Activated Sludge Modelling: Development and Potential Use of a Practical Applications Database

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Abstract

This study aims at synthesizing experiences in the practical application of ASM type models. The information is made easily accessible to model users by creating a database of modelling projects. This database includes answers to a questionnaire that was sent out to model users in 2008 to provide inputs for a Scientific and Technical Report of the IWA Task Group on *Good Modelling Practice – Guidelines for use of activated sludge models*, and a literature review on published modelling projects.

The database is analysed to determine which biokinetic model parameters are usually changed by modellers, in which ranges, and what values are typically used for seven selected activated sludge models. These results should help model users in the calibration step, by providing typical parameter values as a starting point and ranges as a guide. However, the proposed values should be used with great care since they are the result of averaging practical experience and not taking into account specific parameter correlations.

Keywords

Good modelling practice; ASM; Database; Parameter sets; Parameter ranges; Survey

INTRODUCTION

The International Water Association (IWA) Task Group on *Good Modelling Practice – Guidelines for use of activated sludge models* (GMP-TG, https://iwa-gmp-tg.cemagref.fr/) is collecting knowledge and experience on how to use activated sludge (AS) models in engineering practice. The group developed and sent out a first questionnaire to current and potential users of activated sludge models. Ninety-six answers were received that provided useful insights into the use of activated sludge models and highlighted the main limitations of modelling and the expectations of users for improvements (Hauduc *et al.*, 2009). The calibration step was pointed out especially as one of the most time-consuming steps (28% of modelling projects) and is considered as an obstacle for widespread model use (24% of respondents). Half of the respondents also asked for better knowledge transfer.

A second, more detailed, questionnaire was sent out in 2008 to provide inputs for the GMP-TG report such as typical parameter values and case studies from several countries and for different wastewater treatment conditions. In addition and as a second source of information, a literature review was carried out on published modelling projects. The objective of this work was to collect available experiences of practical applications using AS models. A database was therefore constructed to synthesise the answers from the second questionnaire and literature data.

The proposed database includes parameters for seven published activated sludge models: (1) ASM1 (Henze *et al.*, 2000a); (2) ASM2d (Henze *et al.*, 2000b); (3) ASM3 (Gujer *et al.*, 2000); (4) ASM3+BioP (Rieger *et al.*, 2001); (5) ASM2d+TUD (Meijer, 2004); (6) Barker & Dold model (Barker & Dold, 1997); (7) UCTPHO+ (Hu *et al.*, 2007). In order to keep this paper readable, these references will not be repeated each time. The database was analysed to extract as much information as possible in terms of current modelling practice: changed parameters, protocol used and parameter value ranges. Results were further compared to published ranges of parameters.

METHOD

Source of data

Questionnaire. In order to completely describe each modelling study, the questionnaire asked for the objectives of the project, the wastewater treatment plant (WWTP) description and the parameter set used for the biokinetic model. It was sent out in 2008 to the respondents of the first survey (Hauduc *et al.*, 2009), to the attendees of the WWTmod2008 seminar (1st IWA/WEF Wastewater Treatment Modelling Seminar, Mont-St-Anne, Québec, Canada), and it could also be downloaded from GMP-TG sponsor websites.

Probably due to the higher complexity of this questionnaire, only 28 answers were received, among which 18 were usable for this study (i.e. at least one biokinetic model parameter set provided for one of the studied models).

Literature review on published modelling projects. In order to have a homogeneous database that allows comparison of modelling projects, only modelling projects applied to full-scale municipal WWTPs or industrial pilot plants with a major domestic wastewater influent were selected. The review includes 50 articles containing 59 parameter sets.

Database description

Structure. In order to store all the information gathered through the questionnaire and the literature review in an efficient way, a database composed of three main tables was constructed:

1. **Parameter sets** (Main table): model, country, temperature, parameter values
2. **WWTP description**: information on influent, wastewater characteristics, processes and environmental conditions
3. **Model users**: information on the modellers

To limit the number of fields in the parameter sets table, the parameters of all models were renamed with the standardised notation of Corominas *et al*. (2010), therefore allowing the parameters that are similar between models to be gathered.

Classification of parameter sets. Two classes of model parameter sets were distinguished:

- **Optimised parameter sets** obtained for a specific modelling project. These parameter sets were provided with the description of the WWTP under study.
- **Proposed new default parameter sets** from the experience of the modellers conducting the study. Proposed new default parameters values were used as starting points for the calibration step during the project. These parameters were given with an approximate number of WWTPs on which this experience was gained.

Sources of parameter values. According to the way it was obtained, a parameter value could be qualified as:

- **Original**: when the value is set to the value given in the original publication of the model;
- **New Default**: when the value is set to the value given in a proposed new default parameter set;
- **Measured**: when the value is obtained using a dedicated experimental protocol;
- **Calibrated**: when the value is changed either using a manual or an automatic procedure to fit the data collected on the WWTP.

Temperature adjustment. For comparison purposes, the parameter values were standardised at a temperature of 20°C. The correction factor was either provided with the dataset or extracted from the original publication (except for ASM3 where Koch *et al.* (2000) was used as a new default parameter set).

Database analysis

The database was analysed for the three topics described below.

Original/proposed new default parameter sets: The proposed default parameter sets are compared to the original ones. The parameter values that were changed are identified and discussed.

Parameters changed in modelling projects: The parameter values that have been changed from the original value in more than 50% of cases are highlighted.

Parameter ranges and statistics: For each model the median value, the 25th and 75th percentiles and the variability have been calculated. The median values should not be misinterpreted as new default parameters. Actually the median values are not from a single parameter set and some parameters may be highly correlated (e.g. growth and decay rate). The 25th and 75th percentiles were chosen to exclude extreme values and to obtain a representative range of the typical parameter values. The variability (V) is calculated as the difference between these two percentiles divided by the median.

RESULTS

Modelling project characteristics

The database contains 77 parameter sets, which can be differentiated into 58 calibrated parameter sets and 19 default parameter sets, and distributed as shown in Figure 1. ASM1 and ASM2d are the most represented models in the database which is according to the first survey (Hauduc *et al.*, 2009).

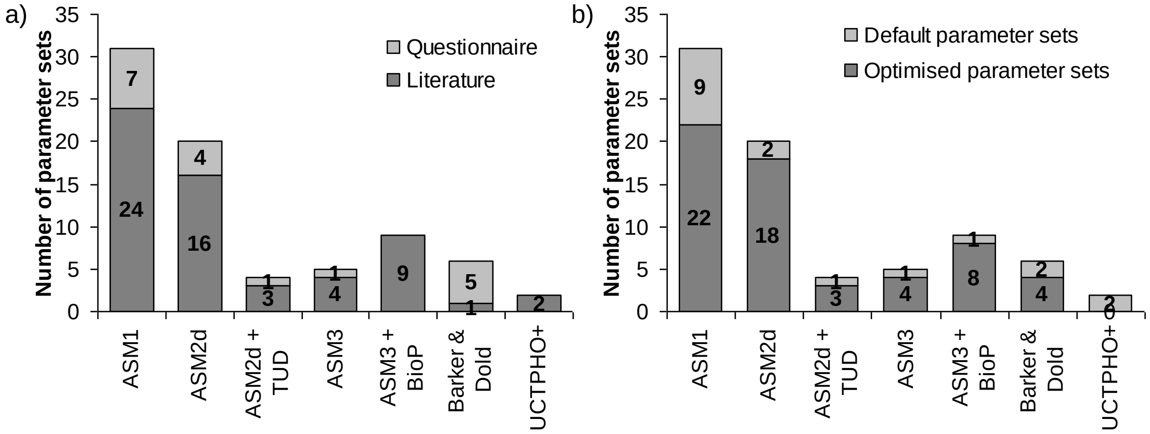

Figure 1. Distribution of parameter sets per model and a) per source b) per class of parameter set

The following paragraphs describe the main information extracted from the current database for ASM1 and ASM2d. An insufficient number of modelling studies is available for the ASM3, ASM3 + BioP and Barker & Dold models and so no comments are given, but their synthesis tables are presented in the appendix. No additional modelling projects beyond their original publication were found for ASM2d + TUD and UCTPHO+ and so they are not presented.

The datasets and the main results for ASM1 and ASM2d are first described. Then the results are discussed according to the three topics presented above.

ASM1

Data description. The database contains 31 parameter sets for ASM1, of which 9 are proposed new default parameter sets and 22 are calibrated parameter sets from specific modelling projects. The modelling studies were mainly carried out at full scale WWTPs (19) with a majority from Europe (18), with only one application in North-America and three in Asia. The sludge age of the specific modelling projects are between 4 and 40 days.

Table 1 presents the main results extracted from the database. In this table, original parameter values are given in column 4. In column 5 the proposed new default parameter sets are given; these values have been ranked in ascending order. In the last columns statistics for optimised data sets, are reported: the number of values for each parameter (n), if it has been modified in more than 50% of the cases compared to the original publication (Modif. >50%), the median value (Med.), the 25th and 75th percentiles and the variability (V).

Original/proposed new default parameter set: 23 parameters (out of 27) have a value that has been modified compared to the original one. A change in ASM1 model structure for the ordinary heterotrophic yield (Y_{OHO}) value by introducing an ordinary heterotrophic yield under anoxic conditions is proposed in three proposed new default parameter sets.

