

Aamr Alalewi1* and Shouwen Chen¹

¹School of Environmental & Biological Engineering, Nanjing University of Science & Technology, Nanjing 210094, China.

Authors' contributions

This work was carried out in collaboration between both authors. Author AA designed the study, performed the statistical analysis, wrote the protocol and wrote the first draft of the manuscript. Author SC managed the analyses of the study. Both authors read and approved the final manuscript.

Article Information

DOI: 10.9734/CJAST/2017/36138 Editor(s): (1) Jakub Kostecki, Faculty of Civil Engineering, Architecture and Environmental Engineering, University of Zielona Góra, Poland. Reviewers: (1) Randa M. Osman, National Research Centre, Egypt. (2) C. R. Ramakrishnaiah, Visvesvaraya Technological University, India. (3) Arnaldo Sarti, Instituto de Quimica (Unesp/Araraquara-SP), Brazil. (4) Saima Fazal, South China University of Technology, China. Complete Peer review History: http://www.sciencedomain.org/review-history/21755

> **Received 14th August 2017 Accepted 14th October 2017 Published 4th November 2017**

Original Research Article

ABSTRACT

Models can play an important role in the evaluation of upgrading strategies for biological nutrient removal. In this paper the calibration of ASM2d to a pilot plant with an intermittent aerobic/anoxic reactor is discussed. The performed modeling study was part of a retrofit study. An existing plant, removing only COD and where phosphorus was chemical precipitated, had to be upgraded towards full biological nutrient removal. Emphasis was put on the practical aspects of calibrating ASM no 2d efficiently. The calibration procedure was based on an 'expert approach' rather than on a system engineering approach. With only changing three parameters (reduction factors, analysis rates for PAOs and the decay rate for autotrophs), the model proved well capable of describing the performance of the pilot plant. A second set of parameter adjustments was tested. Good results were obtained as well, but more parameters had to be changed. New findings are that oxygen entering the treatment plant via the influent has an important influence on the simulated phosphate effluent concentrations. Further, reactions occurring in the final clarifier effect the effluent

concentrations. This is indicated by the necessity to introduce and assign a virtual volume to the settler where reaction can occur. Both factors are extremely important to focus attention to because they are different between a pilot plant and a full scale system.

Keywords: Nutrient removal; ASM2d; phosphorus; sludge.

1. INTRODUCTION

Wastewater treatment plants built in the past were mainly designed for COD removal. Stricter environmental regulations necessitate the removal of nitrogen and phosphorus in the treatment plants. Including biological nutrient removal in existing wastewater treatment facilities means reassigning existing tanks for new purposes, redesigning the flow scheme of the plant and when necessary the installation of new tanks. The high number of reactions, the interaction between the different processes, the very strict regulations and the limited space available for upgrading or building new treatment plants necessitates nowadays the application of models for designing these facilities. An IAWQ task group presented ASM2d for modelling nutrient removal [1].

The parameters in the ASM models are average values often based on laboratory experiments performed under extreme conditions favoring particular processes. These parameters can be very case specific and new values should be assigned based on pilot and or full scale data. Indeed, the quality of the predictions depends on the quality of the parameters of the model and of the quality of the wastewater and plant characterization. In the case of upgrading an installation, investing money in prior pilot scale experiments with different scenarios will result in better modelling results and maximized design knowledge. A good strategic set-up benefits the success of the calibration procedure. Although it is often said that for the application of dynamic processes, default values may be retained for stoichiometry and most kinetic constants, it will be shown in this paper that ASM2d has some shortcomings which can be overcome by adjusting certain parameters. Other parameters will be shown to be process and influent dependent.

Wastewater characterization was performed using the Dutch standards proposed by STOWA [2]. Laboratory experiments were used to obtain a first indication of the fraction of PAOs, to differentiate between denitrifying and nondenitrifying PAOs and to have an idea of the denitrifying capacity of the heterotrophs. In this paper the standard notation of the IAWQ task group has been used [3].

2. MATERIALS AND METHODS

2.1 Installation

The projects involve upgrading an existing plant for COD removal to a full biological nutrient removal plant, including biological nitrogen and phosphorus removal. A pilot plant was built and long-term pilot investigations with different AS processes were carried. An intensive measurement campaign was set up with the pilot plant consisting of an anaerobic tank of 1 m^3 , an aerobic/anoxic tank of 6 $m³$ and a settler of 3.5 m³. Influent was taken from the WWTP after the grit chamber and fed at a constant flow rate of 12 m3/d to the pilot plant without primary settling[4]. The aerobic/anoxic tank was operated intermittently with a complete cycle of 5000 seconds of which 2000 seconds with aeration switched on. The oxygen concentration was regulated at 1 mg O2/ l. Excess sludge was taken from this tank at intermitted intervals to set a sludge retention time of 14 days. The return flow was set to 81.6 m^3 /d.

