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# 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.


**Key words** | ASM, database, good modelling practice, parameter ranges, parameter sets, survey

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## 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 to better define the profile of ASM users and to identify the tools and procedures used. 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 and is considered as an obstacle

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for widespread model use. 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 regarding 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 constructed to synthesise the answers from the second questionnaire and literature data.

The database includes parameters for seven published activated sludge models: (1) ASM1 (Henze *et al.* 2000*a*); (2) ASM2d (Henze *et al.* 2000*b*); (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. Prior to this parameter study, all models were analysed for typos and errors (Hauduc *et al.* 2010).

## METHOD

### Source of data

#### Questionnaire

In order to completely describe each modelling study, the questionnaire asked for the objectives of the project, the description of the wastewater treatment plant (WWTP) and the parameter set used for the biokinetic model. The questionnaire was sent out in 2008 to the respondents of the first survey, to the attendees of the WWTmod2008 seminar in Mont-St-Anne, QC, Canada, and could be downloaded from GMP-TG sponsor websites.

Probably due to the higher complexity of this questionnaire, only 28 answers were received, among which 17 were usable for this study (i.e. at least one model parameter set provided).

#### Literature review

In order to have a homogeneous database, only published modelling projects applied to full-scale WWTPs or 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 in an efficient way, a database composed of three main tables was constructed:

1. **Parameter sets**: model, country, temperature, parameter values
2. **WWTP description**: information on influent, wastewater characteristics, processes and environmental conditions
3. **Model users**: user information

To facilitate parameter comparison, a new standardised notation (Corominas *et al.* 2010) was used.

#### 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. Parameter values may have different sources (see below).
- **Proposed new default parameter sets** based on personal expertise. These parameters were used as starting points for the calibration step during the project and given with an approximate number of WWTPs on which this experience was gained.

#### Sources of parameter values

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

#### Temperature adjustment

For comparison purposes, the parameter values were standardised at 20°C. The correction factor was either provided with the dataset or extracted from the original publication. For instance, in the original ASM1 and ASM2d publications, the kinetic parameters only are given at 10°C and 20°C. The correction factor $\theta_{pow}$ has thus been recalculated following the equation $k_{10°C} = k_{20°C} {*} \theta_{pow}^{10-20}$.

## Database analysis

The database was analysed for the three topics:

Original vs. proposed new default parameter sets: The parameter sets were compared and differences identified and discussed.

Parameters changed in modelling projects: Most often changed parameters (in more than 50% of the projects) are highlighted.

Parameter ranges and statistics: For each model, the following variables have been calculated:

- The median values, which should not be misinterpreted as new default parameters, because the median values are not from a single parameter set and some parameters may be correlated (e.g. growth and decay rate),
- The 25th and 75th percentiles. These percentiles have been chosen to exclude extreme values and to obtain a representative range of the typical parameter values,
- The variability (V), the difference between the two percentiles divided by the median.

These results are discussed and confronted to the knowledge on parameter values and parameter ranges of other published overview studies.

## RESULTS

### Modelling project characteristics

The database contains 76 parameter sets, which can be differentiated into 57 optimised parameter sets and 19 proposed new default parameter sets, and distributed as shown in Figure 1. ASM1 and ASM2d are the most represented models in the database.

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 other models, thus no comments are given on the results for these models. However, synthesis tables are presented in the appendix for ASM3, ASM3 + BioP and Barker & Dold model. Concerning ASM2d + TUD and UCTPHO +, no additional modelling projects than those in the original publication were found, the tables are thus not presented.

### ASM1

#### Data description

The database contains 31 parameter sets for ASM1, of which 9 are "proposed new default parameter" sets and 22 are "optimised parameter sets" from specific modelling projects. The modelling studies were mainly carried out at full scale WWTPs (19) mostly in Europe (18), with only 1 application in North-America and 3 in Asia. The sludge ages of the specific modelling projects are between 4 and 40 days.

Table 1 presents the main results extracted from the database including the original and the proposed new default parameter sets. Basic statistics for optimised parameter sets comprise the number of values for each parameter (n), if the parameter has been modified in more than 50% of the cases (Modif. >50%), the median value (Med.), the 25th and 75th percentiles and the variability (V). The proposed new default parameter sets are by definition based on several simulation studies and therefore present more experience than single

