Brazilian Journal
of Chemical
Engineering

ISSN 0104-6632
Printed in Brazil
www.abeq.org.br/bjche

Vol. 31, No. 03, pp. 649 - 658, July - September, 2014
dx.doi.org/10.1590/0104-6632.20140313s00002541

SIMULATION AND CALIBRATION OF A FULL-SCALE SEQUENCING BATCH REACTOR FOR WASTEWATER TREATMENT

M. C. Oselame*, H. Fernandes and R. H. R. Costa

Department of Sanitary and Environmental Engineering, Federal University of Santa Catarina, UFSC/CTC/ENS, CEP: 88010 970, Florianópolis - SC, Brazil.
Phone: + (55) (48) 3721 7738
E-mail: murilo.oselame@gmail.com

(Submitted: February 13, 2013 ; Revised: June 7, 2013 ; Accepted: June 26, 2013)

Abstract - The aim of this study is to apply the main mathematical models used in activated sludge reactors, the Activated Sludge Model No. 1 (ASM1) and its variations (ASM2d and ASM3), to predict the behavior of a full-scale sequencing batch reactor (SBR) used for the treatment of domestic wastewater employing the software ASIM®. Two cycles were studied, the step-feed cycle and conventional filling. Samples were taken from the raw influent, from the reactor and from the treated wastewater, and these data were used to calibrate the models. The ASM1 model was the best model to represent the cycle with only an input, while model ASM3 was the best for simulating the scaled filling cycle. This work presents calibrated parameters for the two kinds of filling. The results of these simulations indicate that the calibration process succeeded and can be used as a model for future studies.
Keywords: Activated Sludge Models; Sequencing batch reactor; Calibration and simulation.

INTRODUCTION

Currently, the activated sludge system is the most used wastewater treatment process in the world due to its high level of efficiency. In the activated sludge process, suspended biomass is responsible for reducing pollutants. Depending on the project, activated sludge reactors can reduce nitrogen, phosphorus, and/or organic matter. Many types of configurations have been developed over the years, including the sequencing batch reactor (SBR).

Activated sludge models are a group of differential equations that represent the biological and chemical reactions that take place in the reactor. Control, design and simulation of activated sludge reactors are important aspects of the process that can be examined with the models (Gernaey *et al*., 2004). The main models for the activated sludge process were developed by the International Water Association (IWA). The first model was developed in 1986 and was named the activated sludge model (ASM). Later known as ASM1, this model was able to simulate the biological oxidation of carbon, nitrification, and denitrification (USEPA, 2009). Although the ASM1 model had proven itself useful in both industry and academia, it had limitations. For example, the model assumed constant temperature and pH, it did not include the removal of phosphorus, and the biological responses did not depend on the carbon source. Efforts to improve upon the ASM1 model spawned other models. Among them was the ASM2 model, which included the removal of phosphorus. The ASM3 model was designed to deal with limitations such as independence of carbon source and temperature, and it was later extended to include the biological removal of phosphorus (ASM3-Bio-P) (USEPA, 2009).

*To whom correspondence should be addressed

The main difference between the ASM1 and ASM3 models is that the latter recognizes the importance of storage polymers in the heterotrophic conversion of activated sludge processes. In ASM3, it is assumed that all readily biodegradable substrates (S_S) are stored in an internal component of the cell (X_{STO}) before the growth stage. The heterotrophic biomass is modeled as an internal cellular structure similar to phosphorus-accumulating organisms. Finally, the component (X_{STO}) is subsequently used for biomass growth, unlike the ASM1 model where cell growth is directly connected to the external substrate.

Another difference between ASM1 and ASM3 is that the latter is easier to calibrate. This happens by changing the death-regeneration model, which is a model of endogenous growth-respiration. The ASM2d model is based on the ASM2 model but adds denitrification by phosphorus-accumulating organisms, which better describes the dynamics of phosphorus and nitrogen (Gernaey *et al*, 2004). The ASM3 model was tested by Koch *et al*. (2000). Based on data from a pilot plant and several full-scale reactors at wastewater treatment stations in Switzerland, it was demonstrated that the calibrated model could properly model sludge production and denitrification with standardized parameters. When compared to ASM1, ASM3 generates superior results from simulations of the behaviors most common in wastewater treatment plants.

The overall objective of this study was to simulate the removal of organic matter and nutrients from a sequencing batch reactor that operates at full-scale, while maintaining responsiveness and control of the system. For the simultaneous removal of nutrients and organic matter in the wastewater treatment process, the models were calibrated using performance data from the SBR. Utilizing activated sludge model No. 1 (ASM1) and its variations (ASM2d and ASM3), the best model to simulate the behavior of COD, nitrogen, and phosphorus removal from the reactor was determined.

MATERIALS AND METHODS

Full-Scale Treatment System

This study was based on a full-scale wastewater treatment plant (WWTP) that uses activated sludge as the treatment process. The reactor operates in sequencing batches and is presented in Figure 1. The treatment system studied was designed to sustain a population of over 800 residents, as presented in Table 1.

