A systematic approach for model verification: application on seven published activated sludge models

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ABSTRACT

The quality of simulation results can be significantly affected by errors in the published model (typing, inconsistencies, gaps or conceptual errors) and/or in the underlying numerical model description. Seven of the most commonly used activated sludge models have been investigated to point out the typing errors, inconsistencies and gaps in the model publications: ASM1; ASM2d; ASM3; ASM3 + Bio-P; ASM2d + TUD; New General; UCTPHO+. A systematic approach to verify models by tracking typing errors and inconsistencies in model development and software implementation is proposed. Then, stoichiometry and kinetic rate expressions are checked for each model and the errors found are reported in detail. An attached spreadsheet (see http://www.iwaponline.com/wst/06104/0898.pdf) provides corrected matrices with the calculations of all stoichiometric coefficients for the discussed biokinetic models and gives an example of proper continuity checks.

Key words | ASM, composition matrix, continuity, errors, Gujer matrix, model implementation, Petersen Matrix

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INTRODUCTION

The quality of simulation results can be affected by several error sources (Refsgaard *et al.* 2007): (i) context and framing; (ii) input uncertainty; (iii) model structure uncertainty; (iv) parameter uncertainty and (v) model technical uncertainty, e.g. model implementation errors. Gernaey *et al.* (2006) detailed the error sources when models are implemented into a simulation software: (i) simplification of the original model; (ii) typing errors; (iii) incomplete model description in the paper; (iv) scattered description of the model in the paper; (v) misinterpretation of the model description; (vi) errors when coding model; (vii) general programming bugs.

Surprisingly no error report has been published, except for ASM2d and ADM1 in Gernaey *et al.* (2006). Tracking those errors is indeed difficult and time consuming for model users, and the potential publication formats are not adapted to publish such information. Furthermore, some typing errors seem to appear or disappear following the version of the papers describing a given model (e.g. ASM2d where typing errors appeared in the paper Henze *et al.* 2000*b* compared to previous publications: Henze *et al.* 1998, 1999). This work aims thus to provide (i) a systematic approach to track typing errors and inconsistencies in models, (ii) a thorough list of errors in the commonly used activated sludge model publications and (iii) the corrected Gujer Matrices (Takács 2005; also called Petersen Matrix) in original and new standardised notation format (Corominas *et al.* 2010) in a spreadsheet (see http://www.iwaponline.com/wst/06104/0898.pdf). The work does not intend to address model structure problems linked either to modelling concepts or to simplifications used in the models.

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Seven of the most commonly used activated sludge models have been investigated: (1) ASM1 (Henze *et al.* 1987; republished in Henze *et al.* 2000*a*); (2) ASM2d (Henze *et al.* 1999; republished in Henze *et al.* 2000*b*); (3) ASM3 (Gujer *et al.* 1999; corrected version published in Gujer *et al.* 2000); (4) ASM3 + Bio-P (Rieger *et al.* 2001); (5) ASM2d + TUD (Meijer 2004); (6) New General (Barker & Dold 1997); (7) UCTPHO + (Hu *et al.* 2007). To keep the article readable, those references will not be repeated each time.

HOW TO TRACK TYPING ERRORS AND INCONSISTENCIES IN MODEL DEVELOPMENT AND SOFTWARE IMPLEMENTATION

Before using or implementing a published model or when developing a new model one should first verify the model by checking the continuity of the stoichiometry and the consistency of the kinetic rate expressions. Because typing errors could stem from the original model publication or could occur during software implementation, this step should be done directly in the simulation software (simulator). However, not all simulators provide adequate tools to track such errors.

One way of verifying model implementations would consist in performing a ring test between several simulators with independent implementations (by several modellers). The simulation results for the same modelling project are compared to verify the model implementations. This method was chosen by the BSM task group to validate the implementation of their settling and biokinetic models, and ASM1 in particular (Jeppsson *et al.* 2007; Copp *et al.* 2008). The study revealed errors in the model codes, in the simulator codes and in the aeration models of the evaluated simulators. However, this task necessitates considerable effort and different simulators, which is not usually available to ASM users.

A method to automatically isolate model implementation errors by comparison of two independent model implementations has been developed by Yuan *et al.* (2003). Next to detection of model implementation errors, a method based on so-called Feature Matrices has been developed also to diagnose the errors and point to the probable location of the error in the model code. However this promising method has not yet been implemented in any simulator.

The following paragraphs propose functionalities of model editors to allow for model verification. Some alternative ways to track errors are also suggested. However this methodology will not allow for the detection of numerical problems that could appear due to programming errors in simulators or wrong numerical solver settings. These errors should be fixed by the simulator developers through the above mentioned ring test for example.

How to track stoichiometric discontinuities

As state variables are typically expressed in terms of COD, elements (e.g. *N*, *P*) or charge, a composition matrix (Gujer & Larsen 1995) was developed complementary to the Gujer Matrix (Henze *et al.* 1987). It contains the required conversion coefficients for all state variables (in rows) to check the continuity for conservatives (e.g. COD, elements and charge) and observables (e.g. TSS) (in columns) for each process. The continuity check is carried out by multiplying (analytically or numerically) the stoichiometric matrix with the composition matrix as shown in Figure 1. The resulting matrix should contain only zeros, or near zeros in case of rounding problems.

The common way to check continuity is a numerical analysis starting with default parameter values. For this study the tolerance is set to 10^{-15}. The numerical analysis is an option available in most simulators, or can be performed using spreadsheets (see http://www.iwaponline.com/wst/06104/0898.pdf).

