Effects of biomass characterization in computer simulation of BNR processes

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Abstract
Accurate characterization of activated sludge biomass stoichiometric and kinetic parameters is necessary for successful computer simulation of biological nutrient removal (BNR) processes. The simulation research have been performed to test the sensitivity of the model BNR plant to the selected parameters. The purpose was to practically identify and quantify those parameters that have the most effect on the model accuracy and that require much attention during model calibration and those that can be left at their default values or be only roughly calibrated. The focus on the most important parameters during model calibration may allow to shorten time used for model calibration and to increase model accuracy. The results have been presented in form of a matrix that indicates relative effect of specific parameters in the model and can be used as a simple tool for pre-selecting the parameters for further calibration.
Keywords Computer simulation, activated sludge, biomass, model parameters

INTRODUCTION

Computer simulation of biological nutrient removal (BNR) processes requires accurate characterization of influent wastewater and activated sludge biomass. Organic material oxidation, nitrification, denitrification and biological enhanced phosphorus removal are carried on by several groups of microorganisms and require different operational conditions that sometimes are contridactory each to the other. Setting the values of kinetic and stoichiometric parameters for each microorganism group during model calibration is a complex, time consuming and expensive procedure that usually require performing respirometric tests and series of analytical measurements. This procedure may and often even should be keep as simple as possible in order to make the simulation research practical, effective and inexpensive.

Model calibration for BNR processes focuses on the three microorganisms groups: autotrophes, heterotrophes, and phosphorus accumulating organisms (PAO) that sometimes are named P-heterotrophes. Theses microorganisms are characterized with different kinetic and stoichiometric parameters. The values of some parameters are relatively constant at different plants and they are often set based on literature review, comparative studies or kept at default values as proposed by simulation software. On the other hand the values of other parameters are highly varying among the plants as they are very sensitive to specific operational conditions and they have to be set individually for each investigated plant.

In order to simplify the model calibration procedure the simulation research has been performed to test the sensitivity of a sample BNR plant to the variations in the most important kinetic and stoichiometric parameters that are usually set during model calibration. The results of research presented in this paper in any case should not be taken as a definite rule for selecting or omitting any specific parameter during model calibration but only as an indication about a model sensitivity to some model parameters.

METHODS

A sample BNR process simulation model comprising influent, biological reactor configured according to Johannesburg scheme with recirculation and a secondary clarifier was defined with GPS-X v. 5.02 software during the research. The biological reactor used ASM 2d model. The clarifier was modeled as non-reactive simple one-dimensional model. The influent composition was based on *tsscod* model. The influent flow and composition as well as starting operational parameters used during the research are presented in Table 1.

Table 1. Influent characteristics and initial operational parameters used during the research.

		Units	Value
Influent	Flow	m^3/d	5,000
	COD	gO_2/m^3	480
	TSS	g/m^3	400
	TKN	gN/m^3	40
	NOx	gN/m^3	1
	PO4	gP/m^3	10
Operational parameters	MLSS	g ds/m3	3,500
	SRT	days	9,6
	HRT	hours	18,2
	Internal recirculation	%	200

The parameters investigated during the research included most of typical kinetic and stoichiometric ones that are usually calibrated or set during simulation research such as growth and decay rates, half saturation constants, yield coefficients, and some others that are typical for specific microorganism groups. The detail list of investigated parameters is presented in Table 2. Typical values are those used in ASM2d model (Henze 1999) or the default values proposed in the simulation software. The range of values tested has been decided based on values proposed in technical reports on activated sludge models or on personal experience from many years of performing computer simulations at different plants.

Table 2. The parameters selected for investigation and the range of values tested

Parameter	Unit	Typical value in ASM2d	Range tested
Biomass COD/VSS	gCOD/g	1.48	1.26÷1.70
N conent of active biomass	gN/gCOD	0.07	0.06÷0.08
P conent of active biomass	gP/gCOD	0.02	0.015÷0.025
Autotrophic yield	gCOD/gN	0.24	0.07÷0.28
Autotrophic specific growth rate	d^{-1}	1.0	0.5÷1.5
Autotrophic decay	d^{-1}	0.15	0.05÷0.20
Half saturation coefficient for ammonium	gN/m^3	1.0	0.5÷2.0
Heterotrophic yield	gCOD/gCOD	0.625	0.460÷0.690
Heterotrophic specific growth rate	d^{-1}	6.0	3.0÷13.2
Heterotrophic decay	d^{-1}	0.4	0.1÷1.6
Heterotrophic half saturation coefficient for VFA	$gCOD/m^3$	4.0	1÷10
PAO yield	gCOD/gCOD	0.625	0.460÷0.690
PAO specific growth rate	d^{-1}	1.0	0.67÷1.6
PAO decay	d^{-1}	0.2	0.1÷0.3
PAO half saturation coefficient for VFA	$gCOD/m^3$	4.0	1÷10

