Sensitivity analysis of simultaneous nitrification-denitrification process by simulation with activated sludge model number one

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Nitrogen removal by Simultaneous Nitrification-Denitrification (SND) has invited much attention in recent years due to possible reduction in capital and operating costs associated with wastewater treatment. The potential of biological nitrogen removal through this process and optimization of its operating parameters were investigated by simulations using Activated Sludge Model No. 1 (ASM1). Adopting typical properties of domestic sewage, simulations of SND process were performed in three sequential phases to optimize the operating parameters and assess reliability of the SND process over variation in the kinetic and stoichiometric parameters. Since dissolved oxygen (DO) concentration and solids retention time (SRT) were considered to have the most significant impact on nitrogen removal, the first set of simulations was aimed at identifying an applicable operating window for these parameters. Simulation results indicated that optimum nitrogen removal occurred at a DO concentration of 0.3 mg/L coupled with a SRT of 15 days. A second set of process simulations was run using this combination of operating DO and SRT to examine the effect of other process parameters; specifically the ratio of biodegradable COD to total Kjeldahl nitrogen (BCOD:TKN) in the influent, hydraulic residence time (HRT), and recycle ratio (R) on total nitrogen removal. The influent BCOD:TKN ratio significantly affected overall nitrogen removal, since availability of electron donor is essential to drive denitrification, with optimal nitrogen removal observed at a BCOD:TKN ratio of 11. Neither HRT nor R had a significant effect on nitrogen removal. The third set of simulations considered the natural variability of the kinetic and stoichiometric parameters of ASM1. Monte Carlo analysis was performed to evaluate the performance of an SND system operated at a DO of 0.3 mg/l and an SRT of 15 d using probability density functions developed by Cox (2004) for the model parameters. Results of these simulations were used to assess the potential reliability of an SND process designed using "typical" model parameter values. A sensitivity analysis was also performed to identify the model parameters that had most significant effect of nitrogen removal.

Keywords: Models, Treatment, Wastewater, Water Quality

Introduction

Biological nitrogen removal (BNR) is usually accomplished either by sets of reactors maintaining anoxic and aerobic phases discretely, or in a single reactor where suitable conditions are sequentially developed. Simultaneous nitrification-denitrification (SND) is the process of achieving nitrification and denitrification in a single activated sludge reactor without distinct spatial or temporal delineation in growth environment, by operating at a reduced dissolved oxygen (DO) level which permits both autotrophic nitrification and heterotrophic denitrification to occur simultaneously. This has invited particular attention in the past years over conventional systems by virtue of effective nitrogen removal in extended aeration type activated sludge (AS) systems and potential savings in capital and operational cost. For continuously operated plants, nitrogen removal obtained in a single tank can save the cost of a second tank, and low operating DO requirement can reduce energy cost in maintaining a higher DO level in aeration tank of conventional plants. Such process modifications, if applied effectively to existing plants, can help meet stringent nitrogen discharge standards.

Simultaneous occurrence of nitrification and denitrification in a single reactor need two apparently conflicting environmental conditions. In order for SND to occur, it is necessary that: (1) the operating DO level be correctly poised so that it is not so low that it cannot support autotrophic nitrification, or so high that it inhibits denitrification; (2) sufficient residence be provided to permit the establishment of a stable population of nitrifiers; and (3) adequate electron donor be available for

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heterotrophic denitrification. Rittmann (2001) concluded that that implementation of SND process required the effective combination of solids retention time (SRT), hydraulic retention time (HRT), and DO concentration. Hence, it is critical to examine and identify the operating conditions that these two processes, requiring two seemingly different conditions, can occur side by side leading to effective nitrogen removal.

Control strategies have been successfully implemented to enable AS operations that were designed primarily for organics removal to achieve biological nitrogen removal The DO concentration in the aeration tank has been identified as an important control parameter to achieve nitrogen removal at reduced operating cost (Lukasse et al., 1998; Copp et al., 2002; Sin et al., 2004; Insel et al., 2006). The fine tuning of operating DO, particularly at low concentration, was observed to be an effective approach for promoting simultaneous nitrification and denitrification resulting in increased nitrogen removal efficiency of the process (Drews et al., 1972 and 1973; Applegate et al., 1980; Daigger, et al., 2000).

