ASM1-based Modeling and Simulation of a Full-scale Simultaneous Nitrification and Denitrification Plant

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Abstract

Simultaneous nitrification and denitrification (SND) caused by insufficient oxygen supply into the flocs has been found to take place in many activated sludge processes in wastewater treatment plants (WWTP). Although SND may not be favorable in the WWTP design as it leads to decrease in the reaction rates of both nitrification and denitrification, it can be an option of WWTP operation to increase total nitrogen (TN) removal rate or reduce the cost of liquid cycle from aeration tank to anoxic tank. In many publications of modeling and simulation of WWTPs involving nitrification and denitrification, the emphasis has mainly been focused on the processes where nitrification and denitrification occur alternatively. In the present contribution, we developed a model of activated sludge process by modifying the ASM1 model and introducing a factor to account for the anoxic zone which was resulted from the low dissolved oxygen (DO) in either the macro or micro levels. The developed model was used for a full-scale wastewater treatment plant (WWTP) operating at low DO, and the simulation of the model was performed for an operation of 90 days. In comparison with the standard ASM1 model with default kinetic constants, the resultant NOx, NH3 and total nitrogen from our model were in better agreements with the plant measurements, while both models led to very close Chemical Oxygen Demand (COD) trajectories which also matched the plant measurements. The model developed in this work would be helpful for process engineers to investigate different configurations or operating strategies for the existing plant. It also benefits the operators by predicting the plant behavior under various operations and exploring different what-if situations.

Keywords: Simulation; Activated sludge; Simultaneous nitrification and denitrification; wastewater treatment plant; ASM1.

1. Introduction

The activated sludge process is the most generally applied biological wastewater treatment method. In such process, organic degradation, nitrification and denitrification may take place simultaneously. The time varying nature of influent flow rate, substrate load and physical characteristics make the activated sludge process complicated [Nuhoglu A, 2005]. Mathematical modeling provides a powerful tool for design, operation, prediction and control of the activated sludge process. Considerable effort has been invested in the modeling of the activated sludge process since early 1970s. The international water association (IWA) task group on Mathematical Modeling and Operation of Biological Wastewater Treatment has presented several Activated Sludge Models (ASM), i.e. ASM1, ASM2, ASM2d and ASM3 [IWA, 2000]. Because of the comprehensiveness of the bioconversion processes in ASM, it is applicable for simulating a wide range of activated sludge processes.

In many wastewater treatment plants (WWTPs) of nitrogen removal, the nitrification and denitrification occur in aerobic and anoxic tanks respectively. Thus the existing modeling and simulation often focused on the processes where nitrification and denitrification occur either during different phases or in different tanks. However, the phenomenon of aerobic denitrification has also been found in various systems in WWTPs [Munch et. al., 1996]. One of the main arguments is that the denitrification occurs in the local anoxic zones due to non-uniform distribution of DO concentration in the aeration tank. It was found [Pochana et. al. 1999] that high stir intensity, breaking big flocs and increasing oxygen concentration could obviously decrease or eliminate denitrification in an aeration tank. The anoxic zones, in the macro level, may be formed if the hydraulics of the reactor is not properly designed or the stir intensity is not sufficiently high which lead to longer hydraulic residence time and incomplete mass transfer. In the micro level, the anoxic cores can be formed within bigger bio-flocs as oxygen is depleted in the half way when diffusing from the bulk liquid to the center of the flocs.

In the present work, by modifying the ASM1 we developed a model for the simulation of a full-scale WWTP treating municipal wastewater and operating under low DO condition [Liu F., 2004]. A factor (between 0 and 1) was introduced to correct the aerobic and anoxic reaction rates. The kinetics of the resultant model consisted of 6 processes and 12 components. Comparing to the ASM1, the organic nitrogen compounds were not treated as independent variables but evaluated as dependent variables of COD so as to simplify the model. Since the aeration tank was composed of 4 compartments in series, the hydraulics was modeled as a series of completely stirred tank reactors (CSTR).

To compare the performance of the developed model, the standard ASM1 model was re-produced and the default kinetic constants were used. The dynamic simulation of the WWTP operating over 90 days was performed by using the two models. The results showed that our model reflected the patterns observed in the effluent ammonia (NH_3-N) and nitrate (NO_3-N), while the ASM1 model overestimated the nitrate and underestimated the ammonia. Both models were in good agreements with the plant measurements of COD.

