ASM1 LIMITATIONS FOR MODELING OF WASTEWATER TREATMENT PROCESSES#

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[#]This paper is dedicated to Professor Roman Modic on the occasion of his 90th celebration.

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Abstract

In modern wastewater reactor technology dynamic modelling proved to be a valuable tool for the simulation of wastewater treatment performance, especially in cases of problematic inflow characteristics and no optimal process conditions. Due to stringent EU legislation the Domžale-Kamnik WWTP of 200,000 PE is confronted with the need to upgrade the plant in the sense of nutrient removal.

As the full-scale plant is also subject to changing process conditions, a CSTR pilot plant of 15 liters was installed. The system was operated in the single sludge mode at the specified process conditions (temperature, dissolved oxygen, flow, recycle ratio), and was fed with artificial wastewater. The effluent composition (organic nitrogen, ammonium, nitrate, COD), some stoichiometric and kinetic parameters, and operation parameters of the pilot plant were determined in the laboratory by standard laboratory methods. These results served as input parameters for the calibration of the steady-state model based on real conditions according to IAWQ model No.1.

The dynamic response to a step disturbance of the input flow was measured and comparison between dynamic response of the calibrated ASM1 model and experimental data is represented. The disagreement between the experimental and by model predicted results can be explained with ASM1 limitations.

Introduction

Understanding, describing and predicting the dynamic behavior of the activated sludge process for removing carbonaceous and nitrogenous compounds from wastewater needs to account for a large number of reactions between a considerable number of components. In the past many different models were introduced and presented in the literature using different process kinetics and model components. To create a uniform model structure in 1987 the IAWQ Task Group on Mathematical Modelling introduced ASM1¹, which became a major reference for many scientific and practical projects, and describes all the necessary reactions and components. Many authors have reported

results of practical modelling according to ASM1 (simulations, determination of kinetic and stoichiometric constants)^{14,15,16}. Our aim was to set up a dynamic model based on ASM1 for a laboratory scale pilot plant and to obtain answer to two questions:

- 1. What is the reliability of the laboratory determined kinetic and stoichiometric constants compared to process parameters? In other words, which parameters should be chosen as calibration parameters?
- 2. Can the dynamic model based on ASM1, successfully calibrated at steady-state conditions, correctly predict the dynamic behavior of the activated sludge process at nonsteady-state conditions?

Experimental

The CSTR pilot plant of 15 liters including nitri-denitrification was operated at the following volumetric relations: anoxic stage Vanx = 5 L, oxic stage Vaer = 10 L, settler Vs = 5 L (Figure 1). It was runing for a few months under constant operating conditions (flow, recycle ratio, oxygen concentration, temperature,...).

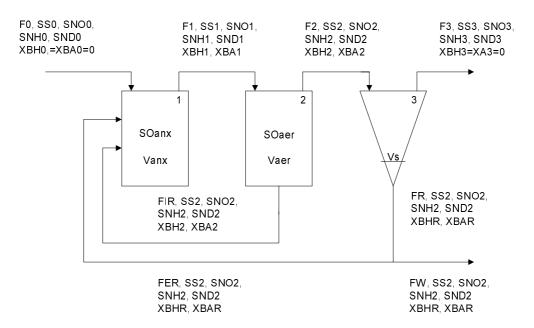


Figure 1: Scheme of the pilot plant

The pilot plant was fed with artificial wastewater of known chemical composition (yeast extract, meat extract, casein peptone, sodium acetate, ammonium chloride, potassium hydrogen phosphate, some inorganic compounds such us magnesium carbonate, sodium chloride, etc., and up to 20 vol % of settled municipal wastewater)^{10,11}. The chemical composition of the artificial wastewater is presented in Table 1.