However, when some parameters are fixed to zero (e.g. $f_{SU\_XB,hyd}$, the fraction of inert COD generated in hydrolysis in ASM2d, ASM3, ASM3 + Bio-P and ASM2d + TUD), a stoichiometric coefficient could be forgotten without any impact on continuity (see hydrolysis process in ASM3 + Bio-P and processes 5 to 12 in UCTPHO +). Furthermore, errors could be compensated by other parameter values (e.g. when using rounded values everywhere in the model). Thus, another check has to be done by changing parameter values one after the other to track any discontinuity. To change values of parameters calculated from elemental molecular weights (see Table 14

ASM1 Composition matrix

		Elements		
		COD	N	Charge
1	S_I	1	0	0
2	S_S	1	0	0
3	X_I	1	0	0
4	X_S	1	0	0
5	$X_{B,H}$	1	0.086	0
6	$X_{B,A}$	1	0.086	0
7	X_P	1	i_{ci}	0
8	S_O	−1		0
9	S_{NO}	−4.57	1	−0.071
10	S_{NH}	0	1	0.071
11	S_{ND}	0	1	0
12	X_{ND}	0	1	0
13	S_{ALK}	0	0	−1
14	S_{N2}	−1.71	1	0

ASM1 Gujer matrix
(S_{N2} has been added for continuity)
i: state variable
j: process
v_{ij}: stoichiometric coefficient (calculated from parameter values of Henze *et al.*, 2000)

i		1	2	3	4	5	6	7	8	9	10	11	12	13	14
j		S_I	S_S	X_I	X_S	$X_{B,H}$	$X_{B,A}$	X_P	S_O	S_{NO}	S_{NH}	S_{ND}	X_{ND}	S_{ALK}	S_{N2}
1	Aerobic growth of heterotrophs		−1.49			1			−0.49		−0.09			−0.006	
2	Anoxic growth of heterotrophs		−1.49			1				−0.17	−0.09			0.006	0.172
3	Aerobic growth of autotrophs						1		−18.04	4.17	−4.25			−0.60	
4	Decay of heterotrophs				0.92	−1		0.08	v_{ji}				0.081		
5	Decay of autotrophs				0.92		−1	0.08					0.081		
6	Ammonification of soluble organic										1	−1		00.07	
7	Hydrolysis of entrapped organic		1		−1										
8	Hydrolysis of entrapped organic N											−1	1		

10^{-15}	10^{-15}	10^{-15}	
10^{-15}	10^{-15}	10^{-15}	
10^{-15}	10^{-15}	10^{-15}	
	$\Sigma_i\ v_{ij}.i_{ci} = 10^{-15}$		
10^{-15}	10^{-15}	10^{-15}	
10^{-15}	10^{-15}	10^{-15}	

Figure 1 | How to check continuity of Gujer Matrix.

in appendix), the molecular weight of the element has to be changed for all the concerned parameters at once.

A better way to track discontinuity that avoids numerical problems is to use a symbolic analysis. Symbolic analysis allows the recalculation of stoichiometric coefficients from the basic stoichiometric coefficients (e.g. yields) and the composition matrix. The symbolic analysis could be carried out by appropriate tools such as Maple (Maplesoft).

How to track kinetic inconsistencies

Some simulators provide the kinetic rates in symbolic form, which allows an easy check of the proper implementation (mainly parentheses errors). However, it is not possible to track kinetic inconsistencies in model editors so far. A tool to check kinetic rate expressions that could be implemented in simulators is proposed. This tool is based on four questions that modellers should answer for every process.

- Which are the consumed components (every state variable with a negative stoichiometric coefficient)? For every consumed component the kinetic rate expression should include a limitation function (e.g. Monod term). Concerning alkalinity, see the discussion in the section on "Common published errors".
- Which biomass is involved in the process as biocatalyst? The kinetic rate expression is typically proportional to this biomass concentration.
- Are other components required for the process (e.g. an electron acceptor that is not consumed: oxygen in ASM2d aerobic hydrolysis)? The kinetic rate expression should include a limitation function for those components (e.g. Monod term).
- Are other components inhibitory (e.g. oxygen in an anoxic process)? The kinetic rate expression should include an inhibitory function for those components (e.g. inhibitory Monod term).

In the attached spreadsheet (see http://www.iwaponline.com/wst/06104/0898.pdf) it is proposed to perform this analysis by colouring the Gujer Matrix cells with different colours for each question. The two first questions could be easily automated in a model editor through the stoichiometric values of the Gujer Matrix. Nevertheless, the two last questions must involve the model developer to indicate electron acceptor conditions of the processes and

inhibitors. This kind of matrix should be provided in model publications and implemented in simulators. With those pieces of information, model editors should be able to automatically check whether the kinetic rate expression includes a term for each coloured component.

In the presented work, the kinetic rate expressions were checked carefully to ensure that (i) every reactant of the process is limiting (to stop a reaction when a reactant is limiting and to prevent the calculation of negative concentrations); (ii) every switching function or kinetic parameter is coherent; and (iii) kinetic rate expressions are consistent from one model to another.

COMMON PUBLISHED ERRORS

Rounding parameters

An error that occurs systematically and that may hinder the continuity of a model is to round parameters to 2 significant figures or even to use rounded and "exact values" of parameters (i.e. fractions in calculated parameters, see Table 14 in appendix) in the very same model. To avoid an accumulation of rounding problems, it is recommended to keep "exact values" everywhere in the model.

The "exact values" of conversion coefficients can be calculated from theoretical (conceptual) COD of elements as defined by Gujer & Larsen (1995) (see Table 13 in appendix) and from molecular weights (periodic table of elements). Table 14 in the appendix summarizes the main conversion coefficients, their calculation explanation and their exact values to be used in ASM-type models.