RESULTS

The research allowed to identify the parameters that have the most important effect on operation and effluent quality of the model plant. There are few such parameters for organic material oxidation, nitrification, denitrification and enhanced P removal. Identification of the relationships between changes in some specific parameters and plants operation and effluent quality is not simple and easy as the processes in the reactor are integrated in the reactor. In details the following effects of individual tested parameters have been identified:

Biomass COD/VSS

Biomass COD/VSS ratio can be easily calculated from theoretical formula $C_{60}H_{87}O_{23}N_{12}P$ assuming complete oxidation to carbon dioxide and water. This theoretical value is 1.42 gCOD/g (Melcer *et al.*, 2003). However in practice the COD/VSS ratio may be somewhat different from its theoretical value. With some relatively simple analytical measurement it can be easily calculated with the following equation (1):

$$\text{COD/VSS}=\frac{COD/VSS = MixedLiquorUnfilteredCOD - EffluentFilteredCOD}{MixedLiquorVSS} \quad (1)$$

The performed simulations showed that the simulation results are not very sensitive to changes in the this parameter value. The variable affected the most by this parameter is MLSS and consequently effluent VSS/TSS and effluent BOD.

N content of biomass (i_{XN})

The theoretical value of this stoichiometric coefficient is 0.086 gN/gCOD. In practice this value is smaller as inert particulate products usually contain less nitrogen than active biomass (Henze 1987). The ASM2d model proposes value of 0.07 gN/gCOD (Henze 1999). The research has shown that simulation results are sensitive to this parameter. Even small inaccuracy in setting its value may especially affects the concentration of orthophosphates in effluent and thus it is important the its value was set correctly in the systems that model phosphorus removal. However if this value is not measured for a specific case it is recommended to keep it at its default vale.

P content of biomass (i_{XP})

This stoichiometric coefficient may also be easily calculated from the above presented theoretical formula $C_{60}H_{87}O_{23}N_{12}P$ as 0.02 gP/gCOD and this value is used as default in ASM2d (Henze 1999). This parameter's value strongly affects concentration of orthophosophates in effluent. If this value is not analytically measured for a specific case it is recommended to keep it at its default vale.

Autotrophic yield (Y_A)

This a composite value for the combined growth of *Nitrosomonas* and *Nitrobacter* under aerobic conditions. Although there are different values cited in the literature the theoretical value is 0.24 gCOD/gN and this value is used in ASM2d by default (Henze 1987, 1999). despite that the above value seems to be very constant for various plants the sensitivity of the system have also been tested for this parameter. It is not surprising that variables the most sensitive to this parameter are those related to nitrification process: effluent ammonia and autotrophic biomass. However value of autotrophic yield also strongly affects orthophosphate concentration in effluent. This parameter should be kept at its default value if no detail information is available for the specific plant.

Autotrophic specific growth rate (μ_A)

This is an essential parameter for nitrification – its value highly varies among the plants and it must be very carefully measured in each case. This value is associated mostly with *Nitrosomonas* bacteria as process limiting microorganisms in nitrification process (Henze 1987). There are two methods of estimating μ_A value: (i) with bioassays at low and high F/M and with computer simulation (ii) by matching the dynamic activated sludge model's response to experimental observations. These methods are detail described in literature (Melcer *et al.*, 2003).The μ_A was tested in the range from 0.5 to1.5 during the research. Its value affects the nitrification process and extremely strongly the effluent ammonia concentration and somehat less the autotrophic biomass concentration and effluent nitrate concentration. Other variables that are very sensitive to μ_A value however in the indirect way are soluble BOD orthophosphates in effluent.

Autotrophic decay rate (b_A)

This parameter is difficult to accurate and reliable measure however there are some methods to presented in the literature (Melcer *et al.*, 2003). In most cases this parameter 's value may be assumed. The typical value of b_A in ASM2d is 0.15 d^{-1}. The performed simulations showed strong relationship between the bA value and effluent ammonia concentration and autotrophic biomass concentration. Other parameters are not or little affected by autotrophic decay rate value.

Half saturation coefficient for ammonia (K_{NH4})

This coefficient affects the nitrification process and in each case should be determined with analytical methods with use of fed-batch reactors (Henze 1987). Its value has been set at 1 gN/m3 in ASM2d. The sensitivity analysis has shown that changes in KNH4 value strongly affect effluent ammonia concentration and much less other nitrogen forms.