Parameters changed in modelling projects (compared to original values): For each parameter set, a majority of parameters are kept to their default values. Only one parameter is always kept to its original value: the autotrophic growth yield (Y_{ANO}). Nine parameters were changed in more than half of the modelling studies. Six of these parameters concern temperature correction factors, and the three others are the heterotrophic yield (Y_{OHO}) and the autotrophic growth and decay rate pair ($\mu_{ANO,Max}$, b_{ANO}).

Only a few parameter sets contain measured parameters (Makinia and Wells, 2000; Nuhoglu *et al.*, 2005; Stamou *et al.*, 1999 and Petersen *et al.*, 2002). Most of the measured values are close to the values used in other modelling projects, except for Stamou *et al.* (1999) who determined very low values for the heterotrophic and autotrophic growth related parameters.

Parameter ranges and statistics: All median values are the same as the original publication values. The variability is quite narrow (<33%), except for the half-saturation coefficient for substrate ($K_{SB,OHO}$), the half-saturation coefficient for nitrate ($K_{NOx,OHO}$) and the autotrophic decay rate (b_{ANO}).

Table 1. Synthesis of database results for ASM1 model, only modified parameters are mentioned. The parameter values are standardised at a temperature of 20°C.

Parameter *	**Unit**	**Original parameter set**		**Proposed new default parameters**	**Optimised parameter sets**					
		notation	**value (a)**	Parameter sets: b / c / d / e / f / g / h / i	**n**	**Modif >50%**	**Med.**	**Perc. 25%**	**Perc. 75%**	**V (%)**
Stoichiometric parameters										
Y_{OHO}	g X_{OHO}.g XC_B^{-1}	Y_H	**0.67**	0.6(*c;i*) $Y_{OHO.Ox}$: 0.67 and $Y_{OHO.Ax}$: 0.54 (b;f;h)	26	X	0.67	0.62	0.67	7
Conversion coefficient										
i_{N_XBio}	g N.g X_{Bio}^{-1}	$i_{X,B}$	**0.086**	0.08(*c;g*)	31		0.086	0.079	0.086	8
Kinetic parameters										
Hydrolysis										
$q_{XCB\_SB,hyd}$	g XC_B.g X_{OHO}^{-1}.d^{-1}	k_h	**3**	2(*c*) / 2.21(*i*) / 5.2(*g*)	31		3.0	2.2	3.0	26
$\theta_{qXCB\_SB,hyd}$	-	θ_{kh}	**1.116**	1.072(*f*)	11	X	1.116	1.072	1.120	4
$K_{XCB,hyd}$	g XC_B.g X_{OHO}^{-1}	K_X	**0.03**	0.02(*c*) / 0.17(*g*) / 0.15(*i*)	30		0.030	0.030	0.030	0
$\theta_{KXCB,hyd}$	-	θ_{KX}	**1.116**	1(*f*)	10	X	1.116	1.116	1.120	0
$\eta_{qhyd,Ax}$	-	η_h	**0.4**	0.5(*g*)/ 0.6(*d*) $n_{qhyd.An}$: 0.75(*d*)	31		0.40	0.40	0.50	25
Ordinary Heterotrophic Organisms										
$\mu_{OHO,Max}$	d^{-1}	μ_H	**6**	4(*d*) / 5.7(*g*)	31		6.0	5.7	6.0	6
$\theta_{\mu OHO,Max}$	-	$\theta_{\mu H}$	**1.072**		11	X	1.072	1.071	1.090	2
$\eta_{\mu OHO,Ax}$	-	η_g	**0.8**	0.6(*c*)	31		0.800	0.800	0.800	0
$K_{SB,OHO}$	g S_B.m^{-3}	K_S	**20**	5(*d*) / 10(*g*)	31		20.0	10.0	20.0	50
b_{OHO}	d^{-1}	b_H	**0.62**	0.4(*d*) / 0.41(*i*) / 0.5(*c*) / 0.53(*g*)	31		0.62	0.61	0.62	2
θ_{bOHO}	-	θ_{bH}	**1.12**	1.029(*f*)/ 1.071(*c;d*)	11	X	1.100	1.029	1.120	8
$K_{O2,OHO}$	g S_{O2}.m^{-3}	K_{OH}	**0.2**	0.05(*f*) / 0.1(*i*)	31		0.200	0.200	0.200	0
$K_{NOx,OHO}$	g S_{NOx}.m^{-3}	K_{NO}	**0.5**	0.1(*f*) / 0.2(*i*)	31		0.50	0.10	0.50	80
Autotrophic Nitrifying Organisms										
$\mu_{ANO,Max}$	d^{-1}	μ_A	**0.8**	0.77(*i*) / 0.82(*g*)/ 0.85(*c*) / 0.9(*b; d*)	30	X	0.80	0.66	0.90	30
$\theta_{\mu ANO,Max}$	-	$\theta_{\mu A}$	**1.103**	1.059(*f; h*)/ 1.072(*b*)	14	X	1.103	1.059	1.110	5
b_{ANO}	d^{-1}	b_A	**0.5-0.15**	0.07(*g*) / 0.096(*i*) / 0.17(*b; f; h*)	30	X	0.10	0.08	0.15	70
θ_{bANO}	-	θ_{bA}	**1.072**	1.027(*f; h*) / 1.083(*d*) / 1.103(*c*)	12	X	1.070	1.029	1.072	4
q_{am}	m^3.g $X_{CB,N}^{-1}$.d^{-1}	k_a	**0.08**	0.05(*g*) / 0.16(*i*)	29		0.08	0.07	0.08	12
θ_{qam}	-	θ_{ka}	**1.072**	1.071(*d; c*)	11		1.070	1.070	1.070	0
$K_{O2,ANO}$	g S_{O2}.m^{-3}	K_{OA}	**0.4**	0.2(*f*) / 0.5(*c*) / 0.75(*i*)	31		0.40	0.40	0.40	0
$K_{NHx,ANO}$	g S_{NHx}.m^{-3}	K_{NH}	**1**	0.1(*f*) / 0.5(*d*)	31		1.00	0.75	1.00	25

a: Henze *et al.* (2000a); b: Questionnaire; c: Questionnaire; d: Bornemann *et al.* (1998); e: Hulsbeek *et al.* (2002); f: Marquot (2006); g: Spanjers *et al.* (1998); h: Choubert *et al.* (2009b); i: Grady *et al.* (1999).
*Standardised notation from Corominas *et al.* (2010) is used. n: number of parameter values in the database.
Please refer to the appendix for the parameter definitions.

Discussion

Original/proposed new default parameter sets: The need to change the ASM1 model structure by introducing a heterotrophic yield under anoxic conditions ($Y_{OHO,Ax}$) to properly model the nitrate and COD consumption was experimentally proven by Orhon *et al.* (1996). A new default value of 0.54 g X_{OHO}.g XC_B^{-1} is proposed by Choubert *et al.* (2009a), based on full-scale modelling studies.

The change of the maximum autotrophic growth rate ($\mu_{ANO,Max}$) and decay rate (b_{ANO}) is discussed in Dold *et al.* (2005). This study proved that it was no longer necessary to modify $\mu_{ANO,Max}$ when the sludge retention time (SRT) varies if a higher b_{ANO} value is used (experimentally measured to 0.19 ±0.4 d^{-1}). Choubert *et al.* (2009b) propose the values of $\mu_{ANO,Max}=0.8\ d^{-1}$ and $b_{ANO}=0.17\ d^{-1}$ at 20°C as new default values validated on 13 full-scale WWTPs.

Parameters changed in modelling projects (compared to original values): Similarly to the proposed new default parameter sets a reduced heterotrophic growth rate (Y_{OHO}) is often associated with plants with an anoxic and/or an anaerobic zone. This confirms the need to differentiate an aerobic and an anoxic growth yield. The couple ($\mu_{ANO,Max}$, b_{ANO}) is modified in most studies. However, in the analysed modelling projects a high maximum growth rate was not always compensated by a high decay rate.

In addition, the temperature correction factor values are often re-evaluated in the course of a project. They are deduced from the parameter determination at a different temperature and therefore include measurement uncertainties.

Parameter ranges and statistics: The ranges provided by the 25th and 75th percentiles of the database are in agreement with other overview studies (Weijers and Vanrolleghem, 1997; Bornemann *et al.*, 1998; Hulsbeek *et al.*, 2002; Cox, 2004 and Sin *et al*., 2009), except for the following parameters:

- $\mu_{OHO,Max}$ and b_{OHO} ranges proposed by Weijers and Vanrolleghem (1997), are narrower in the database
- $K_{SB,OHO}$, b_{OHO} and $K_{NHx,ANO}$ in Bornemann *et al.* (1998) have wider and not overlapping ranges
- The median values provided by Cox (2004) are quite different from the database ones; whereas the 25th and 75th percentiles are in agreement. An exception is for the heterotrophic growth and decay rates ($\mu_{OHO,Max}$, b_{OHO}) and the half-saturation coefficient for substrate ($K_{SB,OHO}$) for which the ranges provided by Cox (2004) are wider and not overlapping the database ones.
- Sin *et al.* (2009) provided "uncertainties" (or better variability) based on expert knowledge. Two parameter variabilities ($\mu_{ANO,Max}$, b_{ANO}) are narrower than the observed variability in this study and 8 much wider (i_{N_XBio}, $K_{XCB,hyd}$, $\mu_{OHO,Max}$, $\eta_{\mu OHO,Ax}$, $K_{O2,OHO}$, q_{am}, $K_{O2,ANO}$, $K_{NHx,ANO}$)

It is noticeable that the above mentioned parameters correspond to the ones with the greatest variability in Table 1 and/or to those modified in more than 50% of the cases, although the observed variations of these parameters are often lower than those provided in these studies.