In this study, SND in a conventional (plug flow) AS system was modeled using Activated Sludge Model No. 1 (ASM1), which incorporates seven (7) soluble and six (6) particulate components, 14 kinetic parameters, and five (5) stoichiometric coefficients. The model was initially used to identify suitable combinations of DO concentrations and solids residence time (SRT), and to discern interrelationships between the three parallel processes of heterotrophic substrate oxidation, autotrophic nitrification, and heterotrophic denitrification. Subsequent simulations were used to assess the effects of other process parameters, i.e. the ratio of biodegradable chemical oxygen demand (BCOD) to total Kjeldahl nitrogen (TKN), the hydraulic retention time (HRT), and recycle ratio (R).

Methodology

SND process simulations were performed using GPS-X (Hydromantis, Inc., Hamilton, Ontario), a simulation package that includes ASM1 modeling. The work has been done in three separate phases. The model system is a conventional activated sludge plant, consisting of a plug flow aeration basin and a secondary clarifier, with solids recycle and wasting. The aeration basin was modeled as four completely mixed compartments in series, while the clarifier was modeled as a point separator with 100% solids removal efficiency. Consequently, the modeling results specifically manifest the effect of parameter changes and variations of the biochemical performance of the system, while eliminating the effects of sludge separation and settleability. The model feed (Table 1) is based on typical domestic wastewater (Grady et al., 1999), except that the BCOD (partitioned between readily and slowly biodegradable fractions) was increased so that the influent BCOD: TKN ratio was 10. This ensured that sufficient electron donor was available to drive denitrification: an influent BCOD: TKN ratio > 10 is reportedly necessary to obtain efficient nitrogen removal (Grady et al., 1999; Rittmann and McCarty, 2001). Kinetic and stoichiometric parameters (Table 2) used for all simulations were based on a statistical analysis of recommended and calibrated parameter values from various sources (Cox, 2004).

Table 1 - Influent characteristics

Component[a]	ASM1 Symbol	Concentration[b], mg/L
Soluble inert organic material	S_I	0
Readily biodegradable substrate	S_S	160
Particulate inert organic material	X_I	30
Slowly biodegradable substrate	X_S	240
Non-biodegradable particulates from cell decay	X_D	0
Free and unionized ammonia	S_{NH}	25
Soluble biodegradable organic nitrogen	S_{ND}	6.5
Particulate biodegradable organic nitrogen	X_{ND}	8.5
Nitrate and nitrite	S_{NO}	0

[a]Typical values based on Grady et al. (1999), except as noted in text. Active biomass was absent from the influent.

[b]Expressed as COD for organics, and as N for various nitrogen species.

Table 2 – Typical parameter values, ranges, and distribution at neutral pH and 20° C for domestic wastewater (Cox, 2004)

Symbol	Units	Statistical Parameters[a] ξ	σ	Mean value[b]
Heterotrophic coefficients				
Y_H	mg biomass COD formed/ mg COD oxidized	-0.45	0.12	0.64
$\hat{\mu}_H$	day^{-1}	1.14	0.60	3.13
K_S	mg COD/L	1.44	0.76	4.22
b_H	day^{-1}	-1.06	0.81	0.35
K_{NO}	mg NO_3^--N/L	-1.55	1.01	0.21
$K_{O,H}$	mg O_2/L	-1.46	0.83	0.23
η_g	Fraction	0.10 [c]	0.90 [c]	0.50
Autotrophic coefficients				
Y_A	mg biomass COD formed/ mg N oxidized	-1.52	0.55	0.22
$\hat{\mu}_A$	day^{-1}	-0.51	0.44	0.60
b_A	day^{-1}	-1.97	0.28	0.14
K_{NH}	mg NH_3-N/L	-0.68	1.00	0.51
$K_{O,A}$	mg O_2/L	-0.82	0.96	0.44
Hydrolysis coefficients				
k_h	mg slowly biodegradable COD/ mg cell COD-day	0.83	0.36	2.29
K_X	mg slowly biodegradable COD/ mg cell COD	-2.82	1.34	0.06
η_h	fraction	-0.86	0.62	0.42
Other coefficients				
f'_D	mg debris COD/ mg biomass COD	*		0.08
$i_{N/XB}$	mg N/ mg COD in active biomass	*		0.086
$i_{N/XD}$	mg N/ mg COD in biomass debris	*		0.06
k_a	L/ mg biomass COD - hour	*		0.1608