2. Materials and methods

2.1 Description of the plant

The WWTP under study was built in 1976 and was designed to treat organics in the municipal wastewater with the capacity of 76000 [m^3 day^{-1}]. A sludge absorption-activation process was used. Since the actual wastewater flow rate was 55000 [m^3 day^{-1}] which was lower than the designed load, it was allowed to operate under lower DO concentration (around 0.7 mg/L) so as to reduce the energy consumption. Although the plant was designed for organics removal, 30-50% total nitrogen was also removed in addition to the removal of 80% COD.

While there were three same reaction tanks in the plant, our study focused only on one of the tanks as the result can be applied to the rest tanks. After the primary settler, the wastewater was fed into the long-channeled reaction tank with the length of 4×45m and cross-section area of 6×6 m^2. A sedimentation tank was used after the tank. The influent of the wastewater was split into three equal amounts of streams and introduced at three points along the length of the tank which divided the tank into 4 equal compartments. Treated effluent was separated from the activated sludge in the settler. A portion of the activated sludge was wasted while a large fraction was returned to the 1st compartment of the tank. This is schematically illustrated in Figure 1.

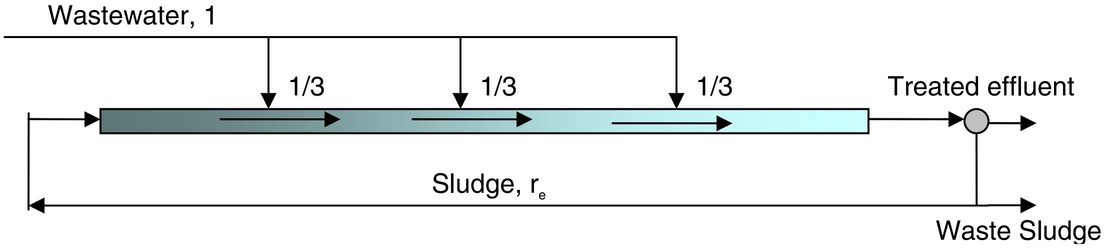

Figure 1. Schematic diagram of the reactor

2.2 Model development

Kinetic Model

ASM1 kinetics was adopted in this work. While other kinetic processes remained unchanged, the ammonification and organic nitrogen hydrolysis were treated as the same process as COD hydrolysis, thus the soluble and particulate organic nitrogen were treated proportional to the related COD. It is noted that many publications of modeling and simulation of WWTPs focused on the processes where nitrification and denitrification occurred either during different phases or in different tanks. In the present work, we took into account the nitrification and denitrification processes simultaneously. Instead of using ‘oxygen switch function’ to deal with the nitrification and denitrification separately, we introduced a factor ‘α’ to account for the SND. The ‘α’ was defined as a constant ratio of anoxic zone volume to the whole reacting volume in the aeration tank. In summary, 6 bio-processes which involve 12 compounds were taken into account and listed in Table 1. And the stoichiometric matrix of processes and the compounds was obtained and presented in Table 2 where all the parameter constants in the above 6 processes were taken from ASM1 except for α.

Table 1. The processes of the model

No.	Process	Rate$_j$
1	Hydrolysis of entrapped organics	$k_h \frac{X_S / X_{BH}}{K_X + (X_S / X_{BH})} X_{BH}$
2	Aerobic growth of heterotrophs	$\hat{\mu}_H (\frac{S_S}{K_S + S_S})(1-\alpha) X_{BH}$
3	Anoxic growth of heterotrophy	$\eta \hat{\mu}_H (\frac{S_S}{K_S + S_S})(\frac{S_{NO}}{K_{NO} + S_{NO}}) \alpha X_{BH}$
4	Decay of heterotrophy	$b_H X_{BH}$
5	Aerobic growth of autotrophy	$\hat{\mu}_A (\frac{S_{NH}}{K_{NH} + S_{NH}})(\frac{S_O}{K_{OA} + S_O})(1-\alpha) X_{BA}$
6	Decay of autotrophy	$b_A X_A$

Table 2. Stoichiometric Matrix $\nu_{j,i}$

Comp No. Processes	S_O 1	S_I 2	S_S 3	S_{NH} 4	S_{N2} 5	S_{NO} 6	S_{ALK} 7	X_P 8	X_S 9	X_{BH} 10	X_{BA} 11	X_I 12
1			1						-1			
2	$1-1/Y_H$		$-1/Y_H$	$i_S/Y_H - i_{XB}$			$(i_S/Y_H - i_{XB})/14$			1		
3			$-1/Y_H$	$i_S/Y_H - i_{XB}$	$(1/Y_H-1)/2.86$	$(1-1/Y_H)/2.86$	$((2.86\ i_S+1)/Y_H-(2.86\ i_{XB}+1))/40.04$			1		
4				$i_{XB} - i_S + f_P(i_S - i_{XP})$			$(i_{XB} - i_S + f_P(i_S - i_{XP}))/14$	f_P	$1-f_P$	-1		
5	$1-4.57/Y_A$			$-i_{XB} -1/Y_A$		$1/Y_A$	$-(i_{XB}+2/Y_A)/14$				1	
6				$i_{XB} - i_S + f_P(i_S - i_{XP})$			$(i_{XB} - i_S + f_P(i_S - i_{XP}))/14$	f_P	$1-f_P$		-1	