The system is comprised of preliminary, primary, and secondary treatment stages. In the pre-treatment unit, the wastewater is settled and incorporated into chambers called baffled reactors. These baffled reactors are septic tanks used to remove coarse solids, as well as for desanding and retaining fats; there are three chambers and the hydraulic detention time is 4 hours. After pre-treatment there is one last chamber for equalization, which occurs during 2.5 hours. The secondary treatment is performed by a SBR. The effluent comes from the sewer system of a residential condominium, which enters the reactor discontinuously after being pumped from the equalization chamber. The reactor is operated at environmental temperatures of 20-30 ºC. After filling, aerobic biological processes begin with artificial aeration. Aeration is performed through a system of air compressors, which send air into the reactor through a membrane to produce fine bubbles. After this phase, aeration is interrupted and the sludge sedimentation phase takes place. After sedimentation, a fraction of treated wastewater is removed and clarified by floating spillways. Then the cycle starts again with a new tank filling.

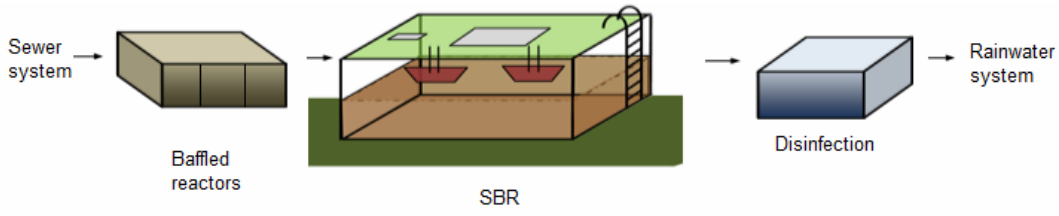

Figure 1: SBR reactor.

Table 1: Treatment system description.

Description	Reactor
Occupation	Residential
Total population	840
Consumption	200 L·(residents·day)$^{-1}$
Daily Output	141.12 m³·day^{-1}

The reactor works with a step-feed system to optimize the conditions for nitrification, denitrification, and phosphorus removal. The filling can be done with one, two, three, or four inputs with varying filling volumes per cycle depending on the volume of wastewater generated in the system. In this study, nineteen cycles were monitored, and two types of cycles were chosen because they were observed more often: step-feed cycle and conventional filling (Figure 2). The step-feed cycle was divided into several phases: 4 input filling (2h), aerobic reaction (4h), sedimentation (1h), and withdrawing (0.5h). The total time per cycle was 7.5 hours. The conventional filling method had only one input and was divided into the following phases: filling (0.5h), aerobic reaction (1h), sedimentation (1h), and withdrawing (0.5h), with a total time per cycle of 3 hours.

The dissolved oxygen concentration was limited to 0.6 $mgO_2 \cdot L^{-1}$. The applied load of total COD was 0.45 $kgCOD \cdot (m^3 \cdot d)^{-1}$ in the step-feed cycle, and 1.32 $kgCOD \cdot (m^3 \cdot d)^{-1}$ for the conventional filling.

The entire process of feeding, aeration, mixing and discharging is automated so as not to require the presence of an operator in the WWTP. In order to prevent compromise to the efficiency of the reactor, internal sensors are used to trigger the pumping system to remove the sludge formed and already settled when it reaches pre-specified concentrations during its operation. The disinfection process is made possible by chlorinating with a 12% sodium hypochlorite solution with application at the outlet of the reactor effluent. After addition of the chemical agent, the effluent passes through the contact tank and then flows to the rainwater system.

Sampling and Monitoring

Monitoring was performed from April, 2011, to July, 2012, and nineteen cycles were completely monitored. Samples were taken from the raw influent (incoming reactor), from the reactor (throughout the cycle, collections made every half hour) and from the treated wastewater (reactor outlet). In all cycles monitored two types occurred more often; they best represent all cycles: one step-feed cycle with a total time per cycle of 8 hours, and one conventional filling with a total time per cycle of 3.5 hours.

Analytical Methods

The samples were stored in vials appropriate for collection and transport and then sent to the laboratory for both physical and chemical analysis. Soluble chemical oxygen demand (COD), ammonium nitrogen (NH_4^+ -N), nitrite (NO_2^--N), nitrate (NO_3^--N), phosphate (PO_4^{-3}-P), total suspended solids (TSS), and volatile suspended solids (VSS) were analyzed according to standard methods (APHA, 2005). Inside the reactor, dissolved oxygen (DO) and pH were measured on-line with a multiparameter probe (YSI 6620). Respirometric tests were carried out to determine the oxygen uptake rate (OUR) of the mixed liquor according to the methods described by Schmidell (2001).

Calibration

Calibration is the selection of values for the kinetic parameters and stoichiometry of the model. Calibration was performed manually using the method described by Henze *et al*. (2000) with initial data from the cycles of the SBR. The calibration was performed logically with an iterative process by changing constants, one at a time. Each change corresponded to one iteration. However, it should be emphasized that the calibration was performed with an understanding of the processes involved.

The calibration was performed with influent and effluent data from the SBR. The soluble COD, NH_4^+-N, NO_3^--N, and PO_4^{-3}-P in the effluent allowed accurate calibration of the growth kinetics. The calibration heterotrophic growth rate (μ_H) was based on laboratory analysis of each parameter. If the values of soluble COD differed by more than five times the normal range of the coefficients of saturation, then the calibration was performed only via μ_H. Thus, the respirometric data were used for μ_H calibration.