Table 1: Artificial wastewater composition in the first and second experiment

Component	Unit	First experiment (17.629.9.1999)	Second experiment (10.517.5.2000)
COD	mg O ₂ /L	650	450
N-Kjel	mg N/L	65	65
N-NH ₄	mg N/L	20	45
N-org	mg N/L	45	20
Total phosphorus	mg P/L	6	6

At steady state conditions we analyzed the influent, effluent and the water of the anoxic and oxic reactor for the following compounds: COD (SS), ammonium nitrogen (SNH), Kjeldahl nitrogen (SNH + SND) and nitrate nitrogen (SNO) according to ISO standards. Influent and effluent were analyzed on daily average samples, anoxic, oxic stage and settler were analyzed on spot samples. Spot samples were also analyzed for MLSS, total COD and total N-Kjeldahl which served as an estimate of active heterotrophic (XBH) and autotrophic biomass (XBA). At the same time, we also determined the kinetic and stoichiometric constants using respirometry and batch tests^{1,5,7,8,9}. All these data were used in the model calibration.

After first stationary experiment (17.6.-29.9.1999) we performed second experiment (10.5.-17.5.2000) under different initial conditions. We measured and analyzed the same parameters and compounds as in the first experiment. These data served us for model verification. All experimental results are presented in Table 2.

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Table 2: Experimental results

First experiment (17.6-29.9.1999)

Second experiment (10.5.-17.5.2000)

	(1	7.6-29.9.1999)		(10.	<u>317.3.2000</u> ,	,	
			Day: 1	2	3	5	7
Symbol	UNIT	I. STATIONARY STATE - Average value	II. STAT. STATE	II. STAT. STATE	1.DAY AFTER STEP FLOW CHANGE	3. DAY AFTER STEP FLOW CHANGE	5. DAY AFTER STEP FLOW CHANGE
F0	L/h	1.5 ± 0.1	1.47	1.44	2.75	2.5	2.5
FIR	L/h	3.9 ± 0.1	3.64	3.53	3.54	3.54	3.54
FR	L/h	1.5 ± 0.1	3.13	3.2	3.2	3.1	3.1
FW	L/h	0.017 ± 0.002	0.0125	0.0125	0.0125	0.021	0.021
XB1	mg CODc/L	5400	3038	3160	1626	2222	2716
XB2	mg CODc/L	5033 ±1180	2994	3130	1724	2250	2736
XBR	mg CODc/L	6869 ± 1728	4622	3980	6986	5490	5210
SS0+XS0	mg COD/L	689 ± 63	451	388	439	514	366
SS0	mg COD/L						
SS1	mg COD/L	48.6 ± 13.6	19.2	40.3	49.6	74	
SS2 = SS3	mg COD/L	33.4 ± 5.8	19.7	22.4	25.6	32.1	33.2
SNO0	mg N-NO ₃ /L	3.2 ± 0.6	0	0	0	0	0
SNO1	mg N-NO ₃ /L	0.3 ± 0.3	0.027	0.08	0	0	0
SNO2 = SNO3	mg N-NO ₃ /L	6.3 ± 2.1	10.2	10.7	9.15	8.42	9.6
SNH0	mg N-NH ₄ /L	20.7 ± 4.0	55.1	48.3	44.7	68.8	53.5
SNH1	mg N-NH ₄ /L	6.1 ± 0.9	9.83	7.64	20	29.6	35.5
SNH2 = SNH3	mg N-NH ₄ /L	0.6 ± 0.3	0.17	0.17	7.03	14.1	16.4
SND0+X ND0	mg N-org/L	46.5 ± 7.7	9.4	14.6	21.0	22.3	
SND0	mg N-org/L						
SND1	mg N-org/L	3.2 ± 1.9	1.2	2.4	2.3	4.2	
SND2 = SND3	mg N-org/L	2.6 ± 2.0	0.9	0.7	4.3	6.5	

Simulation model

A mathematical model was built up according to ASM1 for activated sludge, including nitrogen removal. For each reactor we wrote mass balance Equations (Equation 1 to 19) based on the known concentrations (SS, SNO, SNH, SND, XA, XH).