Material balance

A model of 4-CSTR in-series was established. Let i (1 – 6), j (1 – 12), and k (1 – 4) denote the indexes of bio-processes, compounds and compartments, respectively. The general material balance for jth compound in the kth compartment is given as following.

$$\frac{dC_{j,k}}{dt} = \frac{q_k}{V_k}(Cin_{k,j} - C_{j,k}) + \sum_{i=1}^{4} \nu_{j,i}\rho_i \tag{1}$$

where q_k is the wastewater flow rate entering the k^{th} compartment and V_k is the volume of the k^{th} compartment. Let Q, Cw_j and r_e denote the total flow rate and concentration of j^{th} compound in the wastewater and the recirculation ratio respectively. The concentrations at the point proceeding to each compartment were obtained as below. Note that the dissolved oxygen (j = 1) was not included in the material balance as it was known from the sample assay.

$k = 1$

$$q_k = Qr_e \tag{2}$$

$$Cin_{j,1} = C_{j,4} \qquad \text{j = 2, …, 7 (soluble compounds)} \tag{3}$$

$$Cin_{j,1} = [\frac{1+r_e}{r_e} - \frac{HRT\sum_{k=1}^{4}(\sum_{j=8}^{12} C_{j,k})}{4r \times SRT} \times \frac{1}{\sum_{j=8}^{12} C_{j,4}}] \times C_{j,4} \qquad \text{j = 8, …, 12 (particulate compounds)} \tag{4}$$

$k = 2$

$$q_k = Q(r_e + 1/3) \tag{5}$$

$$Cin_{j,2} = \frac{Cw_j/3 + r_e C_{j,1}}{r_e + 1/3} \qquad \text{j = 2, …, 12} \tag{6}$$

$k = 3$

$$q_k = Q(r_e + 2/3) \tag{7}$$

$$Cin_{j,3} = \frac{Cw_j/3 + (r_e + 1/3)C_{j,2}}{r_e + 2/3} \quad \text{j = 2, …, 12} \tag{8}$$

$k = 4$

$$q_k = Q(r_e + 1) \tag{9}$$

$$Cin_{j,4} = \frac{Cw_j/3 + (r_e + 2/3)C_{j,3}}{r_e + 1} \quad \text{j = 2, …, 12} \tag{10}$$

3. Results and Discussion

Transformation of variables

To perform the simulation of the above model, we had to deal with the first challenge, i.e. determination of the input concentrations of the 12 model compounds. It is noted that since the data of influent were measured after the primary sedimentation tank, the tank was not included in the present model. The available plant data are the routine measurements, i.e. the flowrate and temperature of the influent wastewater, the concentration of BOD_5, total COD, suspended solid (SS), NH3 and total nitrogen (TN) in the influent and effluent, as well as NOx in the effluent. The input concentrations of S_I, S_S, S_{NH}, X_I and X_S were transformed from the above assay data by the procedures detailed as below.

Bio-degradable COD: $S_S + X_S = 1.71 \times BOD_5$

Inert COD: $S_I + X_I = COD_t - (S_S + X_S)$

The sample assay [Liu F., 2004] showed that the soluble COD took 55% - 59% of total COD, therefore with the average value of 57%, we obtained $S_S + S_I = 0.57 \times COD_t$

The effluent COD comprises both soluble and particulate COD, i.e. COD_s and COD_p. Since $COD_p = 1.5 \times SS$ and assuming S_I taking 90% of soluble COD in the effluent (COD_s), then $S_I = 0.9 \times (COD_{t,eff} - 1.5 \times SS)$. The S_I in the effluent was assumed unchanged as in the influent.

Consequently, the concentrations of S_I, S_S, X_I and X_S in the influent were estimated. The dissolved oxygen *S*o and S_{NH} were obtained directly from the assay. The initial concentrations of the rest 6 compounds, i.e. S_{N2}, S_{NO}, S_{ALK}, $X_{B,A}$, $X_{B,H}$ and X_P, were assumed to be zero. The resulting effluent concentrations of S_{NO} and S_{NH} were directly obtained from the model, while the total *COD* and *TN* were evaluated as below: $COD_t = S_S + S_I + 1.5 \times SS$ and $TN = S_{NO} + S_{NH} + 7\% COD_t$ where it was assumed that the organic nitrogen was 7% of total COD.