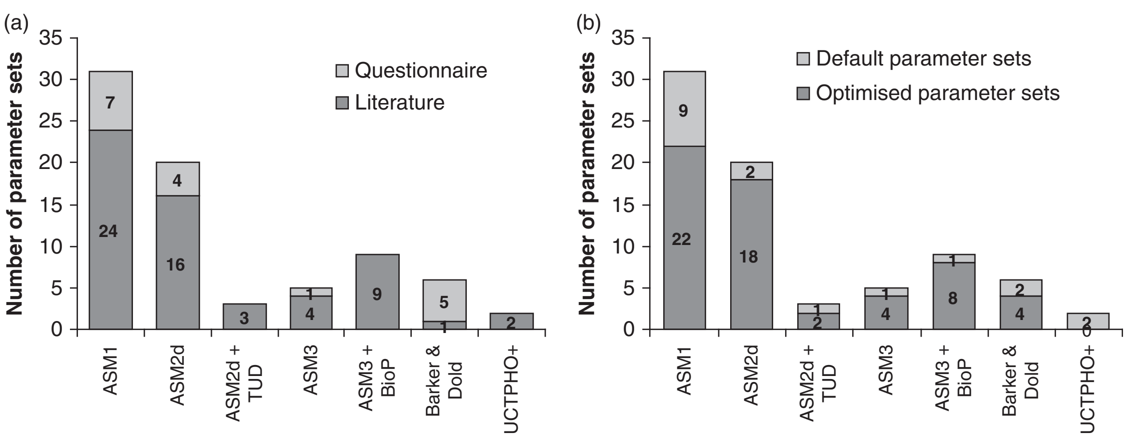


**Figure 1** | Distribution of parameter sets per model: a) per source; b) per class of parameter set.

**Table 1** | Synthesis of database results for ASM1, only modified parameters are mentioned. Parameter values are standardised at a temperature of 20°C

