

New Framework for Standardized Notation in Wastewater Treatment Modelling

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Abstract

Many unit process models are available in the field of wastewater treatment. All of these models use their own notation, causing problems for documentation, implementation and connection of different models (using different sets of state variables). The main goal of this paper is to propose a new notational framework which allows unique and systematic naming of state variables and parameters of biokinetic models in the wastewater treatment field. The symbols are based on one main letter that gives a general description of the state variable or parameter and several subscript levels that provide greater specification. Only those levels that make the name unique within the model context are needed in creating the symbol. The paper describes specific problems encountered with the currently used notation, presents the proposed framework and provides additional practical examples. The overall result is a framework that can be used in whole plant modelling, which consists of different fields such as activated sludge, anaerobic digestion, sidestream treatment, membrane bioreactors, metabolic approaches, fate of micropollutants and biofilm processes. The main objective of this consensus building paper is to establish a consistent set of rules that can be applied to existing and most importantly, future models. Applying the proposed notation should make it easier for everyone active in the wastewater treatment field to read, write and review documents describing modelling projects.

Keywords

Wastewater treatment; modeling; nomenclature; ASM; ADM

INTRODUCTION

Mathematical modelling of wastewater treatment (WWT) processes has become a widely accepted tool in the past decade, and is used for research, plant design, optimization, training, and model-based development and testing of process control. Starting with the activated sludge system and now moving into whole plant modelling, the modelling community has produced a significant number of models describing the processes occurring in wastewater treatment plants (WWTPs).

New models and model extensions are constantly being developed in response to changing requirements, e.g. stricter effluent limits, or new processes such as side-stream treatment.

One of the milestones in dynamic modelling of WWTPs was the research carried out by the University of Cape Town (Ekama and Marais, 1977; Dold *et al.*, 1980). With this research a specific notation was introduced (further referred to as the ‘UCT system’) and several research groups are still using this naming system (e.g. Barker and Dold, 1997; Lee *et al.*, 2006). In 1987, a task group, chaired by Prof. Henze, of the International Association on Water Pollution Research and Control (IAWPRC originally, and since 2000 the International Water Association, IWA) introduced the first Activated Sludge Model for biological carbon and nitrogen removal (ASM1). ASM1 was based on the South African work but was presented in a new format (the Gujer or Petersen table, composed of a stoichiometric matrix, a rate vector and extra information as units and names) and with a new and standardized notation (in this paper referred to as the ‘IWA system’). The latter notation had its roots in the work of another IAWPRC/IUPAC task group, led by Prof. Grau (Grau *et al.*, 1982a, 1982b, 1987).

The need to widen the model boundaries and to include other process units led to the development of several other models such as ADM1 for anaerobic treatment (Batstone *et al.*, 2002), fixed biomass (Rittmann and McCarty, 1980; Wanner and Gujer, 1986; Horn *et al.*, 2003) and membrane bioreactors (MBRs; Lu *et al.*, 2001; Jiang *et al.*, 2008). Nitrite as an intermediate compound is included in several models (Sin *et al.*, 2008). Increased microbiological and biochemical insights led to the development of so-called metabolic models (e.g. Smolders *et al.*, 1995; Murnleitner *et al.*, 1997; Lavallée *et al.*, 2009; Lopez-Vazquez *et al.*, 2009). An emerging field is the modelling of the fate of micropollutants, where a number of models were proposed by several researchers (e.g. Joss *et al.*, 2006; Schönerklee *et al.*, 2009). All of these models are published with their own notation, sometimes using different names for the same compound or parameter, or the same name for different compounds/parameters.

Motivation

The need for a common international notation standard in biological wastewater treatment was already highlighted in Henze *et al.* (1982), where examples were given of abuse of notation (e.g. double notation, double meaning, misdirection, etc.). It was concluded that notation is a common cause of confusion due to the absence of a universally-agreed system of terminology. At the same time a proposal for unifying the notation used in the description of biological wastewater treatment processes was presented by Grau *et al.* (1982a, 1982b, 1987). This proposal was presented by a Working Group set up by the IAWPRC and the Commission on Water Quality of the International Union of Pure and Applied Chemistry (IUPAC). In this report, several symbols are listed together with their description, dimensions and some specifications as footnotes. This notation standard has been followed for many years. However, the complexity of WWT models has significantly increased over the last 25 years (Gujer, 2006) and new modelling concepts have been introduced. Moreover, in the work of Grau *et al.* (1982a, 1982b, 1987) no clear framework was given for future developments.

The need to re-address this problem arose during the work of the IWA task group on ‘Good Modelling Practice – Guidelines for Use of Activated Sludge Models’ (GMP TG 2008) as well as during the work on a book on Biological Wastewater Treatment (Henze *et al.*, 2008). The IWA task group on ‘Benchmarking of Control Strategies for Wastewater Treatment Plants’, implementing and describing the details of a plant-wide WWTP model, was confronted with the issue as well. A working group involving several experts was set up in connection with the 1st IWA/WEF

Wastewater Treatment Modelling Seminar (WWTmod2008), where the state-of-the-art in wastewater treatment modelling was discussed. It was decided to address the following problems:

- i) The same state variables and parameters used in different models or different platforms are named differently.
- ii) Several specific pitfalls prevail in the existing notations (e.g. colloidal matter, see next section).
- iii) No internationally accepted framework is available to name new state variables and parameters.
- iv) Model documentation (including notation) is time consuming and can lead to implementation errors.
- v) Model exchange is a problematic issue especially for complex models (Gernaey *et al.*, 2006).
- vi) Coupling different models is becoming common such as for plant-wide modelling (Grau *et al.*, 2009) making the use of one notation indispensable.
- vii) Different notations in reporting and coding can cause implementation errors and make double-checking difficult.

Given all of the above, it appears that a new and extendable notational framework is needed, that should:

- a. be as similar as possible to the existing notations,
- b. be simple,
- c. be straightforward and easy to understand,
- d. provide unique names within a model context,
- e. describe physical, biological and chemical properties important within the model context,
- f. be extendable for future developments.

To present the new framework, this paper is organized as follows; first, the general objectives for the framework are laid out and general notation rules are introduced. Then, separate sections for state variables and parameters are presented. They include a discussion on problems currently encountered and a description of the proposed new framework with some examples. Finally, the contributions of the new framework and the conclusions are described.

GENERAL FRAMEWORK

The proposed notation should be valid for the different subfields of WWT modelling, and is mainly focused on biokinetic models. Therefore, the new notation has been developed considering models for activated sludge, anaerobic digestion, sidestream treatment, membrane bioreactors, micropollutant fate and biofilm processes, etc. In addition, the notation also considers metabolic modelling approaches. The main objective of this consensus building paper is, first to create a consistent set of notation rules that can be applied to existing and more importantly, future models and second, to promote the establishment of a consensus on variable/parameter names.

