

# ACTIVATED SLUDGE MODEL NO. 3

by

**IAWQ TASK GROUP ON MATHEMATICAL MODELLING FOR DESIGN AND  
OPERATION OF BIOLOGICAL WASTEWATER TREATMENT**

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# 1. Introduction

With the introduction of the Activated Sludge Model No. 1 (ASM1) the IAWPRC (later IAWQ and now IWA) Task Group on Mathematical Modelling for Design and Operation of Biological Wastewater Treatment Processes introduced a new paradigm for the mathematical modelling of activated sludge systems. ASM1 as it was introduced in 1987 (Henze *et al.*, 1987) has become a major reference for many scientific and practical projects. Today, mathematical models related to ASM1 are implemented in various computer codes for the simulation of the behaviour of activated sludge systems treating municipal wastewater of mainly domestic origin.

With over ten years of experience with the application of ASM1, some defects of this model have become apparent, including:

- ASM1 does not include kinetic expressions that can deal with nitrogen and alkalinity limitations of heterotrophic organisms. The result is that computer code cannot be based on the original form of ASM1, where under some circumstances negative concentrations of, for example, ammonium may occur. This led to the development of computer codes based on different versions of ASM1, which can hardly be differentiated any more.
- ASM1 includes biodegradable soluble and particulate organic nitrogen as model compounds. These cannot easily be measured and made the use of ASM1 unnecessarily complicated. Therefore this distinction of nitrogen compounds has in the meantime been eliminated in many models based on ASM1.
- The kinetics of ammonification in ASM1 cannot easily be quantified, moreover the process is fast and therefore hardly affects model predictions. Again in many versions of ASM1 assuming a constant composition of all organic compounds (constant N to COD ratio) has eliminated this process.
- ASM1 differentiates inert particulate organic material depending on its origin, influent or biomass decay, but it is impossible to differentiate these two fractions in reality.
- In the structure of ASM1, the process of hydrolysis has a dominating effect upon the predictions of oxygen consumption and denitrification by heterotrophic organisms. In reality this process stands for some coupled processes such as hydrolysis, lysis of organisms and storage of substrates. Therefore the identification of the kinetic parameters for this combined process is difficult.
- Lysis combined with hydrolysis and growth is used to describe the lumped effects of endogenous respiration of, for example, storage compounds, death, predation and lysis of the biomass. This leads to further difficulties in the evaluation of kinetic parameters.
- With elevated concentrations of readily biodegradable organic substrates, storage of poly-hydroxy-alkanoates and sometimes lipids or glycogen is observed under aerobic and anoxic conditions in activated sludge plants. This process is not included in ASM1.
- ASM1 does not include the possibility to differentiate decay rates of nitrifiers under aerobic and anoxic conditions. At high solids retention times (SRT) and high fractions of anoxic reactor volumes this leads to problems with the prediction of maximum nitrification rates.
- ASM1 does not directly predict the frequently measured mixed liquor suspended solids concentration.
- In respiration tests frequently high biomass yield coefficients are obtained. Even if only soluble, readily biodegradable substrates such as acetate are added, it appears from respiration tests that this substrate includes a slowly biodegradable fraction.

Considering all these defects and the advance in experimental evidence on storage of organic compounds, the Task Group has proposed the Activated Sludge Model No. 3 (ASM3) (Gujer *et al.*, 1999) which should correct for these defects and which could become a new standard for future modelling. ASM3

relates to the same dominating phenomena as does ASM1: oxygen consumption, sludge production, nitrification and denitrification in activated sludge systems treating wastewater of primarily domestic origin.

ASM3 is designed to be the **core** of many different models. Modules for biological phosphorus removal (as contained in the Activated Sludge Model No. 2 (ASM2 and ASM2d) (Henze *et al.*, 1995, 1999), chemical precipitation, growth of filamentous organisms or pH calculations are not part of ASM3 but can easily be connected as add on modules. With increasing experience with ASM3 the Task Group may well suggest such modules which would serve many purposes in practical simulation work.

Introduction of ASM1 has spurred and focused research internationally. Based on a common platform it became possible to discuss rather complex results of careful research. Today interest is with topics such as modelling population dynamics, biological phosphorus

removal and structured biomass (storage products). ASM3 may provide the backbone, which describes the processes of minor interest in research, such that we can concentrate on new frontiers again. In this we should realize that scientific research and model application in engineering practice have different goals. Whereas the detailed structure of the models is used to convey the message on new mechanisms which have been identified in our advanced research projects, model application in engineering must rely on manageable models with a moderate number of parameters but a high potential to predict system behaviour. ASM3 is designed to satisfy primarily the requirements of model application. Nevertheless, the Task Group has tried to fulfil the didactic requirement to keep as many details as are necessary to obtain some insight into the interconnected processes. ASM3 may well become a basis for teaching advanced biological wastewater treatment courses.



## 2. Comparison of ASM1 and ASM3

In ASM1 a single decay process (lysis) was introduced to describe the sum of all decay processes under all environmental conditions (aerobic, anoxic). The reason was that in 1985, when ASM1 was first published, computing power was still scarce. The simplest description possible saved computation time. Today, as computation is not limiting simulation to the same extent, a more realistic description of decay processes is introduced in ASM3: endogenous respiration is close to the phenomena observed (we typically measure a respiration rate) and the relevant rate constants can be obtained directly and independent of stoichiometric parameters (from the slope of  $\ln(r_{O_2, \text{endog}})$  versus time).

The flow of COD in ASM1 is rather complex. The death (decay) regeneration cycle of the heterotrophs and the decay process of nitrifiers are strongly interrelated (Figure 2.1). The two decay processes differ significantly in their details. This results in differing and confusing meanings of the two decay rates in ASM1. In ASM3 all the conversion processes of the two groups of organisms are clearly separated and decay processes are described with identical models (Figure 2.1).

The complexity of ASM3 is comparable to ASM1. There is a shift of emphasis from hydrolysis to storage of organic substrates, a process, which has been postulated and observed by many researchers. Characterization of wastewater must consider this change. Readily available organic substrates ( $S_S$ ) must now be estimated based on the storage rather than the growth process. Differentiation of soluble and particulate substrates ( $S_S$  and  $X_S$ ) remains somewhat arbitrary as in ASM1 and is mainly based on time constants for degradation. Correct characterization of wastewater for the use of ASM3 might still rely on bioassays, which relate to respiration.

Similarly to ASM2 (Henze *et al.* 1995) ASM3 includes cell internal storage compounds. This requires the biomass to be modelled with cell internal structure. Decay processes (which include predation) must include both fractions of the biomass, hence four decay processes are required (aerobic and anoxic loss of  $X_H$  as well as  $X_{STO}$ ) and the kinetics of the growth processes (aerobic and anoxic) must relate to the ratio of  $X_{STO}/X_H$ .

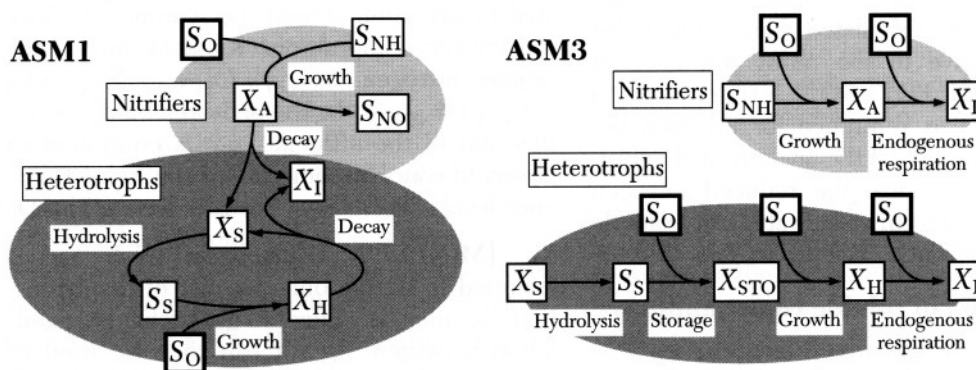


Figure 2.1. Flow of COD in ASM1 and ASM3. In ASM1 (left) heterotrophic organisms use COD in a cyclic reaction scheme: Decay feeds into hydrolysis and triggers additional growth. Nitrifiers decay and thereby enhance heterotrophic growth. Autotrophic and heterotrophic organisms cannot be entirely separated. Only two entry points for oxygen exist. In ASM3 (right) nitrifiers and heterotrophs are clearly separated, no COD flows from one group to the other. Many entry points for oxygen exist. For definitions of state variables see later.

### 3. ASM3: definition of compounds in the model

The following compounds are used in ASM3. Concentrations of soluble compounds are characterized by  $S$  and particulate compounds by  $X$ . Within the activated sludge systems the particulate compounds are assumed to be associated with the activated sludge (flocculated onto the activated sludge or contained within the active biomass). Particulate compounds can be concentrated by sedimentation/thickening in clarifiers whereas soluble compounds can only be transported with the water. Only soluble compounds may carry ionic charge. As in ASM1 and ASM2 filtration over  $0.45\ \mu\text{m}$  membrane filters cannot be used to differentiate model soluble from model particulate compounds in the influent (typically primary effluent): particulate, slowly biodegradable substrates ( $X_S$ , see later) will partially not be retained on the filter membrane. In the activated sludge reactors, where large amounts of surfaces exist, these substrates will rapidly adsorb to the suspended solids, resulting in a better differentiation of soluble and particulate compounds.