| | | | Original parameter set | | Optimised parameter sets | | | | | | Proposed new default parameters |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Parameter* | Unit | Description | Notation | Value (a) | n | Modif >50% | Med. | Perc. 25% | Perc. 75% | V (%) | Parameter sets: b/c/d/e/f/g/h/i |
| **Stoichiometric parameters** | | | | | | | | | | | |
| $Y_{OHO}$ | g $X_{OHO}$ g $XC_B^{-1}$ | Yield for $X_{OHO}$ growth | $Y_H$ | **0.67** | 26 | X | **0.67** | 0.62 | 0.67 | 7 | 0.6(*c;i*) $Y_{OHO.Ox}$: 0.67 and $Y_{OHO.Ax}$: 0.54 (b;f;h) |
| **Conversion coefficient** | | | | | | | | | | | |
| $i_{N\_XBio}$ | g N g $X_{Bio}^{-1}$ | N content of biomass ($X_{OHO}$, $X_{ANO}$) | $i_{X,B}$ | **0.086** | 31 | | **0.086** | 0.079 | 0.086 | 8 | 0.08(*c;g*) |
| **Kinetic parameters** | | | | | | | | | | | |
| **Hydrolysis** | | | | | | | | | | | |
| $q_{XCB\_SB,hyd}$ | g $XC_B$ g $X_{OHO}^{-1}$ $d^{-1}$ | Maximum specific hydrolysis rate | $k_h$ | **3** | 31 | | **3** | 2.2 | 3 | 26 | 2(*c*)/2.21(*i*)/5.2(*g*) |
| $\theta_{qXCB\_SB,-hyd}$ | - | Temperature correction factor for $q_{XCB\_SB,hyd}$ | $\theta_{kh}$ | **1.116** | 11 | X | **1.116** | 1.072 | 1.12 | 4 | 1.072(*f*) |
| $K_{XCB,hyd}$ | g $XC_B$ g $X_{OHO}^{-1}$ | Half-saturation coefficient for $XC_B/X_{OHO}$ | $K_X$ | **0.03** | 30 | | **0.03** | 0.03 | 0.03 | 0 | 0.02(*c*)/0.17(*g*)/0.15(*i*) |
| $\theta_{KXCB,hyd}$ | - | Temperature correction factor for $K_{XCB,hyd}$ | $\theta_{KX}$ | **1.116** | 10 | X | **1.116** | 1.116 | 1.12 | 0 | 1(*f*) |
| $\eta_{qhyd,Ax}$ | - | Correction factor for hyd. under anoxic cond. | $\eta_h$ | **0.4** | 31 | | **0.4** | 0.4 | 0.5 | 25 | 0.5(*g*)/ 0.6(*d*) $n_{qhyd.An}$: 0.75(*d*) |
| **Ordinary Heterotrophic Organisms** | | | | | | | | | | | |
| $\mu_{OHO,Max}$ | $d^{-1}$ | Maximum growth rate of $X_{OHO}$ | $\mu_H$ | **6** | 31 | | **6** | 5.7 | 6 | 6 | 4(*d*)/5.7(*g*) |
| $\theta_{\mu OHO,Max}$ | - | Temperature correction factor for $\mu_{OHO,Max}$ | $\theta_{\mu H}$ | **1.072** | 11 | X | **1.072** | 1.071 | 1.09 | 2 | |
| $\eta_{\mu OHO,Ax}$ | - | Reduction factor for anoxic growth of $X_{OHO}$ | $\eta_g$ | **0.8** | 31 | | **0.8** | 0.8 | 0.8 | 0 | 0.6(*c*) |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $K_{SB,OHO}$ | g $S_B$ $m^{-3}$ | Half-saturation coefficient for $S_B$ | $K_S$ | **20** | 31 | | **20** | 10 | 20 | 50 | 5(*d*)/10(*g*) |
| $b_{OHO}$ | $d^{-1}$ | Decay rate for $X_{OHO}$ | $b_H$ | **0.62** | 31 | | **0.62** | 0.61 | 0.62 | 2 | 0.4(*d*)/0.41(*i*)/0.5(*c*)/0.53(*g*) |
| $\theta_{bOHO}$ | - | Temperature correction factor for $b_{OHO}$ | $\theta_{bH}$ | **1.12** | 11 | X | **1.1** | 1.029 | 1.12 | 8 | 1.029(*f*)/ 1.071(*c;d*) |
| $K_{O2,OHO}$ | g $S_{O2}$ $m^{-3}$ | Half-saturation coefficient for $S_{O2}$ | $K_{OH}$ | **0.2** | 31 | | **0.2** | 0.2 | 0.2 | 0 | 0.05(*f*)/0.1(*i*) |
| $K_{NOx,OHO}$ | g $S_{NOx}$ $m^{-3}$ | Half-saturation coefficient for $S_{NOx}$ | $K_{NO}$ | **0.5** | 31 | | **0.5** | 0.1 | 0.5 | 80 | 0.1(*f*)/0.2(*i*) |
| **Autotrophic Nitrifying Organisms** | | | | | | | | | | | |
| $\mu_{ANO,Max}$ | $d^{-1}$ | Maximum growth rate of $X_{ANO}$ | $\mu_A$ | **0.8** | 30 | X | **0.8** | 0.66 | 0.9 | 30 | 0.77(*i*)/0.82(*g*)/ 0.85(*c*)/ 0.9(*b; d*) |
| $\theta_{\mu ANO,Max}$ | - | Temperature correction factor for $\mu_{ANO,Max}$ | $\theta_{\mu A}$ | **1.103** | 14 | X | **1.103** | 1.059 | 1.11 | 5 | 1.059(*f; h*)/ 1.072(*b*) |
| $b_{ANO}$ | $d^{-1}$ | Decay rate for $X_{ANO}$ | $b_A$ | **0.5-0.15** | 30 | X | **0.1** | 0.08 | 0.15 | 70 | 0.07(*g*)/0.096(*i*)/0.17(*b; f; h*) |
| $\theta_{bANO}$ | - | Temperature correction factor for $b_{ANO}$ | $\theta_{bA}$ | **1.072** | 12 | X | **1.07** | 1.029 | 1.072 | 4 | 1.027(*f; h*)/1.083(*d*)/ 1.103(*c*) |
| $q_{am}$ | $m^3$ g $X_{CB,N}^{-1}$ $d^{-1}$ | Rate constant for ammonification | $k_a$ | **0.08** | 29 | | **0.08** | 0.07 | 0.08 | 12 | 0.05(*g*)/0.16(*i*) |
| $\theta_{qam}$ | - | Temperature correction factor for $q_{am}$ | $\theta_{ka}$ | **1.072** | 11 | | **1.07** | 1.07 | 1.07 | 0 | 1.071(*d; c*) |
| $K_{O2,ANO}$ | g $S_{O2}$ $m^{-3}$ | Half-saturation coefficient for $S_{O2}$ | $K_{OA}$ | **0.4** | 31 | | **0.4** | 0.4 | 0.4 | 0 | 0.2(*f*)/0.5(*c*)/0.75(*i*) |
| $K_{NHx,ANO}$ | g $S_{NHx}$ $m^{-3}$ | Half-saturation coefficient for $S_{NHx}$ | $K_{NH}$ | **1** | 31 | | **1** | 0.75 | 1 | 25 | 0.1(*f*)/0.5(*d*) |

a: Henze *et al*. (2000a); b, c: 2 answers from the 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.

studies. Consequently, they are presented on the same level as the median of all the optimised parameter sets.

Original vs. proposed new default parameter set: Only 3 parameters (out of 26) have not been changed compared to the original value: the autotrophic growth yield ($Y_{ANO}$), the fraction of particulate unbiodegradable organics generated in biomass decay ($f_{XU\_Bio,lys}$) and the nitrogen content of unbiodegradable organics generated in biomass decay ($i_{N\_XUE}$).