Estimation of α

To perform the simulation with the developed model, all the constants took the default values of ASM1 except the α which can be estimated by fitting the simulated and observed trajectories of four components in the effluent, i.e. total COD, S_{NO}, S_{NH} and *TN*. In particular, a optimization procedure of minimizing the error term defined below was performed where $C_{p,q}^{real}$ and $C_{p,q}^{simu}$ are the measured and simulated concentrations of p^{th} sample of the q^{th} (q = 1-4) component, $\overline{C}_q^{real}$ is the measured average concentration of the q^{th} component, and N_q is the sample number of q^{th} component.

$$error = \sum_{q=1}^{4} [\frac{\sqrt{\sum_{p=1}^{N_q} (C_{p,q}^{real} - C_{p,q}^{simu})^2 / N_q}}{\overline{C}_q^{real}}] \tag{11}$$

Ideally, a steady state is needed to start the dynamic simulation. However, since the influent of wastewater varied frequently, a real steady state was seldom achieved. Therefore, a pseudo steady state which was generated by taking the daily average values of the routine measurements within one month was employed as the initial condition of the simulation.

The resultant value of α is 0.267, and the time-dependent concentrations of COD, S_{NO}, S_{NH} and TN in the effluent, from both plant assay and the simulation, are presented in Figure 2. The deviations of our model from the assay effluent data as defined in Eq. (11) are listed in Table 3 (Column 2).

Comparison with ASM1 model

In order to assess the performance of the developed model, we reproduced the standard ASM1 with the default values of the kinetic constants (Table 4). The resultant error terms defined in Eq.(11) are listed in Table 3 (Column 3). It is showed that our model outperformed the ASM1 model with an obviously smaller sum of the errors. In particular, the error in S_{NO} is less than half of that of ASM1 model. The errors in total COD is close to that of the ASM1 model, while the error in TN and S_{NH} are slightly smaller than those of ASM1 model. For visual examination, the time course resultant concentrations of COD, S_{NO}, S_{NH} and TN in the effluent are plotted in Figure 2. Clearly, the ASM1 model over estimated the NOx and underestimated the NH3-N.

Table 3. Comparison the error terms from α model and ASM1 model

Error	α model	ASM1 model
Total COD	0.205	0.195
NOx-N	0.474	0.913
NH3-N	0.526	0.577
TN	0.139	0.146
sum	1.345	1.830

Table 4. The parameter values of ASM1 (at 20°C)

Model parameters	**Symbol**	**Unit**	**Value**
Stoichiometric parameters			
Autotrophic yield	Y_A	g cell COD formed (g N oxidized)$^{-1}$	0.24
Heterotrophic yield	Y_H	g cell COD formed (g COD oxidized)$^{-1}$	0.67
Fraction of inert products from biomass decay	f_P	dimensionless	0.08
Nitrogen fraction of COD in biomass	i_{XB}	g N (g COD)$^{-1}$ in biomass	0.086
Nitrogen fraction of COD in endogenous mass	i_{XP}	g N (g COD)$^{-1}$ in endogenous mass	0.06
Kinetic parameters			
Heterotrophic maximum specific growth rate	$\hat{\mu}_H$	day^{-1}	6.0
Half saturation constant for assimilation of carbon	K_S	g COD m^{-3}	20
Heterotrophic oxygen half saturation constant	$K_{O,H}$	g O2 m^{-3}	0.2
Half saturation constant for nitrate	K_{NO}	g NO3-N m^{-3}	0.5
Heterotrophic decay rate	b_H	day^{-1}	0.62
Correction factor for anoxic growth of heterotrophs	η_g	dimensionless	0.8
Correction factor for anoxic hydrolysis	η_h	dimensionless	0.8
Maximum specific hydrolysis rate	k_h	g slowly biodegradable COD (g cell COD . day)$^{-1}$	3.0
Hydrolysis half saturation constant	K_X	g slowly biodegradable COD (g cell COD)$^{-1}$	0.03
Autotrophic maximum specific growth rate	$\hat{\mu}_A$	day^{-1}	0.8
Half saturation constant for ammonium	K_{NH}	g NH3-N m^{-3}	1.0
Autotrophic decay rate	b_A	day^{-1}	0.2
Autotrophic oxygen half saturation constant	$K_{O,A}$	g O2 m^{-3}	0.4
Specific ammonification rate	ka	m3 . COD(g.day)-1	0.05