Heterotrophic yield (Y_H)

The typical value of heterotrophic yield in activated sludge models is 0.666 gCOD of biomass per gCOD utilized (Melcer *et al.*, 2003). Under anoxic conditions the Y_H value is reduced and this is represented by the appropriate reduction factor incorporated in the model. In the ASM2d the Y_H value is set at 0.625 gCOD/gCOD as default. This parameter's value is relatively constant but if possible Y_H value should be measured in individual cases. This can be relatively easily done by observing the mass of cell material formed during removal of soluble substrate in a lab test. The simulations have shown that heterotrophic yield value affects many variables in the activated sludge system. Its effect is strong on effluent orthophosphates and TP, and to smaller extent on heterotrophic biomass and effluent BOD. Other parameters are less sensitive to changes in Y_H value.

Heterotrophic specific growth rate (μ_H)

Also this parameter is relatively constant from case to case but should be measured whenever possible however this is not easy. The measurement should be based on respirometric prediction of the maximum OUR and specific procedures for this is in detail presented in literature (Henze 1987, Melcer *et al.*, 2003). The default value of μ_H in ASM2d is set at 6 d^{-1}. The results of sensitivity analysis show that μ_H the most affects effluent orthophosphates and soluble BOD. It effect on other parameters such as herterotrophic and PAO biomass is much smaller.

Heterotrophic decay rate (b_H)

This parameter is very important to predictions of sludge production and oxygen requirements (Henze 1987). Its value can be relatively easy measured in a laboratory batch test. In the ASM2d model it is set at value of 0.20 d^{-1}. The performed simulations showed that b_H value much affects heterotrophic biomass concentration and effluent soluble BOD.

Half saturation coefficient for VFA (K_{HVFA})
This coefficient is relatively constant from case to case in integrated biological reactors and often it does not require detailed calibration. Its default value in ASM2d is 4 $gCOD/m^3$. Its value affect orthophosphates and BOD in effluent. It also has some effect on PAO biomass concentration and nitrates and TN in effluent.

PAO yield (Y_{PAO})
PAO yield coefficient in ASM2d is the same under both aerobic and anoxic conditions despite that bioenergetically, the anoxic yield should be reduced compared to the aerobic yield (Zhi-rong 2003). This parameter may be calibrated by using observed phosphate concentrations in effluent from the anaerobic tank. The default value is 0.625 gCOD/gCOD. The variables that are highly sensitive to Y_{PAO} value are effluent orthophosphates and TP and also PAO biomass.

PAO specific growth rate (μ_{PAO})
Also this parameter is relatively constant from case to case. If possible this parameter should be calibrated with OUR tests. However, if this is not possible then it should be kept unchanged unless it is necessary for the calibration. In the ASM2d the default value is 1.0 d^{-1}. The PAU growth rate extremely strongly affects the phosphorus removal process and in particular effluent orthophosphate and TP concentrations.

PAO decay rate (b_{PAO})
The decay rate of PAO is significantly smaller that this for other heterotrophic bacteria. In the ASM2d model it is set at 0.2 d^{-1} as default. Its value significantly affects effluent orthophosphate and TP and also PAO biomass and effluent ammonia concentration.

Half saturation coefficient for VFA (K_{PAOVFA})
This coefficient is relatively constant from case to case in integrated biological reactors. Often the detailed calibration is not needed. Its default value in ASM2d is 4 $gCOD/m^3$. Phosphorus removal process is very sensitive to changes in this parameter. This especially applies to effluent orthophosphate and TP and also PAO biomass and effluent ammonia concentration.

The overall sensitivity of the integrated BNR process to the selected parameters can be presented quantitatively as shown in Fig. 1. The rows represent the kinetic and stoichiometric parameters that are usually calibrated during simulation research while the columns represent plants operational parameters and effluent characteristics that are affected by kinetics and stoichiometric parameters' values. Numbers in individual cells represent the relative effect of a change in specific parameters value (in percent) in relation to typical default value used in ASM2d. In addition the strength of the response is represented by colour of a cell—the darker colour the stronger response. If the relative change in the plants operational parameter was smaller the 3 percent the cell was left blank and the effect of such kinetic or operational parameter was considered as negligible.