A change in ASM1 model structure for the ordinary heterotrophic yield ($Y_{OHO}$) value by introducing an ordinary heterotrophic yield under anoxic conditions is suggested in three of the proposed new default parameter sets.

Parameters changed in modelling projects (compared to original values): for each parameter set, a majority of parameters are kept at their default values. Only the autotrophic growth yield ($Y_{ANO}$) is always kept at its original value. Nine parameters were changed in more than half of the modelling studies: 6 temperature correction factors, 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 (Stamou et al. 1999; Makinia & Wells 2000; Petersen et al. 2002; Nuhoglu et al. 2005). 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 in the original parameter set. The variability is quite narrow (<33%), except for the half-saturation coefficients for substrate ($K_{SB,OHO}$) and nitrate ($K_{NOx,OHO}$) and the autotrophic decay rate ($b_{ANO}$).

## Discussion

Original vs. 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). The authors showed 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 $0.19 \pm 0.4$ $d^{-1}$). Choubert et al. (2009b) proposed 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 in France.

Parameters changed in modelling projects (compared to original values): Similar to the proposed new default parameter sets a reduced heterotrophic growth rate ($Y_{OHO}$) is often associated with plants with anoxic and/or anaerobic zones. This confirms the need to differentiate aerobic and anoxic growth yields.

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 sometimes 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 generally in agreement with other overview studies, which ranges were not included in the database (Weijers & Vanrolleghem 1997; Bornemann et al. 1998; Hulsbeek et al. 2002; Cox 2004; Sin et al. 2009). However, the ranges from the database differ from these studies for the following parameters:

- $\mu_{OHO,Max}$ and $b_{OHO}$ ranges proposed by Weijers & Vanrolleghem (1997) are wider (respectively 2–10 $d^{-1}$; 0.1–1.5 $d^{-1}$);
- $K_{SB,OHO}$, $b_{OHO}$ and $K_{NHx,ANO}$ in Bornemann et al. (1998) have different and not overlapping ranges (respectively 1–5 g $S_B$ $m^{-3}$; 0.3–0.5 $d^{-1}$; 0.1–0.7 g $S_{NHx}$ $m^{-3}$);
- The median values provided by Cox (2004) are quite different from the database ones (up to 100% of relative difference); 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 not overlapping the database ones (respectively 2.06–4.69 $d^{-1}$; 0.2–0.6 $d^{-1}$; 2.54–7.06 g $S_B$ $m^{-3}$);
- Sin et al. (2009) provided "uncertainties" (or better variabilities) based on expert knowledge. Two parameter variabilities ($\mu_{ANO,Max}$, $b_{ANO}$) are narrower than the observed variability in this study (respectively 5% and 25%) and 8 much wider (50% of variability for $i_{N\_XBio}$, $K_{O2,OHO}$, $q_{am}$, $K_{NHx,ANO}$; 25% of variability for $K_{XCB,hyd}$, $\mu_{OHO,Max}$, $\eta_{\mu OHO,Ax}$, $K_{O2,ANO}$).

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 its value was modified in none of the 22 modelling projects.

## 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 supported by the literature data although the chosen 25$^{th}$ and 75$^{th}$ 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 "optimised parameter sets" from specific modelling projects. The modelling studies were mainly carried out in Europe (16), with only two applications in Asia; and mainly on full scale WWTPs (12). Table 2 synthesises the main results for ASM2d. The sludge ages of the specific modelling projects are between 7 and 22 days.

Original vs. 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 in fact ASM2 and not ASM2d.

Parameters changed in modelling projects (compared to original values): The majority of the parameters are kept at their original values, from which 33 (of the 83 parameters) have never been changed:

- 4 of the 11 stoichiometric parameters: 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: $i_{N\_SF}$, $i_{N\_XBio}$, $i_{P\_SF}$, $i_{P\_SU}$, $i_{TSS\_XCB}$, $i_{TSS\_XPAO,PHA}$ and $i_{TSS\_XPAO,PP}$.
- 22 of the 57 kinetic parameters: the alkalinity half-saturation parameters ($K_{Alk,OHO}$, $K_{Alk,PAO}$, $K_{Alk,ANO}$); heterotrophic half-saturation parameters for nutrients ($K_{NHx,OHO}$, $K_{PO4,OHO}$); autotrophic half-saturation parameters for nutrients ($K_{PO4,ANO}$); 5 phosphorus accumulating organism half-saturation parameters ($K_{S,fPP\_PAO}$, $K_{O2,PAO}$, $K_{NOx,PAO}$, $K_{NHx,PAO}$, $K_{PO4,PAO,upt}$); the half-saturation parameters for dissolved oxygen and nitrates in the hydrolysis process ($K_{O2,hyd}$, $K_{NOx,hyd}$); 6 of the 12 temperature correction factors ($\theta_{q\_XCB\_SB,hyd}$, $\theta_{\mu\_OHO,Max}$, $\theta_{q\_SF\_Ac,Max}$, $\theta_{b\_OHO}$, $\theta_{\mu\_ANO,Max}$, $\theta_{b\_ANO}$); and the chemical phosphorus precipitation parameters ($q_{P,pre}$, $q_{P,red}$, $K_{Alk,pre}$).

