

Elemental Balances in Activated Sludge Modelling

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Abstract Activated sludge models, based on COD and N balances and presented using the Gujer (Petersen) matrix description are investigated from the standpoint of maintaining elemental (C, O, H, N) balances. ASM1 is used as an example. The ASM1 Gujer matrix is extended with N₂, CO₂ and H₂O state variables to close elemental balances. Typical composition of state variables is determined using standard COD, TOC, VSS and TKN measurements. Chemical reactions are derived for each process in the ASM1 model for general composition and stoichiometric parameters, as well as for the most likely composition of state variables and best estimates for stoichiometric parameters (yield, endogenous fraction, etc.). For more accurate evaluations, "traditional" data is needed on total and filtered influents, mixed liquor and effluents (VSS or VS, COD, TOC or DOC, N, and P with and without filtration). The method can be used to verify model integrity and is necessary in linking different models using the CBIM transformer method, in view of plant-wide modelling and simulation.

Keywords Elemental composition, elemental balances, modelling, ASM, ADM, wastewater treatment

Introduction

Engineers and operators have to consider the whole treatment plant and the effect of individual processes, recycles on each other in their work. One of the approaches to full-plant modelling is to link existing process models (e.g. ASM1, ADM1 and others) through transformers to each other. The continuity-based interface method (CBIM, Vanrolleghem et al., 2005) was recently proposed and applied to construct such interfaces. This systematic method of building model transformers is based on elemental composition (C, H, O, N, P, S content) of organic and inorganic matter in the models to be connected. The transformer must preserve mass balances (continuity) on all elements when mapping state variables between models. Thus, the CBIM requires information on the elemental composition of all state variables. The insight that specification of elemental composition is useful in modelling is not new; see for instance, Hellings et al., 1995; Henze et al., 2000; Reichert et al., 2001; Batstone et al., 2002.

The objective of this paper is to investigate, using the example of ASM1, if existing models preserve elemental material balances, and to describe how to determine elemental composition of state variables. The Gujer (Petersen) matrix method is extended to ensure that these balances are preserved. Maple (from Maplesoft, www.maplesoft.com) was used for most symbolic equation manipulations.

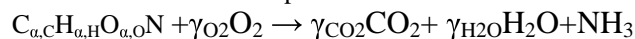
Do COD-based Models Preserve Elemental Balances?

The ASMx and ADM1 models were constructed using COD and N mass balances. The models in their current form do not close the balance on C, H, O and N. Consideration of dissolved nitrogen gas, CO₂ and water as reaction products is necessary to close elemental balances in these models. These state variables, particularly water, as a reaction product, do not need to be calculated (integrated) in the model but are necessary to write the complete reaction of the particular process (e.g. heterotrophic growth) according to accepted chemical reaction principles. Thus, the ASM1 model matrix, which is used here as the illustrative example since it considers only COD, N and charge balances, was extended with three new columns: dissolved N₂ gas (S_{N2}, gN.m⁻³), total CO₂, (S_{CO2}, mole.m⁻³), and water, (S_{H2O}, mole.m⁻³).

Charge balance is maintained in ASM1 using alkalinity as a state variable and the effect of charged reactants on it (e.g. nitrification using NH₄⁺ and producing NO₃⁻). This aspect was not included in this paper, since there is a contemporary and more accurate way of calculating the pH effects of conversion processes, through an equilibrium pH-model outside the kinetic matrix. This was introduced in the River Water Quality Model No. 1 (Reichert et al., 2001), and then adopted in ADM1 (Batstone et al., 2002) and ASM models (Takács et al., 2004; Volcke et al., 2006). The new method incorporates the effect of other processes (e.g. CO₂ gas transfer) on alkalinity, and does not depend on an approximate charge balance (e.g. the charge of total CO₂ is pH dependent, at pH=7 and typical wastewater ionic strength is 0.819). For these reasons charge balances will not be considered in this paper focussing on elemental balances. Consequently, the alkalinity state variable was not included in this analysis and all state variables will be represented in their unionized form (i.e. NH₃ and HNO₃). These state variables represent the complete mass of the compound, e.g. the sum of ammonia (NH₃) and ammonium (NH₄⁺).