Conservation of **Theoretical Oxygen Demand** (ThOD) will be used extensively in the development of process stoichiometry. For organic materials COD may analytically approximate this ThOD. For some inorganic materials ThOD must be calculated based on redox equations relative to the redox reference of  $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ,  $\text{NH}_4^+$ ,  $\text{PO}_4^{3-}$ ,  $\text{SO}_4^{2-}$ .  $\text{NH}_4$  rather than  $\text{NO}_3^-$  is chosen as reference for nitrogen because the standard COD analysis with chromate does not oxidize the reduced nitrogen compounds present in wastewater. An example of calculation of ThOD is given in Table 3.1.

#### 3.1. Definition of soluble compounds, $S_i$

**$S_{\text{O}_2}$  [M(O<sub>2</sub>) L<sup>-3</sup>]: Dissolved oxygen, O<sub>2</sub>.** Dissolved oxygen can directly be measured and is subject to gas exchange. In stoichiometric computations  $S_{\text{O}_2}$  is introduced as negative ThOD.

**$S_1$  [M(COD) L<sup>-3</sup>]: Inert soluble organic material.** The prime characteristic of  $S_1$  is that these organics cannot be further degraded in the treatment plants dealt with in this report. This material is assumed to be part of the influent and may be produced in the context of hydrolysis of particulate substrates  $X_S$ . It can

readily be estimated from the residual soluble COD in the effluent of a low loaded activated sludge plant.

**$S_S$  [M(COD) L<sup>-3</sup>]: Readily biodegradable organic substrates (COD).** This fraction of the soluble COD is directly available for consumption by heterotrophic organisms. In ASM3, for simplification, it is assumed that all these substrates are first taken up by heterotrophic organisms and stored in the form of  $X_{\text{STO}}$ .  $S_S$  is preferentially determined with the aid of a bioassay (respiration test). Measuring the sum of  $S_1 + S_S$  in the form of the total soluble COD in wastewater as determined with  $0.45\ \mu\text{m}$  membrane filtration may lead to gross errors. This is due to the fact that some  $X_S$  (see later) in wastewater (e.g. starch) cannot adsorb to the small amount of biomass present in the influent and therefore contributes to the analytically determined soluble material.

**$S_{\text{NH}_4}$  [M(N) L<sup>-3</sup>]: Ammonium plus ammonia nitrogen (NH<sub>4</sub><sup>+</sup>-N + NH<sub>3</sub>-N).** For the balance of the ionic charges,  $S_{\text{NH}_4}$  is assumed to be all  $\text{NH}_4^+$ . Because ASM3 assumes that organic compounds contain a fixed fraction of organic nitrogen ( $\iota_{\text{N},i}$ , see Table 8.2), the influent  $S_{\text{NH}_4,0}$  cannot be observed directly (measured analytically) but should be computed from wastewater composition: Kjeldahl nitrogen - organic nitrogen ( $S_{\text{NH}_4,0} = C_{\text{TKN},0} - \sum \iota_{\text{N},i} \cdot C_{i,0} + S_{\text{N}_2,0} + S_{\text{NOX},0}$ ). In the activated sludge reactors and in the effluent  $S_{\text{NH}_4}$  is equivalent to observed concentrations. With the redox reference level chosen,  $S_{\text{NH}_4}$  does not have a ThOD.

**$S_{\text{N}_2}$  [M(N) L<sup>-3</sup>]: Dinitrogen (N<sub>2</sub>).**  $S_{\text{N}_2}$  is assumed to be the only product of denitrification.  $S_{\text{N}_2}$  may be subject to gas exchange, parallel with oxygen,  $S_{\text{O}_2}$ . It can then be used to predict problems due to supersaturation with  $\text{N}_2$  in secondary clarifiers. Alternatively the  $\text{N}_2$  contained in the influent and gas exchange can be neglected.  $S_{\text{N}_2}$  may then be used to calculate the amount of nitrogen lost due to denitrification.  $S_{\text{N}_2}$  has a negative ThOD.

**$S_{\text{NOX}}$  [M(N) L<sup>-3</sup>]: Nitrate plus nitrite nitrogen (NO<sub>3</sub><sup>-</sup>-N + NO<sub>2</sub><sup>-</sup>-N).**  $S_{\text{NOX}}$  is assumed to include nitrate as well as nitrite nitrogen, since nitrite is not included as a separate model

Table 3.1. Computation of Theoretical Oxygen Demand ThOD. Each reactive electron is equivalent to a ThOD of 8 g mole<sup>-1</sup>. Therefore each element can be associated with a ThOD which relates to the redox reference of ThOD (H<sub>2</sub>O, CO<sub>2</sub>, NH<sub>4</sub><sup>+</sup>, SO<sub>4</sub><sup>2-</sup>, PO<sub>4</sub><sup>3-</sup>). ThOD may then be computed by adding the individual contributions to each molecule.

Element	Equivalent ThOD	Examples
Carbon	C + 32 g ThOD (mol C) <sup>-1</sup>	<i>What is the ThOD of 1 mole of NO<sub>3</sub><sup>-</sup>?</i> N: - 24 g mole <sup>-1</sup> 3 O: - 48 -: + 8 g mole <sup>-1</sup> Total: -64 g ThOD (mole NO <sub>3</sub> <sup>-</sup> ) <sup>-1</sup>
Nitrogen	N - 24 g ThOD (mol N) <sup>-1</sup>	
Hydrogen	H + 8 g ThOD (mol H) <sup>-1</sup>	
Oxygen	O - 16 g ThOD (mol O) <sup>-1</sup>	<i>What is the ThOD of 1 mole of SO<sub>4</sub><sup>2-</sup>?</i> S: + 48 g mole <sup>-1</sup> 4 O: - 64 g mole <sup>-1</sup> 2-: + 16 g mole <sup>-1</sup> Total: 0 g ThOD (mole SO <sub>4</sub> <sup>2-</sup> ) <sup>-1</sup>
Sulphur	S + 48 g ThOD (mol S) <sup>-1</sup>	
Phosphorus	P + 40 g ThOD (mol P) <sup>-1</sup>	
Negative charge	- + 8 g ThOD (mol (-)) <sup>-1</sup>	
Positive charge	+ - 8 g ThOD (mol (+)) <sup>-1</sup>	

compound. For all stoichiometric computations (ThOD conservation),  $S_{\text{NOX}}$  is considered to be NO<sub>3</sub>-N only.  $S_{\text{NOX}}$  has a negative ThOD.

**$S_{\text{ALK}}$  [mole(HCO<sub>3</sub>) L<sup>-3</sup>]: Alkalinity of the wastewater.** Alkalinity is used to approximate the conservation of ionic charge in biological reactions. Alkalinity is introduced in order to obtain an early indication of possible low pH conditions, which might inhibit some biological processes. For all stoichiometric computations,  $S_{\text{ALK}}$  is assumed to be bicarbonate, HCO<sub>3</sub>, only.

### 3.2. Definition of particulate compounds, $X_p$

**$X_{\text{I}}$  [M(COD) L<sup>-3</sup>]: Inert particulate organic material (COD).** This material is not degraded in the activated sludge systems for which ASM3 has been developed. It is flocculated onto the activated sludge.  $X_{\text{I}}$  may be a fraction of the influent and is produced in the context of biomass decay.

**$X_{\text{S}}$  [M(COD) L<sup>-3</sup>]: Slowly biodegradable substrates (COD).** Slowly biodegradable substrates are high molecular weight, soluble, colloidal and particulate organic substrates which must undergo cell external hydrolysis before they are available for degradation. It is assumed that the products of hydrolysis of  $X_{\text{S}}$  are either readily biodegradable ( $S_{\text{S}}$ ) or inert ( $S_{\text{I}}$ ) soluble organics. As compared to ASM1 this fraction has a different origin. In ASM3 all  $X_{\text{S}}$  is contained in the influent and none is generated in decay processes. In ASM1 a large fraction of  $X_{\text{S}}$  is assumed to originate from decay processes.

**$X_{\text{H}}$  [M(COD) L<sup>-3</sup>]: Heterotrophic organisms (COD).** These organisms are assumed to be the 'allrounder' heterotrophic organisms, they can grow aerobically and many of them also anoxically (denitrification). These organisms are responsible for hydrolysis of particulate substrates  $X_{\text{S}}$  and can metabolize all degradable organic substrates. They can form organic storage products in the form of poly-hydroxy-alkanoates or glycogen.  $X_{\text{H}}$  are assumed to have no anaerobic activity except cell external hydrolysis, which is the only anaerobic process in ASM3.

hydrolysis, which is the only anaerobic process in ASM3.

**$X_{\text{STO}}$  [M(COD) L<sup>-3</sup>]: A cell internal storage product of heterotrophic organisms (COD).** It includes poly-hydroxy-alkanoates (PHA), glycogen, etc. It occurs only associated with  $X_{\text{H}}$ ; it is, however, not included in the mass of  $X_{\text{H}}$ .  $X_{\text{STO}}$  cannot be directly compared with analytically measured PHA or glycogen concentrations;  $X_{\text{STO}}$  is only a functional compound required for modelling but not directly identifiable chemically.  $X_{\text{STO}}$  may, however, be recovered in COD analysis and must satisfy ThOD conservation. For stoichiometric considerations,  $X_{\text{STO}}$  is assumed to have the chemical composition of poly-hydroxy-butyrate (C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>)<sub>n</sub>.

**$X_{\text{A}}$  [M(COD) L<sup>-3</sup>]: Nitrifying organisms (COD).** Nitrifying organisms are responsible for nitrification; they are obligate aerobic, chemo-litho-autotrophic. It is assumed that nitrifiers oxidize ammonium,  $S_{\text{NH}_4}$ , directly to nitrate,  $S_{\text{NOX}}$ . Nitrite as an intermediate compound of nitrification is not considered in ASM3.