Two types of modelling studies could be distinguished:

- Studies with a calibrated parameter subset (12 studies). These are mainly composed of kinetic parameters;
- Studies with measured parameters (6 studies), among which 4 studies use the calibration protocol of Penya-Roja *et al.* (2002) (Penya-Roja *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 phosphorus accumulating organisms.

Among the 18 modelling studies, 8 parameters - all of which are kinetic parameters - were changed in more than half of the cases: the heterotrophic and autotrophic maximum growth rates ($\mu_{OHO,Max}$, $\mu_{ANO,Max}$), the autotrophic half-saturation coefficient for ammonia ($K_{NHx,ANO}$), the rate constants for volatile fatty acids (VFA) uptake ($q_{PAO,VFA\_Stor}$) and for polyphosphate storage ($q_{PAO,PO4\_PP}$) of the PAO and their storage pools' decay ($m_{PAO}$, $b_{PP\_PO4}$, $b_{Stor\_VFA}$).

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

### Discussion

Parameters changed in modelling projects (compared to original values): Among the eight parameters that were changed most, two have a particularly wide range of values: the rate constants for VFA uptake ($q_{PAO,VFA\_Stor}$) and polyphosphate storage ($q_{PAO,PO4\_PP}$). Furthermore, the users of the Penya-Roja *et al.* (2002) protocol observed large parameter ranges for PAO growth and polyphosphates storage yields ($Y_{PAO}$, $Y_{PP\_Stor,PAO}$). This could indicate a problem in the ASM2d model structure, such as the simplification of not

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

| Parameter* | Unit | Description | Original notation | Original parameter set j | Optimised parameter sets n | Modif. >50% | Median | Perc. 25% | Perc. 75% | V (%) |
|---|---|---|---|---|---|---|---|---|---|---|
| **Kinetic parameters** | | | | | | | | | | |
| **Hydrolysis** | | | | | | | | | | |
| $\eta_{qhyd,Ax}$ | - | Correction factor for hydrolysis under anoxic conditions | $\eta_{NO3}$ | **0.6** | 20 | | **0.6** | 0.6 | 0.8 | 33 |
| $\eta_{qhyd,A\eta}$ | - | Correction factor for hydrolysis under anaerobic conditions | $\eta_{fe}$ | **0.4** | 20 | | **0.4** | 0.2 | 0.4 | 50 |
| **Ordinary Heterotrophic Organisms** | | | | | | | | | | |
| $\mu_{OHO,Max}$ | $d^{-1}$ | Maximum growth rate of $X_{OHO}$ | $\mu_H$ | **6** | 20 | X | **6** | 4 | 6 | 33 |
| $\eta_{\mu OHO,Ax}$ | - | Reduction factor for anoxic growth of $X_{OHO}$ | $\eta_{NO3}$ | **0.8** | 20 | | **0.8** | 0.8 | 0.8 | 0 |
| **Phosphorus Accumulating Organisms** | | | | | | | | | | |
| $q_{PAO,VFA\_Stor}$ | g $X_{Stor}$ g $X_{PAO}^{-1}$ $d^{-1}$ | Rate constant for $S_{VFA}$ uptake rate ($X_{PAO,Stor}$ storage) | $q_{PHA}$ | **3** | 20 | X | **3.4** | 3 | 6 | 90 |
| $q_{PAO,PO4\_PP}$ | g $X_{PP}$ g $X_{PAO}^{-1}$ $d^{-1}$ | Rate constant for storage of $X_{PAO,PP}$ | $q_{PP}$ | **1.5** | 20 | X | **1.5** | 1.5 | 3.3 | 120 |
| $\mu_{PAO,Max}$ | $d^{-1}$ | Maximum growth rate of $X_{PAO}$ | $\mu_{PAO}$ | **1** | 20 | | **1** | 1 | 1.04 | 4 |
| $\theta_{\mu PAO,Max}$ | - | Temperature correction factor for $\mu_{PAO,Max}$ | $\theta_{\mu PAO}$ | **1.041** | 3 | | **1.041** | 1.0-41 | 1.0-58 | 2 |
| $m_{PAO}$ | $d^{-1}$ | Endogenous respiration rate of $X_{PAO}$ | $b_{PAO}$ | **0.2** | 20 | X | **0.2** | 0.15 | 0.2 | 25 |
| $b_{PP\_PO4}$ | $d^{-1}$ | Rate constant for lysis of $X_{PAO,PP}$ | $b_{PP}$ | **0.2** | 20 | X | **0.2** | 0.15 | 0.2 | 25 |
| $b_{Stor\_VFA}$ | $d^{-1}$ | Rate constant for respiration of $X_{PAO,Stor}$ | $b_{PHA}$ | **0.2** | 20 | X | **0.2** | 0.15 | 0.2 | 25 |
| **Autotrophic Nitrifying Organisms** | | | | | | | | | | |
| $\mu_{ANO,Max}$ | $d^{-1}$ | Maximum growth rate of $X_{ANO}$ | $\mu_{AUT}$ | **1** | 20 | X | **1** | 1 | 1.15 | 15 |
| $b_{ANO}$ | $d^{-1}$ | Decay rate for $X_{ANO}$ | $b_{AUT}$ | **0.15** | 20 | | **0.15** | 0.15 | 0.16 | 7 |
| $K_{NHx,ANO}$ | g $S_{NHx}$ $m^{-3}$ | Half-saturation coefficient for $S_{NHx}$ | $K_{NH4}$ | **1** | 20 | X | **1** | 0.5 | 1 | 50 |