Finally, all of the overview studies present a parameter range or an "uncertainty" for the autotrophic yield (Y_{ANO}), whereas none of the 22 modelling projects has modified its value.

Conclusion. Regarding ASM1, six parameters have been pointed out as subject to changes: Y_{OHO}, $K_{SB,OHO}$, $K_{NOx,OHO}$, $\mu_{ANO,Max}$, b_{ANO} and $K_{NHx,ANO}$. In addition to the variability of Y_{OHO}, $\mu_{ANO,Max}$ and b_{ANO} already discussed, the three other parameters are half-saturation coefficients, suspected to depend on environmental conditions. These results are confirmed by the literature data although the chosen 25th and 75th percentiles provide a narrower range for some of the parameters than specified in literature.

ASM2d

Data description. The database contains 20 parameter sets for ASM2d, of which 2 are proposed new default parameter sets and 18 are calibrated in a modelling project. The modelling studies were mainly carried out in Europe (16), with only two applications in Asia; and mainly on full scale WWTP (12). Table 2 synthesises the main results for ASM2d and is structured as Table 1. The sludge age of the specific modelling projects are between 7 and 22 days.

Original/proposed new default parameter sets: Only the original parameter set is presented. A new default parameter set was proposed by Cinar *et al.* (1998) but it concerns ASM2 and not ASM2d. The parameter differences in comparison with the originally published values (Henze *et al.*, 2000b) could be caused by the missing description of anoxic PAO processes in ASM2.

Table 2 Synthesis of database results for ASM2d model, only modified parameters are mentioned. The parameter values are standardised at a temperature of 20°C.

Parameter*	**Unit**	**Original notation**	**Original parameter values**	**Optimised parameter sets**					
Parameter sets			**j**	**n**	**changed >50%**	**Median**	**Perc. 25%**	**Perc. 75%**	**V (%)**
Kinetic parameters									
Hydrolysis									
$\eta_{qhyd,Ax}$	-	η_{NO3}	**0.60**	20		0.60	0.60	0.80	33
$\eta_{qhyd,A\eta}$	-	η_{fe}	**0.40**	20		0.40	0.20	0.40	50
Ordinary Heterotrophic Organisms									
$\mu_{OHO,Max}$	d^{-1}	μ_H	**6.0**	20	X	6.0	4.0	6.0	33
$\eta_{\mu OHO,Ax}$	-	η_{NO3}	**0.8**	20		0.8	0.8	0.8	0
Phosphorus Accumulating Organisms									
q_{PAO,VFA_Stor}	$g\ X_{Stor}.g\ X_{PAO}^{-1}.d^{-1}$	q_{PHA}	**3**	20	X	3.4	3.0	6.0	90
$q_{PAO,PO4\_PP}$	$g\ X_{PP}.g\ X_{PAO}^{-1}.d^{-1}$	q_{PP}	**1.50**	20	X	1.50	1.50	3.30	120
$\mu_{PAO,Max}$	d^{-1}	μ_{PAO}	**1.00**	20		1.00	1.00	1.04	4
$\theta_{\mu PAO,Max}$	-	$\theta_{\mu PAO}$	**1.041**	3		1.041	1.041	1.058	2
m_{PAO}	d^{-1}	b_{PAO}	**0.20**	20	X	0.20	0.15	0.20	25
b_{PP_PO4}	d^{-1}	b_{PP}	**0.20**	20	X	0.20	0.15	0.20	25
b_{Stor_VFA}	d^{-1}	b_{PHA}	**0.20**	20	X	0.20	0.15	0.20	25
Autotrophic Nitrifying Organisms									
$\mu_{ANO,Max}$	d^{-1}	μ_{AUT}	**1.00**	20	X	1.00	1.00	1.15	15
b_{ANO}	d^{-1}	b_{AUT}	**0.15**	20		0.15	0.15	0.16	7
$K_{NHx,ANO}$	$g\ S_{NHx}.m^{-3}$	K_{NH4}	**1.00**	20	X	1.00	0.50	1.00	50

j: Henze *et al.* (2000b). Please refer to the appendix for the parameter definitions.
*Standardised notation from Corominas *et al.* (2010) is used. n: number of parameter values in the database.

Parameters changed in modelling projects (compared to original values): The majority of parameters are kept to their original value in the modelling projects. 33 of the 83 parameters were always kept to their original value:

- 4 of the 11 stoichiometric parameters were never changed: the inert fractions generated in hydrolysis and biomass decay processes ($f_{SU\_XCB,hyd}$, $f_{XU\_Bio,lys}$); the yield of polyphosphate storage per organic stored compound used (Y_{PHA_PP}) and the autotrophic growth yield (Y_{ANO}).
- 7 of the 15 conversion coefficients were never changed: i_{N_SF}, i_{N_XBio}, i_{P_SF}, i_{P_SU}, i_{TSS_XCB}, $i_{TSS\_XPAO,PHA}$ and $i_{TSS\_XPAO,PP}$.

- 22 of the 57 kinetic parameters were never changed: the alkalinity half-saturation parameters ($K_{\mathrm{Alk,OHO}}$, $K_{\mathrm{Alk,PAO}}$, $K_{\mathrm{Alk,ANO}}$); heterotrophic half-saturation parameters for nutrients ($K_{\mathrm{NHx,OHO}}$, $K_{\mathrm{PO4,OHO}}$); autotrophic half-saturation parameters for nutrients ($K_{\mathrm{PO4,ANO}}$); five phosphorus accumulating organism half-saturation parameters ($K_{\mathrm{S,fPP\_PAO}}$, $K_{\mathrm{O2,PAO}}$, $K_{\mathrm{NOx,PAO}}$, $K_{\mathrm{NHx,PAO}}$, $K_{\mathrm{PO4,PAO,upt}}$); the half-saturation parameters for dissolved oxygen and nitrates in the hydrolysis process ($K_{\mathrm{O2,hyd}}$, $K_{\mathrm{NOx,hyd}}$); six of the twelve temperature correction factors ($\theta_{\mathrm{q\_XCB\_SB,hyd}}$, $\theta_{\mathrm{\mu\_OHO,Max}}$, $\theta_{\mathrm{q\_SF\_Ac,Max}}$, $\theta_{\mathrm{b\_OHO}}$, $\theta_{\mathrm{\mu\_ANO,Max}}$, $\theta_{\mathrm{b\_ANO}}$); and the chemical phosphorus precipitation parameters ($q_{\mathrm{P,pre}}$, $q_{\mathrm{P,red}}$, $K_{\mathrm{Alk,pre}}$).

Two types of studies could be distinguished:

- modelling studies with a calibrated parameter subset (12 studies). These are mainly composed of kinetic parameters
- modelling studies with measured parameters (6 studies). Among these 6 studies, 4 use the calibration protocol of Penya-Roya *et al*. (2002) (Penya-Roya *et al*., 2002; 2 by Ferrer *et al.*, 2004; Garcia-Usach *et al.,* 2006). This protocol is based on batch tests that allow the measurement of many stoichiometric and kinetic coefficients for autotrophs, ordinary heterotrophs and phosphorous accumulating organisms.

Among the 16 modelling studies, eight exclusively kinetic parameters were changed in more than half of the cases: the heterotrophic and autotrophic maximum growth rates ($\mu_{\mathrm{OHO,Max}}$, $\mu_{\mathrm{ANO,Max}}$), the autotrophic half-saturation coefficient for ammonia ($K_{\mathrm{NHx,ANO}}$), the rate constants for volatile fatty acids (VFA) uptake ($q_{\mathrm{PAO,VFA\_Stor}}$) and for polyphosphate storage ($q_{\mathrm{PAO,PO4\_PP}}$) of the PAO and their storage pools' decay (m_{PAO}, $b_{\mathrm{PP\_PO4}}$, $b_{\mathrm{Stor\_VFA}}$).

Parameter ranges and statistics: The median values are the same as the original publication values except for the rate constant for VFA uptake ($q_{\mathrm{PAO,VFA\_Stor}}$). The ranges of kinetic parameter values between 25th and 75th percentiles are quite narrow (<33%), except for the reduction factor for hydrolysis under anaerobic conditions ($\eta_{\mathrm{qhyd,A\eta}}$), for the rate constants for VFA uptake ($q_{\mathrm{PAO,VFA\_Stor}}$) and polyphosphate storage ($q_{\mathrm{PAO,PO4\_PP}}$) and the half-saturation coefficient for ammonia ($K_{\mathrm{NHx,ANO}}$).

Discussion

Parameters changed in modelling projects (compared to original values): Applying the Penya-Roja *et al.* (2002) protocol results in large parameter ranges, especially for the phosphorus accumulating organisms growth yield ($\mathrm{Y}_{\mathrm{PAO}}$), for the yield of phosphate release per stored organic compound ($\mathrm{Y}_{\mathrm{PP\_Stor,PAO}}$), for the rate constants for VFA uptake ($q_{\mathrm{PAO,VFA\_Stor}}$) and polyphosphate storage ($q_{\mathrm{PAO,PO4\_PP}}$).

Among the eight parameters that were changed most, two have a particularly wide range of values: the rate constants for VFA uptake ($q_{\mathrm{PAO,VFA\_Stor}}$) and polyphosphate storage ($q_{\mathrm{PAO,PO4\_PP}}$).