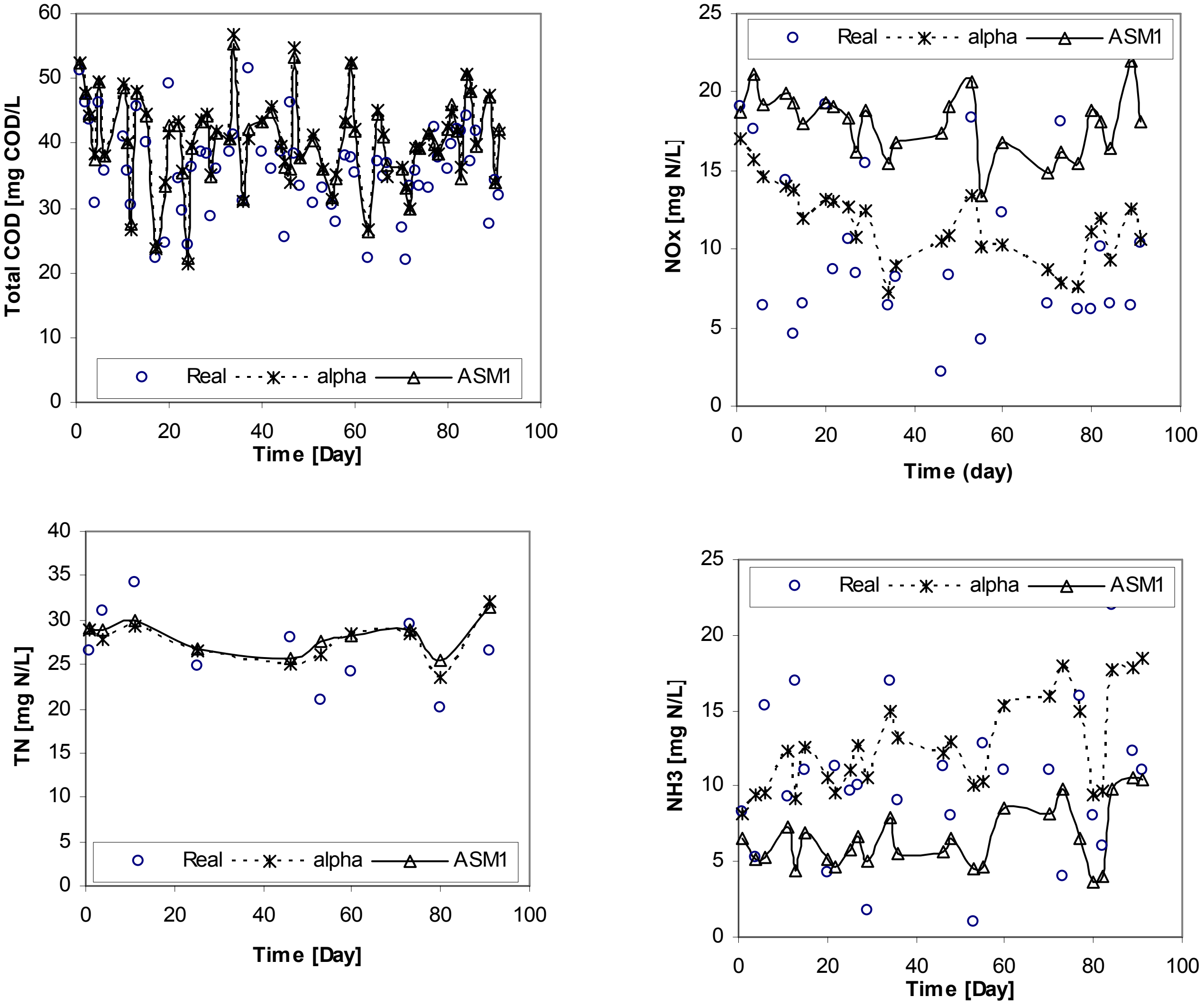

Figure 2. Comparison of the concentrations of the simulation results from our model and ASM1 model with the plant data for total COD, NOx, NH3-N, and Total Nitrogen.

4. Conclusions

It was shown that the developed SND model outperformed the ASM1 model with default kinetic constants in reflecting the patterns observed in the effluent COD, ammonia (NH$_3$-N) and nitrate (NO$_3$-N). Therefore, the model developed in this work would be helpful for process engineers to investigate different configurations or operating strategies for the existing plant. It also benefits the operators by predicting the plant behavior under various operations and exploring different what-if situations.

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