j: **Henze *et al.* (2000*b*)**. 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.

taking into account glycogen storage and glycogen accumulating organisms in ASM2d (Penya-Roja *et al.* 2002).

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 link both yields to energy production (in metabolic models, e.g.: Meijer 2004) or model PAO growth and polyphosphate storage as a single process (Barker & Dold model, UCTPHO+). Fixing the ratio between growth and phosphate storage would then assist ASM2d calibration.

Parameter ranges and statistics: Based on expert knowledge, Brun *et al.* (2002) assigned an uncertainty to each parameter. The database is in agreement with the low uncertainties (between 5% and 20%) attributed to stoichiometric parameters and conversion coefficients parameters by Brun *et al.* (2002). In Brun *et al.* (2002), high uncertainty is attributed to kinetic parameters (between 20% and 50% of uncertainty), which are overestimated based on the database results for all the parameters, except for the reduction factors for hydrolysis under anoxic and anaerobic conditions ($\eta_{qhyd,Ax}$, $\eta_{qhyd,An}$), the rate constants for VFA uptake ($q_{PAO,VFA\_Stor}$) and polyphosphate storage ($q_{PAO,PO4\_PP}$).

### Conclusion

The main potential pitfalls in calibrating ASM2d seem to come from the determination of the rate constants for VFA uptake ($q_{PAO,VFA\_Stor}$) and polyphosphate storage ($q_{PAO,PO4\_PP}$). These two parameters are used in organic compound storage and consumption processes, and their high variability could indicate a problem in the model structure leading to difficulties in the calibration process.

## GENERAL DISCUSSION

### Inter-model comparison

In both ASM1 and ASM2d, few parameters have been changed in more than half the cases considered. This shows that either 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 the 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
- Autotrophic half-saturation coefficient ammonia.

The half-saturation coefficients are thought to be dependent on specific 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: tank configuration, tank dimensions, 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 for data validation and reconciliation;
- method used to optimise the parameter set: protocol, parameters set to original value;
- temperature for which the optimised parameter set is provided.

This lack of information prevents further analysis of the database, such as an investigation of correlations. It also makes it difficult to evaluate the quality of the modelling projects. Thus, the modelling projects included in the database had to be considered to be of equal quality. The differences within parameter values therefore are supposed to be linked to the WWTP conditions and not to a wrong calibration or poor data quality.

It should also be noted that there seems to be a lack of (published) experimental data with respect to parameter values. If parameters were measured it is often difficult to evaluate the results due to missing information on the measurement method.

### Potential use of the database

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

The database has been designed to allow future extensions with new data sets. 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;
- provide a synthesis of practical modelling experiences that could help model users to find appropriate case studies similar to their simulation project;
- examine correlation between parameters and analyse its impact on calibration practice (e.g. $b_{ANO}$ and $\mu_{ANO}$);
- examine correlations between changes in parameter values and WWTP conditions;
- determine practical model limits from various modelling experiences;
- identify 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 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 or specific environmental conditions.