**$X_{\text{SS}}$  [M(SS) L<sup>-3</sup>]: Suspended solids (SS).** Suspended solids are introduced into the biokinetic models in order to compute their concentration via stoichiometry. Treatment plant operators typically follow SS in day to day analysis. In the influent, SS ( $X_{\text{SS},0}$ ) include an inorganic fraction of SS and the 'soluble' fraction of  $X_{\text{S},0}$ , which passes membrane filters. SS measured in the influent are therefore smaller than  $X_{\text{SS},0}$  used to describe the influent in the terms of the model compounds. Describing influent SS correctly should allow predicting MLSS as observed in the activated sludge reactors. If chemicals are added in order to precipitate phosphorus, the precipitates formed must in ASM3 be added to the concentration of SS computed in the influent ( $X_{\text{SS},0}$ ). Alternatively  $X_{\text{SS}}$  may be used to model volatile suspended Solids (VSS). This requires the relevant choice of absolute numbers for the composition parameters for SS ( $i_{\text{SS},p}$  in Table 8.2).



## 4. ASM3: definition of processes in the model

ASM3 includes only the microbiological transformation processes. Chemical precipitation processes are not included, but may easily be added based on the information provided for ASM2 (Henze *et al.*, 1995). ASM3 considers the following transformation processes:

1. Hydrolysis. This process makes available all slowly biodegradable substrates  $X_S$  contained in the influent to an activated sludge system. Hydrolysis is assumed to be active independently of the electron donor. This process is different from the hydrolysis process in ASM1; it is of less dominating importance for the rates of oxygen consumption and denitrification.
2. Aerobic storage of readily biodegradable substrate. This process describes the storage of readily biodegradable substrate  $S_S$  in the form of cell internal storage products  $X_{STO}$ . This process requires energy, which is obtained from aerobic respiration. It is assumed that all substrates first become stored material and later are assimilated to biomass. This is definitely not observed in reality, however at this moment no reliable model is available which can predict the substrate flux into storage, assimilation and dissimulation respectively. Therefore the Task Group suggests for the time being this simplest assumption. However using a low yield coefficient for storage ( $Y_{STO}$ ) and a higher one for subsequent growth ( $Y_H$ ) allows to approximate the consequences of direct growth rather than storage followed by growth.
3. Anoxic storage of readily biodegradable substrate. This process is identical to aerobic storage, but denitrification rather than aerobic respiration provides the energy required. Only a fraction of the heterotrophic organisms  $X_H$  in activated sludge is capable of denitrification. ASM3 considers this by reducing the anoxic heterotrophic storage rate as compared to the aerobic rate.
4. Aerobic growth of heterotrophs. The substrate for the growth of heterotrophic organisms is assumed to consist entirely of stored organics  $X_{STO}$ . This assumption simplifies ASM3 considerably.
5. Anoxic growth of heterotrophs. This process is similar to aerobic growth but respiration is based on denitrification. Only a fraction of the heterotrophic organisms  $X_H$  in activated sludge is capable of denitrification. ASM3 considers this by reducing the anoxic heterotrophic storage rate as compared to the aerobic rate.
6. Aerobic endogenous respiration. This process describes all forms of biomass loss and energy requirements not associated with growth by considering related respiration under aerobic conditions: decay, (maintenance), endogenous respiration, lysis, predation, motility, death, and so on. The model of this process is significantly different from the decay (lysis) process introduced in ASM1.
7. Anoxic endogenous respiration. This process is similar to aerobic endogenous respiration but typically slower. Especially protozoa (predation) are considerably less active under denitrifying than under aerobic conditions.
8. Aerobic respiration of storage products. This process is analogous to endogenous respiration. It assures that storage products,  $X_{STO}$ , decay together with biomass.
9. Anoxic respiration of storage products. This process is analogous to the aerobic process but under denitrifying conditions.

As compared with ASM1, ASM3 includes a more detailed description of cell internal processes (storage) and allows for better adjustment of decay processes to environmental conditions. The importance of hydrolysis has been reduced and degradation of soluble and particulate organic nitrogen have been integrated into the hydrolysis, decay and growth process.

## 5. ASM3: stoichiometry

Table 5.1 introduces the stoichiometric matrix  $\nu_{j,i}$  of ASM3 together with the composition matrix  $\iota_{k,i}$  as proposed by Gujer and Larsen (1995). Whereas the stoichiometric matrix  $\nu_{j,i}$  is well known since the introduction of ASM1, the composition matrix is less well known. Relating to Table 5.1 the composition matrix may be read as follows:  $\iota_{2,3}$  is filled with the symbol  $i_{N,SS}$  and indicates that any g COD in the form of  $S_S$  contains  $i_{N,SS}$  g of N. The index  $k = 2$  relates to the second conservative which is nitrogen, the index  $i = 3$  relates to the third compound which is  $S_S$ .  $S_S$  is measured in terms of g COD (as indicated below the symbol  $S_S$ ) and the conservative 'nitrogen' is expressed in g N (as indicated to the right of nitrogen in the composition matrix).  $i_{N,SS}$  therefore indicates the composition of  $S_S$  relative to nitrogen, hence  $\iota_{k,i}$  is called the composition matrix.

All empty elements of  $\nu_{j,i}$  or  $\iota_{k,i}$  indicate values of 0. All values of  $x_j$ ,  $y_j$  and  $z_j$  can be obtained from the conservation Equation 5.1 for the three conservatives  $k$ : ThOD, nitrogen and ionic charge:

$$\sum_i \nu_{j,i} \cdot \iota_{k,i} = 0 \quad \text{for } i = 1 \text{ to } 12 \quad (5.1)$$

As introduced earlier, ThOD stands for Theoretical Oxygen Demand and is the conservative form of COD. In most cases ThOD of organic compounds may analytically be approximated by standard dichromate COD analysis. ThOD is a conservative quantity since it effectively accounts for the electrons involved in the biological redox processes.

The stoichiometric coefficient for  $S_{N_2}$  in any denitrification process is the negative of the coefficient for  $S_{NOX}$ . The composition coefficients for ThOD for  $S_{N_2}$  ( $-1.71 \text{ g ThOD (g } N_2)^{-1}$ ) and  $S_{NOX}$  ( $-4.57 \text{ g ThOD (g } NO_3^- \text{-N)}^{-1}$ ) as well as  $S_{O_2}$  ( $-1 \text{ g ThOD (g } O_2)^{-1}$ ) are negative for electron donors relative to the redox reference for ThOD.

The stoichiometric coefficients for the obser-

vable  $X_{SS}$  can be obtained from the Composition Equation 5.2:

$$\nu_{j,13} = \sum_i \nu_{j,i} \cdot \iota_{4,i} \quad \text{for } i = 8 \text{ to } 12 \quad (5.2)$$

It is known that the biochemical energy (ATP) yield of anoxic respiration is smaller than in aerobic respiration. This leads to the fact that aerobic yield coefficients ( $Y_{STO,O_2}$  and  $Y_{H,O_2}$ ) exceed the anoxic yield coefficients ( $Y_{STO,NOX}$  and  $Y_{H,NOX}$ ). Assuming the anoxic energy yield to be  $\eta_{anoxic} = 0.70$  of the aerobic energy yield the following energy relationship (Equation 5.3) applies:

$$\frac{1 - Y_{STO,O_2}}{Y_{STO,O_2}} = \frac{\eta_{anoxic} \cdot (1 - Y_{STO,NOX})}{Y_{STO,NOX}} \quad \text{and} \\ \frac{1 - Y_{O_2}}{Y_{O_2}} = \frac{\eta_{anoxic} \cdot (1 - Y_{NOX})}{Y_{NOX}} \quad (5.3)$$

It is suggested that Equation 5.3 is used to relate anoxic and aerobic yields in ASM3.

The net (true) yield of heterotrophic biomass  $X_H$  produced per unit of substrate  $S_S$  removed in ASM3 is obtained from:

$$Y_{net,O_2} = Y_{STO,O_2} \cdot Y_{H,O_2} \quad \text{and} \\ Y_{net,NOX} = Y_{STO,NOX} \cdot Y_{H,NOX} \quad (5.4)$$

All stoichiometric parameters are defined together with their units and a typical value in Table 8.2. A numeric example of all stoichiometric coefficients is given in Table 8.4.

In the composition matrix  $\iota_{k,i}$  of Table 5.1 the composition of all organic fractions relative to ThOD is assumed to be unity. These values have units however ( $i_{ThOD,S_i} = 1 \text{ g ThOD (g COD)}^{-1}$ , ...) and it should be realized that these values are actually model parameters which here have been assumed to be unity whereas in reality COD analysis recovers only a fraction of ThOD, typically 95% in domestic wastewater.

**Activated Sludge Model No. 3**

Table 5.1. Stoichiometric matrix  $v_{j,i}$  and composition matrix  $u_{k,i}$  of ASM3. The values of  $x_j$ ,  $y_j$ ,  $z_j$  and  $t_j$  can be obtained in this sequence from mass and charge conservation (Equation 5.1) and composition (Equation 5.2).