Naming system established for the new notation

The main goal of the new notation is to provide a framework which allows unique naming of state variables (the compounds or components used in the model's mass balances) and parameters. The resulting name is kept as short and mnemonic as possible and previously accepted notation is applied whenever feasible. An important element of the new notation is that the symbols are

consistently defined as a main symbol with different subscript levels, which accounts for the increasing complexity of the models. Elements in the subscript are separated by a comma or underscores. The authors suggest using only the subscript levels required to make the name unique within the model context (e.g. for understanding the behaviour/role of the compound or parameter, or to prevent misinterpretation). **Thus, all levels of subscripts are optional and only those required should be used in a given model context.** Additional levels can be added by the model developer if further specifications are required (e.g. compartment or units of expression). The naming system also allows the use of superscripts under certain conditions (e.g. biofilm modeling) if this makes the symbol more comprehensible or better readable. The resulting symbols have to be properly documented in each of the models used and they are always presented with their units and their values. A list of the proposed abbreviations and symbols is given in Table 4 of the Appendix. In the preparation of the proposed list, existing abbreviations were favored over new ones.

STATE VARIABLES

While analysing current models, the most obvious problems were encountered with respect to the naming of state variables. New models, model extensions, the connection of models using different sets of state variables (e.g. in whole WWTP and other fields of integrated modelling) were driving forces to develop the new notational framework. The new notation should provide the information required in the context of the model used (e.g. on the physical, chemical and biological properties of the compounds).

Specific problems encountered

Different naming systems: Looking at the most common models one can observe that there is no real consensus with respect to the use of standardized symbols (Table 1).

- Main letter: In the IWA system the main letter is used to differentiate between the particulate ('X') variables that will settle out of the bulk liquid and soluble ('S') variables that will remain dissolved. The former UCT system uses the main letter to differentiate between units of measurement where 'S' represents substrate, 'Z' volatile solids in COD units, 'X' volatile solids in VSS units and 'N' nitrogen (e.g. $S_{bs,c}$, Z_{BH} , N_{obs}).
- Subscripts:
 - Degradability: In the UCT system 'B' stands for biodegradable and 'U' for unbiodegradable (e.g. S_{US}). In the IWA notation they are given as 'S' (substrate) and 'I' (inert) (e.g. S_I). Conversion processes that do not depend on biodegradation, such as precipitation, acid-base reactions or adsorption, lack a clear notational framework to deal with these 'abiotic' (non biological) reactions.
 - Structured biomass: With the introduction of structured biomass models (e.g. Smolders *et al.*, 1995; Wild *et al.*, 1995; Lavallée *et al.*, 2009) it becomes necessary to link cell-internal products (e.g. PHA, RNA) to a specific biomass group (e.g. X_{PHA} in ASM2d is not linked to an organism group).
- Specification system:
 - Subscripts are not standardized with respect to upper and lower case (e.g. S_{BC} in GenASDM and $S_{bs,c}$ in UCTPHO).
 - The order of specifications is not standardized.
- Units: Different models use different units for the same state variables. For example, ADM1 model uses $\text{kg COD}\cdot\text{m}^{-3}$ as the basis in addition to $\text{kmol C}\cdot\text{m}^{-3}$ (for HCO_3^- and CO_2) and $\text{kmol N}\cdot\text{m}^{-3}$ (for NH_4^+ and NH_3). ASM models use $\text{g COD}\cdot\text{m}^{-3}$, $\text{g N}\cdot\text{m}^{-3}$ and $\text{mol HCO}_3^-\cdot\text{m}^{-3}$ for alkalinity.

Another example is S_{ND} in ASM1 and N_{OS} in GenASDM which represent soluble biodegradable organic nitrogen. Both symbols use ‘S’ for soluble and ‘N’ for nitrogen, but they are combined in a different way.

Different names used: ammonia, nitrate, oxygen, volatile fatty acids and other compounds have different symbols or abbreviations in different models (see Table 1). Moreover, biomass names are abbreviated differently (e.g. nitrifying organisms in Table 1).

Non-meaningful names: Some state variable names do not provide a clear and unique meaning (e.g. S_A in ASM2d does not provide a clear meaning, unless the letter ‘A’ would be considered a standardized abbreviation for acetate. However, the letter ‘A’ is also used in ASM2d to abbreviate autotrophic, e.g. Y_A).

Colloidal matter: The first structured activated sludge models divided the organic substrate according to degradability (readily [S_S] and slowly [X_S] biodegradable compounds). For these models there is an incoherent use of ‘X’ and ‘S’ that refer to the particle size. S_S is mostly soluble, while X_S contains both particulate and soluble (colloidal) compounds in these models. This S - X distinction is frequently confusing modellers as it cannot be directly converted to soluble and particulate compounds, which were required later for primary and secondary settler and whole plant modelling. Introducing a colloidal fraction (which is both soluble and slowly degradable) solves this problem. Filtrates containing both soluble and colloidal fractions can be properly distinguished. The WERF and STOWA influent fractionation methods (Melcer *et al.*, 2003; Roeleveld and van Loosdrecht, 2002) contain a specific flocculation step to discriminate between a colloidal fraction and truly soluble compounds.

Table 1. Selection of state variable symbols used in different models

Description	ASM1 ¹⁾	ASM2d ¹⁾	ASM3 ¹⁾	GenASDM ²⁾	UCTPHO ³⁾	UCTPHO+ ⁴⁾	TU Delft-P ⁵⁾	ADMI ⁶⁾
Fermentable organic matter		S_F		S_{BSC}	$S_{bs,c}$	S_F	S_F	$S_{su}+S_{aa}+S_{fa}$
Volatile fatty acids		S_A		S_{BSA}		S_A	S_A	$S_{va}+S_{bu}+S_{pro}+S_{ac}$
Propionate				S_{BSP}				S_{pro}
Dissolved methane				S_{CH4}				S_{ch4}
Soluble inert organic matter	S_I	S_I	S_I	S_{US}	S_{US}	S_I	S_I	S_I
Dissolved oxygen	S_O	S_{O2}	S_O	DO	O	S_{O2}	S_O	
Particulate inert endogenous products	X_P	X_I	X_I	Z_E	Z_E	X_E		X_I
Particulate inert organic matter from influent	X_I			X_I	Z_I	X_I		X_I
Soluble biodegradable organic N	S_{ND}			N_{OS}	N_{obs}			
Total ammonia	S_{NH}	S_{NH4}	S_{NH}	S_{NH3}	N_a	S_{NH4}	S_{NH}	S_{IN}
Total nitrite + nitrate	S_{NO}	S_{NO3}	S_{NO}	$S_{NO2}+S_{NO3}$	N_{O3}	S_{NO3}	S_{NO}	
Ordinary heterotrophic organisms	$X_{B,H}$	X_H	X_H	Z_{BH}	Z_{BH}	X_H	X_H	
Nitrifying organisms (NH_4 to NO_3)	$X_{B,A}$	X_{AUT}	X_A	$Z_{AOB}+Z_{NOB}$	Z_{BA}	X_{NIT}	X_A	
Stored poly- β -hydroxyalkanoates in PAOs		X_{PHA}		S_{PHA}	X_{PHA}	X_{PHA}	X_{PHA}	

¹⁾ IWA Activated Sludge Models, Henze *et al.* (2000), ²⁾ ‘General Activated Sludge Digestion Model’ proprietary model in simulation software BioWin 3 (ESA, 2007), ³⁾ University of CapeTown model, Wentzel *et al.* (1992), ⁴⁾ latest version of UCT model, Hu *et al.* (2007), ⁵⁾ TU Delft phosphorus removal model, Meijer (2004), ⁶⁾ IWA Anaerobic Digestion Model No.1, Batstone *et al.* (2002).