Temperature adjustment of kinetic parameters

Kinetic parameter values depend on temperature. Three different ways have been proposed to provide temperature adjustment of kinetic parameters (with θ being the temperature adjustment coefficient, $k_{20°C}$ the kinetic coefficient at 20°C and k_T the kinetic coefficient at temperature T):

- in ASM1 and ASM2d, kinetic parameters are given at 10 and 20°C
- in ASM3, ASM3 + Bio-P and ASM2d + TUD, θ values are provided using the following equation: $k_T = k_{20°C} \times e^{\theta \times (T-20)}$
- in New General and UCTPHO + , θ values are provided using: $k_T = k_{20°C} \times \theta^{T-20}$

The two last equations are similar: the temperature adjustment e^{θ} in equation $k_T = k_{20°C} \times e^{\theta \times (T-20)}$ is equivalent to θ in the equation $k_T = k_{20°C} \times \theta^{T-20}$. It is thus easy to convert temperature coefficient from one equation to the other. Unfortunately the same symbol (θ) is given to these two different parameters. As suggested in Corominas *et al.* (2010), an extended notation should be used. The first parameter could be noted θ_{exp} and the second one θ_{pow}. Then $\theta_{pow} = \exp(\theta_{exp})$. However, it should be easier for model comparison to use a single temperature adjustment equation among the modelling community. The second Equation ($k_T = k_{20°C} \times \theta_{pow}^{T-20}$) is chosen in this work as it is the simplest one and the most commonly used (Vavilin 1982).

Impact of alkalinity on kinetic rates

Alkalinity is introduced in several models to guarantee the continuity in ionic charge of the biological processes, and to predict possible pH changes. Alkalinity is usually measured in molar concentration of HCO_3^- or in concentration of $CaCO_3$ ($1\,mol\,HCO_3^-\,m^{-3} = 50\,g\,CaCO_3\,m^{-3}$). Low alkalinity concentration causes unstable pH, which could reach inhibiting levels (Henze *et al.* 2000*a*). Three ways to deal with alkalinity have been proposed in the models:

- alkalinity is not taken into account in the model at all (New General and UCTPHO +);
- alkalinity is taken into account in the stoichiometry but does not limit the kinetic rates (ASM1);
- alkalinity is taken into account in both stoichiometry and kinetic rates (ASM2d, ASM3, ASM3 + Bio-P and ASM2d + TUD).

For the latter models, the stoichiometric coefficients for alkalinity were compared using the parameter sets from the original publications (see http://www.iwaponline.com/wst/06104/0898.pdf). Those calculations reveal two major problems that are illustrated through practical examples.

- **The use of alkalinity as a limiting factor for kinetic rates is not consistent**. Table 1 summarises models that involve alkalinity. For each process, it is checked

Table 1 | The use of alkalinity as a limiting factor for kinetic rates. Stoichiometric coefficients have been calculated with published parameter values

	Nb of processes	Nb of proc. with: -Alk consumed, -Alk limiting	Nb of proc. with: -Alk produced, -Alk limiting	Nb of proc. with: -Alk consumed, -Alk not limiting	Nb of proc. with: -Alk produced, -Alk not limiting	Nb of proc. without Alk. stoichiom
ASM2d	21	8	7	0	6	
ASM3	12	2	1	0	8	1
ASM3 + Bio-P	23	6	4	0	11	2
ASM2d + TUD	22	3	4	3	12	

whether alkalinity is consumed or produced and whether alkalinity is considered as a limiting factor or not. It reveals that alkalinity is a limiting factor for all processes in those models where alkalinity is consumed, except in process 11, 21 and 15 of ASM2d + TUD (see paragraph concerning ASM2d + TUD below). Alkalinity may also be considered as a limiting factor or not in the processes where it is produced.

- **The stoichiometric coefficients for alkalinity highly depend on parameter values** (e.g. yield values or conversion coefficients that change the proportions of consumed or released nutrients). To illustrate this point, a test has been carried out on ASM2d + TUD by changing two stoichiometric parameter values (i_{NBM} and i_{NSF}). Table 2 shows that these parameter values impact the sign of the stoichiometric coefficient of alkalinity. Thus, a process that consumes alkalinity with one parameter set could produce alkalinity with another parameter set.

The way of inclusion of alkalinity in the kinetic rates is a structural model problem and therefore out of the scope of this paper. The reason to discuss it was to raise awareness of inconsistencies. Hence, the kinetic rates for alkalinity in the attached spreadsheets have not been changed (see http://www.iwaponline.com/wst/06104/0898.pdf).

TYPING ERRORS, INCONSISTENCIES AND GAPS IN PUBLISHED MODELS

During the checks performed on the stoichiometric continuity and the evaluation of the kinetic rate expressions, several implementation errors and inconsistencies were identified. They are presented below for each model and separated into 3 different error types: (i) typing errors; (ii) inconsistencies when it is not clearly an error but a potentially risky simplification; and (iii) gaps in stoichiometry and kinetics due to oversight or purposeful omission to keep the model simple.

ASM1

ASM1 was first published by Henze *et al.* (1987), but here we shall examine the later version published as Henze *et al.* (2000*a*). The first version contained other errors than the 2000 version but they are not discussed here.

Inconsistencies

There is no term in the kinetic rate expression to model nutrient (ammonia) limitation in the heterotrophic growth process, which could induce negative ammonia concentration values (Table 3).

Table 2 | Examples of changes in stoichiometric coefficient values of ASM2d + TUD depending on parameter values

	Default parameter values		Tested parameter values	
Processes	Parameter value	Alkalinity stoichiometric coefficient sign	Parameter value	Alkalinity stoichiometric coefficient sign
Process 15	$i_{NBM} = 0.07$	−	$i_{NBM} = 0.08$	+
Processes 1, 2, 3	$i_{NSF} = 0.03$	+	$i_{NSF} = 0.045$	−
Process 4	$i_{NSF} = 0.03$	−	$i_{NSF} = 0.045$	+

Table 3 | Inconsistencies in kinetic rate expressions in ASM1 model publication (Henze *et al.* 2000)

Process	Description	Missing Monod term	Correct Monod term
1, 2	Heterotrophic growth	Ammonia limitation	$\frac{S_{NH}}{K_{NH,H}+S_{NH}}$

The coefficient $K_{NH,H}$ is introduced and the same default value as in ASM2d is chosen ($0.05\,g\,S_{NH_4}\,m^{-3}$).