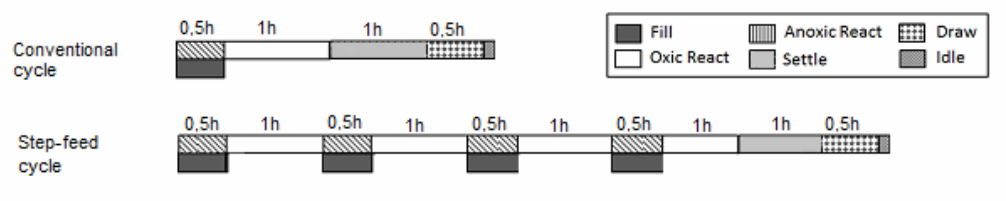

Figure 2: Operational scheme for the monitored cycles.

Normally the Monod term for oxygen and COD is the limiting factor, but in this case μ_H was not changed. Calibration parameters for the autotrophic portion are similar to the process recommended for the heterotrophic growth constant. The ammonia in the effluent was used to calibrate, autotrophic growth rate (μ_A), which is the autotrophic constant. If the amounts of oxygen and ammonia were five times greater than the normal range of constant saturation, then the calibration could be performed by μ_A. To calibrate the denitrification, μ_H was not changed, in case it had already been used to calibrate the oxygen and COD. The kinetics of phosphorus was calibrated using the data of the effluent. The parameters for growth rate of phosphorus-accumulating organisms (μ_{PAO}) and storage of phosphorus-accumulating organisms (q_{PHA}) were calibrated. If data were not available, then the respirometric μ_{PAO} and μ_H were not changed.

Data

The final data of the cycle were selected as the initial conditions of the reactor. For the initial conditions of the reactor and simulations, the following ASM1 model variables were considered: S_S (readily biodegradable substrate), X_S (slowly biodegradable substrate), S_{NO3} (nitrogen as nitrate), and S_{NH4} (nitrogen as ammonia). In ASM2d and ASM3, the X_{SST} variable (referring to the suspended solids) was also considered. The S_{PO4} variable (phosphate), was only considered in ASM2d because there is no S_{PO4} in ASM1 and ASM3. The module for removing phosphorus from ASM3, ASM3-bio-P, was not used.

Simulation

The simulation was performed with the ASIM® program, where the initial data of the reactor, operating conditions cycles, and specific models were identified. The program allows the use of a model library, which included the ASM1, ASM2d and ASM3 models. The type of reactor was also set, which in this case was the sequencing batch reactor.

For the simulation, it was considered that the SBR had a concentration of dissolved oxygen (DO) that was constant at each point of the cycle. The oxygen data used in the simulation was obtained from the DO profile within the reactor at each cycle period. However, in the settling step, the DO was considered to be equal to zero to create an anoxic zone and simulate denitrification in the reactor. The inflow was verified using data from the pump drive and the level of the reactor. The filling occurred in steps and three input volumes were checked in one cycle (step-feed), and one input in the other.

The simulations were performed using equations from the ASM1, ASM2d, and ASM3 models. After calibration, the data were set to the steady state. Finally, the calculations were performed for the reactor dynamics over the cycle with the ASIM® program. These data were compared with the actual data obtained during the SBR cycle monitoring.

ASIM®

Using the ASIM® software, the type of hydraulic reactor must first be defined, which in this case was an SBR. After defining the reactor, models were chosen, including ASM1, ASM2 and ASM3. Afterwards, the conditions of the cycle were defined, such as input and output volumes, time elapsed for each step, DO concentration and the reactor volume. The effluent data from the reactor was entered into the program. After the first simulations, cycle data could be changed to fit the selected model, which allows for calibration. The stoichiometry and kinetics were standard for each model. After the simulations, the results were available in graphic and spreadsheet format.

RESULTS AND DISCUSSION

Calibration

As indicated by Henze *et al*. (2000), based on default parameter values the simulations did not satisfactorily reproduce the data obtained; therefore, it was necessary to calibrate the ASM1, ASM2d, and ASM3 models. The calibrated parameters include the aerobic and anoxic heterotrophic growth rate (μ_H), autotrophic growth rate (μ_A), storage rate (k_{STO}), anaerobic hydrolysis reduction factor (η_{fe}), growth rate of phosphorus-accumulating organisms (μ_{PAO}), and storage of phosphorus-accumulating organisms (q_{PHA}). Other adopted parameters are standard for each model. Since the reactor did not significantly remove phosphorus, the results obtained in the calibration were not satisfactory. This was neither a flaw in the procedure nor in the model. In Table 2, the default and calibrated parameters are presented in the step-feed cycle.

Depending on the model, the parameters can simultaneously affect more than one component. Because of this, each parameter was changed separately and iteratively until it reached the goal of the simulation. For the ASM2 model, 5 parameters had to be

Table 2: Parameters of the step-feed cycle.