Framework

In the proposed notational framework, the main symbol is related to the particle size and should always be given. In the subscript, four levels can be provided, each referring to different information:

1. Degradability
2. Organic/inorganic compound
3. Name of compound or organism
4. Additional specifications.

The main symbol is in upper case and italics, the different elements of the subscript are in upper case (or combined with lower case if needed to make the name clearer, e.g. AcCoA) and not italicised, as defined in Table 4 of the Appendix. Figure 1 shows the proposed framework and some examples that illustrate the notational procedure.

In most cases, one or several of the subscript levels are not required (as illustrated in Figure 1), and therefore, are not included in the symbol. Generally, if the name of the compound is provided (e.g. Volatile Fatty Acids, abbreviated as VFA), it is not necessary to write the preceding levels (i.e. degradability or organic/inorganic). Finally, depending on the model or on the context for describing the model, it may be necessary to add specifications, as the final elements of the subscript. An example is X_I in the ASM1 model, which becomes $X_{U,Inf}$ when applying the proposed notation, with the subscript ‘Inf’ referring to the fact that this fraction originates from the influent of the WWTP.

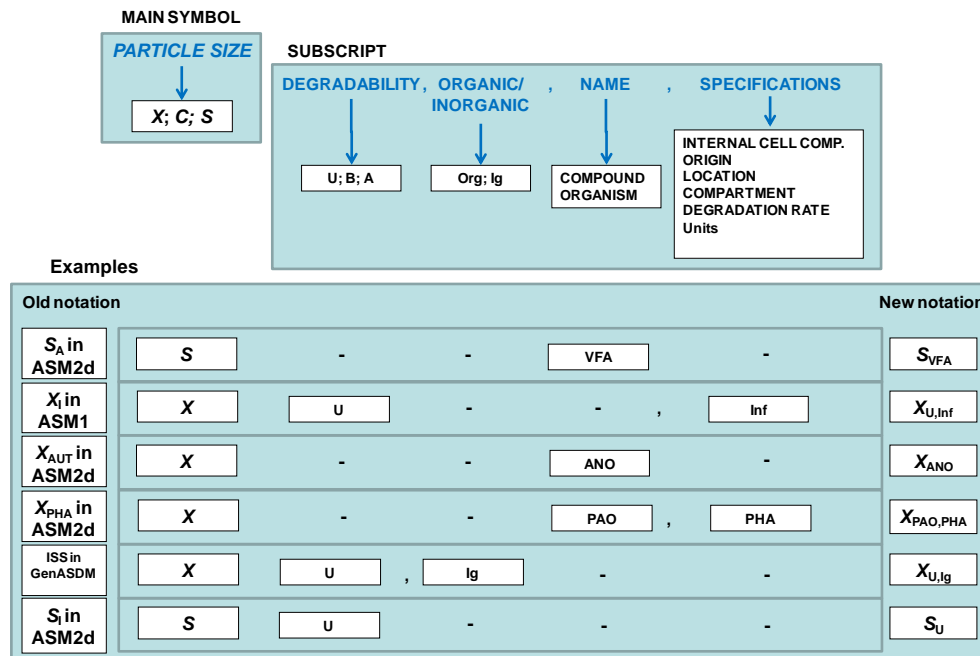


Figure 1. Description of the proposed notation for state variables

Notational procedure

Particle size: The first upper case letter of the notation is related to the particle size. It is proposed to differentiate between soluble (*S*), particulate (*X*) and colloidal (*C*) matter. The novelty here is that the colloidal fraction is included explicitly, as was already proposed by Melcer *et al.* (2003). The filter size to distinguish between soluble, particulate and colloidal compounds cannot be specified at this stage, considering that MBR researchers need to adapt it according to the membrane pore size used. Therefore, the particle size used in a particular model (or study) should be specified and

documented. Care should be taken not to confuse the use of ‘C’ for colloidal and for total material concentration (as defined in Grau *et al.*, 1987). It is proposed to use the symbol ‘Tot’ for total material concentration.

Degradability: This is one of the most important aspects of WWT models. It is proposed to distinguish between undegradable (U), biodegradable (B) and abiotically convertible (A) compounds. The last symbol was already used in Howard *et al.* (1991) and refers to compounds that can be involved in conversion processes that are not related to the metabolism of an organism (e.g. photolysis, chemical reactions, adsorption, etc.).

Organic/inorganic: This differentiation is useful, notably, to distinguish between autotrophic and heterotrophic metabolism, where the carbon is obtained from inorganic (Ig) or organic (Org) compounds.

Name: For biomasses, all variables that contain an ‘X’ (as an upper case letter) and a subscript that finishes with an ‘O’, represent an organism (e.g. X_{OHO} for ordinary heterotrophic organisms).

For simple state variables describing specific molecules, there are two ways to specify names:

- a. An abbreviation of the compound’s name if the chemical formula is too long. Examples are given in Table 4 of the Appendix. Upper and lower cases will be used as follows:
 - For acronyms: Upper case is used for all letters (e.g. OHO)
 - For initial and syllabic abbreviations: The first letter is upper case and the rest is lower case (e.g. Inf, Org, Ig), except for abbreviations that refer to a process (e.g. hyd for hydrolysis) where all letters are lower case.
- b. The chemical formula itself if it is sufficiently short (e.g. NH_4 , CH_4 , NO_2). The IUPAC recommendations for nomenclature on organic and inorganic chemistry can be found in Hellwinkel (2001; The Blue Book) and Connelly *et al.* (2005; The Red Book), respectively.

If chemical species are part of the model, it is necessary to differentiate between protonated and non protonated molecules, which may be uncharged or ionic molecules depending on specific compounds, as well as ion activity and concentration. In accordance with established chemical notation, we propose to use:

- Brackets for the ion concentration (e.g. $S_{[NH_4]}$ or $S_{[Ac]}$). Standard units should be $[kmol.m^{-3}]$
- Parentheses for ion activity (e.g. $S_{(NH_4)}$) in $[kmol.m^{-3}]$
- Use of ‘H’ for undissociated acids (e.g. acetic acid concentration would be $S_{[HAc]}$)
- No brackets or parentheses for total compounds (e.g. S_{NH_x} $[g N.m^{-3}]$ for total ammonia consisting of NH_3 and NH_4 (the x is used to lump both) or S_{Ac} $[g COD.m^{-3}]$ for the sum of acetate and acetic acid)

For example, the description of total ammonia in the system is frequently required (e.g. in ASM1, S_{NH_x} , as substrate for autotrophic nitrifying organisms, ANOs). Other times the model needs to consider one of the ionic species (e.g. inhibition by ammonia, $S_{[NH_3]}$).

