissolved oxygen in the model; nitrate is reduced only when the dissolved oxygen is depleted.

The model was then applied to more recent dynamic studies with different sets of air-on/off periods for model verification. Considering the simplicity of the model, the

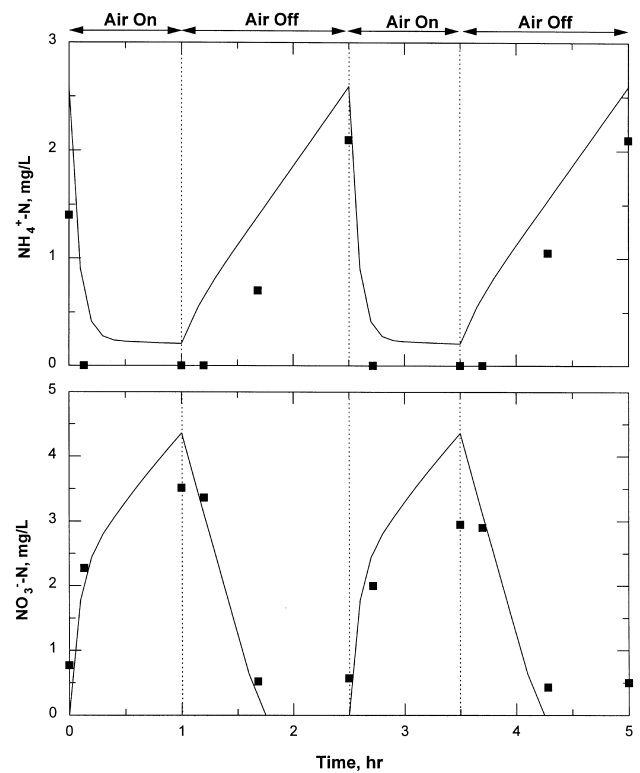


Fig. 2. Comparison of linearized model prediction with experiment data used for model calibration. $\theta = 12$ h, $\tau = 12$ days, air on/off = 1.0 h/1.5 h.

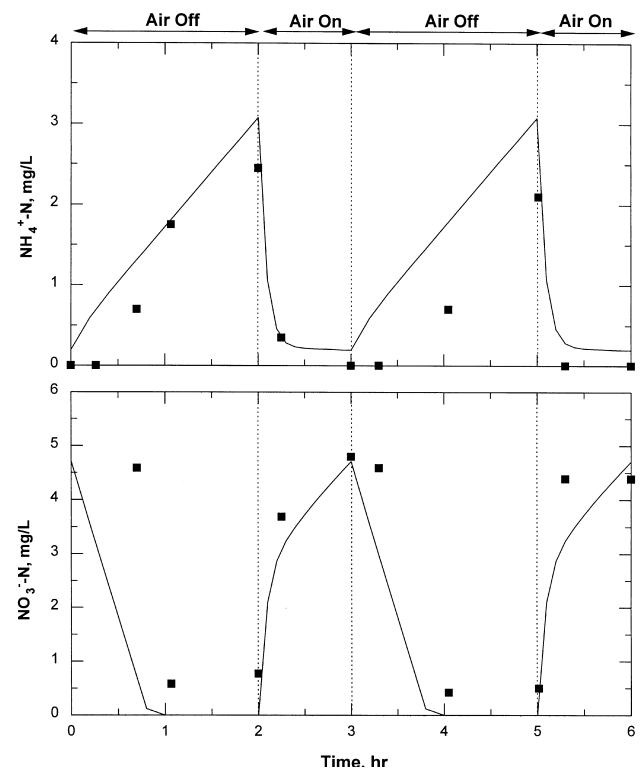


Fig. 3. Comparison of linearized model prediction with experiment data. $\theta = 12$ h, $\tau = 12$ days, air on/off = 1.0 h/2.0 h.