2.2 Measurement Campaign

Three automatic samplers (AS900, Sigma) were located respectively at the entrance of the biological unit, at the end of the anaerobic compartment and at the effluent 24h composite samples were taken during a period of 48 days. Within that period, 2h composite samples were collected for 48 hours. VFA determination was performed only for these 2h samples. All samples were cooled at 4°C and transported to the laboratory every day for analysis.

Influent samples were analyzed for COD, CODf, BOD, BODf, SS, VSS, KjN, NH4-N, NO3-N, NO2-N, TP and PO4-P. Samples of the effluent of the anaerobic tank were analyzed for COD, CODf, SS, VSS, KjN, KjNf, NH4-N, NO3-N, NO2- N and TP. Within the biological reactors ammonia, nitrate and dissolved oxygen were monitored on-line. The effluent samples were

analyzed for COD, CODf, BOD, SS, KjN, NH4-N, NO3-N, NO2-N, TP and PO4-P.

3. SLUDGE CHARACTERIZATION

Two jacketed laboratory fermenters of 2 liters were used to perform batch tests to determine the fraction of phosphate removing organisms and the reduction factors for anoxic acetate uptake and anoxic phosphate uptake. The activated sludge used was taken from the aerobic basin of the pilot installation preferably one day prior to the batch experiments.

The values resulting from the experiments are used as indication for increasing or decreasing the relevant parameters. The tests were performed at a controlled temperature of 20°C and pH of 7.0 ± 0.1 .

Prior to the experiments phosphate is added to the sludge to allow for eventual aerobic phosphate uptake. Then the sludge is subjected to an anaerobic stage with acetate feed, followed by an aerobic or anoxic period. To this end the mixed liquor is divided in two equal amounts after the anaerobic period. Phosphate, ammonium, nitrate, VSS and MLSS are measured following a pre-set sampling program.

3.1 Influent Characterizations

Since the IAWQ models (ASM1, ASM2, and ASM2d) were published, a variety of methods emerged to characterize the different

Measured value Conversion equations for model values

components of the wastewater. This method is based on a physic-chemical method to characterize the soluble and particulate fractions, combined with a BOD-measurement for characterizing the biodegradable fraction of the influent COD. In Table 1 the average measurement data obtained during the measurement campaign are presented along with their standard deviations (34 measurement points). In the last column the set of equations needed for the influent characterization according to the STOWA guidelines are presented. Since for ASM2d no soluble inert production is included in the model, i.e. fSI being the stoichiometric parameter for production of SI in the hydro analysis process is set to zero, the proposed equation, $SI = 0.9$ CODefflux, was replaced by $SI = CODeffI$.

4. SIMULATION ENVIRONMENT

For simulation purposes the software package Simba 3.2+ (c), based on Matlab and Simulink, was used. The plant lay-out consists of one anaerobic tank, one intermittent aerobic/anoxic tank and one settler. A proportional controller was used to set the oxygen concentration at 1 mg O2/ l . To account for the processes taking place in the settler, a virtual anoxic reactor is implemented in the return sludge line of the model of the plant. Indeed, during the passage through the settler, biological processes continue. These processes are not accounted for in the model as it is when a standard point settler model is used.

Measured value			Conversion equations for model values				
Influent measurement data							
	Average	Stdv					
COD	524.7	188.4	$COD = SA + SF + SI + XI + XS$ (gives XI)				
BOD ₅	203.4	76.1	$BCOD = \frac{1}{1 - f_{\text{non}}} * \frac{1}{1 - e^{-k_{\text{non}}}} * BOD_s = S_A + S_F + X_s$ $(giveX_{s})$				
CODf	221.6	109.8	$COD f = S A + S F + S I (gives SF)$				
VFA	16.5	6.7	SA (gives SA)				
Ki-N	46.1	5.9	$SNH4 = Kj-N - (INSI *SI + iNSF *SF + iNXI *XI + iNXS *XS + iNXBIO$ *XBIO)				
TP	7.6	1.5	$SPO4 = TP - (IPSI *SI + IPSF *SF + IPXI *XI + IPXS *XS + IPXBIO$ *XBIO)				
SNH4	31.1	5.5					
SNO ₃	Ω						
SPO ₄	4	0.8					
Effluent measurement data							
CODf	38	4	$SI = CODf$ (gives SI)				

Table 1. Average measurement data and conversion formulas [5]

The virtual reactor has a volume corresponding to the residence time of the sludge in the settler. To calculate the residence time of the sludge in the settler the settling velocity and the return flow rate have been used. With a return flow rate of 81.6 m³/d and a superficial area of 5 m², the underflow velocity equals 0.68 m/h. Considering an average settling velocity of 2 m/h, an overall velocity of 2.68 m/h is obtained. This value was rounded to 2.5 m/h. As the sludge enters the settler at approximately half its height, a residence time of the sludge in the settler of 15 minutes is obtained. A virtual reactor with a volume resulting in such a residence time was implemented. The reactor volume was set at $0.95 \; \text{m}^3$.