Specifications: In certain cases it is necessary to include extra information in the name of the variable (fourth and next levels). The following cases are considered:

- Structured biomass compounds will appear in the symbol next to the name of the organism, separated by a comma. With cell internal storage products, different levels of detail can be considered. For example, $X_{PAO,PHA}$ would be preferred when glycogen is included in the

model as another state variable (i.e. modelling more than one storage polymer), while $X_{\text{PAO,Stor}}$ would be fine in cases where glycogen is not considered (i.e. only one organic storage polymer is modeled).

- The origin of the products can be specified to indicate whether the compound is originating from endogenous processes (E) or from the influent (Inf) (e.g. $X_{\text{U,E}}$ or $X_{\text{U,Inf}}$ to describe the ASM1 state variables X_{P} and X_{I} , respectively).
- For some models it is important to specify the compartment. For instance, in the case of biofilm or anaerobic digestion models, different compounds are in equilibrium between different compartments/phases. The symbols considered for the compartments are the following (Morgenroth, 2008): L for liquid, G for gas, F for the inner biofilm, LF for the biofilm surface (e.g. $S_{\text{CO}_2,\text{L}}$ or $S_{\text{CO}_2,\text{G}}$). If all variables of the model belong to the same compartment, there may be no need to specify the compartment.
- If required, the valence of an ion, e.g. in the case that $S_{\text{Fe},2}$ and $S_{\text{Fe},3}$ are considered in the same model.
- If required, the units can be defined as an additional subscript. They should be written as shown in Grau *et al.* (1987), indicating the power (can be negative or positive) in the superscript (e.g. $\text{g COD}\cdot\text{m}^{-3}$).

Naming lumped variables

A lumped variable is the single variable obtained after grouping several variables. The first two levels proposed in the new framework allow the grouping of variables according to the degradability and the organic-inorganic properties (e.g. see in Figure 2, $X_{\text{U,Org}}$ and $X_{\text{B,Org}}$). It is also possible within this framework to lump variables according to their particle size. In this case, the main symbol will contain the different particle size letters, following the sequence $X \rightarrow C \rightarrow S$ (for example, X_{S} in ASM1 is X_{C_B} according to the new notation). For some of the lumped variables, the specific name is normally provided (e.g. ‘Stor’ for storage products or ‘Bio’ for total biomass). Composite variables (calculated from multiple state variables, facilitating the comparison of model results with experimental measurements) are not discussed in this paper.

Example

ASM2d using the new framework

Figure 2 shows an example for the use of the new state variable notational framework for ASM2d (Henze *et al.*, 2000). The variables are organized according to particle size, organic/inorganic properties and degradability.

Table 2 presents a comparison of the symbols used for ASM2d according to the former and new notational systems. It can be seen that the main symbols are kept identical (except for the former X_{S} , which becomes X_{C_B}) in the proposed framework and that some modifications are introduced in the subscripts. For simple variables describing specific molecules, the chemical formula is used in both notational systems (e.g. S_{N_2} , S_{O_2} , S_{PO_4}). For total ammonia an ‘x’ is added at the end of the subscript with the new notation (the ‘x’ combines NH_4^+ and NH_3); the same applies for S_{NO_x} , where the ‘x’ combines NO_2^- and NO_3^- . Regarding volatile fatty acids, the subscript ‘VFA’ is used in the new notation instead of the abbreviation ‘A’ used previously. For variables that do not have a specific name or formula, the degradability is specified in the subscript (e.g. X_{U} , X_{C_B}). Organism variable symbols have the main symbol ‘X’ and the subscript finishes with an ‘O’ (e.g. X_{ANO} for ammonium nitrifying organisms, X_{OHO} for ordinary heterotrophic organisms). Internal cell compound symbols are linked to the organism ($X_{\text{PAO,Stor}}$).

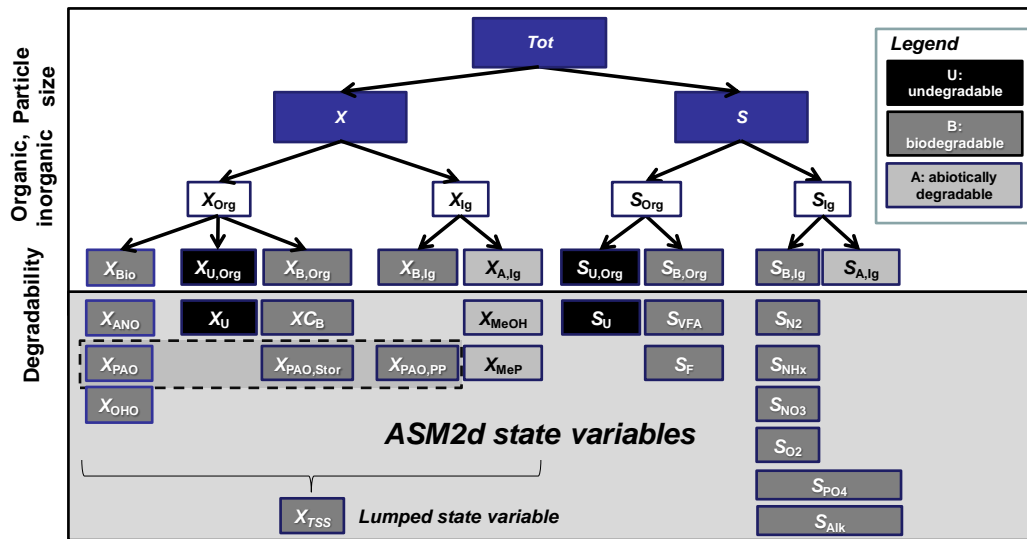


Figure 2. ASM2d state variables using the proposed notational framework

Table 2. Comparison of the former and new notational systems for ASM2d. Bold signifies a proposed change to the state variable name. (1) In the ASM2d definitions X_S includes colloidal substrates and (2) X_I does not include colloidal substrates; (3) normally NO_3 stands for nitrate only; (4) X_{PHA} is not directly the measured PHA.