Gaps

In order to close mass balances, N_2 should be included in the Gujer Matrix in process 2 (anoxic growth of heterotrophic biomass). This variable is only useful to verify the model continuity but has no impact on model results.

To perform a full nitrogen balance, variables S_{NI} (soluble non-biodegradable organic nitrogen) and X_{NI} (particulate non-biodegradable organic nitrogen) should be estimated in the influent. As non-biodegradable compounds, they do not appear in the Gujer Matrix. S_{NI} should be added to total soluble nitrogen in the effluent and X_{NI} should be added to total nitrogen in activated sludge.

ASM2d

Typing errors

Table 4 summarises ASM2d typing errors (Henze *et al.* 2000*b*). Those typing errors have previously been pointed out by Gernaey *et al.* (2006).

Stoichiometric coefficients for S_O, S_{NH_4}, S_{N_2}, S_{NO_3}, S_{PO_4}, S_{ALK} and X_{TSS} are not given in detail, so that users have to apply continuity equations to implement them. The corrected matrix provided in the attached spreadsheet details these coefficients (see http://www.iwaponline.com/wst/06104/0898.pdf).

Inconsistencies

The same parameter name is given to many kinetic parameters common for hydrolysis, precipitation, heterotrophic, phosphorus-accumulating and nitrifying organisms processes, although some of these parameters have different values in the parameter set provided in the publication (e.g. η_{NO_3}(hydrolysis) = 0.6 and η_{NO_3}(heterotrophs) = 0.8). A suffix (respectively: HYD, PRE, H, PAO, AUT) has been added to these parameters to avoid any confusion. These problems are fixed when defining extended symbols using the standardised notation (Corominas *et al.* 2010).

ASM3

Typing errors

The original publication (Gujer *et al.* 1999) had several typing errors. The corrected version (Gujer *et al.* 2000) should be used.

The coefficient $i_{SS,STO}$ is missing in the parameter list, the same default value as in ASM3 + Bio-P is chosen ($0.6\,g\,TSS\,g\,XStor^{-1}$).

Stoichiometric coefficients for S_O, S_{NH_4}, S_{N_2}, S_{NO_x}, S_{PO_4}, S_{ALK} and X_{TSS} are not given in detail, so that users have to apply continuity equations to implement them. The corrected matrix provided in the attached spreadsheet details these coefficients (see http://www.iwaponline.com/wst/06104/0898.pdf).

Table 4 | Typing errors in ASM2d model publication (Henze *et al.* 2000*b*)

Process	Description	Kinetic or stoichiometry	Wrong	Correct
6, 7	Anoxic growth of heterotrophs on S_F and S_A	Kinetic rate	$\frac{K_{NO_3}}{K_{NO_3}+S_{NO_3}}$	$\frac{S_{NO_3}}{K_{NO_3}+S_{NO_3}}$
7	Anoxic growth of heterotrophs on S_A	Stoichiometry of S_{N_2}	$-\frac{1-Y_H}{40/14\cdot Y_H}$	$\frac{1-Y_H}{40/14\cdot Y_H}$
8	Fermentation	Kinetic rate	K_F	K_{fe}
11	Aerobic storage of X_{PP}	Kinetic rate	K_{PP}	K_{IPP}
13, 14	Aerobic and anoxic growth of X_{PAO}	Stoichiometry of X_{PHA}	$-1/Y_H$	$-1/Y_{PAO}$

Table 5 | Typing errors in ASM3 + Bio-P model publication (Rieger *et al.* 2001)

Process	Description	Kinetic or stoichiometry	Wrong	Correct
1	Hydrolysis	Stoichiometry of S_I	No coefficient	f_{SI}
1	Hydrolysis	Stoichiometry of S_{PO_4}	$i_{P,XS} - i_{P,SS}$	$-(1 - f_{SI}) \times i_{P,SS} - f_{SI} \times i_{P,SI} + i_{P,XS}$
8, 9	Aerobic and anoxic respiration of internal storage	Kinetic rate	b_H	b_{Sto}
11, 12	Aerobic and anoxic endogenous respiration of X_{AUT}	Kinetic rate	$K_{O,H}$	$K_{O,A}$
P9, P11	Anoxic lysis of X_{PP} and anoxic respiration of X_{PHA}	Kinetic rate	$\frac{S_{NO}}{K_{NO,PAO}}$	$\frac{S_{NO}}{K_{NO,PAO}+S_{NO}}$

Table 6 | Typing errors in ASM2d + TUD model publication (Meijer 2004)

Process	Description	Kinetic or stoichiometry	Wrong	Correct
5, 7, 10, 12	OHO growth on S_A and PAO growth on S_A	Kinetic rate	K_A	K_{Ac}
21	Autotrophic growth	Stoichiometry of X_{TSS}	$-i_{TSS,BM}$	$i_{TSS,BM}$
21	Autotrophic growth	Kinetic rate	K_O	$K_{A,O}$
21	Autotrophic growth	Kinetic rate	K_{PO}	S_{PO}

ASM3 + Bio-P

Typing errors

Table 5 summarises ASM3 + Bio-P typing errors (Rieger *et al.* 2001).

Inconsistencies

The kinetic parameter $K_{NO,A}$ is missing: the kinetic rate in process 12 (Anoxic endogenous respiration) uses $K_{NO,H}$.