5. RESULTS

5.1 Sludge Characterization

From the experiments an uptake rate of 5.4 mg P/g VSS/h was determined. For enhanced cultures of PAOs a value of 55 mg P/g VSS/h is measured [6], indicating that about 10% of the sludge population can be considered to be PAOs. The ratio between acetate uptake under aerobic conditions and acetate uptake under anoxic conditions revealed a value of 0.40 for the reduction factor. In ASM2d the default value for ηHNO3 is 0.8. The experiment thus indicates that the number of denitrifying heterotrophic bacteria is probably lower for this plant than the average assumed value. For the reduction factor for denitrification by PAOs a similar value was found.

5.2 Influent Characterizations

The rate constant of the BOD test (kBOD , measured by an external laboratory) resulted in a value of 0.38 d-1 for the 24 hour grab samples and a value of 0.28 d-1 for the period in which 2 hour grab samples were collected. Using these values, the influent concentrations of the different fractions were calculated. However, the calculated values revealed high concentrations for the particulate inert fraction in the influent XI. The actual value of this component in the reaction basins depends on the influent concentration via XI, reaction basin = XI, influent *SRT/HRT, supplemented with the formation of inert in the analysis process. Only taking the XIinfluent gave a higher value than the observed total sludge concentration of 4.63 g COD/. The estimation of kBOD has in practice proven to be

difficult. At the same time this value has a large influence on the fraction of inert in the sludge, and thereby on the total sludge production. It was decided to start with a value of 0.23 d-1 or kBOD, this value is used in the Netherlands as an average value when reliable measurements are lacking. In Table 2the obtained influent composition is given.

Table 2. Calculated influent concentration

 $X1$ SS = 11SSXI *XI + 11SSXS *XS +11 as suggested as default in ASM2d. $SS = XI + XS + XH + XPAO + XAUT$, based on a COD/VSS ratio of 1.33 and a VSS/SS ratio of 0.75 as observed for the plant

5.3 Calibration Procedures

5.3.1 Ste1: Using the default parameters of ASM2d

The calibration procedure was started using the default values of ASM2d and using the influent concentrations as given in Table 3. With the standard kBOD value of 0.23 d-1 reasonably good match between simulated and measured total solids concentration was obtained. The concentrations for the soluble components, however, did not correspond satisfactorily. In Table 3 the effluent concentrations as measured during an extensive measurement campaign are summarized. In Table 4 the simulated effluent concentrations are given. It can be seen from these tables that ammonium is far too high and nitrate and phosphate are too low if ASM2d default values are used.

Component	Average	Stdv	Unit
BOD			g BOD/ m^3
COD	51	9	g COD/ $m3$
CODf	38		g COD/ $m3$
SS	18	9	g/m ³
TKN	3.97	2	g N/m ³
NH ₄	1.79	2	g N/m ³
NO ₃	4.13	3	g $N/m3$
	2.23		qP/m^3

Table 3. Effluent measurement data during extensive measurement

5.3.2 Step 2: Determining a set of parameters subject to calibration

A range of parameters which are unknown or plant specific can be proposed a priori. These parameters are the most logical to change in the calibration procedure.

The reduction factors for anoxic acetate and phosphate uptake (ηHNO3 and ηPNO3) are considered to be plant and influent dependent. The experimentally obtained values were used as an indication, not as exact values since the experimental conditions in the lab might have been somewhat different than in the real plant. In the activated sludge models cell analysis is incorporated. This analysis is modelled such that it leads to generation of particulate substrate, which by a hydro analysis process is converted into soluble substrate. The substrate is then converted to biomass again by growth processes. Aside whether this proposed mechanism is correct or not, a good description of the activated sludge process is obtained [7]. Analysis of heterotrophic bacteria leads to new heterotrophic bacteria using this "death-regeneration concept". In ASM2d, however, analysis of autotrophic and phosphorus removing bacteria also leads to the creation of new heterotrophic biomass, instead of new respectively autotrophic and phosphorus removing bacteria. Pure and enriched culture experiments used to determine the analysis rates of PAOs and nitrifies (bPAO, bPP, bPHA and bAUT), will give different values as those which will have to be used in the model of the pilot plant. The value proposed by [8] or by [6] calculated

from a maintenance coefficient is indeed lower than suggested for ASM2d.