These large variations of parameter values concerning the storage and consumption of organic compounds highlighted by the users of the protocol of Penya-Roja *et al.* (2002) (for yields) and by this database (for rates) could indicate a problem in the ASM2d model structure. Penya-Roja *et al.* (2002) suggest that this could be due to the simplification of not taking into account glycogen storage and glycogen accumulating organisms in ASM2d.

Another explanation could be that the ASM2d model describes polyphosphate uptake and the growth of PAOs as two independent kinetic processes. However, experimental results show that oxidation of organic stored compounds provides energy for both PAO growth and polyphosphate storage (Wentzel *et al.,* 1989). Consequently, PAO growth and polyphosphate storage yield are linked and depend on the oxidation of organic stored compounds. Therefore some models are linking both yields to energy production (in metabolic models, e.g.: Meijer, 2004) or are modelling PAO growth and polyphosphate storage as a single process (Barker & Dold model, UCTPHO+). Fixing the ratio between growth and phosphate storage would then facilitate ASM2d calibration.

Parameter ranges and statistics: Based on expert knowledge, Brun *et al.* (2002) assigned a class of uncertainty (class 1: 5%, class 2: 20% or class 3: 50%) to each parameter. These uncertainties are compared with the variability observed in the database. Stoichiometric parameters and conversion coefficients were mainly classified into class 1 and 2 (respectively 5% and 20% of uncertainty). The database shows no major modification for these parameter values, which is in agreement with the low uncertainties attributed to these parameters by Brun *et al.* (2002).

In Brun *et al.* kinetic parameters were classified into class 2 or 3 (respectively 20% and 50% of uncertainty). The kinetic parameters classified into class 2 had no or few parameter values variation in the database, except for the reduction factors for hydrolysis under anoxic and anaerobic conditions ($\eta_{\mathrm{qhyd,Ax}}$, $\eta_{\mathrm{qhyd,An}}$). The uncertainty of 50% attributed to other kinetic parameters seems to be overestimated based on the database results, apart from the rate constants for VFA uptake ($q_{\mathrm{PAO,VFA\_Stor}}$) and polyphosphate storage ($q_{\mathrm{PAO,PO4\_PP}}$) which have a variability of around 100%.

Conclusion. The main potential pitfalls in calibrating ASM2d seem to come from the determination of the rate constants for VFA uptake ($q_{\mathrm{PAO,VFA\_Stor}}$) and polyphosphate storage ($q_{\mathrm{PAO,PO4\_PP}}$). These two parameters are used in organic compounds storage and consumption processes. Their high variability could indicate a problem in the model structure, due to the absence of a glycogen storage pool for polyphosphate accumulating organisms and of the glycogen accumulating organisms. Another explanation could be the description of PAO growth and polyphosphates storage as two independent processes leading to difficulties in the calibration.

DISCUSSION

Inter-model comparison

In both ASM1 and ASM2d few parameters have been changed in more than half the cases considered. This shows that model users are in most cases relying on the original values, or that the model outputs are not sensitive to these parameters. In an inter-model comparison taking into account the results for other models presented in appendix (ASM3, ASM3 + BioP, ASM2d + TUD, Barker & Dold), the following parameters are most often modified:

- growth and decay rates of autotrophs,
- PAO storage processes rates,
- Heterotrophic half-saturation coefficients for substrate and oxygen and autotrophic half-saturation coefficient ammonia.

The variability of PAO storage process rates may reveal a problem in the ASM2d model structure describing the PAO processes. Concerning autotrophic growth and decay rates and half-saturation coefficients, these parameters are known as dependent of the environmental conditions.

Several modelling protocols suggest measuring some kinetic and stoichiometric parameters: WERF (Melcer *et al.*, 2003), BIOMATH (Vanrolleghem *et al.*, 2003) and HSG (Langergraber *et al.*, 2004). However, in current practice few, if any, biokinetic parameters are measured.

Limitations of modelling project articles

The large literature review on modelling projects revealed that important information is often missing from these articles to enable them to be fully used. Lacking information included:

- information on plant: design, tank size, aeration time;
- information on environmental conditions: temperature, rain events, diurnal variations;
- information on measurement campaign: duration, number of samples, measurement methods;
- information on influent characteristics and characterisation method used;
- method used to optimise the parameter set: protocol, parameters set to original value;
- temperature for which the optimised parameter set is provided.

Unfortunately no exhaustive description of the modelling project is available for any of the parameter sets in the database. This means that some of this information has to be assumed to make the study usable, which in turn lowers the quality of the database results. Furthermore this lack of information prevents further analysis of the database, such as an investigation of correlations.

Potential use of the database

A number of correlations were searched for in the database including: correlations between parameters; correlations between changed values; correlations between parameters and WWTP conditions (Food/Microorganism ratio, nitrogen loads, Sludge Retention Time). Probably because of the limited number of datasets no significant correlations were found.

The database has been designed to allow future extensions with new modelling project data. A larger database could allow further analysis to determine:

- model parameter ranges and typical values to define current practice and help model users in the calibration step for the commonly used models (ASM1, ASM2d, ASM3, ASM3+BioP, ASM2d+TUD, Barker & Dold model, UCTPHO+);
- a synthesis of practical modelling experiences that could help model users to find the appropriate case studies similar to their simulation project;
- correlations between changes in parameter values and WWTP conditions;
- practical model limits from various modelling experiences;
- identification of research needs.

CONCLUSION

This study synthesises the practical knowledge of activated sludge models through a database that combines experience from modelling projects and expert knowledge. For now this database provides parameter ranges and typical values for ASM1 and ASM2d. These values should help model users in the calibration step, by showing typical practice in model calibration. However, these parameters should be used with great care since they are the result of averaging practical experience without taking into account parameter correlations.

These results contribute to the knowledge transfer on activated sludge modelling that was requested by respondents of the first survey (Hauduc *et al.*, 2009). This database can be expanded with more modelling projects which would enable further analysis to be carried out. The authors would like to make this database accessible to the AS modelling community and several solutions are currently under study.

The questionnaire provides further information that has not been presented in this study, but will be included in the Scientific and Technical Report of the *Good Modelling Practice – Guidelines for use of activated sludge models* (GMP-TG), such as typical ratios and key numbers currently measured at WWTPs.

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REFERENCES

Barker P.S. and Dold P.L. (1997) General model for biological nutrient removal activated-sludge systems: Model presentation. *Water Environment Research*, **69**(5), 969-984.

Bornemann C., Londong J., Freund M., Nowak O., Otterpohl R. and Rolfs T. (1998) Hinweise zur dynamischen Simulation von Belebungsanlagen mit dem Belebtschlammodell Nr. 1 der IAWQ. *Korrespondenz Abwasser*, **45**(3), 455-462, [in German].

Brun R., Kuehni M., Siegrist H., Gujer W. and Reichert P. (2002) Practical identifiability of ASM2d parameters - Systematic selection and tuning of parameter subsets. *Water Research*, **36**(16), 4113-4127.

Choubert J.-M., Marquot A., Stricker A.-E., Racault Y., Gillot S. and Héduit A. (2009a) Anoxic and aerobic values for the yield coefficient of the heterotrophic biomass: Determination at full-scale plants and consequences on simulations. *Water SA*, **35**(1), 103-110.

Choubert J.-M., Stricker A.-E., Marquot A., Racault Y., Gillot S. and Héduit A. (2009b) Updated Activated Sludge Model n1 parameter values for improved prediction of nitrogen removal in activated sludge processes: Validation at 13 full-scale plants. *Water Environment Research*, **81**, 858-865.

Cinar O., Daigger G.T. and Graef S.P. (1998) Evaluation of IAWQ Activated Sludge Model No. 2 using steady-state data from four full-scale wastewater treatment plants. *Water Environment Research*, **70**(6), 1216-1224.

Corominas L., Rieger L., Takács I., Ekama G., Hauduc H., Vanrolleghem P.A., Oehmen A., Gernaey K.V. and Comeau Y. (2010) New framework for standardized notation in wastewater treatment modelling. *Water Science and Technology*, **61**(4), 841–857.

Cox C.D. (2004) Statistical distributions of uncertainty and variability in activated sludge model parameters. *Water Environment Research*, **76**(7), 2672-2685.

Dold P.L., Jones R.M. and Bye C.M. (2005) Importance and measurement of decay rate when assessing nitrification kinetics. *Water Science and Technology*, **52**(10-11), 469-477.

Ferrer J., Morenilla J.J., Bouzas A. and Garcia-Usach F. (2004) Calibration and simulation of two large wastewater treatment plants operated for nutrient removal. *Water Science and Technology*, **50**(6), 87-94.

Garcia-Usach F., Ferrer J., Bouzas A. and Seco A. (2006) Calibration and simulation of ASM2d at different temperatures in a phosphorus removal pilot plant. *Water Science and Technology*, **53**(12), 199-206.

Grady C.P.L J., Daigger G.T. and Lim H.C. (1999) *Biological Wastewater Treatment - Second Edition, revised and expanded*, 1076 pp., Marcel Dekker, New York.

Gujer W., Henze M., Mino T. and Van Loosdrecht M. (2000) Activated Sludge Model No.3, in *Activated Sludge Models ASM1, ASM2, ASM2d and ASM3*. edited by M. Henze, *et al*., IWA Publishing, London, UK.