These results contribute to the knowledge transfer on activated sludge modelling that was requested by respondents of the first survey. 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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# 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 $m^{-3}$ | | $X_{PP}$ | | $X_{PP}$ | |

**Table 3** | (continued)

| Description | Parameter* | Unit | ASM1 | ASM2d | ASM3 | ASM3 + BioP | Barker & Dold |
|---|---|---|---|---|---|---|---|
| **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 $q_{XCB\_SB,hyd}$ | $\theta_{qXCB\_SB,hyd}$ | - | $\theta_{kh}$ | | | | |
| Half-saturation coefficient for $XC_B/X_{OHO}$ | $K_{XCB,hyd}$ | g $XC_B$ g $X_{OHO}{}^{-1}$ | $K_X$ | | | | |
| Temperature correction factor for $K_{XCB,hyd}$ | $\theta_{KXCB,hyd}$ | | $\theta_{KX}$ | | | | |
| Correction factor for hydrolysis under anoxic conditions | $\eta_{qhyd,Ax}$ | - | $\eta_h$ | $\eta_{NO3}$ | | | $\eta_{gro}$ |
| Correction factor for hydrolysis under anaerobic conditions | $\eta_{qhyd,An}$ | - | | $\eta_{fe}$ | | | |
| **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 $X_{OHO}$ | $\mu_{OHO,Max}$ | $d^{-1}$ | $\mu_H$ | $\mu_H$ | $\mu_H$ | | |
| Temperature correction factor for $\mu_{OHO,Max}$ | $\theta_{\mu OHO,Max}$ | - | $\theta_{\mu H}$ | | | | |
| Reduction factor for anoxic growth of $X_{OHO}$ | $\eta_{\mu OHO,Ax}$ | - | $\eta_g$ | $\eta_{NO3}$ | $\eta_{NOX}$ | | |
| 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 $X_{OHO}$ | $b_{OHO}$ | $d^{-1}$ | $b_H$ | | | | |

**Table 3** | *(continued)*

| Description | Parameter* | Unit | ASM1 | ASM2d | ASM3 | ASM3 + BioP | Barker & Dold |
|---|---|---|---|---|---|---|---|
| Temperature correction factor for $b_{OHO}$ | $\theta_{bOHO}$ | | $\theta_{bH}$ | | | | |
| 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 $X_{PAO}$ | $\mu_{PAO,Max}$ | $d^{-1}$ | | $\mu_{PAO}$ | | | |
| 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 $X_{ANO}$ | $\mu_{ANO,Max}$ | $d^{-1}$ | $\mu_A$ | $\mu_{AUT}$ | $\mu_A$ | $\mu_A$ | $\mu_A$ |
| 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 $b_{ANO}$ | $\theta_{bANO}$ | | $\theta_{bA}$ | | | | |
| 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 $q_{am}$ | $\theta_{qam}$ | - | $\theta_{ka}$ | | | | |
| 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 1 is a "proposed new default parameter sets", and 3 are "optimised parameter sets". The modelling studies were exclusively carried out in the North of Europe (Belgium, Finland, Germany) on full scale WWTPs. Table 4 synthesises the main results for ASM3.

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

| Parameter* | Unit | Original parameter set | | Proposed new default parameter set | Optimised parameter sets | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Parameter sets | | Notation | Value (k) | l | n | Modif >50% | Median | Perc. 25% | Perc. 75% | V (%) |
| **Stoichiometric parameters** | | | | | | | | | | |
| $Y_{Stor\_OHO,Ox}$ | $g\ X_{OHO}\ g\ X_{Stor}^{-1}$ | $Y_{H,O2}$ | **0.85** | 0.8 | 5 | | 0.80 | 0.80 | 0.80 | 0 |
| $Y_{Stor\_OHO,Ax}$ | $g\ X_{OHO}\ g\ X_{Stor}^{-1}$ | $Y_{H,NOX}$ | **0.8** | 0.7 | 5 | | 0.70 | 0.70 | 0.70 | 0 |
| $Y_{SB\_Stor,Ox}$ | $g\ X_{Stor}\ g\ S_B^{-1}$ | $Y_{STO,O2}$ | **0.63** | 0.8 | 5 | | 0.80 | 0.63 | 0.80 | 21 |
| $Y_{SB\_Stor,Ax}$ | $g\ X_{Stor}\ g\ S_B^{-1}$ | $Y_{STO,NOX}$ | **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 |
| $i_{N\_XCB}$ | $g\ N\ g\ X_{CB}^{-1}$ | $i_{N,XS}$ | **0.04** | 0.03 | 5 | | 0.030 | 0.030 | 0.030 | 0 |
| **Kinetic parameters** | | | | | | | | | | |
| **Hydrolysis** | | | | | | | | | | |
| $q_{XCB\_SB,hyd}$ | $g\ X_{CB}\ g\ X_{OHO}^{-1}\ d^{-1}$ | $k_H$ | **3** | 9 | 5 | | 9.0 | 3.0 | 9.0 | 67 |
| $q_{SB\_Stor}$ | $g\ X_{CB}\ g\ X_{OHO}^{-1}\ d^{-1}$ | $k_{STO}$ | **0.1** | | 5 | | 12.0 | 10.0 | 12.0 | 17 |
| **Ordinary Heterotrophic Organisms** | | | | | | | | | | |
| $\mu_{OHO,Max}$ | $d^{-1}$ | $\mu_H$ | **2** | 3 | 5 | | 3.0 | 2.0 | 3.0 | 33 |
| $\eta_{\mu OHO,Ax}$ | - | $\eta_{NOX}$ | **0.6** | 0.5 | 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 |
| $K_{Stor\_OHO}$ | $g\ X_{Stor}\ g\ X_{OHO}^{-1}$ | $K_{STO}$ | **1** | 0.1 | 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** | | | | | | | | | | |
| $\mu_{ANO,Max}$ | $d^{-1}$ | $\mu_A$ | **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, 1 original parameter set and 8 optimised parameter sets. The modelling studies were exclusively carried out in Germany. Half of them were carried out on full scale WWTPs.