As such the rates for analysis of autotrophic and phosphorus removing bacteria are considered to be subject to changes during calibration procedures.

In the model, the hydro analysis process is assumed to be carried out by heterotrophic bacteria. However, the exact mechanisms are totally unknown. Since only heterotrophic bacteria are considered in ASM2d, the hydro analysis rate can be adjusted by changing the not known parameters for ηLNO3 and ηfe.

Oxygen concentration gradients in the reactors due to non homogeneous mixing will affect the overall observed conversions in the anaerobic and anoxic reactors. Floc internal oxygen gradients will also influence the process in the aerobic and anoxic compartments. These effects are compensated for by the 'affinity' and 'inhibition' constants for oxygen. This means that the parameters KHNO3 and KNO2 are process dependent and influenced by the type of flocs formed and the mixing intensity in the system. When a pilot plant is compared to a full scale possible changes in these affinity constants have therefore to be envisaged. The calibration was thus started taking the following parameters into account: ηLNO3, ηfe, ηHNO3, ηPNO3, bPAO, bPP, bPHA and bAUT (reduced set). A second calibration sequel was done incorporating KHNO3 and KNO2 (full set).

5.3.3 Step 3: Parameter adjustments

The calibration procedure is started by adjusting the nitrification kinetics to decrease the ammonia concentration. This can be achieved by decreasing the decay rate for nitrifiers (bAUT). Lowering the saturation coefficient for oxygen (KNO2) will also decrease the ammonia concentration. It was found that adjusting the nitrification kinetics had little impact on the concentrations for nitrate and phosphate.

The next step in the calibration procedure consisted of adjusting the denitrification kinetic

Table 4. Summary of calibration results using ASM2d default values

	$SNH4$ (mg N/)			$SNO3$ (mg $N/$)		SPO4 (mg N/)		
low	0k	high	low	οĸ	high	low	οĸ	high
		2.99	0.63			14		

parameters. Decreasing the saturation/inhibition coefficient for nitrate (KHNO3) is one way of decreasing the nitrate concentration. In ASM2d denitrification can be performed by heterotrophic as well as phosphorus removing bacteria. So, reducing denitrification, as was necessary in this case, can also be obtained by lowering the available COD amount. This was achieved by decreasing the hydro analysis rate. However, decreasing the available COD also has an impact on the phosphate removal capacity of the plant. As such, starting with adjusting denitrification, necessitated the simultaneous adjustment of the parameters for phosphorus removal. Where initially the effluent phosphate concentration was too low, this shifted while adjusting for the effluent nitrate concentration.

To increase the effluent nitrate concentration the reduction factor for Denitrification (ηHNO3) was decreased and hydro analysis was lowered by decreasing the reduction factors for hydro analysis (ηLNO3, ηfe).

Finally, to increase phosphorus removal, the rates for analysis of XPAO, XPP and XPHA (bPAO, bPP and bPHA) were decreased. From own experimental evidence it was found indeed that the reduction factor for anoxic activity of the PAOs should be lowered. The value was changed in approximately the same way as the other reduction parameters in the model.

In Table 5 and Table 6 the initial and final parameters are given along with the resulting effluent concentrations for both calibration exercises.

Calibration efforts should preferable result in as few parameters to be changed as possible. Indeed, changing many parameters will probably always lead to a set of values giving satisfactory results. For interpretation reasons and to facilitate the comparison between results of different authors, a selected set of parameter adjustments is to be preferred. As such the reduced set of parameters was chosen for the model to be used in testing upgrading scenarios. In Fig. 1 the dynamic concentration profiles in the intermittent reactor and for the effluent are shown for this set of parameters.

Table 5. Effluent prediction by the calibrated model

SNH4 (mg N/) SNO³ (mg N/) SPO⁴ (mg N/) low ok high low ok high low ok high

Fig. 1. Dynamic concentration profiles in the anoxic/aerobic reactor and in the influent

	LNO3	l fe	HNO3	PNO3	- 1 bPAO (d-1)	bPP (d-1)	bPHA bAUT (d-1)	(d-1)	KHNO3 (gN m-3)	KNO ₂ $(qO2 m-3)$
ASM _{2d} full set reduced set	0.60 0.25 0.25		$0.40\quad 0.80$ $0.15 \quad 0.20$ $0.15 \quad 0.26$	0.60 0.20 0.20	0.20 0.03 0.069	0.20 0.03 0.069	0.20 0.03 0.069	0.15 0.1175 0.2 0.065	0.5 ASM _{2d}	0.5 0.2 ASM _{2d}