Hauduc H., Gillot S., Rieger L., Ohtsuki T., Shaw A., Takács I. and Winkler S. (2009) Activated Sludge Modelling in Practice - An International Survey. *Water Science and Technology*, **60**(8), 1943-1951.

Henze M., Grady C.P.L J., Gujer W., Marais Gv R. and Matsuo T. (2000a) Activated Sludge Model No.1, in *Activated Sludge Models ASM1, ASM2, ASM2d and ASM3*. edited by M. Henze, *et al*., IWA Publishing, London, UK.

Henze M., Gujer W., Mino T., Matsuo T., Wentzel M.C., Marais G.v.R. and van loosdrecht M. (2000b) Activated Sludge Model No.2d, in *Activated Sludge Models ASM1, ASM2, ASM2d and ASM3*. edited by M. Henze, *et al*., IWA Publishing, London, UK.

Hu Z.R., Wentzel M.C. and Ekama G.A. (2007) A general kinetic model for biological nutrient removal activated sludge systems: Model development. *Biotechnology and Bioengineering*, **98**(6), 1242-1258.

Hulsbeek J.J.W., Kruit J., Roeleveld P.J. and van Loosdrecht M.C.M. (2002) A practical protocol for dynamic modelling of activated sludge systems. *Water Science and Technology*, **45**(6), 127-136.

Koch G., Kühni M., Gujer W. and Siegrist H. (2000) Calibration and validation of Activated Sludge Model no. 3 for Swiss municipal wastewater. *Water Research*, **34**(14), 3580-3590.

Langergraber G., Rieger L., Winkler S., Alex J., Wiese J., Owerdieck C., Ahnert M., Simon J. and Maurer M. (2004) A guideline for simulation studies of wastewater treatment plants. *Water Science and Technology*, **50**(7), 131-138.

Makinia J. and Wells S.A. (2000) A general model of the activated sludge reactor with dispersive flow - I. Model development and parameter estimation. *Water Research*, **34**(16), 3987-3996.

Meijer S.C.F. (2004) *Theoretical and practical aspects of modelling activated sludge processes*. PhD thesis, Department of Biotechnological Engineering, Delft University of Technology, Delft, The Netherlands.

Melcer H., Dold P.L., Jones R.M., Bye C.M., Takacs I., Stensel H.D., Wilson A.W., Sun P., Bury S., (2003), Methods for wastewater characterisation in activated sludge modeling, Water Environment Research Foundation (WERF), Alexandria, VA, US.

Nuhoglu A., Keskinler B. and Yildiz E. (2005) Mathematical modelling of the activated sludge process - The Erzincan case. *Process Biochemistry*, **40**(7), 2467-2473.

Obara T., Yamanaka O. and Yamamoto K. (2006) A sequential parameter estimation algorithm for activated sludge model no.2d based on mathematical optimization and a prior knowledge for parameters. In: Proceedings IWA World Water Congress, Beijing, CHN, 10-14 septembre 2006

Penya-Roja J.M., Seco A., Ferrer J. and Serralta J. (2002) Calibration and validation of Activated Sludge Model No.2d for Spanish municipal wastewater. *Environmental Technology*, **23**(8), 849-862.

Petersen B., Gernaey K., Henze M. and Vanrolleghem P.A. (2002) Evaluation of an ASM1 model calibration procedure on a municipal-industrial wastewater treatment plant. *J. Hydroinformatics*, **4**(1), 15-38.

Rieger L., Koch G., Kuhni M., Gujer W. and Siegrist H. (2001) The EAWAG Bio-P module for Activated Sludge Model No. 3. *Water Research*, **35**(16), 3887-3903.

Sin G., Gernaey K.V., Neumann M.B., van Loosdrecht M.C.M. and Gujer W. (2009) Uncertainty analysis in WWTP model applications: A critical discussion using an example from design. *Water Research*, **43**(11), 2894-2906.

Stamou A., Katsiri A., Mantziaras I., Boshnakov K., Koumanova B. and Stoyanov S. (1999) Modelling of an alternating oxidation ditch system. *Water Science and Technology*, **39**(4), 169-176.

Vanrolleghem P.A., Insel G., Petersen B., Sin G., Pauw D.D., Nopens I., Dovermann H., Weijers S. and Gernaey K. (2003) A comprehensive model calibration procedure for activated sludge models. In: *Proceedings 76th Annual WEF Conference and Exposition.* Los Angeles, USA, October 11-15, 2003. (on CD-ROM).

Weijers S.R. and Vanrolleghem P.A. (1997) A procedure for selecting best identifiable parameters in calibrating Activated Sludge Model No. 1 to full-scale plant data. *Water Science and Technology*, **36**(5), 69-79.

Wentzel M.C., Ekama G.A., Loewenthal R.E., Dold P.L. and Marais Gv R. (1989) Enhanced polyphosphate organism cultures in activated sludge systems. Part II: Experimental behaviour. *Water S.A.*, **15**(2), 71-88.

APPENDIX
Parameter definitions

Table 3. Parameter definitions and original notation of the studied models.

Description	Parameter*	Unit	ASM1	ASM2d	ASM3	ASM3 + BioP	Barker & Dold
State Variables							
COD soluble							
Soluble biodegradable organics	S_B	g COD.m^{-3}	S_S		S_S	S_S	
Fermentable organic matter	S_F	g COD.m^{-3}		S_F			S_{BSC}
Fermentation product (volatile fatty acids)	S_{VFA}	g COD.m^{-3}		S_A			S_{BSA}
Soluble undegradable organics	S_U	g COD.m^{-3}	S_I	S_I	S_I	S_I	S_{US}
Dissolved oxygen	S_{O2}	- g COD.m^{-3}	S_O	S_{O2}	S_O	S_O	S_O
COD particulate and colloidal							
Particulate biodegradable organics	X_{CB}	g COD.m^{-3}	X_S	X_S	X_S	X_S	S_{ENM}
Adsorbed slowly biodegradable substrate	X_{Ads}	g COD.m^{-3}					
Particulate undegradable organics	X_U	g COD.m^{-3}		X_I	X_I	X_I	
Particulate undegradable organics from the influent	$X_{U,Inf}$	g COD.m^{-3}	X_I				S_{UP}
Particulate undegradable endogenous products	$X_{U,E}$	g COD.m^{-3}	X_P				Z_E
Nitrogen and Phosphorus							
Ammonium and ammonia nitrogen (NH_4 + NH_3)	S_{NHx}	g N.m^{-3}	S_{NH}	S_{NH4}	S_{NH}	S_{NH}	N_{H3}
Nitrate and nitrite (NO_3 + NO_2) (considered to be NO_3 only for stoichiometry)	S_{NOx}	g N.m^{-3}	S_{NO}	S_{NO3}	S_{NO}	S_{NO}	N_{O3}
Particulate biodegradable organic N	$X_{CB,N}$	g N.m^{-3}	X_{ND}				N_{BP}
Soluble biodegradable organic N	$S_{B,N}$	g N.m^{-3}	S_{ND}				N_{BS}
Soluble inert organic N	$S_{U,N}$	g N.m^{-3}					N_{US}
Soluble inorganic phosphorus	S_{PO4}	g P.m^{-3}		S_{PO4}		S_{PO4}	P_{O4}
Biomasses							
Ordinary heterotrophic organisms	X_{OHO}	g COD.m^{-3}	X_{BH}	X_H	X_H	X_H	Z_H
Autotrophic nitrifying organisms (NH_4 to NO_3)	X_{ANO}	g COD.m^{-3}	X_{BA}	X_{AUT}	X_A	X_A	Z_A
Phosphorus accumulating organisms	X_{PAO}	g COD.m^{-3}		X_{PAO}		X_{PAO}	Z_P
Organisms (biomass)	X_{Bio}	g COD.m^{-3}					
Storage compound in OHOs	$X_{OHO,Stor}$	g COD.m^{-3}			X_{STO}	X_{STO}	
Storage compound in PAOs	$X_{PAO,Stor}$	g COD.m^{-3}		X_{PHA}		X_{PHA}	S_{PHB}
Stored glycogen in PAOs	$X_{PAO,Gly}$	g COD.m^{-3}					
Stored polyphosphates in PAOs	$X_{PAO,PP}$	g P.m^{-3}		X_{PP}		X_{PP}	
Stoichiometric parameters							
Yield for X_{OHO} growth	Y_{OHO}	g X_{OHO}.g XC_B^{-1}	Y_H				
Yield for X_{OHO} growth per $X_{OHO,Stor}$ (Aerobic)	$Y_{Stor\_OHO,Ox}$	g X_{OHO}.g X_{Stor}^{-1}			$Y_{H,O2}$		
Yield for X_{OHO} growth per $X_{OHO,Stor}$ (Anoxic)	$Y_{Stor\_OHO,Ax}$	g X_{OHO}.g X_{Stor}^{-1}			$Y_{H,NOX}$		
Yield for $X_{OHO,Stor}$ formation per S_B (Aerobic)	$Y_{SB\_Stor,Ox}$	g X_{Stor}.g S_B^{-1}			$Y_{STO,O2}$		
Yield for $X_{OHO,Stor}$ formation per S_B (Anoxic)	$Y_{SB\_Stor,Ax}$	g X_{Stor}.g S_B^{-1}			$Y_{STO,NOX}$		
Conversion coefficient							
N content of S_U	i_{N_SU}	g N.g S_U^{-1}					$f_{N,SEP}$
N content of X_U	i_{N_XU}	g N.g X_U^{-1}			$i_{N,XI}$		
N content of XC_B	i_{N_XCB}	g N.g XC_B^{-1}			$i_{N,XS}$		
N content of X_{OHO}	i_{N_OHO}	g N.g X_{OHO}^{-1}					$f_{N,ZH}$
N content of biomass (X_{OHO}, X_{PAO}, X_{ANO})	i_{N_XBio}	g N.g X_{Bio}^{-1}	$i_{X,B}$				
N content of products from X_{OHO}	$i_{N\_XUE,OHO}$	g N.g X_{UE}^{-1}					$f_{N,ZEH}$
N content of products from X_{PAO}	$i_{N\_XUE,PAO}$	g N.g X_{UE}^{-1}					$f_{N,ZEP}$
N content of products from X_{ANO}	$i_{N\_XUE,ANO}$	g N.g X_{UE}^{-1}					$f_{N,ZEA}$