ASM2d + TUD

Typing errors

Table 6 summarises ASM2d + TUD typing errors (Meijer 2004).

Inconsistencies

The kinetic check reveals missing Monod terms to ensure consistency with the process. Table 7 summarises ASM2d + TUD inconsistencies in kinetic rate expressions.

Another theoretical inconsistency was identified in the anoxic glycogen formation process (process 15). This process turns PAO matter into glycogen and uses nitrate as the energy source. However, PAO matter is more oxidised than glycogen and no compound with reducing power is used in this process. To match the continuity mathematically, it results in a production of nitrate and a consumption of N_2. Note that this inconsistency has a negative effect on denitrification. As this is a structural inconsistency, the process has not been changed and no kinetic limitation function has been added for N_2 in the attached spreadsheet (see http://www.iwaponline.com/wst/06104/0898.pdf).

As in ASM2d, the same parameter name is given to many kinetic parameters common for hydrolysis and organisms processes. A suffix has been added to these parameters to avoid any confusion.

New General

Typing errors

The unit of K_{SP} (Saturation constant for $P_{PP\text{-}LO}$) should be $g\,P\,m^{-3}$ instead of $g\,P\,g\,COD^{-1}$ (Barker & Dold 1997).

Table 7 | Inconsistencies in kinetic rate expressions in ASM2d + TUD model publication (Meijer 2004)

Process	Description	Missing Monod term	Correct Monod term
1	Aerobic hydrolysis	Oxygen limitation	$\frac{S_O}{K_O+S_O}$

Table 8 | Inconsistencies in kinetic rate expressions in New General model publication (Barker & Dold 1997)

Process	Description	Missing Monod term	Correct Monod term
1 to 4	Heterotrophic growth on S_{BSC}	Substrate preference switch function	$\frac{S_{BSC}}{S_{BSC}+S_{BSA}}$
5 to 8	Heterotrophic growth on S_{BSA}	Substrate preference switch function	$\frac{S_{BSA}}{S_{BSC}+S_{BSA}}$
15	Fermentation of S_{BSC} to S_{BSA} (Anaerobic growth)	Phosphate and ammonia limitation	$\frac{N_{H3}}{K_{NA}+N_{H3}} \cdot \frac{P_{O4}}{K_{LP,GRO}+P_{O4}}$
16	Autotrophic growth	Phosphate limitation	$\frac{P_{O4}}{K_{LP,GRO}+P_{O4}}$
20 and 21	Aerobic growth of PAO, PO_4 limited	$P_{PP\text{-}LO}$ limitation (phosphorus source in case of PO_4 depletion)	$\frac{P_{PP-LO}}{K_{XP}+P_{PP\text{-}LO}}$

Inconsistencies

In the kinetic rate expressions of processes 1 to 8 (growth on S_{BSC} or S_{BSA}) there is no substrate preference switch function (as e.g. in ASM2d) such as $S_{BSC}/(S_{BSC}+S_{BSA})$. This substrate preference switch function prevents the heterotrophic specific growth rate from increasing above a maximum value if both substrates are present in high concentration (Henze *et al.* 2000*b*). Even if Barker & Dold (1997) specify that the S_{BSA} concentration entering the anoxic and aerobic zones is usually very low, this substrate preference switch function could be added to enhance the robustness of the model. The preference switch function $S_{BSC}/(S_{BSC}+S_{BSA})$ is proposed (as e.g. used in ASM2d and in ADM1 (Batstone *et al.* 2002)); other function types are described in Dudley *et al.* (2002).

The kinetic check reveals other missing Monod terms to ensure consistency with the stoichiometry of the process. Table 8 summarises New General inconsistencies in kinetic rate expressions.

Gaps

In order to keep the continuity, N_2 (processes 2, 4, 6, 8, 22 and 27) should be included in the Gujer Matrix as a state variable. As in ASM1, this variable is only useful to verify the model continuity but has no impact on model results.

Table 9 | Gaps in stoichiometry in New General model publication (Barker & Dold 1997)

Process	Description	Gap in stoichiometry	Corrected stoichiometry*
2, 4, 6, 8	Anoxic growth of heterotrophs	S_{N_2} variable	$(1-Y_{H.ANOX})/(i_{NO_x,N_2}\times Y_{H.ANOX})$
22	Anoxic growth of PolyP organisms	S_{N_2} variable	$(1-Y_P)/(i_{NO_x,N_2}\times Y_P)$
27	Anoxic decay of PolyP organisms	S_{N_2} variable	$(1-f_{EP.P}-f_{ES.P})/i_{NO_x,N_2}$
11	Anoxic hydrolysis of stored/enmeshed COD	S_H variable	$(1-E_{ANOX})/i_{COD\_SH}$
12	Anaerobic hydrolysis of stored/enmeshed COD	S_H variable	$(1-E_{ANA})/i_{COD\_SH}$
15	Fermentation of S_{BSC} to S_{BSA}	S_H variable	$(1-(1-Y_{H,ANA})\times Y_{AC}-Y_{H,ANA})/i_{COD\_SH}$
36	Sequestration of S_{CFA} by PolyP organisms	S_H variable	$(1-Y_{PHB})/i_{COD\_SH}$
3, 7	Aerobic growth of heterotrophs on S_{BSC}/S_{BSA} with N_{O_3}	Oxygen from consumed N_{O_3} not included in S_O	$-(1-Y_{H.AER})/Y_{H.AER}-i_{COD\_NO_x}\times f_{N.ZH}$
19, 21	Aerobic growth of PolyP organisms on S_{PHB} with N_{O_3} without and with P_{O_4} limited	Oxygen from consumed N_{O_3} not included in S_O	$-(1-Y_P)/Y_P-i_{COD\_NO_x}\times f_{N.ZP}$
4, 8	Anoxic growth of heterotrophs on S_{BSC}/S_{BSA} with N_{O_3}	Different yield for S_{BSC} or S_{BSA} consumption with N_{O_3}	$-1/Y_{H.ANOX}+i_{COD\_NO_x}\times f_{N.ZH}$

*The new parameters and variables introduced in this study are named according to the standardised notation rules (Corominas *et al.* in press) and thus may not be consistent with the original model notation. The conversion factors are described in Table 14 in appendix.

