Modelling of Sequencing Batch Reactors for Wastewater Treatment in Malaysia Implementing ASM2 as a Model Structure and Using AQUASIM

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Abstract The objective of this paper is to use modelling as a tool to investigate the use of sequencing batch reactors (SBRs) for wastewater treatment in Malaysia. A modified form of the Activated Sludge Model No. 2 (ASM2) was implemented using AQUASIM 2.0 as a modelling platform to simulate the microbial activities in a 10 litre single tank SBR reactor. The model results were compared to observed results in a real 10-litre system. The model indicated a steady state mixed liquor suspended solid (MLSS) of 3260 mgSS/l. Removal efficiencies of COD, TN, NH₄⁺ and NO_x⁻ were 89%, 91.5%, 99% and 100% respectively for the modelling compared with 89.5(±1.2)%, 91(±1.0)%, 98.5(±0.5)% and 98.75(±0.8)% respectively for the experiments. The rates of Nitrification and denitrification were 13.7 and 18.3 [mgNO_x⁻-N/(l.h)] respectively for the modelling compared with 13.95(±1.0) and 18.1(±0.3) [mgNO_x⁻-N/(l.h)] respectively for the experiments. The study indicated that for design, operating and monitoring purposes, modelling can help in implementing a sludge control to determine the required biomass concentration with a given react phase time.

Key Words AQUASIM, ASM2, Malaysia, react time, removal efficiency, sequencing batch reactor (SBR).

INTRODUCTION

The upgrading of the wastewater treatment (WWT) infrastructure in Malaysia is consistent with the intention of the Government to introduce more stringent effluent quality criteria. Under the latest sewerage master plan, approximately US\$1.6 billion was approved to upgrade the WWT infrastructure (IWK, 1997). This has created a need to evaluate different options for the WWT plants in order to determine the feasibility of implementing these options, in terms of reliance and efficiency under Malaysian conditions.

Sequencing batch reactors (SBRs) are one of the proposed systems to upgrade the existing low-technology systems such as waste stabilization ponds in Malaysia, to mechanical plants (Ujang *et al.*, 2001). This paper is part of a multiphase study "*Feasibility Study on sequencing batch Reactor System for Upgrading Wastewater Treatment in Malaysia* (Al-Shididi et al., 2002)". Theoretical, field and laboratory investigations respectively were carried out as the preliminary phases of the study in the last phase, modelling of the proposed systems. The goal of this study was to determine the feasibility of implementing the SBR system in Malaysia by evaluating the reliability, flexibility, robust, and partly the economical feasibility of the system (Al-Shididi et al., 2002).

This paper puts emphasis on the final phase of the study, the modelling investigation phase. The information collected by the previous investigations lacked data resolution, particularly information on microbial activities in the mixed liquor, where 16 SBR experiments were carried out. Figure 1 presents the nitrification-denitrification data of the last 2 experiments.



Figure 1: NO_x development over nitrification and denitrification in experiments 14, 15 and 16. The removal efficiencies data for the same experiments are presented in table 1. A need appeared for subsequent analysis that can determine the influence of microbial activity on efficiency, processes rates and optimal operation. Modelling was used as a tool to fill these information gaps for the feasibility study. This paper presents the methodology, results and conclusions of the modelling.

METHODOLOGY

The results of mainly the last two SBR experiments in the previous phase of the study were used as a reference (observed data) of the parameter estimation (calibration) for the model. The SBR was modelled using AQUASIM 2.0 (Reichert, 1998), implemented as a fully mixed compartment, with variable volume of maximum 10 litres as in the experiments. The ASM2 (Henze et al., 2000) was implemented as a model structure for the microbiological activities using ASM2 processes kinetics and stoichiometry with the following modification: Without phosphorous removal, since the scheduled tasks of the study were confined to the carbon and nitrogen removals. Therefore, within ASM2 processes, the aerobic processes and the anoxic processes were included and the anaerobic processes were excluded. Specifically, anaerobic hydrolysis, both growth and fermentation of heterotrophs on fermentation products, fermentation, phosphorous-accumulating organisms (PAO) and simultaneous precipitation of phosphorous with ferric hydroxide Fe(OH)₃ were excluded. Ammonification process was included. Initial conditions were repeatable response to a set cycle, from average measured data in the experiments. 100 cycles were modelled. Figure 2 illustrates the configuration of the modelling investigation. The concept and the general assumptions of the modelling will be presented in this section as the procedure of the modelling.



Figure 2: Schematic presentation of the modelling investigation.