It can be seen from the matrix that organic material oxidation process is the most sensitive to μ_H, b_H, K_{HVFA}; nitrification process to μ_A, K_{NH4}, b_A, Y_A; denitrification to: μ_A, K_{NH4}, b_A, Y_A; and enhanced phosphorus removal to μ_{PAO}, K_{PAOVFA}, b_{PAO}, Y_{PAO}, μ_H, Y_H. The enhanced P removal process is strongly affected by majority of the tested parameters. It is not surprising as the process is complex and requires changing operational conditions. Nitrification is extremely sensitive to autotrophic growth rate and much attention must be paid to setting value of this parameter during calibration. Heterotrophic decay rate is another parameter that must be set very carefully as it affects organic material oxidation and denitrification process.

VARIABLES

PARAMETERS	MLSS	VSS/ TSS	XAUT	XH	XPAO	COD	SCOD	BOD5	SBOD5	TN	SNH	NOx	TP	SPO4	
XCOD/ VSS	-12	-19						8							XCOD/ VSS
iXN												-4		-41	iXN
iXP														-69	iXP
YA			76							3	79		-16	-32	YA
μA			69	17	-42			-8	-82	-225	-4420	86	48	97	μA
bA			-81							14	258	-4	7	16	bA
KNH4										15	296	-6			KNH4
YH	13	19		45	13	3		22		-6		-8	-164	-322	YH
μH				14	-33			-19	-238				196	398	μH
bH	-16	34	19	-164	-53	7	4		461						bH
KHVFA					18			78		16		20	-119	-240	KHVFA
YPAO					-33								217	438	YPAO
μPAO	-6	6			7								508	1030	μPAO
bPAO	-7	-2		16	-93			-11		0	-59	5	308	613	bPAO
KPAOVFA	10				56			9		-1	44	-5	-493	-995	KPAOVFA
	MLSS	VSS/ TSS	XAUT	XH	XPAO	COD	SCOD	BOD5	SBOD5	TN	SNH	NOx	TP	SPO4	

Fig. 1 The matrix of simulated relative effect of changes in individual parameters on operational and effluent parameters in the model plant in relation to default parameters' values (in percent).

CONCLUSIONS

The simulation research on a model BNR plant allowed to identify the parameters that are the most important for successful calibration of a integrated nutrient removal process. The results show that the following parameters should be especially carefully calibrated as the BNR model is especially sensitive to their values: μ_A, μ_{PAO}, K_{PAOVFA}, b_{PAO}, b_H, Y_{PAO}, μ_H, Y_H, K_{NH4}, b_A, and K_{HVFA}. The values of many other parameters must also be set very carefully during model calibration as their effect on model quality is significant. The model sensitivity matrix (Fig. 1) that has been developed with use of simulation results may be helpful to identify the parameters that more and less important for the BNR process modeling. It indicates the parameters that require much attention during calibration and must be set with very high accuracy and the parameters that at least during preliminary model calibration can be easily left at their default values. However it must be noted the due to the limited scope and simple methodology of the research that the information from the matrix should not be taken as a definite rule for selecting or omitting any specific parameter during model calibration but only as an indication about a model sensitivity to some model parameters.

REFERENCES

Hu Z., Wentzel, M. C. and Ekama G. A. (2003) Modelling biological nutrient removal activated sludge systems—a review Water Research, Volume 37, Issue 14, Pages 3430-3444

Jeppsson U. (1996) „Modelling Aspectes of Wastewater Treatment Processes". Doctoral dissertation. Lund Institute of Technology, Department of Industrial Electrical Engineering and Automation, Lund, Sweden.

Henze, M., C. P. L. Grady Jr., W. Gujer, G. v. R. Marais and T. Matsuo (1987). Activated sludge model no. 1. Scientific and Technical Report No. 1. IAWPRC, London.

Henze, M., W. Gujer, T. Mino, T. Matsuo, M. C. Wentzel and G. v. R. Marais (1995b). Activated sludge model no. 2. Scientific and Technical Report No. 3. IAWQ, London, Great Britain.

Henze M, Gujer W, Mino T, *et al*. (1999) Activated sludge model No. 2d, ASM2D [J]. Water Sci Technol, 39(1): 165–182.

Liu J. , Zou L. Stoichiometric deduction of activated sludge process for organic carbon and nitrogen removal, J Shanghai Univ (Engl Ed), 2009, 13(1): 88–94

Melcer H, Dold P., Jones, R.M., Bye C.M., Takacs I. *et al.* (2003) Methods for water characterization in activated sludge modeling, Water Environment Research Foundation, Alexandria, VA, USA

Watson B. *et al.* (1994) Modelling of Full-Scale Wastewater Treatment Plants: How Detailed Should It Be? *Wat.Sci.Tech*., 30(2), 141-147.