Table 10 | Typing errors in UCTPHO + model publication (Hu *et al.* 2007)

Process	Description	Kinetic or stoichiometry	Wrong	Correct
14, 17	Heterotrophic and autotrophic decay	Stoichiometry of X_{ENM}	$f_{XI,H}$	$f_{XE,H}$
14, 17	Heterotrophic and autotrophic decay	Stoichiometry of S_{NH_4}	No coefficient	$i_{NBM} - (1 - f_{XE-H}) \times i_{NENM} - f_{XE-H} \times i_{NXE}$ or $i_{NBM} - (1 - f_{XE-NIT}) \times i_{NENM} - f_{XE-NIT} \times i_{NXE}$
5 to 8	Heterotrophic growth on S_F	Stoichiometry of S_{PO_4}	$-i_{PBM}$ No P contained in S_F	$-i_{PBM} + i_{PSF}/Y_{H_1}$ or $-i_{PBM} + i_{PSF}/Y_{H_2}$
9 to 12	Heterotrophic growth on X_{ads}	Stoichiometry of S_{PO4}	$-i_{PBM}$ No P contained in X_{ads}	$-i_{PBM} + i_{PENM}/Y_{H_1}$ or $-i_{PBM} + i_{PENM}/Y_{H_2}$
15	Conversion of S_F to S_A	Stoichiometry of S_{PO_4}	No coefficient	i_{PSF}
18	Aerobic growth of X_{PAO} on X_{PHA} with S_{NH_4}	Stoichiometry of S_{PO_4}	No coefficient	$-i_{PBM} - Y_{PP1}/Y_{PAO1}$
24, 27, 30	Decay of X_{PAO}	Stoichiometry of S_{NH4}	In coefficients A, B and C, nitrogen fraction of X_E is i_{NBM} instead of i_{NXE}	A: $i_{NBM} - f_{XE.PAO} \times i_{NXE} - f_{SI.PAO} \times i_{NSI}$ B: $i_{NBM} - f_{XE.PAO} \times i_{NXE} - f_{SI.PAO} \times i_{NSI} - i_{NENM} \times (1 - \eta_{PAO}) \times (1 - f_{XE.PAO} - f_{SI.PAO})$ C: $i_{NBM} - f_{XE.PAO} \times i_{NXE} - f_{SI.PAO} \times i_{NSI} - i_{NENM} \times (1 - f_{XE.PAO} - f_{SI.PAO})$
14, 17, 24, 27, 30	OHO, ANO and PAO decay	Stoichiometry of S_{PO_4}	$i_{PBM} \times (1 - f_{XE})$ P fraction of X_E is i_{PBM} instead of i_{PXE}	$i_{PBM} - f_{XE.H} \times i_{PXE}$ or $i_{PBM} - f_{XE.NIT} \times i_{PXE}$ or $i_{PBM} - f_{XE.PAO} \times i_{PXE}$
24, 27, 30	Decay of X_{PAO}	Stoichiometry of S_{PO_4}	$i_{PBM} - f_{XE.PAO} \times i_{PXE}$ No P contained in S_I	$i_{PBM} - f_{XE.PAO} \times i_{PXE} - f_{SI.PAO} \times i_{PSI}$
14, 17, 26, 27, 29, 30, 32	OHO and ANO decay, anoxic and anaerobic PAO decay, X_{PHA} lysis	Stoichiometry of S_{PO_4}	No P contained in X_{ENM}	Depends on X_{ENM} stoichiometry: $\nu_{ij,XENM} \times i_{PENM}$ should be added (see http://www.iwaponline.com/wst/06104/0898.pdf)

Table 11 | Inconsistencies in kinetic rate expressions in UCTPHO + model publication (Hu *et al.* 2007)

Process	Description	Missing Monod term	Correct Monod Term
1 to 4	Heterotrophic growth on S_A	Substrate preference switch function	$\frac{S_A}{S_F+S_A+X_{ADS}}$
5 to 8	Heterotrophic growth on S_F	Substrate preference switch function	$\frac{S_F}{S_F+S_A+X_{ADS}}$
9 to12	Heterotrophic growth on X_{Ads}	Substrate preference switch function	$\frac{X_{Ads}}{S_F+S_A+X_{ADS}}$
3, 7, 11	Anoxic growth with S_{NH_4}	Nitrate limitation	$\frac{S_{NO_3}}{K_{NO_3}+S_{NO_3}}$
26, 29, 32	X_{PHA} lysis during (aerobic, anoxic, anaerobic) PAO decay	Ammonia and phosphate limitation (X_{PHA} is turned into X_{ENM}, which contains nitrogen and phosphorus. Ammonia and phosphate have thus to be consumed)	$\frac{S_{NH_4}}{K_{NH_4}+S_{NH_4}} \cdot \frac{S_{PO_4}}{K_{PO_4\text{-}lys}+S_{PO_4}}$
		Parameter K_{PO_4-lys} is introduced, the value of K_{PO_4-gro} is kept	
20 and 21	Aerobic growth of PAO, PO_4 limited	X_{PP} limitation (phosphorus source in case of PO_4 depletion)	$\frac{X_{PP}}{K_{PP}+X_{PP}}$

The "COD losses" mentioned in Barker & Dold (1997) (processes 11, 12, 15 and 36) have been detected based on experimental data. This is modelled through the introduction of an efficiency parameter in hydrolysis processes (11, 12) and a yield parameter in fermentation and sequestration processes (15, 36). However the fate of the resulting COD is not described by the model and leads to a lack of continuity. In the model ASDM (as implemented in BioWin, EnviroSim 2009), the "COD loss" is considered to be due to H_2 gas formation (Kraemer *et al.* 2008). A state variable S_H is therefore added to the model (Table 9).