[a] Represent the mean ξ and the standard deviation σ of a log-normal PDF, unless specified.

[b] Recommended parameter values, representing 10^{ξ} in a log-normal PDF and the central value in a uniform PDF

[c] η_g follows a uniform PDF with the tabulated values representing lower and upper limits, respectively.

An initial set of simulations was performed to identify appropriate combinations of DO concentration and SRT to support SND process were identified. A second set of simulations was then performed at a selected DO and SRT to examine the effect of other operating parameters (influent BCOD: TKN ratio, HRT, and R) on total nitrogen removal, where each of these process parameters was varied individually while holding all other process parameters were held constant. In both of these simulation sets, the listed mean parameter values for ASM1 (Table 3) were used.

Table 3. Values/ranges a of operating parameters used in SND process simulations

Parameter [b]	Set 1	Set 2	Set 3
SRT (θ_X), day	1 – 30	15	15
DO concentration, mg/L	0.1 – 2.0	0.3	0.3
HRT (θ), hr.	6	4 – 24	6
R	0.5	0.25 – 3.0	0.5
Influent BCOD: TKN	10	4 – 20	10

a Selected ranges typical of a range of SND process configuration (Rittman, 2001)

b Parameter symbols: DO – dissolved oxygen concentration in aeration tank, θX – solids residence time, θ – hydraulic retention time, and R – recycle ratio