Description	Former notation	New notation
Fermentable organic matter	S_F	S_F
Fermentation products, considered to be acetate	S_A	S_{VFA}
Soluble undegradable organics	S_I	S_U
Dissolved oxygen	S_{O2}	S_{O2}
Slowly biodegradable substrates ⁽¹⁾	X_S	X_{C_B}
Particulate undegradable organics ⁽²⁾	X_I	X_U
Ammonium plus ammonia nitrogen	S_{NH4}	S_{NHx}
Nitrate plus nitrite nitrogen ⁽³⁾	S_{NO3}	S_{NOx}
Dissolved nitrogen gas	S_{N2}	S_{N2}
Soluble inorganic phosphorus	S_{PO4}	S_{PO4}
Ordinary heterotrophic organisms	X_H	X_{OHO}
Autotrophic nitrifying organisms	X_{AUT}	X_{ANO}
Phosphorus accumulating organisms	X_{PAO}	X_{PAO}
Cell internal storage product of phosphorus-accumulating organisms ⁽⁴⁾	X_{PHA}	$X_{PAO,Stor}$
Stored polyphosphates in PAOs	X_{PP}	$X_{PAO,PP}$
Metal-hydroxides	X_{MeOH}	X_{MeOH}
Metal-phosphates	X_{MeP}	X_{MeP}
Alkalinity	S_{ALK}	S_{Alk}
Total suspended solids	X_{TSS}	X_{TSS}

MODEL PARAMETERS

It is an insurmountable task to define a framework that covers the naming of every parameter used in all present and future biokinetic models. Therefore, the authors' goal was to provide a framework for standard, frequently used parameters or for cases where problems were encountered in current practice. The comparison of the parameter symbols used in different models (see Table 3) reveals some challenges that the new notation faces (e.g. avoiding the use of different main symbols and subscripts for the same parameter).

This section describes the stoichiometric and kinetic parameters separately, in accordance with the setup of the Gujer matrix.

Table 3. Parameter symbols used in different models

Description		ASMI ¹⁾	ASM2d ¹⁾	ASM3 ¹⁾	GenASDM ²⁾	UCTPHO ³⁾	UCTPHO+ ⁴⁾	TU Delft-P ⁵⁾	ADMI ⁶⁾
Yield for autotrophic biomass	$g X_{ANO} \cdot (g N)^{-1}$	Y_A	Y_A	Y_A		Y_{ZA}	Y_{NIT}	Y_A	
Correction factor for max growth rate under anoxic conditions	-	η_g	η_{NO3}	$\eta_{NO,H}$	η_G	η_G	η_H	η_{NO}	
Saturation/inhibition coeff. for oxygen	$g O_2 \cdot m^{-3}$	$K_{O,H}$	K_{O2}	$K_{O,H}$	K_{OH}	K_{OH}	K_{OH}	K_O	
Rate constant for storage of X_{PHA} (base X_{PP})	$g X_{PAO,PHA} \cdot (g X_{PAO})^{-1} \cdot d^{-1}$		q_{PHA}	q_{PHA}	K_{SCFA}	K_P	q_{PHA}	q_{Ac}	
Saturation coeff. for phosphate (nutrient)	$g P \cdot m^{-3}$		K_P	$K_{PO4,PAO}$	K_P	K_{PS}	$K_{PO4-gro}$	K_P	
Saturation coeff. for ammonium (substrate)	$g N \cdot m^{-3}$	K_{NH}	K_{NH4}	$K_{NH,A}$	K_{NH}	K_{SA}	K_{NH4}	K_{NH}	
Max. rate for fermentation	$g S_F \cdot (g X_{OHO})^{-1} \cdot d^{-1}$		q_{fe}		$\mu_{ZBH,ANA}$	K_C	K_{FE}	q_{fe}	
Max. specific hydrolysis rate	d^{-1}	k_h	k_h	k_h	k_h	K_{MP}		k_h	$k_{hyd,i}$

¹⁾ IWA Activated Sludge Models, Henze *et al.* (2000), ²⁾ 'General Activated Sludge Digestion Model' proprietary model in simulation software BioWin 3 (ESA, 2007), ³⁾ University of Cape Town model, Wentzel *et al.* (1992), ⁴⁾ latest version of UCT model, Hu *et al.* (2007), ⁵⁾ TU Delft phosphorus removal model, Meijer (2004), ⁶⁾ IWA Anaerobic Digestion Model No.1, Batstone *et al.* (2002).

Stoichiometric Parameters

Yield

In the proposed notation a 'yield' represents a stoichiometric parameter describing the amount of a specified product that is obtained from specified amounts of reactants.

Specific problems encountered

- For the biomass growth yield coefficients, there is no standardization to specify the substrate source (not considered in the evaluated models) and the environmental conditions (e.g. for aerobic conditions, O is used in TU Delft-P and the subindex 1 in UCTPHO⁺).
- Naming yields, such as for cell-internal storage (e.g. Y_{PO4} in ASM2, which represents the requirement of X_{PP} per X_{PHA} storage during P-release), is not straightforward and does not allow a clear understanding of the parameter on the basis of the symbol only.

Framework

The main symbol for yield is *Y* (upper case letter and italics). Subscripts start with the reactant (or substrate source) and, through an underscore, describe the product (e.g. the cell-internally stored compounds). They continue with the name of the organism followed by the environmental conditions, which allows differentiating yields depending on the availability of oxygen and nitrate/nitrite (Ox: oxic; Ax: anoxic; Ax2: anoxic, nitrite present; Ax3: anoxic, nitrate present; and An: anaerobic). The ‘reactant_product’ subscript with the underscore between the two compounds for the yield is used in other fields as well. For instance in Roels (1983), Y_{SX} represents the yield of biomass on substrate and Y_{SP} the yield of product on substrate. Figure 3 shows the proposed framework and some examples that illustrate the notational procedure. In the cases when only one substrate is consumed for direct growth the ‘reactant_product’ pair is not required (e.g. Y_{OHO}).