Compound $i \rightarrow$		1	2	3	4	5	6	7	8	9	10	11	12	13
$j$ Process		$S_{O_2}$	$S_I$	$S_S$	$S_{NH_4}$	$S_{N_2}$	$S_{NOX}$	$S_{ALK}$	$X_I$	$X_S$	$X_H$	$X_{STO}$	$X_A$	$X_{SS}$
$\downarrow$ Expressed as $\rightarrow$		$O_2$	COD	COD	N	N	N	Mole	COD	COD	COD	COD	COD	SS
1 Hydrolysis			$f_{S_I}$	$x_1$	$y_1$			$z_1$		-1				$-i_{X_S}$
<i>Heterotrophic organisms, aerobic and denitrifying activity</i>														
2 Aerobic storage of $S_S$		$x_2$		-1	$y_2$			$z_2$				$Y_{STO,O_2}$		$t_2$
3 Anoxic storage of $S_S$				-1	$y_3$	$-x_3$	$x_3$	$z_3$				$Y_{STO,NOX}$		$t_3$
4 Aerobic growth of $X_H$	$x_4$				$y_4$			$z_4$		1		$-1/Y_{H,O_2}$		$t_4$
5 Anoxic growth (denitrific.)					$y_4$	$-x_5$	$x_5$	$z_5$		1		$-1/Y_{H,NOX}$		$t_5$
6 Aerobic endog. respiration	$x_6$				$y_6$			$z_6$	$f_I$		-1			$t_6$
7 Anoxic endog. respiration					$y_7$	$-x_7$	$x_7$	$z_7$	$f_I$		-1			$t_7$
8 Aerobic respiration of $X_{STO}$	$x_8$											-1		$t_8$
9 Anoxic respiration of $X_{STO}$						$-x_9$	$x_9$	$z_9$				-1		$t_9$
<i>Autotrophic organisms, nitrifying activity</i>														
10 Aerobic growth of $X_A$	$x_{10}$				$y_{10}$		$1/Y_A$	$z_{10}$					1	$t_{10}$
11 Aerobic endog. respiration	$x_{11}$				$y_{11}$			$z_{11}$	$f_I$				-1	$t_{11}$
12 Anoxic endog. respiration					$y_{12}$	$-x_{12}$	$x_{12}$	$z_{12}$	$f_I$				-1	$t_{12}$
<i>Composition matrix <math>u_{k,i}</math></i>														
<i>k Conservatives</i>														
1 ThOD	g ThOD	-1	1	1		-1.71	-4.57		1	1	1	1	1	
2 Nitrogen	g N		$i_{N,S_I}$	$i_{N,S_S}$	1	1	1		$i_{N,X_I}$	$i_{N,X_S}$	$i_{N,BM}$			$i_{N,BM}$
3 Ionic charge	Mole +				1/14		-1/14	-1						
<i>Observables</i>														
4 SS	g SS								$i_{SS,X_I}$	$i_{SS,X_S}$	$i_{SS,BM}$	0.60		$i_{SS,BM}$

## 6. ASM3: kinetics

The kinetic expressions of ASM3 are based on switching functions (hyperbolic or saturation terms, Monod equations,  $S/(K+S)$ ) for all soluble compounds consumed. This form of kinetic expression is chosen not because of experimental evidence but rather for mathematical convenience: these switching functions stop all biological activity as educts of a process approach zero concentrations, an important difference between ASM1 and ASM3. Similarly for particulate educts the switching functions relate to the ratio of  $X_{\text{STO}}/X_{\text{H}}$  resp.  $X_{\text{S}}/X_{\text{H}}$ . Inhibition is modelled with  $1 - S/(K + S) = K/(K + S)$ .

Table 6.1 is a summary of all kinetic expressions of ASM3. The kinetic parameters are defined in Table 8.1 together with their units and a typical value at 10 °C and 20 °C. It is recommended to interpolate kinetic paramet-

ers  $k$  to different temperatures  $T$  (in °C) with the following temperature equation:

$$k(T) = k(20\text{ °C}) \cdot \exp(\theta_T \cdot (T - 20\text{ °C})) \quad (6.1)$$

where  $\theta_T$  (in °C) may be obtained from

$$\theta_T = \frac{\ln(k(T_1)/k(T_2))}{t_1 - T_2} \quad (6.2)$$

### 6.1 Estimation of readily biodegradable substrate $S_{\text{S}}$

As indicated earlier, readily biodegradable substrate  $S_{\text{S}}$  in wastewater is best determined from a bioassay. Kinetics of the storage and growth processes are such that the storage process in ASM3 will be related to the additional rapid uptake of oxygen after addition of wastewater to biomass. Therefore the yield of the storage

Table 6.1. Kinetic rate expressions  $\rho_j$  for ASM3. All  $\rho_j \geq 0$ .

$j$ Process	Process rate equation $\rho_j$ , all $\rho_j \geq 0$ .
1 Hydrolysis	$k_{\text{H}} \cdot \frac{X_{\text{S}}/X_{\text{H}}}{K_{\text{X}} + X_{\text{S}}/X_{\text{H}}} \cdot X_{\text{H}}$
<i>Heterotrophic organisms, aerobic and denitrifying activity</i>	
2 Aerobic storage of $S_{\text{S}}$	$k_{\text{STO}} \cdot \frac{S_{\text{O}_2}}{K_{\text{O}_2} + S_{\text{O}_2}} \cdot \frac{S_{\text{S}}}{K_{\text{S}} + S_{\text{S}}} \cdot X_{\text{H}}$
3 Anoxic storage of $S_{\text{S}}$	$k_{\text{STO}} \cdot \eta_{\text{NOX}} \cdot \frac{K_{\text{O}_2}}{K_{\text{O}_2} + S_{\text{O}_2}} \cdot \frac{S_{\text{NOX}}}{K_{\text{NOX}} + S_{\text{NOX}}} \cdot \frac{S_{\text{S}}}{K_{\text{S}} + S_{\text{S}}} \cdot X_{\text{H}}$
4 Aerobic growth	$\mu_{\text{H}} \cdot \frac{S_{\text{O}_2}}{K_{\text{O}_2} + S_{\text{O}_2}} \cdot \frac{S_{\text{NH}_4}}{K_{\text{NH}_4} + S_{\text{NH}_4}} \cdot \frac{S_{\text{ALK}}}{K_{\text{ALK}} + S_{\text{ALK}}} \cdot \frac{X_{\text{STO}}/X_{\text{H}}}{K_{\text{STO}} + X_{\text{STO}}/X_{\text{H}}} \cdot X_{\text{H}}$
5 Anoxic growth (denitrification)	$\mu_{\text{H}} \cdot \eta_{\text{NOX}} \cdot \frac{K_{\text{O}_2}}{K_{\text{O}_2} + S_{\text{O}_2}} \cdot \frac{S_{\text{NOX}}}{K_{\text{NOX}} + S_{\text{NOX}}} \cdot \frac{S_{\text{NH}_4}}{K_{\text{NH}_4} + S_{\text{NH}_4}} \cdot \frac{S_{\text{ALK}}}{K_{\text{ALK}} + S_{\text{ALK}}} \cdot \frac{X_{\text{STO}}/X_{\text{H}}}{K_{\text{STO}} + X_{\text{STO}}/X_{\text{H}}} \cdot X_{\text{H}}$
6 Aerobic endogenous respiration	$b_{\text{H},\text{O}_2} \cdot \frac{S_{\text{O}_2}}{K_{\text{O}_2} + S_{\text{O}_2}} \cdot X_{\text{H}}$
7 Anoxic endogenous respiration	$b_{\text{H},\text{NOX}} \cdot \frac{K_{\text{O}_2}}{K_{\text{O}_2} + S_{\text{O}_2}} \cdot \frac{S_{\text{NOX}}}{K_{\text{NOX}} + S_{\text{NOX}}} \cdot X_{\text{H}}$
8 Aerobic respiration of $X_{\text{STO}}$	$b_{\text{STO},\text{O}_2} \cdot \frac{S_{\text{O}_2}}{K_{\text{O}_2} + S_{\text{O}_2}} \cdot X_{\text{STO}}$
9 Anoxic respiration of $X_{\text{STO}}$	$b_{\text{STO},\text{NOX}} \cdot \frac{K_{\text{O}_2}}{K_{\text{O}_2} + S_{\text{O}_2}} \cdot \frac{S_{\text{NOX}}}{K_{\text{NOX}} + S_{\text{NOX}}} \cdot X_{\text{STO}}$
<i>Autotrophic organisms, nitrifying activity</i>	
10 Aerobic growth of $X_{\text{A}}$ , nitrification	$\mu_{\text{A}} \cdot \frac{S_{\text{O}_2}}{K_{\text{A},\text{O}_2} + S_{\text{O}_2}} \cdot \frac{S_{\text{NH}_4}}{K_{\text{A},\text{NH}_4} + S_{\text{NH}_4}} \cdot \frac{S_{\text{ALK}}}{K_{\text{A},\text{ALK}} + S_{\text{ALK}}} \cdot X_{\text{A}}$
11 Aerobic endogenous respiration	$b_{\text{A},\text{O}_2} \cdot \frac{S_{\text{O}_2}}{K_{\text{A},\text{O}_2} + S_{\text{O}_2}} \cdot X_{\text{A}}$
12 Anoxic endogenous respiration	$b_{\text{A},\text{NOX}} \cdot \frac{K_{\text{A},\text{O}_2}}{K_{\text{A},\text{O}_2} + S_{\text{O}_2}} \cdot \frac{S_{\text{NOX}}}{K_{\text{A},\text{NOX}} + S_{\text{NOX}}} \cdot X_{\text{A}}$

process must be used in order to relate oxygen uptake to substrate consumption:

$$\begin{aligned} S_S (\text{batch}) &= \int \Delta r_{S_S} \cdot dt = \frac{v_{S_S}}{v_{SO_2}} \int \Delta r_{SO_2} \cdot dt \\ &= \frac{\int \Delta r_{SO_2} \cdot dt}{1 - Y_{O_2,STO}} \end{aligned} \quad (6.3)$$

It is recommended to simulate the batch experiment, which is used to identify  $S_S$  with the aid of ASM3. This allows the identification of possible errors that could be introduced by this simple procedure.