Concept

The sludge in the model needs to accumulate as in an ordinary treatment plant. The sludge development process is achieved by the growth of the bacteria inside the reactor, fed with the wastewater flow into the reactor and by the soluble (S) and the particulate (X) contents of the wastewater. A realistic sludge composition can be reached by successive retention and growth until the amount of the biomass is sufficient for the treatment and can simulate effectively observed values. Therefore, 100 full cycles (aerated fill - aerated react - mixed react-draw) were carried out in the model. Figure 3 illustrates this.



Figure 4: The hydraulic cycle and the sludge building up concept in the modelling of the SBR.

Figure 3: Phases of a full cycle of modelled SBR.

Assumptions

The following assumptions were adopted:

1. The reactor was empty of sludge before the first cycle, with no seed. The time set assigned for the operational phases in experiment no. 16 is adopted in the model. The operational phases of a modelled SBR cycle are illustrated in figure 4. The time set for the same cycle is illustrated in figure 5. A full cycle occupies 8.25 hours. Hence, 100 cycles will take 825 operational hours. The only overlapping between the phases is between the aerated fill and the aerated react phases.



Figure 5: Time set of experiment no. 16, which is implemented in the model.

- 2. There is no settle phase, since the settling process is not indicated in the model.
- 3. The effluent will contain only the soluble concentrations (S) at the end of the react phase (aerated aerobic react + mixed anoxic react) and the particulate concentrations (X) are left in the tank to form the accumulation of the sludge (See figure 3).
- 4. The temperature in the reactor is at 28°C (The Malaysian condition).

PARAMETER ESTIMATION

The observed data, which are the target of the parameter estimation, are the nitrate/nitrite development during nitrification and denitrification. This concerns the following:

- 1. *The nitrification parameter estimation*: This was dependent on the aeration condition. The aeration observed data of experiment no. 16 was considered as the target of the estimation. The modelled aeration was simulated to fit the observed oxygen concentration over the aerated react (nitrification + denitrification) phase time. The result of the parameter estimation is illustrated in figure 6.
- 2. *The denitrification parameter estimation*: This parameter estimation was carried out by adding 4 pulses of acetic acid (HAc) during the mixed react phase at 15, 30, 45 and 60 min. after the start of the mixed react as 7.5 g HAc/l MLSS for the first pulse, and 3.75 g Hac/l MLSS for the rest of the pulses. HAc was added as a carbon source for anoxic heterotrophs (X_H) during denitrification in experiments 14, 15 and 16.



Figure 6: The aeration parameter estimation of the simulated oxygen concentration at cycle no. 41 compared with the observed oxygen concentration over the react time (nitrification + denitrificationn).

RESULTS AND DISCUSSION

The observed data for the last two experiments (No. 15, and 16), as the optimised ones, were compared to the results of the model focusing on experiment no. 16 as the modelled experiment. Results include steady state, sludge age, removal efficiencies, processes rates, solid biomass fractions, react time estimation and reliability to the Malaysian condition.

Steady State

At cycle no. 25 (Hour 198 to hour 206.25) the steady state was reached regarding the concentration of heterotrophic bacteria (X_H), slowly biodegradable substrate (X_S), particulate organic Nitrogen (X_N), total nitrogen (TN) removal, ammonium (NH_4^+) removal and Nitrate/nitrite (NO_x^-) generation and removal. At cycle no. 40 (Hour 321.75 to hour 330) the steady state was reached regarding the concentration of autotrophic bacteria (X_A) and Chemical Oxygen Demand (COD) removal. Given this, starting at cycle no. 40, a full steady state operation was achieved at a mixed liquor suspended solid (MLSS) concentration equal to 3260 mgSS/l.

Removal Efficiencies

The results of the removal efficiencies of COD, TN and NH_4^+ are presented in table 1 below together with the efficiencies in experiments no. 15 and no. 16. The ratio of the observed to the modelled removal efficiencies of COD and TN are about 0.92. The 0.08 lower ratio in the observed efficiencies of COD and TN is due to the existence of the particulate matter in the effluent, not included in the model. A correction can be applied as shown in Eq. 1, and the modified model efficiencies are shown in table 1 in parentheses.