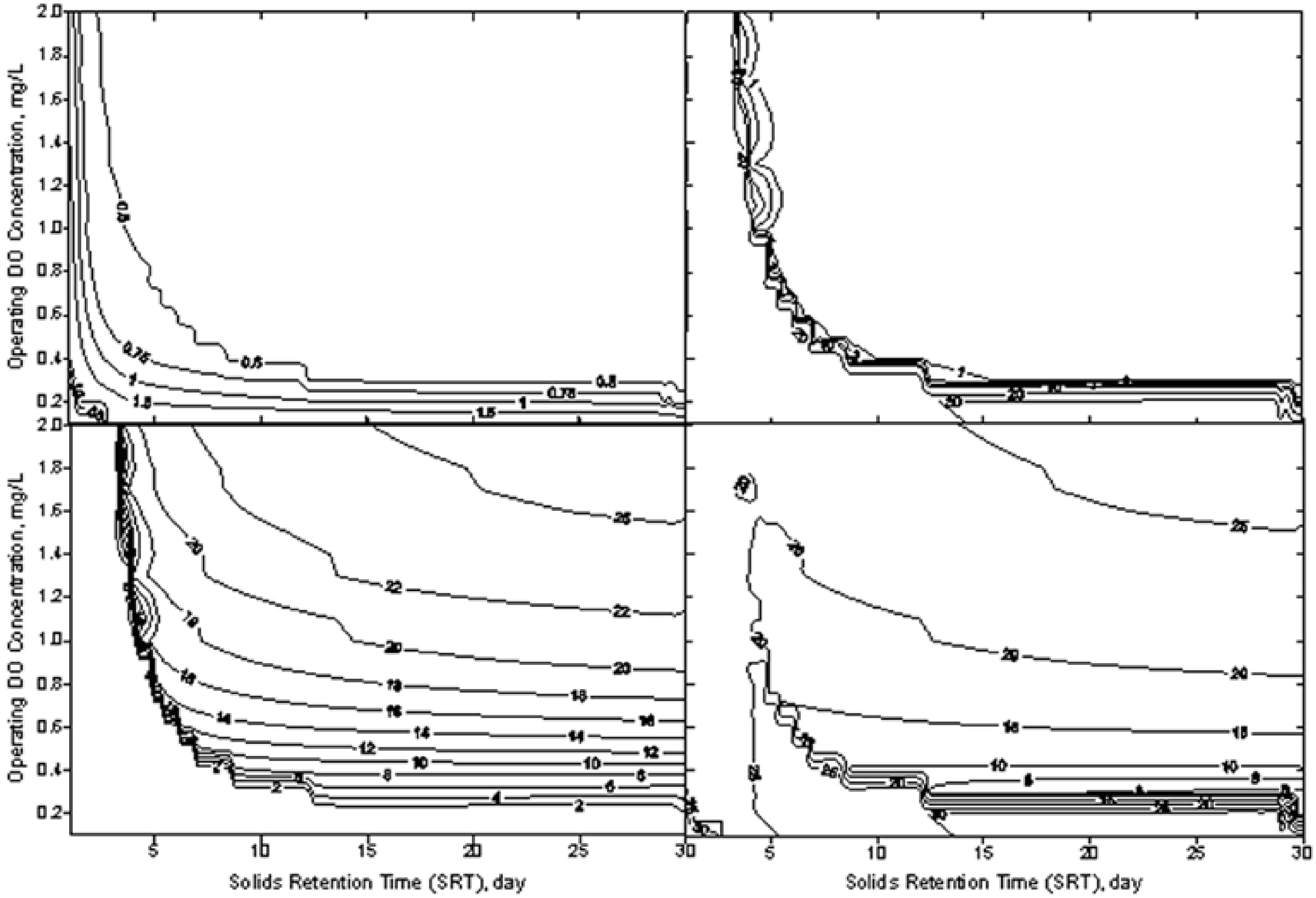
Finally, a set of Monte Carlo simulations was performed, where 15 of the 19 the model parameters were permitted to vary in accordance with reported (Cox, 2004) probability distribution functions (PDFs, Table 2). Output of this third simulation set was used to assess the sensitivity of SND process performance to ASM1 kinetic and stoichiometric parameters, based on a Spearman rank correlation matrix generated with the aid of the CORR procedure of SAS (The SAS Institute, Cary, NC), and to evaluate the inherent uncertainty in SND process performance, based on the empirical cumulative distribution functions (CDFs) of the effluent properties.

Results and Discussion

Identification of Optimal DO and SRT

Oxygen is required for nitrification but inhibits denitrification,hence, it was necessary to identify operating conditions that would permit these two processes to occur simultaneously. An appropriate operating window for the SND process was identified by running exhaustive simulations on different combinations of DO concentration and SRT. Simulation results (Figure 1) indicated that organic material in the wastewater was consumed almost entirely when the SRT was > 5 d and the DO level was ≥ 0.2 mg/L. The effluent total nitrogen (TN) was minimum at 0.3 mg/L and ~12.5 d SRT; higher SRT values provide little discernible improvement in TN removal. Higher DO levels inhibited denitrification, resulting in higher effluent nitrate concentrations. Further reducing the DO, however, prevented effective nitrification and resulted in increased effluent ammonia concentrations, or required operation at a higher SRT to permit the establishment of a nitrifying population. Hence, a DO concentration of 0.3 mg/L and a SRT of 15 d were selected as "optimal" for overall nitrogen removal, and subsequent simulations were performed under these conditions.

Figure 1. Effect of DO concentration and SRT on effluent concentrations of: (a) soluble COD mg/L; (b) ammonia (SNH), mg/L as N; (c) nitrate (SNO), mg/L as N; and (d) total nitrogen, mg/L as N.