Parameter	Unit	ASM1 *Def.	ASM1 **Cal.	ASM2 Def.	ASM2 Cal.	ASM3 Def.	ASM3 Cal.
Heterotrophic growth rate (μ_h)	day^{-1}	6	0.6	6	0.5	2	2
Autotrophic growth rate (μ_a)	day^{-1}	0.8	0. 8	1	4.5	1	1.2
Storage rate (k_{sto})	$mgCOD\cdot(mgCOD\cdot day)^{-1}$	-	-	-	-	5	4.5
Anaerobic hydrolysis reduction factor (η_{fe})	-	-	-	0.4	0.53	-	-
Growth rate of PAO (μ_{pao})	day^{-1}	-	-	1	1.8	-	-
Storage of PAO (q_{pha})	$mgCOD\cdot(mgPAO\cdot day)^{-1}$	-	-	3	0.2	-	-

*Def. = Default **Cal. = Calibrated

changed in the simulation, which led to simultaneous changes in various components such as COD, nitrite, and nitrate. Due to these simultaneous changes, the iterations were longer. The same is true for the ASM1 model, which only needed one parameter to be calibrated. There was simultaneously a great influence on multiple components, which required additional time for calibration. As for the ASM3 model, the calibration was more objective and required a smaller number of iterations.

Currently, there are few studies of simulations with SBR systems; however, Furumai *et al*. (1999) used a modification of the ASM2 model to calibrate a SBR treating wastewater from a restaurant. The calibration results obtained in this study, however, were unlike those obtained for the SBR in the Furumai study, which occurred because the cycle was step-feed. This study obtained a reduction factor for anaerobic hydrolysis (η_{fe}) of 0.2, which is below the standard value of 0.4; the value obtained in the calibration of the SBR in the Furumai study was 0.53.

Krishna and van Loosdrecht (1999) tested the ASM3 model in their experiments using an SBR with acetate as effluent. Defined in the calibration was a constant storage rate (K_{STO}) of 10 mgCOD $(mgCOD\cdot d)^{-1}$. Koch *et al*. (2000) found a value of 12 $mgCOD\cdot(mgCOD\cdot d)^{-1}$ for a batch reactor at the pilot scale. The calibration of the SBR in the study yielded a result of 4.5 $mgCOD\cdot(mgCOD\cdot d)^{-1}$, which is below the standard value of the model. The SBR was step-feed, which differentiates it from other reactors, and yet the value found is close to the default value of 5 $mgCOD\cdot(mgCOD\cdot d)^{-1}$.

Koch *et al*. (2000) calibrated the ASM3 model with experiments on full-scale batch reactors with activated sludge systems in Switzerland and found autotrophic growth rates (μ_A) ranging between 0.9 and 2.0 d^{-1}. For the step-feed with SBR, the rate was 1.2 d^{-1} for the ASM3 model, which was within the optimal value according to the literature. However, for the ASM2 model, the autotrophic growth rate (μ_A) was well above the standard value of 1.0 d^{-1}, whereas in the ASM1 model the rate remained standard. For the heterotrophic aerobic growth rate (μ_H), the ASM3 model had a rate of 3.0 d^{-1}, whereas in the present SBR study the default value of 2.0 d^{-1} was maintained. The ASM1 and ASM2 models had a rate well below the standard, which suggests the difficulty of calibrating these models for influences on the simulation cycle.

For the ASM2 model, a growth rate of 1.8 d^{-1} was found for phosphorus-accumulating organisms (μ_{PAO}). Furumai *et al*. (1999) found a rate of 1.0 d^{-1}, which is the default for the model and close to the standard value. They also found the calibration of the storage rate for phosphorus-accumulating organisms (q_{PHA}) to be 5.0 $mgCOD\cdot(mgPAO\cdot day)^{-1}$, while the default value was 3.0 $mgCOD\cdot(mgPAO\cdot day)^{-1}$. As for the SBR used in this study, we defined it as a rate of 0.2 $mgCOD\cdot(mgPAO\cdot day)^{-1}$. The value found is far from the literature and this difference should be taken into account in the simulation of phosphate. In Table 3, the default and calibrated parameters are presented for the cycle with one input.

Table 3: Parameters of the cycle with one input.

Parameters	Unit	ASM1 *Def.	ASM1 **Cal.	ASM2 Def.	ASM2 Cal.	ASM3 Def.	ASM3 Cal.
Aerobic Heterotrophic growth (μ_H)	day^{-1}	6	6	6	4.5	2	2
Anoxic heterotrophic growth (μ_H)	day^{-1}	4.8	3.2	-	-	-	-
Autotrophic growth (μ_A)	day^{-1}	0.8	0.8	1	1.3	1	1.5
Storage rate (k_{STO})	$mgCOD\cdot(mgCOD\cdot day)^{-1}$	-	-	-	-	5	6.5

*Def. = Default **Cal. = Calibrated

Calibrating the cycle with one input was easier. For the ASM2 model, the simulation was more difficult since two parameters were changed. The same happened with ASM1, but in this model only one parameter was changed. Still, one parameter had a large effect on many components and demanded more time. For the ASM3 model, the calibration was more objective and demanded less iterations because it had a minimal amount of influence on other components when compared to the one-parameter calibration.