 $Effluent \ concentration = Influent \ concentration - 0.92 \times modelled \ efficiency \times Influent \ concentration \qquad (Eq. 1)$

		Model			Experiment no. 15			Experiment no. 16		
Parameter	Unit	Influent	Effluent	Efficiency (%)	Influent	Effluent	Efficiency (%)	Influent	Effluent	Efficiency (%)
COD	MgCO D/l	400	13 (44)**	≤96.75 (89)**	636	59	90.7	398	47	88.2
TN	MgN/l	70.43	0.43 (6)**	≤99.4 (91.5)**	66	5.21	92.1	69	6.86	90.06
NH_4^+	MgN/l	42	0.42	99	39.6	0.7	98.23	43.22	0.4	99.07
NOx	MgN/l	41.14*	0.01	≈100	27.18*	0.11	99.6	25.99*	0.56	97.85

Table 1: The removal efficiencies of COD, TN, NH^{$^+$} *and NO*^{$^-$} *in the modelled SBR compared with experimental efficiencies.*

* This value represent the highest value of the NO_x generated by nitrification. The influent value is approximately 0.43 mgNO_x-N/l.

** The modified efficiency considering a ratio of 0.92 of observed to modelled removal efficiencies, which considers X in the effluent that the model ignored.

Effluent COD has met the requirements of Malaysian standards A and B (50 & 100 mgCOD/l respectively) (Malaysian Standards, 1991). It should be noted in table 1 that the maximum values of the observed NO_x^- concentrations in the experiments are considerably less than the modelled NO_x^- concentrations. This is explained in the next section.

Processes Rates

The model achieved the illustrated nitrate-nitrogen development in figure 7 at cycle no. 40 (Hour198 to hour 206.25). Figure 7 presents the results, which are selected at cycle no. 41 (Hour 321.75 to hour 330), right after the full steady state started.

As shown in Figure 7, simulated nitrate is above experimental nitrate. This may be due to model limitations, analytical problems in nitrite detection, or anoxic conversion during sample preparation and analysis. Unfortunately, we suspect analytical and sample handling errors, as fitted oxygen uptake rates

from all experiments are consistent with model nitrification rates. We have therefore taken the higher result (model) for further analysis. On the other hand, the modelled nitrification and denitrification rates are close to the observed nitrification and denitrification rates in experiments no. 14, 15, and 16.



Nitrate Nitrogen development during nitrification and denitrification

Figure 7: The NO₃⁻N development during the react phase in the SBR modelling at cycle no. 41 compared with the observed data in experiment no. 16.

From figure 7, the linear estimation of the nitrification and denitrification rates could be conducted. Table 2 presents a comparison between the modelled rates and the observed rates.

Table 2: A comparison between the modelled rates and the observed rates of nitrification and denitrification.

Rate: $r_{v,s}$ [mgNO _x ⁻ -N/(l.h)]	Modelled	Experiment no. 15	Experiment no. 16
Nitrification	13.7	13.38	13.28
Denitrification	18.29	17.86	18.41

Biomass Fractions (X)

The values of the biomass fractions, which reached a steady state at cycles no. 25 and 40, are presented in table 3.

Table 3: The fractions of solid biomass at the steady state condition.

Component	Start of steady state [Cycle]	Concentration X _{COD} [mgCOD/l]	Concentration X_{VSS} [mgX/l] = $(X_{COD} \times 0.7 \text{ mgX/mgCOD})^*$	
Autotrophic bacteria (X _A)	40	75	53	
Heterotrophic bacteria (X _H)	25	1290	900	
Slowly biodegradable substrate (X_s)	25	350	245	
Particulate organic nitrogen (X _{ND})	25	27	19	

* This unit conversion is derived from Table 4.5 in Henze et al, 1997.

React Phase Time Estimation

The time estimation of the react phase (t_{total}), which is the summation of the nitrification time ($t_{nitrification}$) and the denitrification time ($t_{denitrification}$), is presented in Table 4.

Experiment		Nitrification rate*	:	Denitrification rate**			
	r _{V,S} [mgN/(1.h)]	$\mu = r_{v,s}/X_{A,COD}$ $[mgN/(gCOD_{XA}.h)]$	$\mu^* = r_{v,s}/X_{A,VSS}$ [mgN/(gX _A .h)]	r _{V,S} [mgN/(l.h)]	$\mu = r_{v.s}/X_{H,COD}$ $[mgN/(gCOD_{XH} .h)]$	$\mu^* = r_{v,s}/X_{H,VSS}$ [mgN/(gX _H .h)]	
Modelled	13.7	182.7	258.5	18.29	14.18	20.32	
No. 15	13.38	178.4	252.4	17.86	13.84	19.84	
No. 16	13.28	177.1	250.6	18.41	14.27	20.46	