In processes 3, 4, 7, 8, 19 and 21, there is another discontinuity for COD that is not mentioned in the paper, due to the potential use of NO_3^- as a nitrogen source by heterotrophs. Indeed, when NO_3^- is used as a nitrogen source, the fate of the oxygen content of NO_3^- is not considered. The O_2 stoichiometric coefficient should be lower for growth with NO_3^- as nitrogen source than O_2 consumption for growth with NH_3 (Grady *et al.* 1999).

To match the continuity of aerobic processes (3, 7, 19 and 21), the authors suggest to decrease the oxygen stoichiometric coefficient by subtracting the COD content in the consumed nitrates (Table 9). This correction is not possible for anoxic processes (4 and 8). The proposed solution is to consider that more substrate is needed for the same growth: the stoichiometric coefficient of the substrate (S_{BSC} or S_{BSA}) is increased by the COD consumed when using nitrates as nitrogen source (Table 9).

Polyphosphate accumulating organisms (PAOs) (Z_P in the model's notation) do not have the same nitrogen content as autotrophs (Z_A) and heterotrophs (Z_H) ($f_{N,ZP} = 0.07$ and $f_{N,ZA}$ and $f_{N,ZH} = 0.068$). In the decay process, all organisms turn into endogenous mass (Z_E) that has the same nitrogen content as the biomass it comes from ($f_{N,ZEP} = 0.07$ and $f_{N,ZEA}$ and $f_{N,ZEH} = 0.068$). Thus, the model structure allows different nitrogen fractions for the endogenous masses. However all the biomasses are turned into a single Z_E, which only has a single nitrogen fraction. Consequently, with the published parameter values, there is a lack in nitrogen continuity of -5×10^{-4} g N for processes 23, 27 and 31 (aerobic, anoxic and anaerobic decay of PAOs). All biomass nitrogen fractions $f_{N,ZEP}$, $f_{N,ZEA}$ and $f_{N,ZEH}$ should be corrected with the same value. A value of 0.07 g N g COD^{-1} is proposed.

UCTPHO +

Typing errors

Table 10 summarises UCTPHO + typing errors (Hu *et al.* 2007).

Inconsistencies

The kinetic check reveals some missing Monod terms to ensure consistency with the stoichiometry of the processes. Table 11 summarises UCTPHO + inconsistencies in the kinetic rate expressions.

Table 12 | Gaps in stoichiometry of UCTPHO + model publication (Hu *et al.* 2007)

Process	Description	Gap	Corrected stoichiometry
3, 4, 7, 8, 11, 12	Anoxic growth of heterotrophs	S_{N_2} variable missing	$(1 - Y_{H_2})/(i_{NO_x,N_2} \times Y_{H_2})$
22, 23	Anoxic growth of PolyP organisms	S_{N_2} variable missing	$(1 - Y_{PAO_2})/(i_{NO_x,N_2} \times Y_{PAO_2})$
27	Anoxic decay of PolyP organisms	S_{N_2} variable missing	$\eta_{PAO} \times (1 - f_{XE.PAO} - f_{SI.PAO})/i_{NO_x,N_2}$
2, 6, 10	Aerobic growth of heterotrophs on $S_A/S_F/X_{ads}$ with S_{NO_3}	Oxygen from consumed S_{NO_x} not include in S_{O_2}	$-(1 - Y_{H_1})/Y_{H_1} - i_{COD\_NO_x} \times i_{NBM}$
19, 21	Aerobic growth of PolyP organisms on X_{PHA} with S_{NO_3} without and with S_{PO_4} limited	Oxygen from consumed S_{NO_x} not include in S_{O_2}	$-(1 - Y_{PAO1})/Y_{PAO1} - i_{COD\_NO_x} \times i_{NBM}$
4	Anoxic growth of heterotrophs on S_A with S_{NO_3}	Different yield of S_A consumption with S_{NO_x}	$-1/Y_{H_2} + i_{COD\_NO_x} \times i_{NBM}$
		Different yield of S_F consumption with S_{NO_3}	$-1/Y_{H_2} + i_{COD\_NO_x} \times i_{NBM}$
8	Anoxic growth of heterotrophs on S_F with S_{NO_3}	S_{NH_4} coefficient correction	$i_{NSF} \times (1/Y_{H_2} - i_{COD\_NO_x} \times i_{NBM})$
		S_{PO_4} coefficient correction	$-i_{PBM} + i_{PSF} \times (1/Y_{H_2} - i_{COD\_NO_x} \times i_{NBM})$
		Different yield of X_{Ads} consumption with N_{O_3}	$-1/Y_{H_2} + i_{COD\_NO_x} \times i_{NBM}$
12	Anoxic growth of heterotrophs on X_{Ads} with S_{NO_3}	S_{NH_4} coefficient correction	$i_{NENM} \times (1/Y_{H_2} - i_{COD\_NO_x} \times i_{NBM})$
		S_{PO_4} coefficient correction	$-i_{PBM} + i_{PENM} \times (1/Y_{H_2} - i_{COD\_NO_x} \times i_{NBM})$
23	Anoxic growth of PolyP organisms on X_{PHA} with S_{NO_3}	Different yield of X_{PHA} consumption with S_{NO_3}	$-1/Y_{PAO_2} + i_{COD\_NO_x} \times i_{NBM}$

Gaps

In order to keep the continuity, N_2 as a state variable should be included in the Gujer Matrix for the processes 3, 4, 7, 8, 11, 12, 22, 23 and 27. As in ASM1 and New General, this variable is only useful to verify the model continuity but has no impact on model results.