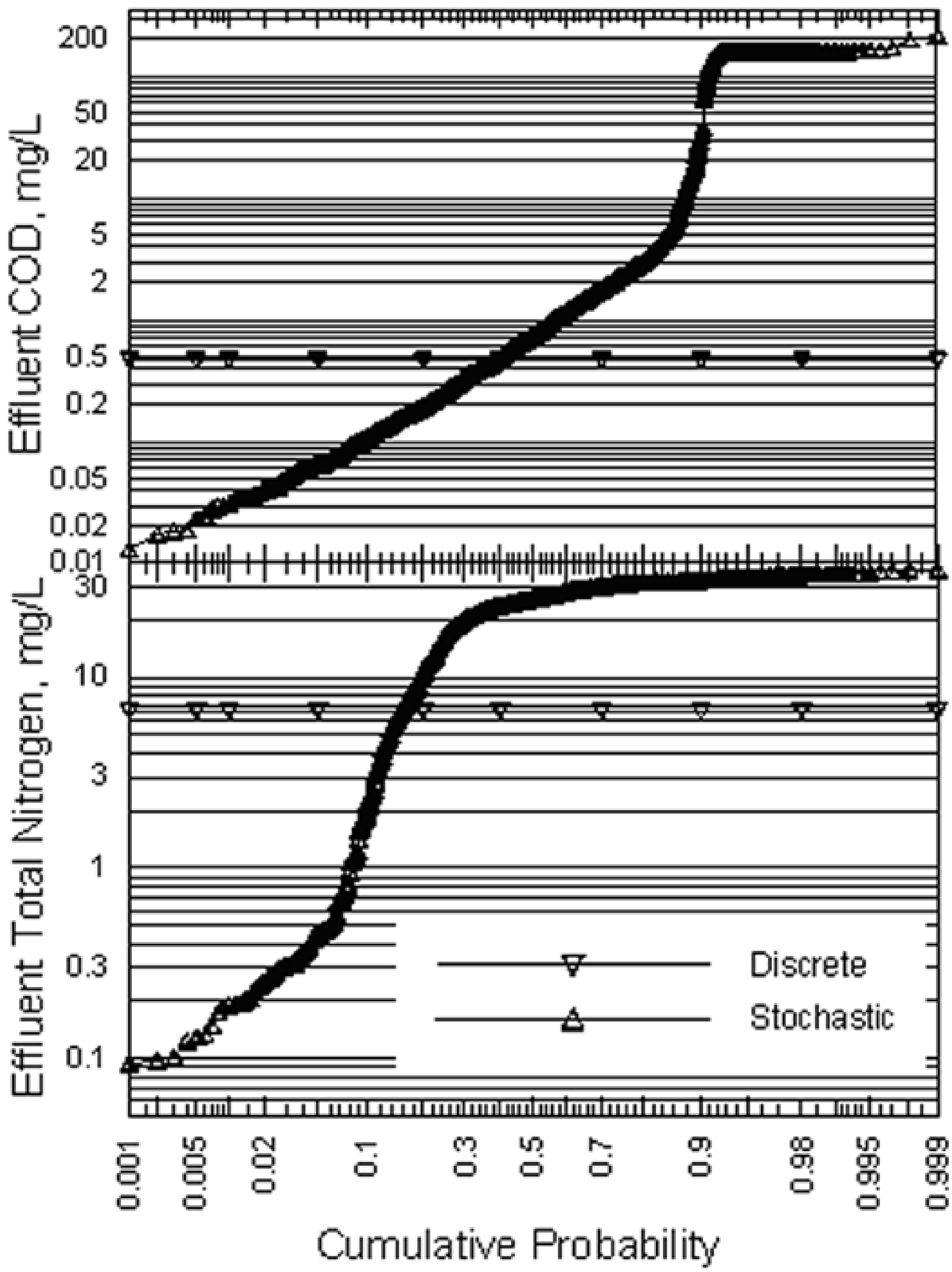
Effect of Additional Process Operating Parameters
Simulations results showed that overall nitrogen removal approached 90% when the influent BCOD: TKN was between 12 and 16, and at least 80% when the influent BCOD: TKN was > 9. Note that these values are much higher than the stoichiometric ratio of 2.86 mg OD/mg NO3--N, since a substantial portion of the influent BCOD is used for cellular growth or is oxidized with oxygen as electron acceptor. Overall nitrogen removal dropped substantially, and effluent nitrate increased, when the influent BCOD: TKN was < 9, indicating that the available electron donor was insufficient to drive denitrification. The recycle ratio had a marginal impact on the overall nitrogen removal. A slight decrease in effluent TN concentration was observed with a rise in R, although overall nitrogen removal was all cases > 80%. The increased R permitted more efficient denitrification by returning effluent to
the reactor at an increased rate, as shown by a rise in COD consumption and a reduction in effluent nitrate concentration. Nonetheless, the impact of variations in the recycle ratio on overall nitrogen removal was not appreciable.