Table 4: Time estimation of the react phase (t_{total}) *for the modelled SBR and experiments no. 15 and 16.*

Experiment	Influent Concentration of ammonium (S _{NH4,in}) [mgN/l]	V _{fill} [1]	V _{total} [1]	$\frac{ \overset{t_{nitrification} =}{S_{NH_{4}^{+},in} \cdot V_{fill} } }{ \mu_{nitrif.} \cdot X_{A} \cdot V_{total} }_{[h]} $	$\frac{ \substack{ t_{denitrification} = \\ S_{NH_{4}^{+},in} \cdot V_{fill} }{ \mu_{denitrif.} \cdot X_{H} \cdot V_{total} }_{[h]} }$	$t_{total} = t_{nitrif.} + t_{denitrif.}$ [h]
Modelled	42	7.5	10	2.3	1.72	≈ 4
No. 15	39.6	7.5	10	2.22	1.66	≈ 3.9
No. 16	43.22	7.5	10	2.25	1.76	≈4

The total best react time is about 4 hours distributed between 2.25 hours for nitrification and 1.75 for denitrification. This procedure can be implemented to control the biomass for the purpose of design and operation.

Reliability

In terms of reliability to the Malaysian condition, the SBR system, according to both the experimental and modelled results, is able to remove efficiently concentrations higher than the average concentrations in the Malaysian wastewater as it is illustrated in table 5.

Table 5: A comparison between different influents and different effluents.

Para	neter	Reference	COD [mgCOD/l]	N [mgN/l]	SS [mgSS/l]
	Malaysian	Christensen et al., (2001)	223	-	146
Influent	Malaysian	SBR field investigation	262 ± 99	28 ± 12	174 ± 56
Influent	Danish	SBR experimental investigation	415 ± 89	67 ± 6.5	243 ± 58
	Modelling	SBR modelling investigation	400	70.43	-
	Malaysian	SBR field investigation	116 ± 50	16 ±7	64 ± 19
Effluent	Danish	SBR experimental investigation	49 ± 11	10.5 ± 2.5	17 ± 4
Ennuent	Modelling	SBR modelling investigation	44	6	-
	Malaysian	Standard A	50	-	50
	Malaysian Standard B		100	-	100

Due to the different effluent results achieved by this study compared to the Malaysian standards of effluent, table 6 is proposed to upgrade for the Malaysian effluent quality standards. The current Danish standards are listed in the same table for the purpose of comparison.

Donomatan	Linit	Standard A		Stand	ard B	Donich standards
Parameter	Unit	Current	Suggested	Current	Suggested	Damsn standards
BOD	mgBOD/l	20	20	50	50	10-30*
COD	mgCOD/l	50	50	100	100	25-75**
TN	mgN/l	-	8	-	15	5-10*
SS	mgSS/l	50	30	100	50	30**

Table 6: The suggested standards for the Malaysian condition, compared with the Danish standards.

* (Christensen et al., 2001).

** (Henze, 2001).

CONCLUSIONS

The SBR system seems able to meet the current Malaysian standards. Modelling the SBR gave further data, in addition to the experimental data, especially concerning the bacterial activities during the removal processes. The computer modelling can be used as a tool to upgrade and monitor the performance of the SBR, particularly, the biomass development and the reaction rates. Given the biomass at steady state and the removal rates of nitrification and denitrification, the optimal time of the react phase (nitrification time) can be determined taking into consideration the ammonium concentration in the influent. In this study, for measured ammonium concentration in the influent of 42 mgN/l, and with adding HAc as an additional carbon source during denitrification + 1.75 hour for denitrification). For design, operating and monitoring purposes, modelling can help to implementing a sludge control to determine the required biomass concentration within a given react phase time. This control can be achieved practically by de-sludging to remove the surplus biomass

A standard for TN concentration in the Malaysian effluent could be suggested by the study, according to the SBR performance. In specific 8 mg N/l is suggested for Standard A and 15 mg N/l is suggested for Standard B of effluents.

Further studies are required on a pilot scale or/and a industrial scale in order to investigate and model more than one tank SBR systems, to optimise control requirement for the SBR plant, to optimise different shapes and sizes of the tanks, and to detect different strategies of operational phases. The modelling can also be integrated into various technical aspects, including socio-economic dimension of the Malaysian condition. Further studies are also needed to investigate the feasibility in terms of cost-effectiveness and flexibility on industrial scales before the design stage. Considering phosphorous removal in further studies gives more credible data concerning sludge building up and may allow implementation of effluent phosphorous standards in Malaysia.

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