## 7. Limitations of ASM3

ASM3 (and ASM1) was developed for the simulation of the aerobic and anoxic treatment of domestic wastewater in activated sludge systems. It is not advised to apply it to situations where industrial contributions dominate the characteristics of the wastewater.

ASM3 (and ASM1) has been developed based on experience in the temperature range of 8–23 °C. Outside of this range model application may lead to very significant errors and even model structure may become unsatisfactory.

ASM3 (and ASM1) does not include any processes that describe biomass behaviour in an anaerobic environment. Simulation of systems with large fractions of anaerobic reactor volume may therefore lead to gross errors.

Development of ASM3 is based on experience in the range of pH values from 6.5 to 7.5. The concentration of bicarbonate alkalinity ( $S_{ALK}$ ) is supplied to give early warnings when pH values below this range are to be expected.

Alkalinity must be dominated by bicarbonate. ASM3 cannot deal with elevated concentrations of nitrite.

ASM3 (and ASM1) is not designed to deal with activated sludge systems with very high load or small SRT (<1 day) where flocculation/adsorption of  $X_S$  and storage may become limiting.

ASM3 provides the structure of a model but not absolute values of model parameters. It is the responsibility of the user of this model to identify the applicable parameters and the relevant characterization of the wastewater.

Neither the Task Group nor IWA can under any circumstances accept any liability for damages of any sort that may result from the application of this model. It is provided here as a service for the scientific and practical engineering community and it is hoped to serve as a reference for future scientific work.

## 8. Aspects of application of ASM3

It is the responsibility of the user of ASM3 to determine the concentrations of relevant compounds in the wastewater, as well as the stoichiometric and kinetic parameters, which apply to the specific case to be dealt with. **Absolute values of these parameters are not part of ASM3.** They are necessary, however, if ASM3 is to be applied to any specific case.

In Tables 8.1–8.4 a set of typical model parameters and concentrations of model compounds in a primary effluent is provided for convenience. This neither indicates that ASM3 is meant to be reliable with these parameters in

any case, nor that these parameters are the state of the art. They are merely presented here as a reference for testing computer code and as a first estimate for the design of possible experiments that may be used to identify these parameters more accurately.

Table 8.1 contains a list of typical kinetic parameters; Table 8.2 suggests some typical stoichiometric parameters. Table 8.3 indicates the composition of a typical primary effluent and finally Table 8.4 is a stoichiometric matrix, based on Table 5.1 and the specific values introduced in Table 8.2.

Table 8.1. Typical values of kinetic parameters for ASM3. These values are provided as examples and are not part of ASM3.

Symbol	Characterization	Temperature		Units
		10 °C	20 °C	
$k_H$	Hydrolysis rate constant	2	3	$\text{g COD}_{X_S} (\text{g COD}_{X_H})^{-1} \text{d}^{-1}$
$K_X$	Hydrolysis saturation constant	1	1	$\text{g COD}_{X_S} (\text{g COD}_{X_H})^{-1}$
<i>Heterotrophic organisms <math>X_H</math>, aerobic and denitrifying activity</i>				
$k_{STO}$	Storage rate constant	2.5	5	$\text{g COD}_{S_S} (\text{g COD}_{X_H})^{-1} \text{d}^{-1}$
$\eta_{NOX}$	Anoxic reduction factor	0.6	0.6	—
$K_{O_2}$	Saturation constant for $S_{NO_2}$	0.2	0.2	$\text{g O}_2 \text{m}^{-3}$
$K_{NOX}$	Saturation constant for $S_{NOX}$	0.5	0.5	$\text{g NO}_3^- \text{N m}^{-3}$
$K_S$	Saturation constant for substrate $S_S$	2	2	$\text{g COD}_{S_S} \text{m}^{-3}$
$K_{STO}$	Saturation constant for $X_{STO}$	1	1	$\text{g COD}_{X_{STO}} (\text{g COD}_{X_H})^{-1}$
$\mu_H$	Heterotrophic max. growth rate of $X_H$	1	2	$\text{d}^{-1}$
$K_{NH_4}$	Saturation constant for ammonium, $S_{NH_4}$	0.01	0.01	$\text{g N m}^{-3}$
$K_{ALK}$	Saturation constant for alkalinity for $X_H$	0.1	0.1	$\text{mole HCO}_3^- \text{m}^{-3}$
$b_{H,O_2}$	Aerobic endogenous respiration rate of $X_H$	0.1	0.2	$\text{d}^{-1}$
$b_{H,NOX}$	Anoxic endogenous respiration rate of $X_H$	0.05	0.1	$\text{d}^{-1}$
$b_{STO,O_2}$	Aerobic respiration rate for $X_{STO}$	0.1	0.2	$\text{d}^{-1}$
$b_{STO,NOX}$	Anoxic respiration rate for $X_{STO}$	0.05	0.1	$\text{d}^{-1}$
<i>Autotrophic organisms <math>X_A</math>, nitrifying activity</i>				
$\mu_A$	Autotrophic max. growth rate of $X_A$	0.35	1.0	$\text{d}^{-1}$
$K_{A,NH_4}$	Ammonium substrate saturation for $X_A$	1	1	$\text{g N m}^{-3}$
$K_{A,O_2}$	Oxygen saturation for nitrifiers	0.5	0.5	$\text{g O}_2 \text{m}^{-3}$
$K_{A,ALK}$	Bicarbonate saturation for nitrifiers	0.5	0.5	$\text{mole HCO}_3^- \text{m}^{-3}$
$b_{A,O_2}$	Aerobic endogenous respiration rate of $X_A$	0.05	0.15	$\text{d}^{-1}$
$b_{A,NOX}$	Anoxic endogenous respiration rate of $X_A$	0.02	0.05	$\text{d}^{-1}$

Table 8.2. Typical stoichiometric and composition parameters for ASM3. These values are given as examples and are not part of ASM3.

Symbol	Characterization	Value	Units	
$f_{S_1}$	Production of $S_1$ in hydrolysis	0	$\text{g COD}_{S_1} (\text{g COD}_{X_S})^{-1}$	
$Y_{\text{STO},O_2}$	Aerobic yield of stored product per $S_S$	0.85	$\text{g COD}_{X_{\text{STO}}} (\text{g COD}_{S_S})^{-1}$	Equation 5.3
$Y_{\text{STO},\text{NOX}}$	Anoxic yield of stored product per $S_S$	0.80	$\text{g COD}_{X_{\text{STO}}} (\text{g COD}_{S_S})^{-1}$	
$Y_{H,O_2}$	Aerobic yield of heterotrophic biomass	0.63	$\text{g COD}_{X_H} (\text{g COD}_{X_{\text{STO}}})^{-1}$	Equation 5.3
$Y_{H,\text{NOX}}$	Anoxic yield of heterotrophic biomass	0.54	$\text{g COD}_{X_H} (\text{g COD}_{X_{\text{STO}}})^{-1}$	
$Y_A$	Yield of autotrophic biomass per $\text{NO}_3^-$ -N	0.24	$\text{g COD}_{X_A} (\text{g N}_{S_{\text{NOX}}})^{-1}$	
$f_{X_1}$	Production of $X_1$ in endog. respiration	0.20	$\text{g COD}_{X_1} (\text{g COD}_{X_{\text{BM}}})^{-1}$	
$i_{N,S_1}$	N content of $S_1$	0.01	$\text{g N} (\text{g COD}_{S_1})^{-1}$	
$i_{N,S_S}$	N content of $S_S$	0.03	$\text{g N} (\text{g COD}_{S_S})^{-1}$	
$i_{N,X_1}$	N content of $X_1$	0.02	$\text{g N} (\text{g COD}_{X_1})^{-1}$	The values below are suggested if $X_{SS}$ is used to model VSS rather than SS: 0.75 g VSS $(\text{g COD}_{X_1})^{-1}$ 0.75 g VSS $(\text{g COD}_{X_S})^{-1}$ 0.75 g VSS $(\text{g COD}_{X_H \text{ or } X_A})^{-1}$
$i_{N,X_S}$	N content of $X_S$	0.04	$\text{g N} (\text{g COD}_{X_S})^{-1}$	
$i_{N,\text{BM}}$	N content of biomass, $X_H, X_A$	0.07	$\text{g N} (\text{g COD}_{X_{\text{BM}}})^{-1}$	
$i_{SS,X_1}$	SS to COD ratio for $X_1$	0.75	$\text{g SS} (\text{g COD}_{X_1})^{-1}$	
$i_{SS,X_S}$	SS to COD ratio for $X_S$	0.75	$\text{g SS} (\text{g COD}_{X_S})^{-1}$	
$i_{SS,\text{BM}}$	SS to COD ratio for biomass, $X_H, X_A$	0.90	$\text{g SS} (\text{g COD}_{X_{\text{BM}}})^{-1}$	

Table 8.3. Short definition of model compounds and typical wastewater composition (primary effluent) for ASM3. The value of TKN considers the composition of the different model compounds as indicated in Table 8.2:  $\text{TKN} = \sum C_i \cdot t_{2,i}$  over all compounds  $i - S_{\text{NOX}} - S_{\text{N}_2}$ .  $\text{COD}_{\text{tot}} = 260 \text{ g COD m}^{-3}$ ,  $\text{TKN} = 25 \text{ g N m}^{-3}$ .