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Anoxic reactor:

$$Vanx \cdot \frac{dSS1}{dt} = F0 \cdot SS0 + (FIR + FER) \cdot SS2 - F1 \cdot SS1 - \frac{1}{YH} \cdot RHanx \cdot Vanx + PSI \cdot (bH \cdot XBH1 + bA \cdot XBA1) \cdot Vanx$$
(1)

$$Vanx \cdot \frac{dSNO1}{dt} = FO \cdot SNO0 + (FIR + FER) \cdot SNO2 - F1 \cdot SNO1 - \frac{1 - YH}{2,86 \cdot YH} \cdot RHanx \cdot Vanx$$
 (2)

$$Vanx \cdot \frac{dSNH1}{dt} = F0 \cdot SNH0 + (FIR + FER) \cdot SNH2 - F1 \cdot SNH1 - iNx \cdot RHanx \cdot Vanx + ka \cdot SND1 \cdot XBH1 \cdot Vanx$$
(3)

$$Vanx \cdot \frac{dSND1}{dt} = F0 \cdot SND0 + (FIR + FER) \cdot SND2 - F1 \cdot SND1 - ka \cdot SND1 \cdot XBH1 \cdot Vanx + PSI \cdot iNx \cdot (bH \cdot XBH1 + bA \cdot XBA1) \cdot Vanx$$
(4)

$$Vanx \cdot \frac{dXBH1}{dt} = FIR \cdot XBH1 + FER \cdot XBHR - F1 \cdot XBH1 + RHanx Vanx - bH \cdot XBH1 Vanx$$
 (5)

$$Vanx \cdot \frac{dXBA1}{dt} = FIR \cdot XBA1 + FER \cdot XBAR - F1 \cdot XBA1 - bA \cdot XBA1 \cdot Vanx$$
 (6)

Oxic (aerobic) reactor

$$Vaer \cdot \frac{dSS2}{dt} = F1 \cdot SS1 - (FIR + F2) \cdot SS2 - \frac{1}{YH} \cdot RHaer \cdot Vaer + PSI \cdot (bH \cdot XBH2 + bA \cdot XBA2) \cdot Vaer$$
(7)

$$Vaer \cdot \frac{dSNO2}{dt} = F1 \cdot SNO1 - (FIR + F2) \cdot SNO2 - \frac{1}{YA} \cdot RAaer \cdot Vaer$$
 (8)

$$Vaer \frac{dSNH2}{dt} = F1 \cdot SNH1 - (FIR + F2) SNH2 - iNx RHaer Vaer - \left(iNx + \frac{1}{YA}\right) \cdot RAaer Vaer$$
(9)

$$Vaer \cdot \frac{dSND2}{dt} = F1 \cdot SND1 - (FIR + F2) \cdot SND2 - ka \cdot SND2 \cdot XBH2 \cdot Vaer + PSI \cdot iNx \cdot (bH \cdot XBH2 + bA \cdot XBA2) \cdot Vaer$$
(10)

$$Vaer \cdot \frac{dXBH2}{dt} = F1 \cdot XBH1 - (FIR + F2) \cdot XBH2 + RHaer \cdot Vaer - bH \cdot XBH2 \cdot Vaer$$
 (11)

$$Vaer \cdot \frac{dXBA2}{dt} = F1 \cdot XBA1 - (FIR + F2) \cdot XBA2 + RAaer \cdot Vaer - bA \cdot XBA2 \cdot Vaer$$
 (12)

<u>Settler</u>

$$V_{S} \cdot \frac{dSS3}{dt} = F_{2} \cdot SS_{2} - F_{3} \cdot SS_{2} - F_{R} \cdot SS_{3}$$
(13)

$$V_{S} \cdot \frac{dSNO3}{dt} = F_{2} \cdot SNO_{2} - F_{3} \cdot SNO_{2} - F_{R} \cdot SNO_{3}$$
 (14)

$$V_{S} \cdot \frac{dSS3}{dt} = F_{2} \cdot SS_{2} - F_{3} \cdot SS_{2} - F_{R} \cdot SS_{3}$$
 (15)

$$V_{S} \cdot \frac{dSNH3}{dt} = F_{2} \cdot SNH_{2} - F_{3} \cdot SNH_{2} - F_{R} \cdot SNH_{3}$$
 (16)

$$V_{S} \cdot \frac{dSND3}{dt} = F_{2} \cdot SND_{2} - F_{3} \cdot SND_{2} - F_{R} \cdot SND_{3}$$
(17)

$$V_{S} \cdot \frac{dXBH3}{dt} = F_{2} \cdot XBH_{2} - F_{R} \cdot XBH_{R}$$
(18)

$$V_{S} \cdot \frac{dXBA3}{dt} = F_{2} \cdot XBA_{2} - F_{R} \cdot XBA_{R}$$
(19)