The calibration results obtained by Furumai *et al*. (1999) were close to the results achieved for the SBR in their study. They obtained a heterotrophic growth rate (μ_H) of 6.0 d^{-1}, and the rate obtained in the calibration was 4.5 d^{-1} for ASM2 and 6.0 d^{-1} for ASM1. For the ASM2 model, Koch *et al*. (2000) acquired a rate of 3.0 d^{-1}, while in the calibration using the ASM3 model the standard value of 2.0 $d^{-1}$was maintained. They also obtained an autotrophic growth rate (μ_A) between 0.9 and 2 d^{-1} for the ASM3 model. For Furumai *et al*. (1999), the μ_A was 1.0 d^{-1}. The rate obtained in this work using ASM2 was 1.3 d^{-1}, and for ASM3 was 1.5 d^{-1}. Thus, the rates found for ASM2 and ASM3 were within the range found in the literature. For the ASM1 model, the rate was maintained at the standard value.

Krishna and van Loosdrecht (1999) defined in their calibration one storage rate (K_{STO}) of 10 $mgCOD \cdot (mgCOD \cdot day)^{-1}$. Koch *et al*. (2000) found 12 $mgCOD \cdot (mgCOD \cdot day)^{-1}$for a batch reactor in the pilot scale. The cycle calibration resulted in 6.5 $mgCOD \cdot (mgCOD \cdot day)^{-1}$, which was higher than the default of the model. The value found for the cycle lies within the range set by the default and those found in literature, which indicates that it was a good result. The remaining parameters used were the standards recommended by Henze *et al*. (2000).

Simulation

The data obtained with the simulations before and after the calibrations were verified and the best results are presented in the figures below. In all of these, the simulations are represented by continuous lines, while the results from the SBR are represented by square data points. The data obtained for soluble COD (S_S) are shown in Figure 3. The values ranged from 15 to 40 $mgCOD \cdot L^{-1}$ for the ASM3 model. In the step-feed cycle the agreement between the experimental and the simulations results was very good for S_S, and it shows that the model ASM3 was ideal to predict this cycle. The last data point for the SBR and the simulation results are at the same point, which is near 20 $mgCOD \cdot L^{-1}$. The simulation with the ASM3 model was the best model to represent S_S in the step-feed cycle.

The simulated data and that obtained for the SBR of nitrate (S_{NO3}) are shown in Figure 4. The values of nitrate, for the ASM3 model, range between 12 and 18 $mgNO_3^-\text{-}N \cdot L^{-1}$. For S_{NO3} in the step-feed cycle, the agreement between the experimental and the simulation results was good, but for the efficiency was not. The final values for nitrate in the simulation and in the actual data were close in number. The ASM3 simulation represented the S_{NO3} well in the step-feed cycle.

The simulated data for ammonium (S_{NH4}) can be observed in Figure 5. The values of ammonium for the ASM3 model ranged between 0 and 7 $mgNH_4^+ \cdot L^{-1}\text{-}N$. As for S_{NH4} in the step-feed cycle, the agreement between the experimental and the simulation results was good, but some points such as 0.5, 2 and 5.5 h were not close to the simulation results. The final value of the simulated and the real data were at the same point. The ASM3 simulation was a good representation of the step-feed cycle. Regarding all components evaluated, particulate COD (X_S), soluble COD (S_S), nitrate (S_{NO3}), and ammonium (S_{NH4}), the ASM3 model was the best to represent the step-feed cycle.

For soluble COD (S_S), the simulated and real data obtained from the cycle with one input are presented in Figure 6. The values ranged between 5 and 45 $mgCOD \cdot L^{-1}$. In the one-input cycle, the agreement between the experimental and the simulation results was almost excellent for S_S; it shows that the ASM1 model was ideal to predict this cycle. The final real and simulated data points remained around 10 $mgCOD \cdot L^{-1}$. The ASM1 simulation was a good representative, and for the one input cycle the ASM1 model best represented S_S.

The real and simulated data obtained for nitrate (S_{NO3}) are presented in Figure 7. The values ranged between 6 and 10 $mgNO_3^-\text{-}N \cdot L^{-1}$ for the ASM1 model. The simulation with ASM1 was excellent for S_{NO3} in the one-input cycle, the agreement between the experimental and the simulation results was great, as well as for the efficiency. The ASM1 model was the best representative of nitrate in the one-input cycle.

The simulated and real data for ammonium (S_{NH4}) are presented in Figure 8. For the ASM1 model the values ranged between 0 and 7 $mgNH_4^+\text{-}N \cdot L^{-1}$. The last data points for the simulation and the collected data were close. The agreement between the experimental and the simulation results was good and showed that the ASM1 model was ideal to predict

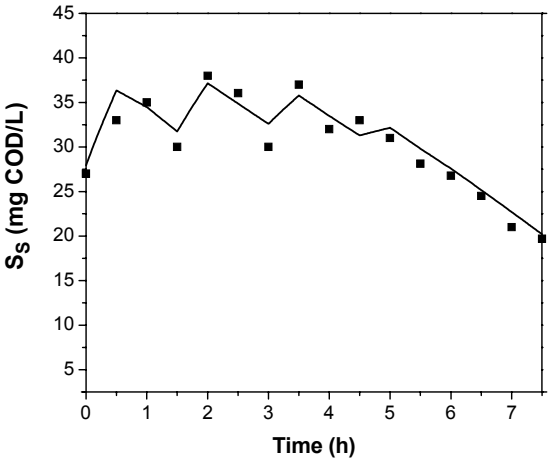

Figure 3: Simulated and experimental data for S_S in the step-feed cycle.