results are again reasonable a match with the experimental results (Figs. 3–5), albeit some predictions were not as good. Since many factors in these experiments certainly differ from the conditions used in model calibration (Fig. 2), such results indicate that the model structure is sufficiently reliable for use in a process control application determining the time duration for aeration. Further improvement on the prediction capability is possible using a corrective feedback loop based on experimental measurements taken on-line. It must be reiterated that the simplifications introduced in this paper are application-motivated and do not result in a model which reflects accurate system behavior for very broad ranges of operating conditions. However, streamlining the model and the rapid turnaround time (a few minutes versus a few hours for ASM1) for computing the model predictions are expected to enhance its application in on-line wastewater process control. This is demonstrated in the accompanying paper in which the linearized model is exploited in an optimization-based control scheme for a bench-scale AAA system. In the control approach, the optimizer conducts many successive simulations of the AAA system in order to estimate the minimum amount of aeration time necessary to maintain the required effluent ammonia concentration. While it would be prohibitively time-consuming to use the full ASM1 equations, the linearized model is sufficiently fast and reliable to be effective for the application.

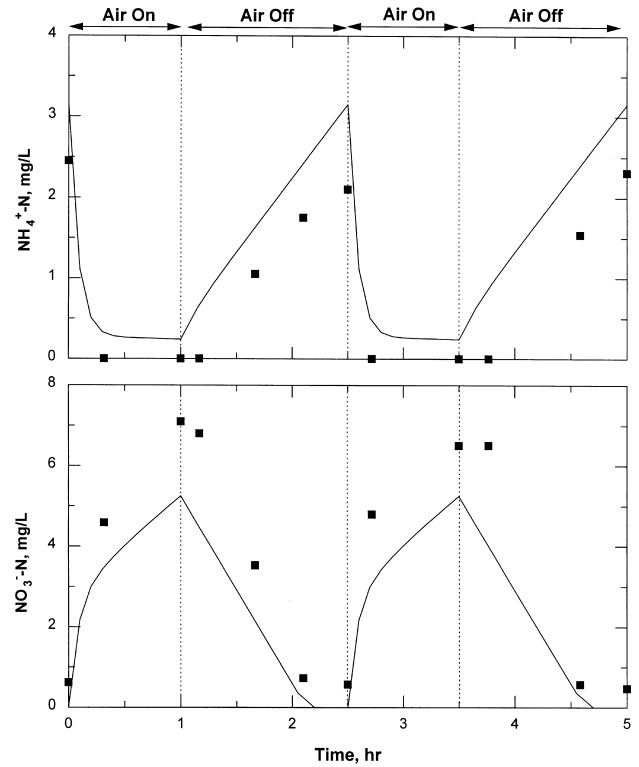


Fig. 5. Comparison of linearized model prediction with experiment data. $\theta = 12$ h, $\tau = 12$ days, air on/off = 1.0 h/1.5 h.

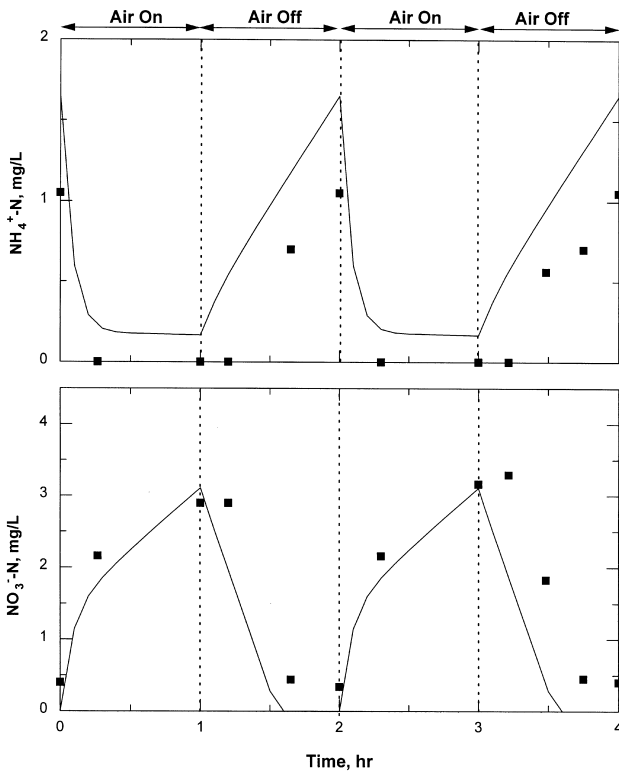


Fig. 4. Comparison of linearized model prediction with experiment data. $\theta = 12$ h, $\tau = 12$ days, air on/off = 1.0 h/1.0 h.

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