Compounds	Concentration	Units	
<i>Dissolved compounds</i>			
$S_{O_2}$	Dissolved oxygen	0	$\text{g O}_2 \text{ m}^{-3}$
$S_I$	Soluble inert organics	30	$\text{g COD m}^{-3}$
$S_S$	Readily biodegradable substrates	60	$\text{g COD m}^{-3}$
$S_{\text{NH}_4}$	Ammonium	16	$\text{g N m}^{-3}$
$S_{\text{N}_2}$	Dinitrogen, released by denitrification	0	$\text{g N m}^{-3}$
$S_{\text{NOX}}$	Nitrite plus nitrate	0	$\text{g N m}^{-3}$
$S_{\text{ALK}}$	Alkalinity, bicarbonate	5	$\text{mole HCO}_3^- \text{ m}^{-3}$
<i>Particulate compounds</i>			
$X_I$	Inert particulate organics	25	$\text{g COD m}^{-3}$
$X_S$	Slowly biodegradable substrates	115	$\text{g COD m}^{-3}$
$X_H$	Heterotrophic biomass	30	$\text{g COD m}^{-3}$
$X_{\text{STO}}$	Organics stored by heterotrophs	0	$\text{g COD m}^{-3}$
$X_A$	Autotrophic, nitrifying biomass	>0	$\text{g COD m}^{-3}$
$X_{\text{SS}}$	Total suspended solids	125	$\text{g SS m}^{-3}$
			The value below is suggested if $X_{SS}$ is used to model VSS rather than SS: 100 g VSS $\text{m}^{-3}$

Table 8.4. Stoichiometric matrix of ASM3 based on the stoichiometric parameters in Table 8.2. This matrix is a typical application of ASM3 but it is not suggested as a reliable form of ASM3.

Compound $i \rightarrow$	1	2	3	4	5	6	7	8	9	10	11	12	13
$j$ Process	$S_{O_2}$	$S_I$	$S_S$	$S_{\text{NH}_2}$	$S_{\text{N}_2}$	$S_{\text{NOX}}$	$S_{\text{ALK}}$	$X_I$	$X_S$	$X_H$	$X_{\text{STO}}$	$X_A$	$X_{\text{SS}}$
$\downarrow$ Expressed as $\rightarrow$	$O_2$	COD	COD	N	N	N	Mole	COD	COD	COD	COD	COD	SS
1 Hydrolysis		0	1	0.01			0.001		-1				-0.75
<i>Heterotrophic organisms, aerobic and denitrifying activity</i>													
2 Aerobic storage of $S_S$	-0.15		-1	0.03			0.002				0.85		0.51
3 Anoxic storage of $S_S$			-1	0.03	0.07	-0.07	0.007				0.80		0.48
4 Aerobic growth of $X_H$	-0.60			-0.07			-0.005			1	-1.60		-0.06
5 Anoxic growth (denitrific.)				-0.07	0.30	-0.30	0.016			1	-1.85		-0.21
6 Aerobic endog. respiration	-0.80			0.066			0.005	0.20		-1			-0.75
7 Anoxic endog. respiration				0.066	0.28	-0.28	0.025	0.20		-1			-0.75
8 Aerobic respiration of $X_{\text{STO}}$	-1										-1		-0.60
9 Anoxic respiration of $X_{\text{STO}}$					0.35	-0.35	0.025				-1		-0.60
<i>Autotrophic organisms, nitrifying activity</i>													
10 Aerobic growth of $X_A$	-18.04			-4.24			4.17	-0.600				1	0.90
11 Aerobic endog. respiration	-0.80			0.066			0.005	0.20				-1	-0.75
12 Anoxic endog. respiration				0.066	0.28	-0.28	0.025	0.20				-1	-0.75

## 9. ASM3C: a carbon-based model

In some countries the chemical determination of COD-Cr in routine analysis is not possible because of the heavy metals (Hg, Cr and Ag) involved in the analytical procedures. The alternative COD-Mn is not very valuable in the context of ASM3 since it greatly underestimates ThOD. This is a severe limitation for the application of models such as ASM3. In order to facilitate the application of ASM3, the Task Group proposes ASM3C as an adapted version of ASM3, where organic state variables are expressed in terms of organic carbon rather than COD. This allows the use of TOC instead of COD-Cr measurements in order to characterize wastewater and activated sludge. Since experience with TOC is rather limited at this time, ASM3C should be used with great care.

### 9.1 Definition and measurement of fractions of organic carbon

TOC [ $M(C) L^{-3}$ ] stands for Total Organic Carbon and is analytically available in wastewater. For samples with suspended solids, careful homogenization of the samples is important. Care has to be taken that sedimentation of coagulating solids does not lead to erroneous results. This is especially relevant if auto-samplers are used where the sample is not stirred before it is injected into the TOC analyser.

Depending on the pretreatment of the sample, the TOC analysis can be used to characterize different fractions of wastewater. In relation to TOC the terms DOC (Dissolved Organic Carbon) and POC (Particulate Organic carbon) are sometimes used. By definition  $TOC = DOC + POC$ . DOC is measured after filtration of the samples. All soluble organic model compounds ( $S_I$ ,  $S_S$ ) may be expressed in terms of DOC.

POC is available from the difference  $TOC - DOC$ . POC may be used to characterize some of the particulate organic model compounds in the influent ( $X_I$ ,  $X_H$ ,  $X_{STO}$ ,  $X_A$ ) but not for others (not  $X_S$ , since a fraction of  $X_S$  passes through the membrane filters).

For the characterization of activated sludge as a whole, standard estimation of TOC may easily lead to gross analytical errors. Here elementary analysis of a dry washed sample or

the use of specialized TOC equipment may be the methods of choice.

Since the fractionation of TOC in DOC and POC is not entirely compatible with the definition of the model compounds ( $X_S$  being the problem), this report will use TOC only, in order to express that a compound is measured in terms of organic carbon.

### 9.2 Transition from ASM3 to ASM3C

Deriving ASM3C from ASM3 is an easy task if the composition of the organic compounds is redefined (COD is replaced by TOC). Introducing new units ( $g \text{ ThOD} (g \text{ TOC})^{-1}$  rather than  $g \text{ ThOD} (g \text{ COD})^{-1}$ ) and accordingly new absolute values for the composition parameters  $i_{\text{ThOD},i}$  for all organic compounds in the composition matrix yields the basis for estimating the unknown stoichiometric coefficients  $x_j$ ,  $y_j$ ,  $z_j$  and  $t_j$  with the aid of Equations 5.1 and 5.2.

Realizing that the values of  $i_{\text{ThOD},??} = 1 g \text{ ThOD} (g \text{ COD})^{-1}$  are actually model parameters chosen to be unity in ASM3 (which is based on the assumption that ThOD is identical to the measured COD), the transition of ASM3 to ASM3C is a rather minor one.

Table 9.1 includes the stoichiometric matrix for ASM3C, revised from Table 5.1. Changes include transition from COD to TOC for expressing the organic state variables, introduction of the  $i_{\text{ThOD},??}$  values in the first row of the composition matrix and adjusting the fixed values for storage compounds ( $X_{STO}$ ) in the composition matrix.

### 9.3 Adjusting kinetic and stoichiometric parameters for ASM3C

With the introduction of TOC based compounds in ASM3C the absolute values and the units of some kinetic and stoichiometric parameters must be adjusted. As an example the aerobic yield of autotrophic biomass  $Y_A$  in ASM3C may be obtained from:

$$\begin{aligned}
 Y_A(\text{ASM3}) \text{ has the units} & \quad [g \text{ COD}_{X_A} (g \text{ NO}_3^- \text{-N})^{-1}] \\
 Y_A(\text{ASM3C}) \text{ has the units} & \quad [g \text{ TOC}_{X_A} (g \text{ NO}_3^- \text{-N})^{-1}] \\
 i_{\text{ThOD,BM}}(\text{ASM3}) \text{ has the units} & \quad [g \text{ ThOD}_{\text{BM}} (g \text{ COD}_{\text{BM}})^{-1}]
 \end{aligned}$$

Table 9.1. Stoichiometric matrix  $v_{j,i}$  and composition matrix  $u_{k,i}$  of ASM3C. The values of  $x_j$ ,  $y_j$ ,  $z_j$  and  $t_j$  can be obtained in this sequence from mass and charge conservation (Equation 5.1) and composition (Equation 5.2). The stoichiometric coefficients ( $f_{S_1}$ ,  $f_1$ ,  $Y_{STO}$  and  $Y_H$ ) must be based on organic carbon (Table 9.3).