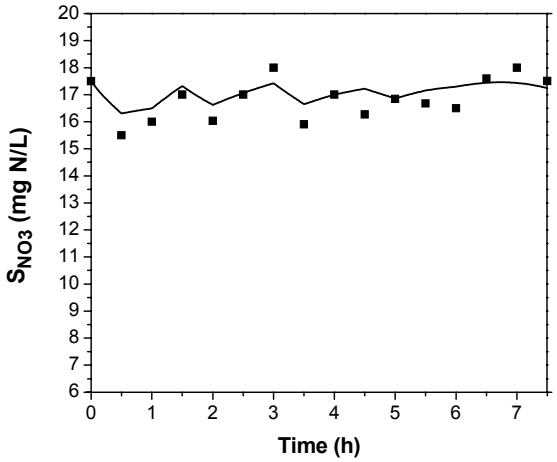

Figure 4: Simulated and experimental data for S_{NO3} in the step-feed cycle.

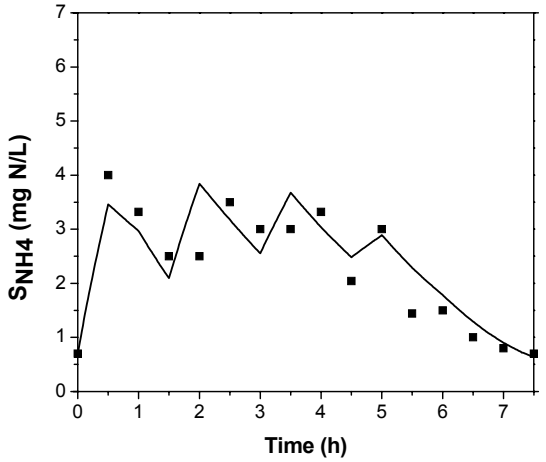

Figure 5: Simulated and experimental data for S_{NH4} in the step-feed cycle.

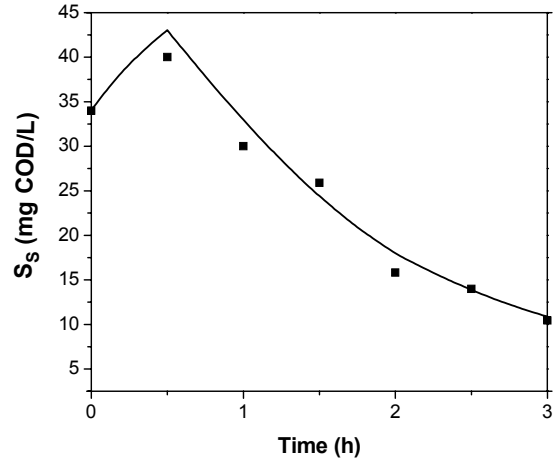

Figure 6: Simulated and experimental data for S_S in the one-input cycle.

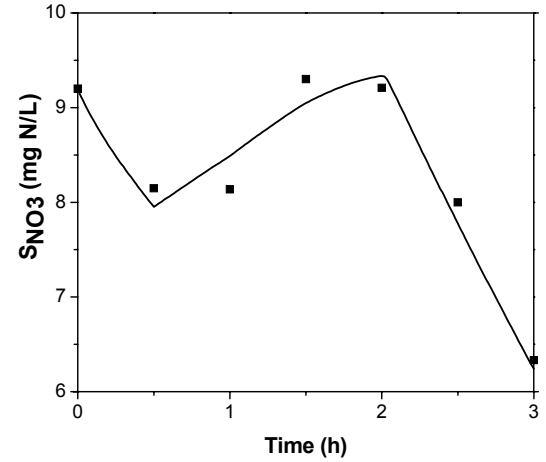

Figure 7: Simulated and experimental data for S_{NO3} in the one-input cycle.

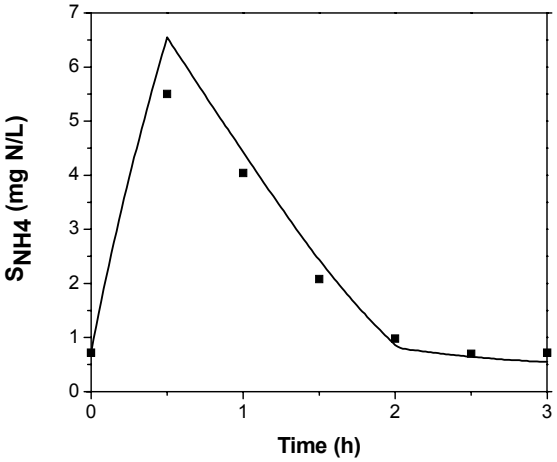

Figure 8: Simulated and experimental data for S_{NH4} in the one-input cycle.

the nitrogen and organic matter in this cycle. The simulation with ASM1 was an excellent representation of S_{NH4} for the cycle with one input. The ASM1 model was the best representative of ammonium in the cycle with conventional filling. The ASM1 model was a good representation of all components of the cycle with conventional filling and can be used to simulate a SBR in these conditions.

Comparison of Experimental and Simulation Data

The last point of the cycle for the simulations and the data obtained while monitoring the SBR are presented in Tables 4 and 5.