Table 6. Summary of calibration parameters

1 the temperature dependence of these parameters as suggested in ASM2d is not changed, only the constant

6. DISCUSSION

The number of parameters involved in the ASM2d along with its non-linear character cause identification problems if a straightforward systems engineering approach is used with a reasonable and cost-effective measuring campaign. For ASM1 with its lower number of reactions taken into account, many authors have investigated through sensitivity analysis which parameters are the most sensitive. Indeed, when a parameter is known to be very difficult to assess through experimental procedure, investing time and money to obtain more reliable values for it is rather senseless when its value has little impact on the simulation results.

From theoretical sensitivity analyses YH, bH, YA, and bA often are reported along with µA and ηg (phosphorus removal is not taken into account in ASM1, so parameters connected to these reactions are not encountered) [9]. Calibration efforts using data from real wastewater treatment plants revealed somewhat different results, meaning that the yield coefficient does not appear to be as important, but µA, µH and KS remain to be important [10]. It should, however, be remembered that the degree of sensitivity is system specific.

The heuristic calibration method used in this study reveals differences compared to the above mentioned results. It was decided from the beginning to use a 'knowledge based' approach rather than a 'black box' approach as e.g. in most

parameter sensitivity studies[11]. It was decided e.g. not to change Y and μ values, considering these values as properly known. A limited set of parameters to be adjusted to obtain satisfactory simulations results was found. It is unclear why in this treatment plant the reduction factors are relatively low. It could be that this was due to some operational conditions, like a relatively high oxygen input in the anaerobic reactor, or a direct feeding of 989anaerobic effluent in the aerobic reactor [12]. All other parameter changes are in accordance with prior experimental evidence or understanding of the model [13].

6.1 Importance of Reactions in Settler

Simulations were performed to evaluate the influence of an increased residence time in the settler. To this end the size of the virtual anoxic basin was increased from 0 to 1.75 m³. From Table 7it can be seen that the size of this reactor indeed has an important impact on the overall results [14]. Due to the increased size of the reactor fewer nitrates is returned to the inlet of the anaerobic reactor, leaving more COD available for the phosphorus removing bacteria [15]. Hence, an increased phosphorus removal capacity is obtained. The effluent nitrate concentration decreased as well. For further calibration purposes, measurement of at least nitrate in the return flows could be considered. This is an important factor when pilot plant data are used for evaluating the full scale operation [16].

Fig. 2. Influent oxygen concentrations (mg O2/l)

6.2 Oxygen Entering the Plant via the Influent

During calibration the importance of oxygen entering the plant was noticed [17]. Initially it was suggested that no oxygen entered the plant. This working hypothesis was checked in practice and turned out to be invalid: influent concentrations were on average 4 mg O2/ l.

This higher oxygen level is due to the aeration action of the influent screw pumps and an aerated grit chamber [18]. In Table 8 the simulation results are given when different inlet oxygen concentrations are considered. From the results it is shown that phosphorus removal increases with decreasing influent oxygen [19]. It is clear that the effect is of such importance that a good measurement of this value is required in a model calibration campaign. Therefore it needs to be evaluated when predictions for the full scale plant are made [20].

Fig. 3. Virtual reactor size (m3)

In Fig. 2 and Fig. 3 the influence of influent oxygen and of the virtual anoxic reactor size on the effluent concentrations are shown. Whereas the influence of the size of the virtual reactor is important on NH4, NO3 as well as PO4, the influence of oxygen penetrating the system via the influent is only noticeable on the effluent PO4 concentration.

7. CONCLUSIONS

It was shown that based on understanding of the model, parameter changed could be proposed leading to a limited set of adjustments necessary in the calibration procedure, allowing a relative quick calibration [20]. There are several aspects of importance when the model of a pilot plant is used for predicting the full scale behavior. These were in this study: (i) oxygen entering the treatment plant via the influent (ii) reactions occurring in the final clarifier, which may be accounted for by e.g. a virtual settler compartment (iii) mixing intensities which might

affect the values of the affinity/inhibition constants for oxygen [21].

Finally it could be that the relatively low reduction factor for anoxic reactions is due to anomalies introduced by the pilot plant set-up (e.g. relative large oxygen diffusion through the air/water interface in the anoxic phase). In general, higher reduction factors are found for full scale applications [22].

ACKNOWLEDGEMENTS

This work was financial supported by foundation Research Program of Damascus city of Syria, Damascus University research institute. The authors would like to thank all the collogues for analyzing and testing.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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