Compound $i \rightarrow$	1	2	3	4	5	6	7	8	9	10	11	12	13
$j$ Process	$S_{O_2}$	$S_I$	$S_S$	$S_{NH_4}$	$S_{N_2}$	$S_{NOX}$	$S_{ALK}$	$X_I$	$X_S$	$X_H$	$X_{STO}$	$X_A$	$X_{SS}$
$\downarrow$ Expressed as $\rightarrow$	$O_2$	TOC	TOC	N	N	N	Mole	TOC	TOC	TOC	TOC	TOC	SS
1 Hydrolysis		$f_{S_1}$	$x_1$	$y_1$			$z_1$		-1				$-i_{X_S}$
<i>Heterotrophic organisms, aerobic and denitrifying activity</i>													
2 Aerobic storage of $S_S$	$x_2$		-1	$y_2$			$z_2$				$Y_{STO,O_2}$		$t_2$
3 Anoxic storage of $S_S$			-1	$y_3$	$-x_3$	$x_3$	$z_3$				$Y_{STO,NOX}$		$t_3$
4 Aerobic growth of $X_H$	$x_4$			$y_4$			$z_4$			1	$-1/Y_{H,O_2}$		$t_4$
5 Anoxic growth (denitrific.)				$y_4$	$-x_5$	$x_5$	$z_5$			1	$-1/Y_{H,NOX}$		$t_5$
6 Aerobic endog. respiration	$x_6$			$y_6$			$z_6$	$f_1$		-1			$t_6$
7 Anoxic endog. respiration				$y_7$	$-x_7$	$x_7$	$z_7$	$f_1$		-1			$t_7$
8 Aerobic respiration of $X_{STO}$	$x_8$										-1		$t_8$
9 Anoxic respiration of $X_{STO}$					$-x_9$	$x_9$	$z_9$				-1		$t_9$
<i>Autotrophic organisms, nitrifying activity</i>													
10 Aerobic growth of $X_A$	$x_{10}$			$y_{10}$		$1/Y_A$	$z_{10}$					1	$t_{10}$
11 Aerobic endog. respiration	$x_{11}$			$y_{11}$			$z_{11}$	$f_1$				-1	$t_{11}$
12 Anoxic endog. respiration				$y_{12}$	$-x_{12}$	$x_{12}$	$z_{12}$	$f_1$				-1	$t_{12}$
<i>Composition matrix <math>u_{k,i}</math></i>													
<i>k Conservatives</i>													
1 ThOD	g ThOD	-1	$i_{ThOD,S_1}$	$i_{ThOD,S_S}$		-1.71	-4.57		$i_{ThOD,X_I}$	$i_{ThOD,X_S}$	$i_{ThOD,BM}$	3.00	$i_{ThOD,BM}$
2 Nitrogen	g N		$i_{N,S_1}$	$i_{N,S_S}$	1	1	1		$i_{N,X_I}$	$i_{N,X_S}$	$i_{N,BM}$		$i_{N,BM}$
3 Ionic charge	Mole +				1/14		-1/14	-1					
<i>Observables</i>													
4 SS	g SS								$i_{SS,X_I}$	$i_{SS,X_S}$	$i_{SS,BM}$	1.80	$i_{SS,BM}$

$i_{ThOD,BM}$ (ASM3C) has the units  
 $[g \text{ ThOD}_{BM} (g \text{ TOC}_{BM}^{-1})]$

From this we obtain (with absolute values from Tables 8.2 and 9.3):

$$\begin{aligned} (\text{ASM3C}) &= Y_A (\text{ASM3}) \cdot \frac{i_{ThOD,BM} (\text{ASM3})}{i_{ThOD,BM} (\text{ASM3C})} \\ &= 0.24 \text{ g COD}_{BM} (g \text{ NO}_3^- \text{ N})^{-1} \cdot \frac{1}{2.8} \\ &= 0.09 \text{ g TOC}_{BM} (g \text{ NO}_3^- \text{ N})^{-1} \end{aligned}$$

Adjustments are best based on careful analysis of the units of the parameter to be adjusted. Even the magnitude of seemingly dimensionless coefficients such as  $Y_H$  must be adjusted.

#### 9.4 Typical kinetic and stoichiometric parameters for ASM3C

Again the following remarks apply to ASM3C as well.

It is the responsibility of the user of ASM3C to determine the concentrations of relevant compounds in the wastewater, as well as the stoichiometric and kinetic parameters, which apply to the specific case to be dealt with.

**Absolute values of these parameters are not part of ASM3C.** They are necessary, however, if ASM3C is to be applied to any specific case.

In Tables 9.2–9.5 a set of typical kinetic and stoichiometric parameters and concentrations

of model compounds in a primary effluent is provided for convenience. This indicates neither that ASM3C is meant to be reliable with these parameters in any case, nor that these parameters are the state of the art. They are merely presented here as a reference for testing computer code and as a first estimate for the design of possible experiments that may be used to identify these parameters more accurately. In comparison to the values given in Tables 8.1–8.4 these values have been adjusted to TOC units based on typical composition parameters in Table 9.4. There may be some rounding errors resulting in slight deviations in model predictions between ASM3 and ASM3C. The extra decimal is not provided because it is thought to be accurate but rather in order to result in better comparison of predictions relative to ASM3.

Table 9.2 provides a list of typical kinetic parameters, Table 9.3 suggests some typical stoichiometric parameters, Table 9.4 indicates the composition of a typical primary effluent and finally Table 9.5 is a stoichiometric matrix, based on Table 9.1 and the specific values introduced in Table 9.3.

#### 9.5 Modelling pH with ASM3C

Including organic carbon in ASM3C allows modelling the pH value in the different reactor compartments. If bicarbonate is assumed to be



**Activated Sludge Model No. 3**

Table 9.2. Typical values of kinetic parameters for ASM3C. These values are provided as examples and **are not part of ASM3**. In comparison to the values given in Table 8.1 these values have been adjusted to TOC units based on typical composition parameters in Tables 8.2 and 9.3. There may be some rounding errors resulting in slight deviations in model predictions between ASM3 and ASM3C. The extra decimal is provided not because it is thought to be accurate but rather in order to result in better comparison of predictions relative to ASM3.

Symbol	Characterization	Temperature		Units
		10 °C	20 °C	
$k_H$	Hydrolysis rate constant	2.3	3.4	$\text{g TOC}_{X_S} (\text{g TOC}_{X_H})^{-1} \text{d}^{-1}$
$K_X$	Hydrolysis saturation constant	1	1	$\text{g TOC}_{X_S} (\text{g TOC}_{X_H})^{-1}$
<i>Heterotrophic organisms <math>X_H</math>, aerobic and denitrifying activity</i>				
$k_{STO}$	Storage rate constant	2.9	5.7	$\text{g TOC}_{S_S} (\text{g TOC}_{X_H})^{-1} \text{d}^{-1}$
$\eta_{NOX}$	Anoxic reduction factor	0.6	0.6	–
$K_{O_2}$	Saturation constant for $S_{NO_2}$	0.2	0.2	$\text{g O}_2 \text{m}^{-3}$
$K_{NOX}$	Saturation constant for $S_{NOX}$	0.5	0.5	$\text{g NO}_3\text{-N m}^{-3}$
$K_S$	Saturation constant for substrate $S_S$	0.6	0.6	$\text{g TOC}_{S_S} \text{m}^{-3}$
$K_{STO}$	Saturation constant for $X_{STO}$	1.1	1.1	$\text{g TOC}_{X_{STO}} (\text{g TOC}_{X_H})^{-1}$
$\mu_H$	Heterotrophic max. growth rate	1	2	$\text{d}^{-1}$
$K_{NH_4}$	Saturation constant for ammonium, $S_{NH_4}$	0.01	0.01	$\text{g N m}^{-3}$
$K_{ALK}$	Saturation constant for alkalinity for $X_H$	0.1	0.1	$\text{mole HCO}_3^- \text{m}^{-3}$
$b_{H,O_2}$	Aerobic endogenous respiration rate of $X_H$	0.1	0.2	$\text{d}^{-1}$
$b_{H,NOX}$	Anoxic endogenous respiration rate of $X_H$	0.05	0.1	$\text{d}^{-1}$
$b_{STO,O_2}$	Aerobic respiration rate for $X_{STO}$	0.1	0.2	$\text{d}^{-1}$
$b_{STO,NOX}$	Anoxic respiration rate for $X_{STO}$	0.05	0.1	$\text{d}^{-1}$
<i>Autotrophic organisms <math>X_A</math>, nitrifying activity</i>				
$\mu_A$	Autotrophic max. growth rate of $X_A$	0.35	1.0	$\text{d}^{-1}$
$K_{A,NH_4}$	Ammonium substrate saturation for $X_A$	1	1	$\text{g N m}^{-3}$
$K_{A,O_2}$	Oxygen saturation for nitrifiers	0.5	0.5	$\text{g O}_2 \text{m}^{-3}$
$K_{A,ALK}$	Bicarbonate saturation for nitrifiers	0.5	0.5	$\text{mole HCO}_3^- \text{m}^{-3}$
$b_{A,O_2}$	Aerobic endogenous respiration rate of $X_A$	0.05	0.15	$\text{d}^{-1}$
$b_{A,NOX}$	Anoxic endogenous respiration rate of $X_A$	0.02	0.05	$\text{d}^{-1}$

Table 9.3. Typical stoichiometric and composition parameters for ASM3C. These values are given as examples and **are not part of ASM3**.