Kinetic parameters							
Hydrolysis							
Maximum specific hydrolysis rate	$q_{XCB\_SB,hyd}$	g XC_B.g X_{OHO}^{-1}.d^{-1}	k_h		k_H		
Temperature correction factor for $q_{XCB\_SB,hyd}$	$\theta_{qXCB\_SB,hyd}$	-	θ_{kh}				
Half-saturation coefficient for XC_B/X_{OHO}	$K_{XCB,hyd}$	g XC_B.g X_{OHO}^{-1}	K_X				
Temperature correction factor for $K_{XCB,hyd}$	$\theta_{KXCB,hyd}$		θ_{KX}				
Correction factor for hydrolysis under anoxic conditions	$\eta_{qhyd,Ax}$	-	η_h	η_{NO3}			η_{gro}
Correction factor for hydrolysis under anaerobic conditions	$\eta_{qhyd,A\eta}$	-		η_{fe}			
Ordinary Heterotrophic Organisms							
Rate constant for $X_{OHO,Stor}$ storage	q_{SB_Stor}	g XC_B.g X_{OHO}^{-1}.d^{-1}			k_{STO}		
Maximum growth rate of X_{OHO}	$\mu_{OHO,Max}$	d^{-1}	μ_H	μ_H	μ_H		
Temperature correction factor for $\mu_{OHO,Max}$	$\theta_{\mu OHO,Max}$	-	$\theta_{\mu H}$				
Reduction factor for anoxic growth of X_{OHO}	$\eta_{\mu OHO,Ax}$	-	η_g	η_{NO3}	η_{NOX}		
Half-saturation coefficient for S_B	$K_{SB,OHO}$	g S_B.m^{-3}	K_S		K_S		
Half-saturation coefficient $X_{OHO,Stor}/X_{OHO}$	K_{Stor_OHO}	g X_{Stor}.g X_{OHO}^{-1}			K_{STO}		
Decay rate for X_{OHO}	b_{OHO}	d^{-1}	b_H				
Temperature correction factor for b_{OHO}	θ_{bOHO}		θ_{bH}				
Endogenous respiration rate of X_{OHO} (Aerobic)	$m_{OHO,Ox}$	d^{-1}			$b_{H,O2}$		
Endogenous respiration rate of X_{OHO} (Anoxic)	$m_{OHO,Ax}$	d^{-1}			$b_{H,NOX}$		
Endogenous respiration rate of $X_{OHO,Stor}$ (Aerobic)	$m_{Stor,Ox}$	d^{-1}			$b_{STO,O2}$		
Endogenous respiration rate of $X_{OHO,Stor}$ (Anoxic)	$m_{Stor,Ax}$	d^{-1}			$b_{STO,NOX}$		
Reduction factor for anoxic endogenous respiration of X_{OHO}	$\eta_{mOHO,Ax}$	-				$\eta_{NO,end,H}$	
Half-saturation coefficient for S_{O2}	$K_{O2,OHO}$	g S_{O2}.m^{-3}	K_{OH}		K_{O2}	$K_{O,H}$	$K_{O,HET}$
Half-saturation coefficient for S_{NOx}	$K_{NOx,OHO}$	g S_{NOx}.m^{-3}	K_{NO}				
Phosphorus Accumulating Organisms							
Rate constant for S_{VFA} uptake rate ($X_{PAO,Stor}$ storage)	q_{PAO,VFA_Stor}	g X_{Stor}.g X_{PAO}^{-1}.d^{-1}		q_{PHA}			
Rate constant for storage of $X_{PAO,PP}$	$q_{PAO,PO4\_PP}$	g X_{PP}.g X_{PAO}^{-1}.d^{-1}		q_{PP}		q_{PP}	
Maximum ratio of $X_{PAO,PP}/X_{PAO}$	$f_{PP\_PAO,Max}$	g X_{PP}.g X_{PAO}^{-1}				$K_{max,PAO}$	
Maximum growth rate of X_{PAO}	$\mu_{PAO,Max}$	d^{-1}		μ_{PAO}			
Temperature correction factor for $\mu_{PAO,Max}$	$\theta_{\mu PAO,Max}$	-		$\theta_{\mu PAO}$			
Endogenous respiration rate of X_{PAO}	m_{PAO}	d^{-1}		b_{PAO}			
Rate constant for lysis of $X_{PAO,PP}$	b_{PP_PO4}	d^{-1}		b_{PP}			
Rate constant for respiration of $X_{PAO,Stor}$	B_{Stor_VFA}	d^{-1}		b_{PHA}			
Half-saturation coefficient for $X_{PAO,PP}$	$K_{PP,PAO}$	g X_{PP}.m^{-3}					K_{XP}
Autotrophic Nitrifying Organisms							
Maximum growth rate of X_{ANO}	$\mu_{ANO,Max}$	d^{-1}	μ_A	μ_{AUT}	μ_A	μ_A	μ_A
Temperature correction factor for $\mu_{ANO,Max}$	$\theta_{\mu ANO,Max}$	-	$\theta_{\mu A}$				
Decay rate for X_{ANO}	b_{ANO}	d^{-1}	b_A	b_{AUT}			b_A
Temperature correction factor for b_{ANO}	θ_{bANO}		θ_{bA}				
Endogenous respiration rate for X_{ANO} (Aerobic)	$m_{ANO,Ox}$	d^{-1}			$b_{A,O2}$		
Endogenous respiration rate for X_{ANO} (Anoxic)	$m_{ANO,Ax}$	d^{-1}			$b_{A,NOX}$		
Rate constant for ammonification	q_{am}	M^3.g $XC_{B,N}^{-1}$.d^{-1}	k_a				
Temperature correction factor for q_{am}	θ_{qam}	-	θ_{ka}				
Half-saturation coefficient for S_{O2}	$K_{O2,ANO}$	g S_{O2}.m^{-3}	K_{OA}			$K_{O,A}$	$K_{O,AUT}$
Half-saturation coefficient for S_{NHx}	$K_{NHx,ANO}$	g S_{NHx}.m^{-3}	K_{NH}	K_{NH4}	$K_{A,NH4}$		K_{NH}

*Standardised notation from Corominas *et al.* (2010) is used.

ASM3

Data description. The database contains 5 parameter sets for ASM3, of which 2 are default parameter sets. The modelling studies were exclusively carried out in the North of Europe (Belgium, Finland, Germany) on full scale WWTP. Table 4 synthesises the main results for ASM3 and is structured as Table 1.

Table 4. Synthesis of database results for ASM3 model, only modified parameters are given