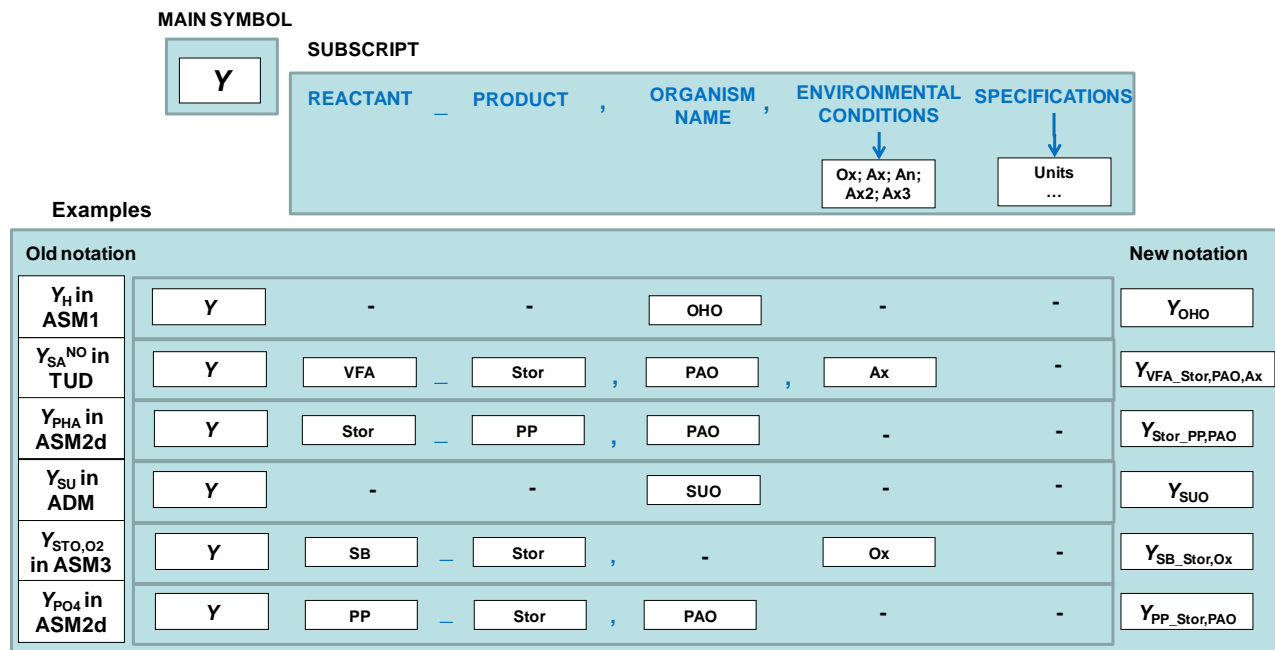


Figure 3. Notational framework and examples for the naming of yield coefficients

Composition and fractionation coefficients

In the proposed framework, composition coefficients refer to the conversion factors used in the continuity equations. Within this context they are defined as a part of a larger entity to explain the composition of a compound. For instance, composition factors are used to specify the content of an element (N, P), charge or any other part (e.g. COD, TSS) of a compound or organism (e.g. nitrogen content of ordinary heterotrophic organisms).

Fractionation coefficients are used to indicate the portion of a state variable that is transformed via a specific process (e.g. f_p in ASM1 describes the fraction of biomass leading to unbiodegradable particulate decay products).

Specific problems encountered:

- Need for clarification of the different use of fractions (composition vs fractionation).
- Order of fraction and organism/main compound in the symbol is not defined.

Framework

The main symbol defines the meaning of the stoichiometric coefficient used. The letter ‘*i*’ is used for composition coefficients and ‘*f*’ for fractionation coefficients. When using ‘*i*’, the first subscript represents the smaller portion (e.g. nitrogen content) and the second subscript represents the main compound or organism (larger entity). When using ‘*f*’, the same order of subscripts is used (“smaller”_”larger”) and the process type can be added in the specifications level. Figure 4 presents the proposed framework and some examples that illustrate the notational procedure. *f* can eventually be used to express ratios (e.g. PP/PAO in ASM2d would become f_{PP_PAO}).

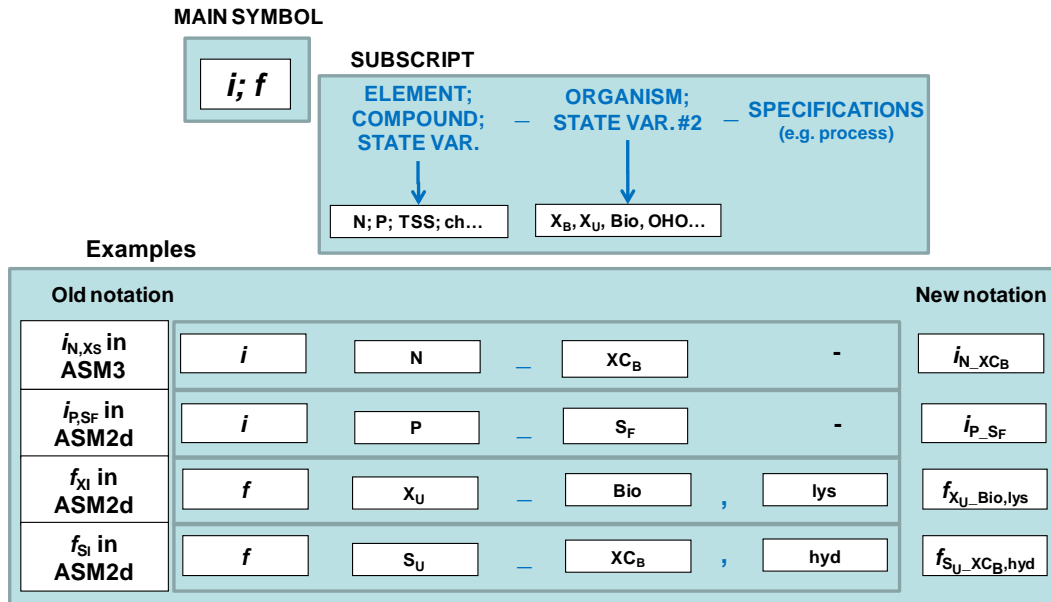


Figure 4. Notational framework and examples for the naming of fractions

As a general rule simplification is recommended for state variables specified in one of the subscript levels of the parameters. The main letter (X,C,S) is used only if the subscript is not meaningful by itself. Normally, the organism names and the chemical compounds can be written without main letter (e.g. Bio). Lumped variables will need the main letter (e.g. XC_B). The comas separating the subscripts of a state variable name will not be used (e.g. i_{P_XUE}). This applies to the rest of the parameters as well.

Kinetic Parameters

Rate coefficients and reduction factors

Reaction rates characterize the kinetics of a process. In ASM-type models, process rate equations (ρ_j) normally include the maximum rate and several saturation terms (e.g. Monod term, Michaelis-Menten...). Reduction factors account for a reduced rate under specific environmental conditions (e.g. anoxic conditions). This framework focuses on the rate coefficients and reduction factors used in these equations.

Specific problems encountered:

- The letter ‘*k*’ was used for both rates (lower case ‘*k*’) and saturation coefficients (upper case ‘*K*’), which could lead to confusion (e.g. for hydrolysis rate k_H and saturation coefficient K_H).
- Not all rate constants were defined in all models (e.g. maintenance was missing in most notational systems)

- A framework to include different substrate sources was missing (e.g. the growth of OHOs on acetate and propionate is usually modelled as two processes).

Framework

The main symbol (lower case letter, italics) specifies growth (μ), decay or endogenous respiration (b) and maintenance (m) (van Loosdrecht and Henze, 1999) and ‘ q ’ is used for all other rates. As additional information, *correction factors* are specified in the framework since they can also be used for these parameters (the main letter is ‘ η ’) and temperature correction (θ) as well.

The first subscript is used for the correction factors to specify the main symbol. The second subscript includes the organism in upper case and in the third level the substrate source or the ‘reactant_product’ pair is specified. Other specifications may be given in the fourth level. Figure 5 provides an overview of the framework and some examples, including one for a reduction factor under anoxic conditions for the heterotrophic growth rate in ASM2d and an example for a temperature correction factor. In the latter case, the equation used for temperature correction should be properly documented (‘pow’ or ‘exp’ can be used in the specifications to indicate the type of equation).