Regarding X_S, ASM3 and ASM2 were close to the actual data, with ASM3 being the closest. For S_S, only ASM3 achieved a good result and, for nitrate, all models obtained a good result. For ASM1 and ASM2, calibration was more difficult. This difficulty is explained by the final data point of the simulation before the calibration. This point is far from the actual data. For these models, the calibration was efficient, and the final results were close to the real data. The same can be said for ammonium, where all models achieved a good result, even though they were distant from the real data before calibrating. The ASM3 model achieved almost the same result as the real data. The phosphate results were close to the real data after calibrating the ASM2d model, but the reactor did not remove phosphate. Only the final data point of the simulation was close to the data obtained.

In the cycle with only one input for X_S, all models experienced excellent results for the final data and the ASM1 and the ASM2 models achieved almost the same results as the real data. For soluble COD, all models were close and the ASM2 model achieved the same result as the real data. For nitrate, all models also achieved a good result for the final data point (ASM1 and ASM3 models almost equaled the real data). For ammonium, all data was close for all models. The phosphate was not calibrated because phosphate was not removed. Even though the final results of some cycles reached the same point as the real data, during the cycle it could still be different.

Ideal Cycle

The reactor consistently showed high efficiency percentages with the step-feed cycle with 88.7% for S_S and 98.5% for ammonium removal. For the one-input cycle, the efficiency was 93.4% for S_S and 98.6% for ammonium removal. The cycle with only one input gave better results, and delivered an effluent with concentrations of 5394 $mg \cdot L^{-1}$ of particulate COD, 10.44 $mg \cdot L^{-1}$ of soluble COD, 6.33 $mgNO_3^-$-$N \cdot L^{-1}$, 0.72 $mgNH_4^+$-$N \cdot L^{-1}$, and 2.02 $mgPO_4^{-3}$-$P \cdot L^{-1}$. For this cycle, the ASM1 model was chosen to simulate the ideal operation of the SBR. Some alterations were made in the cycle, which included altering the oxygen concentration and adding one anoxic phase. In extended aeration activated sludge plants, Bertanza (1997) achieved high total N removal efficiencies (up to 90%) with low DO concentration. This was due to simultaneous nitrification and denitrification. In the reactor of our present study, the same process was observed where low DO led to the simultaneous removal of ammonium and nitrate. When the DO concentration increased, COD removal as well as denitrification became worse, while nitrification improved. The reactor accumulated nitrate, so the DO was limited to 0.5 $mgO_2 \cdot L^{-1}$. With this DO concentration, denitrification was ideal and COD removal improved. Even though there was no simultaneous nitrification and denitrification when using the ASM1 model, the process could be simulated by including one anoxic phase with low DO concentration.

The cycle was altered during the first phase by 30 minutes of filling at a concentration of 0.5 $mgO_2 \cdot L^{-1}$, followed by one 30-minute anoxic phase. Afterwards, one hour of aeration was performed at 0.5 $mgO_2 \cdot L^{-1}$ and, in the end, one hour of sedimentation and 30 minutes of withdrawal were performed. This simulated cycle gave outputs of 5399 $mgCOD \cdot L^{-1}$ of X_S, S_S of 5.38 $mgCOD \cdot L^{-1}$, 6.37 mg NO_3^--$N \cdot L^{-1}$, and 0.68 $mgNH_4^+$-$N \cdot L^{-1}$. The removal of 96.6% of S_S and 98.7% of S_{NH4} was reached with this new cycle. Figures 9 and 10 show the results of the simulation along with the ideal cycle.

Table 4: Final data of the step-feed cycle.

Component	Real data	ASM1 default	ASM1 calibrated	ASM2 default	ASM2 calibrated	ASM3 default	ASM3 calibrated
$X_S(mgCOD \cdot L^{-1})$	6278	6360	6163	6338	6344	6322	6321
$S_S(mgCOD \cdot L^{-1})$	19.71	7.54	4.50	1.51	6.45	11.09	20.21
$S_{NO3}(mgN \cdot L^{-1})$	17.51	7.07	17.12	3.13	17.77	14.09	17.24
$S_{NH4}(mgN \cdot L^{-1})$	0.70	0.00	0.81	1.00	0.59	1.80	0.64
$S_{PO4}(mgP \cdot L^{-1})$	2.87	-	-	0.89	2.60	-	-

Table 5: Final results from the cycle with one input.

Component	Real data	ASM1 default	ASM1 calibrated	ASM2 default	ASM2 calibrated	ASM3 default	ASM3 calibrated
X_S(mgCOD·L^{-1})	5394	5397	5397	5395	5396	5381	5381
S_S(mgCOD·L^{-1})	10.44	5.32	10.89	1.93	10.44	26.67	9.10
S_{NO3}(mgN·L^{-1})	6.33	7.19	6.24	2.60	7.03	11.91	6.42
S_{NH4}(mgN·L^{-1})	0.72	0.32	0.55	3.36	0.64	3.50	0.8
S_{PO4}(mgP·L^{-1})	2.02	-	-		0.05	0.03	-

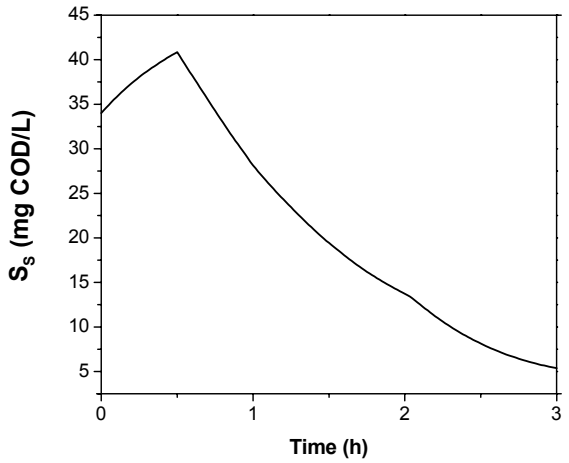

Figure 9: Simulated data for S_S in the ideal cycle.