Nitrogen removal increased from 22% at an HRT of 4 h to more than 84% at when the HRT was 6 h, but was only slightly enhanced by further increases in the HRT. The extent of ammonia and COD oxidation were significantly reduced when the HRT was < 6 h, indicating insufficient contact time between the biomass and the wastewater.

Sensitivity and Uncertainty Analysis
Data generated using the Monte Carlo simulations were used to assess the sensitivity of the effluent COD, ammonia and nitrate concentrations on the ASM1 kinetic parameters and stoichiometric coefficients. Overall nitrogen removal was strongly correlated to the oxygen half-saturation coefficients for autotrophs (KO,A), in

a positive direction, and strongest maximum specific autotrophic growth rate (Aμˆ), in a negative direction. The empirical CDFs of the steady state effluent COD and TN concentrations (Figure 2) suggest that these conform to truncated log-normal PDFs. Comparison of the discrete (deterministic) simulation results using the recommended model parameter values suggests that the certainty of achieving the predicted COD and TN removal are in the order of 40 and 20%, respectively.

Figure 2. Stochastic simulation results of steady state effluent COD and TN in SND system



Comparison of Simulation Results with Measured Performance

In general, laboratory and field results documented in the technical literature report SND at DO levels slightly higher and SRTs comparable to the optimal window determined by these simulations. Elisabeth et al. (1996) reported, at a DO of 0.5 mg/L, TCOD: TKN ratio of 9.4, HRT of 18 h, and SRT of 15 d, the rates of nitrification and denitrification would be similar and this might lead to complete SND. Zeng et al. (2003) achieved < 1 mg/L effluent TN at 0.5 mg/L DO concentration and 15 day SRT in a laboratory AS system. Bertanza (1997) reported significant nitrogen removal in pilot- and full-scale AS plants at 0.3 to 0.5 mg/L DO. Likewise, Münch et al. (1996) and Insel et al. (2005) suggest that SND can be achieved at a DO level of about 0.5 mg/L. Hence, while ASM1 was able to reasonably forecast general trends in the behavior of the SND process in response to variations in the operating parameters, specific values, particularly for the DO concentration, were not so accurately predicted. This suggests that, while the structure of ASM1 is suitable for modeling the SND process, specific model parameters may have to be calibrated for SND to more accurately model and simulate the process. The sensitivity analysis provides some initial suggestions as to specific model parameters that might be adjusted to properly calibrate ASM1 for SND process simulation.

Summary and Conclusions

The simultaneous nitrification de-nitrification (SND) process was simulated using ASM1 to identify an appropriate operating window, and to assess process sensitivity and uncertainty. Simulation results suggested that a DO level of 0.3 mg/L in the aeration tank and an SRT of 15 d were "optimal" for SND. An influent BCOD: TKN ratio > 9 was necessary to ensure that sufficient electron donor was available to drive denitrification and a high level of overall nitrogen removal. The recycle ratio and HRT, on the other hand, had little effect on overall nitrogen removal, provided they exceeded specific threshold values of 0.3 and 6 h, respectively.

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