As previously seen in the New General, a discontinuity for COD in processes 2, 4, 6, 8, 10, 12, 19, 21 and 23 is due to the use of NO_3^- as nitrogen source.

In the same way as in the New General, the authors suggest to lower the oxygen stoichiometric coefficient in aerobic processes (2, 6, 10, 19 and 21) and to increase the stoichiometric coefficient of substrate in anoxic processes (4, 8, 12 and 23). In contrast to the New General, some of the substrates contain a fraction of nitrogen and phosphorus (S_F for process 8 and X_{Ads} for process 12). The stoichiometric coefficients of S_{NH_4} and S_{PO_4} should be corrected to match the continuity (Table 12).

CONCLUSION

Several error sources can impact model quality. This paper points out typing errors, inconsistencies and gaps in the publications of seven selected models. Some of the errors corrected in this paper are mainly theoretical errors and will only have a minor impact on model results in typical conditions, but may have a significant impact in case of peculiar treatment conditions (e.g. near or outside model limits).

It is necessary to verify both a published model and the model implementation in simulators to avoid typing errors and inconsistencies. A simple spreadsheet, as presented in the attached file (see http://www.iwaponline.com/wst/06104/0898.pdf), could be used for continuity checks. The evaluation of the kinetic rate expressions is only possible based on a detailed check of the individual expressions but should be carried out with great care. The attached spreadsheet provides corrected matrices with all stoichiometric coefficients for the discussed biokinetic models and gives an example of a proper continuity and kinetic rate expressions check.

Model verification is a time-consuming task that could be facilitated and automated by appropriate model editor tools as part of a simulator. Albeit model verification is facilitated with these tools, it remains that model users have to redo this work each time they implement a new model.

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APPENDIX

Table 13 | Theoretical COD of electrical charge and main elements (from Gujer & Larsen 1995)

Element description	Symbol	Oxidation number	Theoretical COD (g COD mol^{-1})	Molecular weight (g mol^{-1})
Negative charge	(−)	+1	+8	−
Positive charge	(+)	−1	−8	−
Carbon	C	+4	+32	12
Nitrogen	N	−3	−24	14
Hydrogen	H	+1	+8	1
Oxygen	O	−2	−16	16
Sulphur	S	+6	+48	32
Phosphorus	P	+5	+40	31
Iron	Fe	+3	+24	55.8

Table 14 | Explanation and exact values of the main coefficients used in ASM-type models

Description	Symbol	Calculation	Exact value*	Unit
Conversion factor for NO_3^- into COD	$i_{COD\_NO_x}$	$(-24 + 3 \times (-16) + 8)$ g COD mol^{-1}/ 14 g N mol^{-1}	−64/14	g COD g N^{-1}
Conversion factor for N_2 into COD	$i_{COD\_N_2}$	(-24×2) g COD mol^{-1}/ (14×2) g N mol^{-1}	−24/14	g COD g N^{-1}
Stoichiometric factor for NO_3^- reduction to N_2 (amount of COD provided by reduction)	i_{NO_x,N_2}	$(64 - 24)$ g COD mol^{-1}/14 g N mol^{-1}	40/14	g COD g N^{-1}
Conversion factor for NH_4^+ into charge	$i_{Charge\_NH_x}$	1 Charge mol^{-1}/14 g N mol^{-1}	1/14	Charge g N^{-1}
Conversion factor for NO_3^- into charge	$i_{Charge\_NO_x}$	−1 Charge mol^{-1}/14 g N mol^{-1}	−1/14	Charge g N^{-1}
Conversion factor for Ac (CH_3COO^-) in charge	i_{Charge_Ac}	−1 Charge mol^{-1}/$(2 \times 32 + 3 \times 8 - 2 \times 16 + 8)$g COD mol^{-1}	−1/64	Charge g COD^{-1}
Conversion factor for PolyP into charge $(K_{0.33}Mg_{0.33}PO_3)_n$	i_{Charge_PP}	K^+ and Mg^{2+} not considered: $(PO_3)_n^-$ − 1 Charge mol^{-1}/31 g P mol^{-1}	−1/31	Charge g P^{-1}
Conversion factor for PO_4^{3-} into charge	$i_{Charge\_PO_4}$	PO_4^{3-}: 50% $H_2PO_4^-$ + 50% HPO_4^{2-} $(-1 - 2)$ Charge mol^{-1}/(2×31) g P mol^{-1}	−1.5/31	Charge g P^{-1}
Conversion factor for MeP ($FePO_4$) in P	i_{P_MeP}	$FePO_4$: $55.8 + 31 + 4 \times 16 = 150.8$ g mol^{-1} 31 g P mol^{-1}/150.8 g TSS mol^{-1}	31/150.8	g P g TSS^{-1}
Stoichiometric coefficients for precipitation and redissolution of PO_4^{3-} (ASM2d)	$f_{MeOH\_PO_4,MW}$	$Fe(OH)_3 + PO_4^{3-} \rightleftharpoons FePO_4 + 3HCO_3^-$ $Fe(OH)_3$: $55.8 + 3 \times 16 + 3 = 106.8$ g mol^{-1} $FePO_4$: $55.8 + 31 + 4 \times 16 = 150.8$ g mol^{-1}	−106.8/31	–
	$f_{MeP\_PO_4},MW$	Normalised on PO_4^{3-} ($= 31$ g P mol^{-1})	150.8/31	–

*The molecular weights used are rounded values (e.g. 12 g C mol C^{-1} instead of 12.0107 g C mol C^{-1}) but as the same value is used for each element in the model, the continuity is verified (which is not the case when rounding ratios, since the rounding error is different for each ratio).