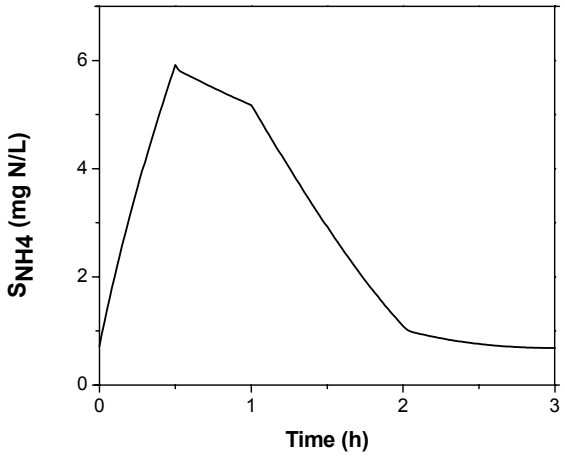

Figure 10: Simulated data for S_{NH4} in the ideal cycle.

CONCLUSIONS

Based on the results from the simulations for the SBR, the ASM1 model best simulates a one-input cycle. The ASM3 model was the best to represent the step-feed cycle. The software ASIM® was ideal to simulate the SBR. Because the library has all models used and the hydraulics of the SBR, it allows editing of the model and manual calibration. The one-input cycle gave better removal of S_S and S_{NH4}, and also was better represented by the three models, whereas the step-feed cycle was harder to calibrate and was not very well represented by the ASM1 and ASM2d models. Finally, the calibration with the ASM3 model was easier and more objective due to smaller effect of varying the parameters on the components.

ACKNOWLEDGEMENTS

The authors would like to thank the team from the Laboratory of Effluents at the Federal University of Santa Catarina, Brazil. In addition, we are grateful to the company Rotária do Brasil who provided the SBR for the study. We would also like to thank FINEP and CNPq for the financial support and for making this study possible.

NOMENCLATURE

ASIM®	Simulation software
ASM	IWA Model (*Activated sludge model*)
COD	Chemical oxygen demand
DO	Soluble oxygen
IWA	International Water Association
k_{STO}	Storage rate
PAO	Phosphorus-accumulating organisms
q_{PHA}	Storage of phosphorus-accumulating organisms
SBR	Sequencing batch reactor
S_{NH4}	NH_4^+-N ammonium
S_{NO3}	NO_3^--N nitrate
S_{PO4}	Phosphate
S_S	Soluble COD
X_S	Particulate COD
X_{STO}	Internal storage products

Greek Letters

η_{fe}	Anaerobic hydrolysis reduction factor
μ_A	Autotrophic growth rate
μ_H	Aerobic and anoxic heterotrophic growth rate
μ_{PAO}	Growth rate of phosphorus-accumulating organisms

REFERENCES

APHA, Standard Methods for the Examination of Water and Wastewater, 21th Ed. American Public Health Association/American Water Works Association/Water Environment Federation, Washington, DC (2005).

Bertanza, G., Simultaneous nitrification denitrification process in extended aeration plants: Pilot and real scale experiences. Water Sci. Tech., 35(6), 53-61 (1997).

Furumai, H., Kazmi, A. A., Fujita, M., Furuya, Y. and Sasaki, K., Modeling long term nutrient removal in a sequencing batch reactor. Water Res., 33(11), 2708-2714 (1999).

Gernaey, K. V., van Loosdrecht, M. C. M., Henze, M., Lind, M. and Jorgensen, S. B., Activated sludge wastewater treatment plant modelling and simulation: State of the art. Environmental Modelling and Software, 19(9), 763-783 (2004).

Henze, M., Gujer, W., Mino, T. and van Loosdrecht, M., Activated sludge models ASM1, ASM2, ASM2d e ASM3. London: IWA Publishing (2000).

Koch, G., Kuhni, M., Gujer, W. and Siegrist, H., Calibration and validation of activated sludge model no. 3 for swiss municipal wastewater. Water Research, 34(14), 3580-3590 (2000).

Krishna, C. and van Loosdrecht, M. C. M., Substrate flux into storage and growth in relation to activated sludge modeling. Water Research, 33(14), 3149-3161 (1999).

Schmidell, W., Agitação e aeração em biorreatores, In: Aquarone, E., Borzani, W., Schmidell, W., Biotecnologia Industrial. 1st Ed. São Paulo: Edgard Blücher Ltda, v. 2, p. 277-331 (2001). (In Portuguese).

USEPA, United States Environmental Protection Agency, Nutrient Control Design Manual, Cincinnati: The Cadmus Group Inc., p. 104 (2009).