Process Rates (anoxic and aerobic growth of heterotrophs and autotrophs)

$$RHanx = MaxH \cdot \left(\frac{SS1}{KS + SS1}\right) \cdot \left(\frac{KOH}{KOH + SOanx}\right) \cdot \left(\frac{SNO1}{KNO + SNO1}\right) \cdot etag \cdot XBH1 \quad (20)$$

RHaer = MaxH
$$\cdot \left(\frac{SS2}{KS + SS2} \right) \cdot \left(\frac{SOaer}{KOH + SOaer} \right) \cdot XBH2$$
 (21)

$$RAaer = MaxA \cdot \left(\frac{SNH2}{KNH + SNH2}\right) \cdot \left(\frac{SOaer}{KOA + SOaer}\right) \cdot XBA2$$
 (22)

Flow rates

$$F1 = F0 + FIR + FR - FW \tag{23}$$

$$F2 = F1 - FIR \tag{24}$$

$$F3 = F2 - FR \tag{25}$$

$$FER = FR - FW \tag{26}$$

Active biomass concentration determined from total biomass concentration

$$XBH = fa (1-deNI) XB$$
 (27)

$$XBA = fa deNI XB$$
 (28)

Table 3: Experimental and modeled values for model parameters determined by the calibration of the first stationary condition at 20 °C.

Symbol of parameter	unit	Experimental value
Vanx	L	5
Vaer	L	10
Vs	L	5
SOanx	mg O ₂ /L	0.0
SOaer	mg O ₂ /L	5.5
F0	L/h	1.5
FIR	L/h	3.9
FR	L/h	1.5
FW	L/h	0.02
XB1	mg MLSS/L	4300
XB2	mg MLSS/L	4900
XBR	mg MLSS/L	6800
XBH1	mg COD/L	2846.2
XBA1	mg COD/L	425.3*
XBH2	mg COD/L	3243.3
XBA2	mg COD/L	484.6*
XBHR	mg COD/L	4500.9
XBAR	mg COD/L	672.5*
SS0	mg COD/L	689.4
SS1	mg COD/L	48.6*
SS2 = SS3	mg COD/L	33.4
SNO0	mg N-NO ₃ /L	3.2
SNO1	mg N-NO ₃ /L	0.3
SNO2 = SNO3	mg N-NO ₃ /L	6.3
SNH0	mg N-NH ₄ /L	20.7
SNH1	mg N-NH ₄ /L	6.1
SNH2 = SNH3	mg N-NH ₄ /L	0.6
SND0	mg N-org/L	46.5
SND1	mg N-org/L	3.2
SND2 = SND3	mg N-org/L	2.6

The model, rebuilt for steady-state operation, can now be used for calibration using appropriate numerical methods¹⁴.

Results and discussion

The sludge process variables (Table 3) and some laboratory determined kinetic and stoichiometric constants (Table 4) served as the input calibration parameters. Calibration was not possible even in the case when all stoichiometric and kinetic constants were free for calibration. For our experimental pilot plant activated sludge process with nitrogen removal included it was shown, that calibration based on the ASM1 model is successful only when some experimental data, namely the

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concentrations of active biomass and readily biodegradable substrate, together with some kinetic and stoichiometric constants were used as calibrated parameters. Those data are shown in Table 3, marked with an asterisk for process variables and in Table 4 for kinetic and stoichiometric constants.

This opens the question of the reliability of some of the analytical methods and the results for activated sludge process variables, especially the active concentration of biomass. On the other hand, the definition of kinetic and stoichiometric constants given by the ASM1 model cannot properly describe the activated sludge process – for example, the heterotrophic yield cannot be fixed as a constant for different reactors. The new concept of ASM3 confirmed our opinion ^{12,13}.