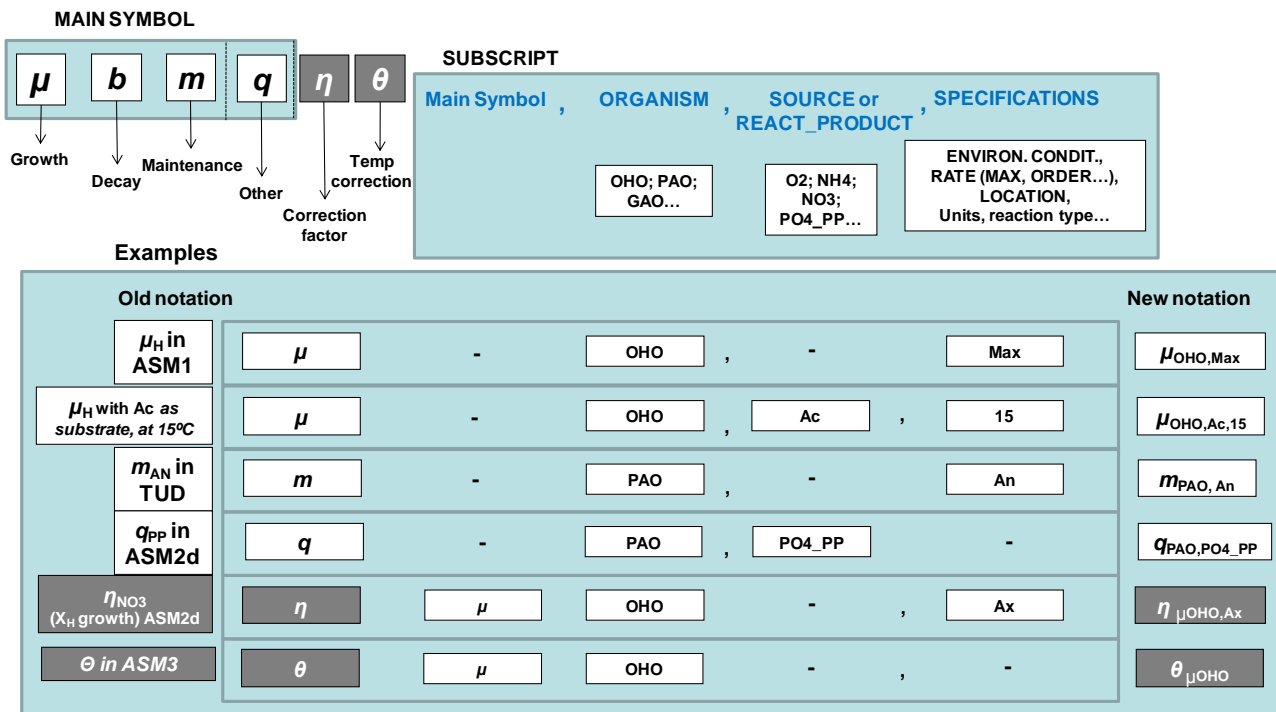


Figure 5. Notational framework and examples for the naming of kinetic rates and reduction factors

Additional explanations and examples

Some common abbreviations for processes (e.g. "hyd" for hydrolysis, "ab" for acid-base reactions) can be found in Table 4 of the Appendix. In the last examples of Figure 5, ‘ η ’ and ‘ θ ’ have been used as main symbols and the parameter symbol to which they refer is found in the subscript.

Saturation or inhibition coefficients

These coefficients are used in reduction terms (e.g. Monod, inhibition Monod, Haldane, etc.) to reduce the maximum process rate according to the existence or limitation of another compound.

Specific problems encountered:

- Non-unique names for some coefficients (e.g. K_{PP} and K_{IPP} in ASM2d or K_{O_2} without reference to specific biomass or a ratio).
- Additional information is sometimes required to understand the meaning of a parameter.

Framework

The main symbol is an upper case K in italics. The first subscript level describes the type of the reduction term (saturation or inhibition). The second level relates to the main compound. The name of the related organism can be given in the third level. For a surface saturation term an underscore is used to highlight the ratio between main compound and organism or second compound (e.g. K_{fPHA_PAO} in $\frac{X_{PAO,PHA}/X_{PAO}}{(K_{fPHA_PAO} + X_{PAO,PHA}/X_{PAO})}$). Figure 6 presents the proposed framework and some examples that illustrate the notational procedure.

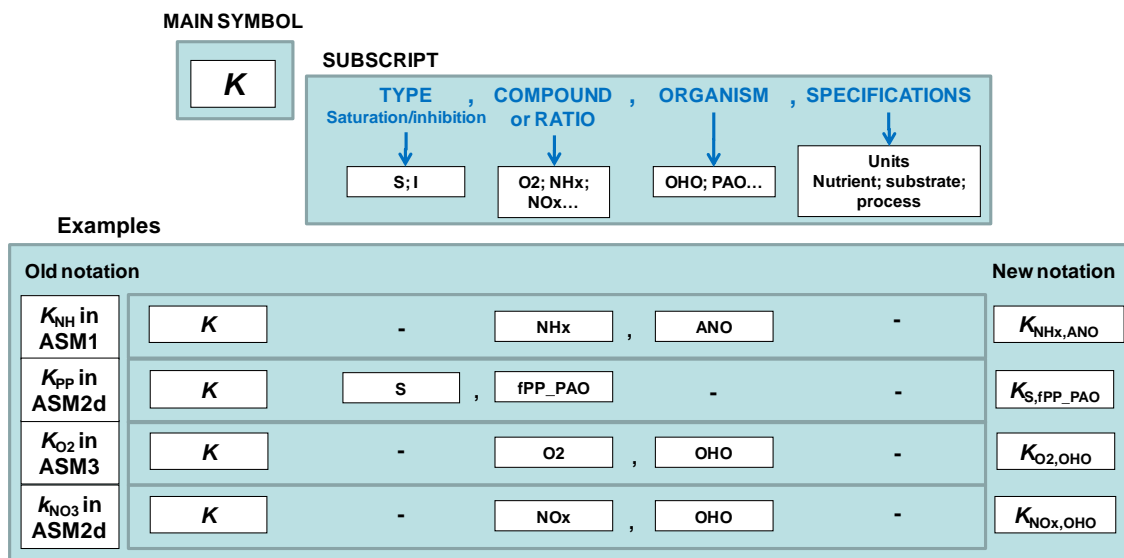


Figure 6. Notational framework and examples for the naming of saturation/inhibition constants

CONTRIBUTIONS OF THE NEW FRAMEWORK

The new framework provides a structured system to specify the symbols for state variables and parameters used in wastewater treatment modelling. Different symbol levels, providing physical, biological and chemical information, are introduced in a systematic and intuitive way with the intention to provide a straightforward, simple and easy to understand framework. Necessarily, there must be compromise in order to keep symbols simple, yet meaningful. This is achieved by providing only those subscript levels that are required to make the symbol unique within the model context. The characters chosen for the framework originated from previously proposed notational examples and the symbols that result are often similar or identical to the ones that were most commonly used in practice. A list of abbreviations is provided as an attempt to standardize selected words and symbols (see Table 4 of the Appendix). The structured framework allows the development of new symbols for new models (in different subfields of WWT modelling) and the extension of the same framework for future developments. The authors have converted state variables and parameters of several accessible models in order to check the applicability of the new framework. The results of this exercise show that conversions are most often straightforward, while

naming gaps or other problems were not encountered. In an effort to assist with the implementation of the proposed framework by model users, a comprehensive list of the former and new notational symbols for the most commonly used models will be available on the Water Science and Technology website.