Symbol	Characterization	Value	Units	
$f_{S_1}$	Production of $S_1$ in hydrolysis	0	$\text{g TOC}_{S_1} (\text{g TOC}_{X_S})^{-1}$	
$Y_{STO,O_2}$	Aerobic yield of stored product per $S_S$	0.91	$\text{g TOC}_{X_{STO}} (\text{g TOC}_{S_S})^{-1}$	
$Y_{STO,NOX}$	Anoxic yield of stored product per $S_S$	0.85	$\text{g TOC}_{X_{STO}} (\text{g TOC}_{S_S})^{-1}$	Equation 5.3
$Y_{H,O_2}$	Aerobic yield of heterotrophic biomass	0.67	$\text{g TOC}_{X_H} (\text{g TOC}_{X_{STO}})^{-1}$	
$Y_{H,NOX}$	Anoxic yield of heterotrophic biomass	0.58	$\text{g TOC}_{X_H} (\text{g TOC}_{X_{STO}})^{-1}$	Equation 5.3
$Y_A$	Yield of autotrophic biomass per $\text{NO}_3\text{-N}$	0.09	$\text{g TOC}_{X_A} (\text{g N}_{S_{NOX}})^{-1}$	
$f_{X_1}$	Production of $X_1$ in endog. respiration	0.20	$\text{g TOC}_{X_1} (\text{g TOC}_{X_{BM}})^{-1}$	
$i_{ThOD,S_1}$	ThOD content of $S_1$	2.8	$\text{g ThOD} (\text{g TOC}_{S_1})^{-1}$	
$i_{ThOD,S_S}$	ThOD content of $S_S$	3.2	$\text{g ThOD} (\text{g TOC}_{S_S})^{-1}$	
$i_{ThOD,X_1}$	ThOD content of $X_1$	2.8	$\text{g ThOD} (\text{g TOC}_{X_1})^{-1}$	
$i_{ThOD,X_S}$	ThOD content of $X_S$	3.2	$\text{g ThOD} (\text{g TOC}_{X_S})^{-1}$	
$i_{ThOD,BM}$	ThOD content of biomass, $X_H, X_A$	2.8	$\text{g ThOD} (\text{g TOC}_{X_{BM}})^{-1}$	
$i_{N,S_1}$	N content of $S_1$	0.03	$\text{g N} (\text{g TOC}_{S_1})^{-1}$	
$i_{N,S_S}$	N content of $S_S$	0.10	$\text{g N} (\text{g TOC}_{S_S})^{-1}$	
$i_{N,X_1}$	N content of $X_1$	0.06	$\text{g N} (\text{g TOC}_{X_1})^{-1}$	
$i_{N,X_S}$	N content of $X_S$	0.13	$\text{g N} (\text{g TOC}_{X_S})^{-1}$	
$i_{N,BM}$	N content of biomass, $X_H, X_A$	0.20	$\text{g N} (\text{g TOC}_{X_{BM}})^{-1}$	
$i_{SS,X_1}$	SS to TOC ratio for $X_1$	2.1	$\text{g SS} (\text{g TOC}_{X_1})^{-1}$	The values below are suggested if $X_{SS}$ is used to model VSS rather than SS: 2.1 g VSS (g $X_1$ ) <sup>-1</sup>
$i_{SS,X_S}$	SS to TOC ratio for $X_S$	2.4	$\text{g SS} (\text{g TOC}_{X_S})^{-1}$	2.4 g VSS (g $X_S$ ) <sup>-1</sup>
$i_{SS,BM}$	SS to TOC ratio for biomass, $X_H, X_A$	2.5	$\text{g SS} (\text{g TOC}_{X_{BM}})^{-1}$	2.4 g VSS (g $X_H$ or $X_A$ ) <sup>-1</sup>

Table 9.4. Short definition of model compounds and typical wastewater composition (primary effluent) for ASM3C. The value of TKN considers the composition of the different model compounds as indicated in Table 9.3:  $TKN = \sum S_i \cdot \iota_{2,i}$  over all compounds  $i$  -  $S_{NOX} - S_{N_2}$ .  $COD_{tot} = 260$  g COD  $m^{-3}$ ,  $TKN = 25$  g N  $m^{-3}$ .

Compounds		Concentration	Units	
<i>Dissolved compounds</i>				
$S_{O_2}$	Dissolved oxygen	0	g $O_2$ $m^{-3}$	
$S_I$	Soluble inert organics	11	g TOC $m^{-3}$	
$S_S$	Readily biodegradable substrates	19	g TOC $m^{-3}$	
$S_{NH_4}$	Ammonium	15.4	g N $m^{-3}$	
$S_{N_2}$	Dinitrogen, released by denitrification	0	g N $m^{-3}$	
$S_{NOX}$	Nitrite plus nitrate	0	g N $m^{-3}$	
$S_{ALK}$	Alkalinity, bicarbonate	5	mole $HCO_3^-$ $m^{-3}$	
<i>Particulate compounds</i>				
$X_I$	Inert particulate organics	9	g TOC $m^{-3}$	
$X_S$	Slowly biodegradable substrates	36	g TOC $m^{-3}$	
$X_H$	Heterotrophic biomass	11	g TOC $m^{-3}$	The value below is suggested if $X_{SS}$ is used to model VSS rather than SS:
$X_{STO}$	Organics stored by heterotrophs	0	g TOC $m^{-3}$	
$X_A$	Autotrophic, nitrifying biomass	>0	g TOC $m^{-3}$	
$X_{SS}$	Total suspended solids	125	g SS $m^{-3}$	

Table 9.5. Stoichiometric matrix of ASM3C based on the stoichiometric parameters in Tables 9.1 and 9.3. This matrix is a typical application of ASM3C but it is not suggested as a reliable form of ASM3C.

Compound $i \rightarrow$	1	2	3	4	5	6	7	8	9	10	11	12	13
$j$ Process	$S_{O_2}$	$S_I$	$S_S$	$S_{NH_4}$	$S_{N_2}$	$S_{NOX}$	$S_{ALK}$	$X_I$	$X_S$	$X_H$	$X_{STO}$	$X_A$	$X_{SS}$
$j$ Expressed as $\rightarrow$	$O_2$	TOC	TOC	N	N	N	Mole	TOC	TOC	TOC	TOC	TOC	SS
1 Hydrolysis		0	1	0.03			0.002		-1				-2.40
<i>Heterotrophic organisms, aerobic and denitrifying activity</i>													
2 Aerobic storage of $S_S$	-0.47		-1	0.10			0.007				0.91		1.64
3 Anoxic storage of $S_S$			-1	0.10	0.23	-0.23	0.023				0.85		1.53
4 Aerobic growth of $X_H$	-1.61			-0.20			-0.014			1	-1.47		-0.15
5 Anoxic growth (denitrific.)				-0.20	0.83	-0.83	0.045			1	-1.72		-0.60
6 Aerobic endog. respiration	-2.24			0.19			0.013	0.20		-1			-2.08
7 Anoxic endog. respiration				0.19	0.78	-0.78	0.069	0.20		-1			-2.08
8 Aerobic respiration of $X_{STO}$	-3										-1		-1.80
9 Anoxic respiration of $X_{STO}$					1.05	-1.05	0.075				-1		-1.80
<i>Autotrophic organisms, nitrifying activity</i>													
10 Aerobic growth of $X_A$	-48.0			-11.3		11.1	-1.60					1	2.50
11 Aerobic endog. respiration	-2.24			0.19			0.013	0.20				-1	-2.08
12 Anoxic endog. respiration				0.19	0.78	-0.78	0.069	0.20				-1	-2.08

the dominating buffer system, pH can be modelled by adding dissolved carbon dioxide ( $CO_2$ ,  $S_{CO_2}$ ) and the proton ( $H$ ,  $S_{H^+}$ ) as additional state variables and two processes describing the equilibrium (forward and backward reaction) of bicarbonate dissociation, with fast reaction rates (the ratio of these reaction rates is given by the equilibrium constant). Further the additional stoichiometric coefficients for  $S_{CO_2}$  can be obtained from conservation of carbon (a fourth conservative). Stripping of  $S_{CO_2}$  must be related to aeration, considering the correct Henry coefficients and possible saturation of rising air bubbles with  $CO_2$ .

It is recommended to derive stoichiometric

coefficients  $z_j$  from a charge balance over bicarbonate rather than the proton. This typically allows for faster numeric integration because the turnover of large amount of charge is modelled via the large pool of  $S_{ALK}$  rather than the very small pool of  $H$ .

Accurate modelling of pH may require expansion of the model to include carbonate, nitrite, ammonium and phosphate buffers as well.

## 9.6 Limitations of ASM3C

The limitations introduced above for ASM3 apply equally to ASM3C. Since experience with TOC is still rather scarce, extra care should be taken in analytical procedures.

## 10. Conclusion

ASM3 and ASM3C correct for most of the defects identified in ASM1. The ASM3 models provide a common base for the simulation of nitrogen removing activated sludge systems for chemical oxygen demand as well as organic carbon based characterization of wastewater and biomass. These two characterization possibilities can analytically be approximated by COD and TOC analysis. The structure of the ASM3 models provides sufficient details such that they may be used in an advanced course on biological wastewater treatment as a didactic tool. These models are designed as the core for further development and inclusion of additional processes and states as may become necessary when biological phosphorus removal, chemical phosphorus precipitation, growth of filaments etc. ought to be included.

The systematic notation, based on an array of state variables, a stoichiometric matrix, a composition matrix, an array of process rates and conservation equations made it especially easy to introduce these models and indicate how a

COD based model may be transformed into another base (here organic carbon, TOC).

Neither ASM3 nor ASM3C has yet been tested against a large variety of experimental data. It is expected that future improvements of model structure may still be required, especially for the description of the storage phenomena. It is obvious that in the beginning experience with ASM3 might be inferior to experience with ASM1. But as our experience will improve the two models might well prove to be equivalent. ASM3 has the advantage that its structure does not have to be adjusted in order to be applicable even if ammonium or bicarbonate limits microbial activity. Therefore if we report in a publication that a simulation was performed with ASM3 or ASM3C, it may be assumed that the model structures introduced in this report have been applied unchanged.

**It is good practice to indicate if model structure has been changed: This would then be a dialect of ASM3 but not ASM3 itself.**



## 11. References

The following limited citations relate to the topic discussed in this report and may be useful to understand the background and the presentation of ASM3. The Task Group would like to apologize for not following the standard rules of citation of scientific work and acknowledges that a vast literature (and communication with peers) has stimulated its work. It appears impossible to explicitly identify the specific source of the elements of ASM3 and ASM3C.

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