Parameter*	Unit	Original notation	default parameters values	Optimised parameter sets characteristics					
Parameter sets			**k** / l	**n**	**changed >50%**	**Median**	**Perc. 25%**	**Perc. 75%**	**V (%)**
Stoichiometric parameters									
$Y_{Stor\_OHO,Ox}$	$g\ X_{OHO}\cdot g\ X_{Stor}^{-1}$	$Y_{H,O2}$	0.8 / **0.85**	5		0.80	0.80	0.80	0
$Y_{Stor\_OHO,Ax}$	$g\ X_{OHO}\cdot g\ X_{Stor}^{-1}$	$Y_{H,NOX}$	0.7 / **0.8**	5		0.70	0.70	0.70	0
$Y_{SB\_Stor,Ox}$	$g\ X_{Stor}\cdot g\ S_{B}^{-1}$	$Y_{STO,O2}$	**0.63** / 0.8	5		0.80	0.63	0.80	21
$Y_{SB\_Stor,Ax}$	$g\ X_{Stor}\cdot g\ S_{B}^{-1}$	$Y_{STO,NOX}$	**0.54** / 0.65	5		0.65	0.54	0.65	17
Conversion coefficient									
i_{N_XU}	$g\ N.g\ X_{U}^{-1}$	$i_{N,XI}$	**0.02** / 0.04	5		0.040	0.035	0.040	13
i_{N_XCB}	$g\ N.g\ X_{CB}^{-1}$	$i_{N,XS}$	0.03 / **0.04**	5		0.030	0.030	0.030	0
Kinetic parameters									
Hydrolysis									
$q_{XCB\_SB,hyd}$	$g\ X_{CB}\cdot g\ X_{OHO}^{-1}.d^{-1}$	k_{H}	**3** / 9	5		9.0	3.0	9.0	67
q_{SB_Stor}	$g\ X_{CB}\cdot g\ X_{OHO}^{-1}.d^{-1}$	k_{STO}	**0.1**	5		12.0	10.0	12.0	17
Ordinary Heterotrophic Organisms									
$\mu_{OHO,Max}$	d^{-1}	μ_{H}	**2** / 3	5		3.0	2.0	3.0	33
$\eta_{\mu OHO,Ax}$	-	η_{NOX}	0.5 / **0.6**	5		0.50	0.50	0.60	20
$K_{SB,OHO}$	$g\ S_{B}.m^{-3}$	K_{S}	**2** / 10	5		10.0	2.0	10.0	80
K_{Stor_OHO}	$g\ X_{Stor}\cdot g\ X_{OHO}^{-1}$	K_{STO}	0.1 / **1**	5		0.10	0.10	0.10	0
$m_{OHO,Ox}$	d^{-1}	$b_{H,O2}$	**0.2** / 0.3	5		0.30	0.20	0.30	33
$m_{OHO,Ax}$	d^{-1}	$b_{H,,NOX}$	**0.1** / 0.15	5		0.15	0.10	0.15	33
$m_{Stor,Ox}$	d^{-1}	$b_{STO,O2}$	**0.2** / 0.3	5		0.30	0.20	0.30	33
$m_{Stor,Ax}$	d^{-1}	$b_{STO,NOX}$	**0.1** / 0.15	5		0.15	0.10	0.15	33
$K_{O2,OHO}$	$g\ S_{O2}.m^{-3}$	K_{O2}	**0.2**	5		0.200	0.200	0.500	150
Autotrophic Nitrifying Organisms									
$\mu_{ANO,Max}$	d^{-1}	μ_{A}	**1** / 1.3	5	X	1.00	1.00	1.30	30
$m_{ANO,Ox}$	d^{-1}	$b_{A,O2}$	**0.15** / 0.2	5		0.20	0.15	0.20	25
$m_{ANO,Ax}$	d^{-1}	$b_{A,NOX}$	**0.05** / 0.1	5		0.10	0.05	0.10	50
$K_{NHx,ANO}$	$g\ S_{NHx}.m^{-3}$	$K_{A,NH4}$	**1** / 1.4	5		1.40	1.00	1.40	29

k: Gujer *et al.* (2000); l: Koch *et al.* (2000). Please refer to the appendix for the parameter definitions.
*Standardised notation from Corominas *et al.* (2010) is used. n: number of parameter values in the database.

ASM3+BioP

Data description. The database contains 9 parameter sets for ASM3 + BioP, of which one is a default parameter set. The modelling studies were exclusively carried out in Germany. Half of them were carried out on full scale WWTP.

Table 5. Synthesis of database results for ASM3 + BioP model, only modified parameters are mentioned

Parameter*	Unit	Original notation	default parameters values	Optimised parameter sets characteristics					
Parameter sets			**m**	**n**	**changed >50%**	**Median**	**Perc. 25%**	**Perc. 75%**	**V (%)**
Kinetic parameters									
Ordinary Heterotrophic Organisms									
$\eta_{mOHO,Ax}$	-	$\eta_{NO,end,H}$	**0.33**	9		0.33	0.33	0.50	52
$K_{O2,OHO}$	$g\ S_{O2}.m^{-3}$	$K_{O,H}$	**0.2**	9		0.200	0.200	0.500	150
Phosphorus Accumulating Organisms									
$q_{PAO,PO4\_PP}$	$g\ X_{PP}\cdot g\ X_{PAO}^{-1}.d^{-1}$	q_{PP}	**1.5**	9	X	1.50	1.50	2.30	53
$f_{PP\_PAO,Max}$	$g\ X_{PP}\cdot g\ X_{PAO}^{-1}$	$K_{max,PAO}$	**0.2**	9	X	1.00	0.24	1.00	76
Autotrophic Nitrifying Organisms									
$\mu_{ANO,Max}$	d^{-1}	μ_{A}	**0.9 - 1.8**	9	X	1.20	1.10	1.60	42
$K_{O2,ANO}$	$g\ S_{O2}.m^{-3}$	$K_{O,A}$	**0.5**	9	X	0.18	0.13	0.50	206

m: Rieger *et al.* (2001). Please refer to the appendix for the parameter definitions.
*Standardised notation from Corominas *et al.* (2010) is used. n: number of parameter values in the database.

Barker & Dold model

The database contains 6 parameter sets for the Barker & Dold model, 2 of which are default parameter sets. Two of the modelling studies were carried out in North-America, one in Africa and one in Oceania. The modelling studies mainly concern full scale WWTP with domestic influent (3).

Table 6. Synthesis of database results for Barker & Dold model, only modified parameters are mentioned

Parameter*	Unit	Original notation	default parameters values	n	Optimised parameter sets characteristics				
Parameter sets			**n** / o		changed >50%	Median	Perc. 25%	Perc. 75%	V (%)
Conversion coefficient									
i_{N_SU}	g N.g S_U^{-1}	$f_{N,SEP}$	0.034 / **0.07**	5		0.070	0.034	0.070	51
i_{N_OHO}	g N.g X_{OHO}^{-1}	$f_{N,ZH}$	**0.07**	6	X	0.069	0.068	0.070	3
$i_{N\_XUE,OHO}$	g N.g X_{UE}^{-1}	$f_{N,ZEH}$	0.034 / **0.07**	6		0.069	0.034	0.070	52
$i_{N\_XUE,PAO}$	g N.g X_{UE}^{-1}	$f_{N,ZEP}$	0.034 / **0.07**	6		0.070	0.034	0.070	51
$i_{N\_XUE,ANO}$	g N.g X_{UE}^{-1}	$f_{N,ZEA}$	0.034 / **0.07**	6		0.068	0.034	0.068	50
Kinetic parameters									
Ordinary Heterotrophic Organisms									
$\eta_{\mu OHO,Ax}$	-	η_{gro}	**0.37**	6		0.37	0.37	0.50	35
$K_{O2,OHO}$	g $S_{O2}.m^{-3}$	$K_{O,HET}$	**0.002** / 0.05	6		0.002	0.002	0.050	2400
Phosphorus Accumulating Organisms									
$K_{PP,PAO}$	g $X_{PP}.m^{-3}$	K_{XP}	0.01 / **0.05**	6	X	0.010	0.010	0.010	0
Autotrophic Nitrifying Organisms									
$\mu_{ANO,Max}$	d^{-1}	μ_A	**0.6** / 0.9	6	X	0.73	0.60	0.90	41
b_{ANO}	d^{-1}	b_A	**0.04** / 0.17	6	X	0.08	0.04	0.17	163
$K_{O2,ANO}$	g $S_{O2}.m^{-3}$	$K_{O,AUT}$	0.25 / **0.5**	6		0.50	0.25	0.50	50
$K_{NHx,ANO}$	g $S_{NHx}.m^{-3}$	K_{NH}	0.5 / **1**	6		1.00	0.50	1.00	50

n: Barker & Dold (1997); o: Questionnaire (based on >100 modelling project studies)
*Standardised notation from Corominas *et al.* (2010) is used. n: number of parameter values in the database.
Please refer to the appendix for the parameter definitions.

Database References

Abusam A., Keesman K.J., Van Straten G., Spanjers H. and Meinema K. (2001) Sensitivity analysis in oxidation ditch modelling: The effect of variations in stoichiometric, kinetic and operating parameters on the performance indices. *J. Chem. Technol. Biot.*, **76**(4), 430-438.

Baetens D. (2001) *Enhanced biological phosphorus removal: Modelling and experimental design*. PhD thesis, BIOMATH Faculteit Landbouwkundige en Toegepaste Biologische Wetenschappen, Ghent University, Gent, Belgium.

Barker P.S. and Dold P.L. (1997) General model for biological nutrient removal activated-sludge systems: Model presentation. *Water Environ. Res.*, **69**(5), 969-984.

Bornemann C., Londong J., Freund M., Nowak O., Otterpohl R. and Rolfs T. (1998) Hinweise zur dynamischen Simulation von Belebungsanlagen mit dem Belebtschlammodell Nr. 1 der IAWQ. *Korrespondenz Abwasser*, **45**(3), 455-462, [in German].

Brun R., Kuehni M., Siegrist H., Gujer W. and Reichert P. (2002) Practical identifiability of ASM2d parameters - Systematic selection and tuning of parameter subsets. *Water Res.*, **36**(16), 4113-4127.

Chachuat B., Roche N. and Latifi M.A. (2005) Optimal aeration control of industrial alternating activated sludge plants. *Biochem. Eng. J.*, **23**(3), 277-289.

Choubert J.-M., Stricker A.-E., Marquot A., Racault Y., Gillot S. and Héduit A. (2009) Updated Activated Sludge Model n1 parameter values for improved prediction of nitrogen removal in activated sludge processes: Validation at 13 full-scale plants. *Water Environ. Res.*, **81**, 858-865.

Cinar O., Daigger G.T. and Graef S.P. (1998) Evaluation of IAWQ Activated Sludge Model No. 2 using steady-state data from four full-scale wastewater treatment plants. *Water Environ. Res.*, **70**(6), 1216-1224.

de la Sota A., Larrea L., Novak L., Grau P. and Henze M. (1994) Performance and model calibration of R-D-N processes in pilot plant. *Water Sci. Technol.*, **30**(6 pt 6), 355-364.

Ferrer J., Morenilla J.J., Bouzas A. and Garcia-Usach F. (2004) Calibration and simulation of two large wastewater treatment plants operated for nutrient removal. *Water Sci. Technol.*, **50**(6), 87-94.