CONCLUSIONS

It is the hope of the authors that the proposed framework combines the advantages of different notational systems, such as the UCT and IWA systems, resulting in a standardised methodology for expressing nomenclature that is useful for the WWT modelling community. Using common notation should facilitate communication amongst modellers and other experts. It should help to achieve better ‘readability’ of new models and help prevent misinterpretation and implementation errors. Since coding is an essential and error-prone part of model implementation, the new notation also provides naming rules for programming.

In view of emerging fields in WWT modelling, like the fate of micropollutants and the inclusion of water chemistry, or new modelling approaches like metabolic or structured biomass models, a standardised framework for notational expression is a highly valuable means of conveying modelling advances to the entire WWT modelling community. With the proposed framework, it should be possible to give meaningful, distinct and commonly accepted names to the new variables and parameters that will inevitably arise from these future advances.

The next step is to convince modellers around the world to adjust their notation and use the new naming rules. The authors believe that these alterations are necessary in order to ease the transfer of knowledge between modelling studies. The structured framework proposed should be directive, yet flexible enough for the benefit of all model users and for the future of modelling.

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APPENDIX

Table 4. Abbreviations proposed for the new notational framework

<i>Lumped variables</i>		<i>Organisms</i>	
A	Abiotically convertible compound	OHO	Ordinary heterotrophic organisms
B	Biodegradable compound (substrate)	AAO	Amino acid degrading organisms
Bio	Organisms (biomass)	ACO	Acetoclastic methanogenic organisms
Ig	Inorganic compound	AMO	Anaerobic ammonia oxidizing organisms
Inh	Inhibitory compound	ANO	Autotrophic nitrifying organisms (NH ₄ ⁺ to NO ₃)
ISS	Inorganic suspended solids	AOO	Ammonia oxidizing organisms
MP	Micropollutant	FAO	Fatty acid degrading organisms
Org	Organic compound	FeOO	Ferrous oxidizing organisms
Stor	Cell-internal storage compound	FeRO	Ferric reducing organisms
Tot	Total	GO	G-Bacteria
Tox	Toxic compound	GAO	Glycogen accumulating organisms
TSS	Total suspended solids	GAO_GB	GAO <i>Competibacter</i>
U	Undegradable compound	GAO_DEF	GAO <i>DeFluviicoccus</i>
VSS	Volatile suspended solids	HMO	Hydrogenotrophic methanogenic organisms
<i>Abbreviations</i>		LOO	Lipid oxidizing organisms
AA	Amino acid	MEOLO	Methylotrophic organisms
Ac	Acetate	NOO	Nitrite oxidizing organisms
AcCoA	Acetyl-CoA	PAO	Phosphorus accumulating organisms
Ads	Adsorbed compound	PRO	Propionic acetogenic organisms
Alk	Alkalinity	SOO	Sulfide oxidizing organisms
BAP	Biomass-associated products	SRO	Sulfate reducing organisms
Bu	Butyrate	SUO	Sugar utilizing organisms
Ca	Calcium	VBO	Valerate and butyrate degrading organisms
CHO	Carbohydrates	<i>Chemical formula</i>	
F	Fermentable organic matter ⁽¹⁾	CH3OH	Methanol
Gly	Glycogen	CH4	Methane
HAc	Acetic acid	CO2	Carbon dioxide
HAP	Hydroxyapatite	CO3	Carbonate
HBu	Butyric acid	H2	Hydrogen
HDP	Hydroxy dicalcium phosphate	H2O	Water
Hi	High Molecular Weight	HCO3	Bicarbonate
HPr	Propionic acid	HNO2	Nitrous acid
Hva	Valeric acid	HNO3	Nitric acid
LCFA	Long chain fatty acid	N	Nitrogen
Li	Lipids	N2O	Nitrous oxide
Lo	Low Molecular Weight	NH3	Ammonia
MAP	Struvite (magnesium ammonium phosphate)	NH4	Ammonium
Me	Metals	NHx	Sum of ammonium and ammonia
MeOH	Metal hydroxide precipitate	NO2	Nitrite
MeP	Metal phosphate compound	NO3	Nitrate
Mg	Magnesium	NOx	Sum of nitrite and nitrate
MW	Molecular Weight	O2	Oxygen
PH2MV	Poly-β-hydroxy-2-methylvalerates	P	Phosphorus
PHA	Poly-β-hydroxyalkanoates	PO4	Phosphate
PHB	Poly-β-hydroxybutyrates	S	Sulfur
PHV	Poly-β-hydroxyvalerates	SO3	Sulfite
PP	Polyphosphate	SO4	Sulfate
Pr	Propionate	<i>Micropollutants</i>	
PrCoA	Propionyl-CoA	BpA	Bisphenol A
Prot	Protein	Def	Diclofenac
Su	Sugar	DEHP	Di(2-ethylhexyl) phthalate
UAP	Utilization-associated product	Ibp	Ibuprofen
Va	Valerate	LAS	Linear alkyl benzene sulfonate (anionic detergent)
VFA	Volatile fatty acid		

Table 4. (continuation)

<i>Main symbols</i>		<i>Processes</i> ⁽²⁾	
<i>Parameters</i>		ab	Acid-base reaction
<i>b</i>	Decay rate	ads	Adsorption
<i>f</i>	Fraction	am	Ammonification
μ	Growth rate	dis	Dissociation
<i>i</i>	Composition coefficient	fe	Fermentation
<i>K</i>	Saturation coefficient	gro	Growth
<i>m</i>	Maintenance rate	hyd	Hydrolysis
η	Reduction factor	lys	Lysis
<i>r</i>	Reaction rate	pre	Precipitation
<i>q</i>	Other rates than μ , <i>b</i> and <i>m</i>	red	Redisolution
<i>Y</i>	Yield	stor	Storage of cell-internal compounds
<i>State variables</i>		<i>Environmental conditions</i>	
<i>C</i>	Colloidal	An	Anaerobic
<i>S</i>	Soluble	Ax	Anoxic (nitrite and nitrate present)
<i>X</i>	Particulate	Ax2	Anoxic (nitrite present)
<i>Origin</i>		Ax3	Anoxic (nitrate present)
<i>E</i>	Endogenous product	Ox	Oxic or aerobic
<i>Inf</i>	Compound originating from the influent	<i>Compartments</i>	
<i>Other</i>		F	Inner biofilm ⁽¹⁾
<i>Max</i>	Maximum	G	Gas
<i>Plim</i>	Rate limited by phosphorus	L	Liquid
		LF	Biofilm surface

(1) The same abbreviation (F) is used for fermentable organic matter and for the inner biofilm compartment. However, the compartment is specified in the last subscript and the variable name in the first subscript, avoiding confusion.

(2) All letters are lower case for process abbreviations to minimize confusion (e.g. Stor and stor)