Table 4: Comparison of stoichiometric and kinetic constants determined experimentally, by calibration and presented by ASM1 at 20°C.

Symbol	Unit	experimentally determined	modeled	ASM1 ¹	
STOICHI	STOICHIOMETRIC CONSTANTS				
YH	mg CODc/mg COD	0,68	0,67	0,67 (0,46 - 0,69)	
YA	mg CODc/mg N		0,27	0,24 (0,07 - 0,28)	
iNx	mg N/mg CODc	0.04 - 0.08	0,1228 *	0,086	
fa		0,634	0,634		
deNI		0,13	0,008		
KINETIC	KINETIC CONSTANTS				
KS	mg COD/L	10 - 65	161,7	20 (10 – 180)	
КОН	mg O ₂ /L		0,2	0.2(0.01-0.15)	
KOA	mg O ₂ /L		0,4	0,4 (0,5 – 2)	
KNO	mg N/L		0,5	0,5 (0,1 – 0,2)	
KNH	mg N/L	1,0	1,0	1,0	
MaxH	1/h	0,22 - 0,38	0,0986 *	0,25 (0,125 - 0,55)	
MaxA	1/h	0,01	0,0377	0,032	
bH	1/h	0,007	0,00927	0,0258 (0,002 - 0,067)	
bA	1/h		0,00616	0,0021 - 0,0063	
ka	L COD/mg.h		0,0003 *	0,0033	
etag			0,07 *	0.8(0.6-1)	

Legend: * - the calibrated value is very different from the value given in the literature

On the basis of the calibration described, the calibrated parameters for steady-state operation of the activated sludge process were used for process simulation based on the dynamic model equations (Equations 1-18).

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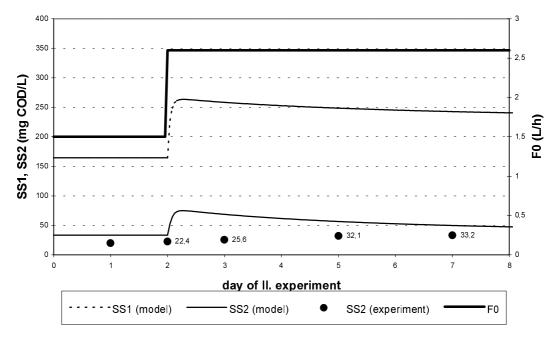


Figure 2: Dynamic model prediction of COD concentration in the anoxic (SS1) and oxic reactors (SS2) compared with experimental data

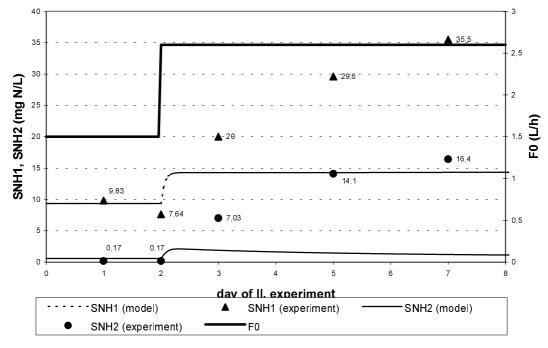


Figure 3: Dynamic model prediction of ammonia concentration in the anoxic (SNH1) and oxic reactors (SNH2) compared with experimental data

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The comparison between experimental and dynamic model response on the step change of the influent flow are presented in Figures 2 and 3. It can be seen that the dynamic model predictions are not in good agreements with the experimental data. Reasons for that could be part of the ASM1 limitations. Although the calibrated ASM1 model can be proved for the steady state operations, the dynamic simulations based on IAWQ model No.1 are questionable. The model, already most parametric sensitive, ¹⁴ anticipates that kinetic and stoichiometric parameters are constants for the aerobic nitrification and anoxic denitrification step. Setting up a new model configuration according to the ASM3 model can solve some of these problems. On the other hand, we have to take into consideration the problems of reliability of experimental results. We should emphasize the difficulties in determing the concentrations of active heterotrophic and autotrophic biomass and the correctness of some kinetic and stoichiometric constants used in the model simulation, which are determined in the laboratory under different process conditions.⁸

Conclusions

A mathematical model was built up according to ASM1 for wastewater treatment process taking place in the pilot wastewater treatment plant including nitrogen removal. The model was successfully calibrated for the steady-state operational conditions and the calculations of the dynamic response on the step change of the influent flow were compared with the experimental data. The deviating between predicted and experimental results was explained with ASM1 limitations and with possible problems of reliability of experimental values. Parameters, the quantities that go alongside the problem, cannot but be lumped, because, were they not, they would have to be treated as variables.