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

| Parameter* | Unit | Original notation | Original parameter set | Optimised parameter sets | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Parameter sets | | | m | n | Modif > 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** | | | | | | | | | |
| $q_{PAO,PO4\_PP}$ | $g\ X_{PP}.g\ X_{PAO}^{-1}.d^{-1}$ | $q_{PP}$ | **1.5** | 9 | X | 1.50 | 1.50 | 2.30 | 53 |
| $f_{PP\_PAO,Max}$ | $g\ X_{PP}.g\ X_{PAO}^{-1}$ | $K_{max,PAO}$ | **0.2** | 9 | X | 1.00 | 0.24 | 1.00 | 76 |
| **Autotrophic Nitrifying Organisms** | | | | | | | | | |
| $\mu_{ANO,Max}$ | $d^{-1}$ | $\mu_A$ | **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, of which 1 is "proposed new default parameter sets" and 4 are "optimised 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 WWTPs with domestic influent (3).

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

| Parameter* | Unit | Original parameter set | | Proposed new default parameter set | n | Optimised parameter sets | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Parameter sets | | Notation | Value (n) | o | | Modif > 50% | Median | Perc. 25% | Perc. 75% | V (%) |
| **Conversion coefficient** | | | | | | | | | | |
| $i_{N\_SU}$ | $g\ N\ g\ S_U^{-1}$ | $f_{N,SEP}$ | **0.07** | 0.034 | 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 |
| $i_{N\_XUE,OHO}$ | $g\ N\ g\ X_{UE}^{-1}$ | $f_{N,ZEH}$ | **0.07** | 0.034 | 6 | | 0.069 | 0.034 | 0.070 | 52 |
| $i_{N\_XUE,PAO}$ | $g\ N\ g\ X_{UE}^{-1}$ | $f_{N,ZEP}$ | **0.07** | 0.034 | 6 | | 0.070 | 0.034 | 0.070 | 51 |
| $i_{N\_XUE,ANO}$ | $g\ N\ g\ X_{UE}^{-1}$ | $f_{N,ZEA}$ | **0.07** | 0.034 | 6 | | 0.068 | 0.034 | 0.068 | 50 |

**Table 6** | *(continued)*

| Parameter* | Unit | Original parameter set | | Proposed new default parameter set | n | Optimised parameter sets | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Parameter sets | | Notation | Value (n) | o | | Modif >50% | Median | Perc. 25% | Perc. 75% | V (%) |
| **Kinetic parameters** | | | | | | | | | | |
| **Ordinary Heterotrophic Organisms** | | | | | | | | | | |
| $\eta_{\mu OHO,Ax}$ | - | $\eta_{gro}$ | **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 $X_{PP}$ $m^{-3}$ | $K_{XP}$ | **0.05** | 0.01 | 6 | X | 0.010 | 0.010 | 0.010 | 0 |
| **Autotrophic Nitrifying Organisms** | | | | | | | | | | |
| $\mu_{ANO,Max}$ | $d^{-1}$ | $\mu_A$ | **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 $S_{O2}$ $m^{-3}$ | $K_{O,AUT}$ | **0.5** | 0.25 | 6 | | 0.50 | 0.25 | 0.50 | 50 |
| $K_{NHx,ANO}$ | g $S_{NHx}$ $m^{-3}$ | $K_{NH}$ | **1** | 0.5 | 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.

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