Funamizu N. and Takakuwa T. (1994) Simulation of the operating conditions of the municipal wastewater treatment plant at low temperatures using a model that includes the IAWPRC activated sludge model. *Water Sci. Technol.*, **30**(4), 105-113.

Garcia-Usach F., Ferrer J., Bouzas A. and Seco A. (2006) Calibration and simulation of ASM2d at different temperatures in a phosphorus removal pilot plant. *Water Sci. Technol.*, **53**(12), 199-206.

Gokcay C.F. and Sin G. (2004) Modeling of a large-scale wastewater treatment plant for efficient operation. *Water Sci. Technol.*, **50**(7), 123-130.

Grady C.P.L J., Daigger G.T. and Lim H.C. (1999) *Biological Wastewater Treatment - Second Edition, revised and expanded*, 1076 pp., Marcel Dekker, New York.

Gujer W., Henze M., Mino T. and Van Loosdrecht M. (2000) Activated Sludge Model No.3, in *Activated Sludge Models ASM1, ASM2, ASM2d and ASM3*. edited by M. Henze, *et al*., IWA Publishing, London, UK.

Henze M., Grady C.P.L J., Gujer W., Marais Gv R. and Matsuo T. (2000a) Activated Sludge Model No.1, in *Activated Sludge Models ASM1, ASM2, ASM2d and ASM3*. edited by M. Henze, *et al*., IWA Publishing, London, UK.

Henze M., Gujer W., Mino T., Matsuo T., Wentzel M.C., Marais G.v.R. and van loosdrecht M. (2000b) Activated Sludge Model No.2d, in *Activated Sludge Models ASM1, ASM2, ASM2d and ASM3*. edited by M. Henze, *et al*., IWA Publishing, London, UK.

Hu Z.R., Wentzel M.C. and Ekama G.A. (2007a) A general kinetic model for biological nutrient removal activated sludge systems: Model development. *Biotechnol. Bioeng.*, **98**(6), 1242-1258.

Hu Z.R., Wentzel M.C. and Ekama G.A. (2007b) A general kinetic model for biological nutrient removal activated sludge systems: Model evaluation. *Biotechnol. Bioeng.*, **98**(6), 1259-1275.

Hulsbeek J.J.W., Kruit J., Roeleveld P.J. and van Loosdrecht M.C.M. (2002) A practical protocol for dynamic modelling of activated sludge systems. *Water Sci. Technol.*, **45**(6), 127-136.

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

Lagarde F. (2003) *Optimisation du traitement de l'azote et du carbone par boues activées en temps de pluie à basse température*. PhD thesis, Sciences et Techniques de l'Environnement, Université Paris XII Val de Marne, Paris, France. [in French].

Lessard P., Tusseau-Vuillemin M.H., Héduit A. and Lagarde F. (2007) Assessing chemical oxygen demand and nitrogen conversions in a multi-stage activated sludge plant with alternating aeration. *J. Chem. Technol. Biot.*, **82**, 367-375.

Lubken M., Wichern M., Rosenwinkel K.H. and Wilderer P.A. (2003) Efficiency of different mathematical models for simulating enhanced biological phosphorus removal in activated sludge systems. *Environmental Informatics Archives*, **1**, 339-347.

Makinia J., Rosenwinkel K.H. and Spering V. (2005a) Long-term simulation of the activated sludge process at the Hanover-Gummerwald pilot WWTP. *Water Res.*, **39**(8), 1489-1502.

Makinia J., Rosenwinkel K.H. and Spering V. (2006a) Comparison of two model concepts for simulation of nitrogen removal at a full-scale biological nutrient removal pilot plant. *J. Environ. Eng.-ASCE*, **132**(4), 476-487.

Makinia J., Rosenwinkel K.H., Swinarski M. and Dobiegala E. (2006b) Experimental and model-based evaluation of the role of denitrifying polyphosphate accumulating organisms at two large scale WWTPs in northern Poland. *Water Sci. Technol.*, **54**(8), 73-81.

Makinia J., Swinarski M. and Rosenwinkel K.H. (2005b) Dynamic simulation as a tool for evaluation of the nitrogen removal capabilities at the "Gdansk-Wschod" WWTP. In: Proceedings IWA Specialized Conference - Nutrient Management in Wastewater Treatment Process and Recycle Streams, Krakow, Poland, 19-21 September 2005.

Makinia J. and Wells S.A. (2000) A general model of the activated sludge reactor with dispersive flow - I. Model development and parameter estimation. *Water Res.*, **34**(16), 3987-3996.

Marquot A. (2006) *Modelling nitrogen removal by activated sludge on full-scale plants: Calibration and evaluation of ASM1*. PhD thesis, Ecole doctorale des Sciences Exactes et de leurs Applications, Université de Pau et des Pays de l'Adour (UPPA), Bordeaux, France.

Marquot A., Stricker A.E. and Racault Y. (2006) ASM1 dynamic calibration and long-term validation for an intermittently aerated WWTP. *Water Sci. Technol.*, **53**(12), 247-256.

Meijer S.C.F. (2004) *Theoretical and practical aspects of modelling activated sludge processes*. PhD thesis, Department of Biotechnological Engineering, Delft University of Technology, Delft, The Netherlands.

Meijer S.C.F., Van Loosdrecht M.C.M. and Heijnen J.J. (2001) Metabolic modelling of full-scale biological nitrogen and phosphorus removing WWTP's. *Water Res.*, **35**(11), 2711-2723.

Nuhoglu A., Keskinler B. and Yildiz E. (2005) Mathematical modelling of the activated sludge process - The Erzincan case. *Process Biochem.*, **40**(7), 2467-2473.

Obara T., Yamanaka O. and Yamamoto K. (2006) A sequential parameter estimation algorithm for activated sludge model no.2d based on mathematical optimization and a prior knowledge for parameters. In: Proceedings IWA World Water Congress, Beijing, CHN, 10-14 September 2006

Penya-Roja J.M., Seco A., Ferrer J. and Serralta J. (2002) Calibration and validation of Activated Sludge Model No.2d for Spanish municipal wastewater. *Environ. Technol.*, **23**(8), 849-862.

Petersen B., Gernaey K., Henze M. and Vanrolleghem P.A. (2002) Evaluation of an ASM1 model calibration procedure on a municipal-industrial wastewater treatment plant. *J. Hydroinform.*, **4**(1), 15-38.

Rieger L., Koch G., Kuhni M., Gujer W. and Siegrist H. (2001) The EAWAG Bio-P module for Activated Sludge Model No. 3. *Water Res.*, **35**(16), 3887-3903.

Ronner-Holm S.G.E., Mennerich A. and Holm N.C. (2006) Specific SBR population behaviour as revealed by comparative dynamic simulation analysis of three full-scale municipal SBR wastewater treatment plants. *Water Sci. Technol.*, **54**(1), 71-80.

Sahlstedt K.E., Aurola A.M. and Fred T. (2003) Practical modelling of a large activated sludge DN-process with ASM3. In: Proceedings Ninth IWA Specialized Conference on Design, Operation and Economics of Large Wastewater Treatment Plants, Praha, Czech Republic, 1-4 September 2003.

Sin G. (2004) *Systematic calibration of activated sludge models*. PhD thesis, BIOMATH Faculteit Landbouwkundige en Toegepaste Biologische Wetenschappen, Ghent University, Gent, Belgium.

Sin G., De Pauw D.J.W., Weijers S. and Vanrolleghem P.A. (2008) An efficient approach to automate the manual trial and error calibration of activated sludge models. *Biotechnol. Bioeng.*, **100**(3), 516-528.

Spanjers H., Vanrolleghem P., Nguyen K., Vanhooren H. and Patry G.G. (1998) Towards a simulation-benchmark for evaluating respirometry-based control strategies. *Water Sci. Technol.*, **37**(12), 219-226.

Stamou A., Katsiri A., Mantziaras I., Boshnakov K., Koumanova B. and Stoyanov S. (1999) Modelling of an alternating oxidation ditch system. *Water Sci. Technol.*, **39**(4), 169-176.

Stricker A.E. (2000) *Application de la modélisation à l'étude du traitement de l'azote par boues activées en aération prolongée : comparaison des performances en temps sec et en temps de pluie*. (Français), PhD thesis, Strasbourg I - Louis Pasteur, Strasbourg, France. [in French].

Sun P. (2006) Numerical modelling COD, N and P removal in a full-scale WWTP of China. *Journal of Applied Sciences*, **6**(15), 3155-3159.

Wentzel M.C., Ekama G.A. and Marai G.V.R. (1992) Processes and modelling of nitrification denitrification biological excess phosphorus removal systems - A review. *Water Sci. Technol.*, **25**(6), 59-82.

Wichern M., Lubken M., Blomer R. and Rosenwinkel K.H. (2003) Efficiency of the Activated Sludge Model no. 3 for German wastewater on six different WWTPs. *Water Sci. Technol.*, **47**(11), 211-218.

Wichern M., Obenaus F., Wulf P. and Rosenwinkel K.H. (2001) Modelling of full-scale wastewater treatment plants with different treatment processes using the Activated Sludge Model no. 3. *Water Sci. Technol.*, **44**(1), 49-56.

Xu S. and Hultman B. (1996) Experiences in wastewater characterization and model calibration for the activated sludge process. *Water Sci. Technol.*, **33**(12), 89-98.