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Symbols

Symbols	,	
Symbol	Unit	Name
bA	1/h	Decay coeff. for autotrophic biomass
bH	1/h	Decay coeff. for heterotrophic biomass
deNI	-	Fraction of autotrophic biomass
etag	-	Correction factor for MaxH under anoxic conditions
etah	-	Correction factor for hydrolysis under anoxic conditions
F	L/h	Volumetric flow
fa	-	Active fraction of the biomass
iNx	mg N/mg CODc	Mass N/mass COD in biomass
ka	L COD/mg.h	Ammonification rate
KNH	mg N/L	Ammonia half-saturation coeff. for autotrophic biomass
KNO	mg N/L	Nitrate half-saturation coeff. for heterotrophic biomass
KOA	$mg O_2/L$	Oxygen half-saturation coeff. for autotrophic biomass
KOH	$mg O_2/L$	Oxygen half-saturation coeff. for heterotrophic biomass
KS	mg COD/L	Half-saturation coeff. for heterotrophic biomass
MaxA	1/h	Max. specific growth rate for autotrophic biomass
MaxH	1/h	Max. specific growth rate for heterotrophic biomass
SND	mg N/L	Soluble organic-N concentration
SNH	mg N/L	Ammonia-N concentration
SNO	mg N/L	Nitrate-N concentration
SO	$mg O_2/L$	Dissolved oxygen concentration
SS	mg COD/L	Readily biodegradable (soluble) substrate concentration
Vaer	L	Volume of aerobic – oxic reactor
Vanx	L	Volume of anoxic reactor
Vs	L	Volume of settler
XB	mg CODc/L	Total biomass concentration in COD units
XBA	mg CODc/L	Active autotrophic biomass concentration in COD units
XBH	mg CODc/L	Active heterotrophic biomass concentration in COD units
YA	mg CODc/mg N	Autotrophic yield
YH	mg CODc/mg COD	Heterotrophic yield

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Povzetek

Dinamično modeliranje procesov čiščenja odpadnih vod se je uveljavilo kot zelo uporabno urodje pri načrtovanju in optimiranju čistilnih naprav ter pri razumevanju kompleksnih procesov čiščenja. Še posebno se uporabnost modeliranja iskaže pri odpadnih vodah zahtevnejših karakteristik in pri ne-optimalnih procesnih pogojih. Stroga zakonodaja Evropske skupnosti in velika vsebnost dušika v odpadni vodi narekujeta nadgradnjo čistilne naprave Domžale-Kamnik z 200,000 PE. V ta namen potekajo študije nitrifikacije in denitrifikacije na pilotni dvostopenjski čistilni napravi, ki vsebuje 5 L anoksični in 10 L aerobni standardni mešalni reaktor ter 5 L usedalnik. Pilotno napravo, ki omogoča spremljanje in nadzor procesnih pogojev (temperatura, raztopljeni kisik, pretok, recikel), smo v našem primeru napajali z umetno odpadno vodo. Vrednosti procesnih spremenljivk med procesom čiščenja (organski dušik, amonijak, nitrat, KPK) in nekaterih stohiometričnih in kinetičnih parametrov smo določili s standardnimi laboratorijskimi metodami. Te rezultate smo uporabili pri kalibraciji s stacionarnim matematičnim modelom, razvitim po ASM1.

Uspešno kalibriran in potrjen model za stacionarno obratovanje smo potem uporabili za napoved dinamičnega odziva pilotne čistilne naprave na stopenjsko motnjo vstopnega toka. Primerjava med eksperimentalnimi rezultati in matematično napovedjo je pokazala na omejitve ASM1 modela.