Determination of Elemental Composition of State Variables

In order to present an example of elemental balancing, the elemental composition of each state variable in the extended ASM1 matrix was determined. The N, (and P and S) components in particulate organic matter can be directly measured by common analytical methods. Typical values in municipal wastewater are: N: 10-12% of VSS, P: 2-3% of VSS, S: 1% of VSS (Grady et al. 1999). To determine the C, O and H content for one particular component, three independent measurements are required, e.g. COD, VSS, TOC. For each additional element (N, P, S) we need one more analytical measurement. In an example case we would have :



This equation has five unknowns, and these can be found from the following balances:

COD/VSS ratio	$iCOD = 2\gamma_{O_2}O / (\alpha_{,C}C + \alpha_{,H}H + \alpha_{,O}O_{\alpha,O} + N)$
C/VSS ratio	$iC = \alpha_{,C}C / (\alpha_{,C}C + \alpha_{,H}H + \alpha_{,O}O_{\alpha,O} + N)$
N/VSS ratio	$iN = N / (\alpha_{,C}C + \alpha_{,H}H + \alpha_{,O}O_{\alpha,O} + N)$
Hydrogen balance	$\alpha_{,H} = 2\gamma_{H_2O} + 3$
Oxygen balance	$\alpha_{,O} + 2\gamma_{O_2} = 2\alpha_{,C} + \gamma_{H_2O}$

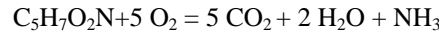
which lead, by using Maple symbolic manipulation software for ease of work, to the chemical composition deduced from simple measurements given in Table 1.

Table 1. Composition of organic matter obtained from simple analytical measurements and atomic weights.

Component considered $C_{\alpha,C}H_{\alpha,H}O_{\alpha,O}N$
$\alpha_C = iC \cdot N / (iN/C)$
$\alpha_H = (3 \cdot C \cdot iN \cdot O_x + 2 \cdot C \cdot iCOD \cdot N - 2 \cdot C \cdot iN \cdot N + 2 \cdot C \cdot N - 2 \cdot iC \cdot N \cdot C - 4 \cdot iC \cdot N \cdot O_x) / iN/C / (2 \cdot H + O_x)$
$\alpha_O = -(2 \cdot C \cdot iCOD \cdot N \cdot H - 4 \cdot iC \cdot N \cdot O_x \cdot H + O_x \cdot C \cdot iN \cdot N + 3 \cdot O_x \cdot C \cdot iN \cdot H - O_x \cdot C \cdot N + O_x \cdot iC \cdot N \cdot C) / iN/O_x/C / (2 \cdot H + O_x)$
$\alpha_N = 1$

Biomass composition

Bailey (1986) reports C and N content for several microorganisms – the average is 49.9% C in VSS, and 13.3% N in VSS. Rittman (2000) presents data for COD/VSS ratios: 1.39 gCOD/gVSS for pure and 1.33 gCOD/gVSS for mixed cultures. ASM3 (Henze et al., 2000) contains a COD/TOC ratio of 2.8. A typically used biomass composition is $C_5H_7O_2N$ after Hoover and Porges (1952), which was subsequently used by many schools (e.g. UCT) and incorporated into almost all modern modelling literature (Henze et al 1995, Henze et al., 2000). This molecular formula, based on the reaction (assumed to occur during the COD test):



results in the following ratios: COD/VSS=1.42, N/VSS=0.124, C/VSS=0.53, and COD/TOC=2.7. Since these are close to typically measured ratios, the $C_5H_7O_2N$ formula is used in this paper for both heterotrophs (X_H) and autotrophs (X_A), as well as their decay products (X_P). X_P is usually thought to contain less N than active biomass, but in lack of precise measurements of N, TOC and COD content the same composition was accepted.

Substrate and inert composition

The elemental composition of biodegradable and inert organic state variables can be deduced using the following logic. COD/VSS ratios for X_S and X_I state variables can be calculated from COD/VSS ratios of influent wastewater and activated sludge mixed liquor, two typical mixtures with available measurements and known composition. Table 2 shows typical compositions of influent and MLSS, from simulation assuming 500 gCOD.m⁻³ and 60% particulates in the influent at 8 d SRT.

Table 2. State variables in influent and MLSS

State	Unit	Influent	MLSS
$X_H + X_E$	gCOD.m ⁻³	15	1722
X_I	gCOD.m ⁻³	65	891
X_S	gCOD.m ⁻³	220	88

Table 3. COD/VSS ratios for X_I and X_S

Measured		Assumed	Calculated	
Influent	MLSS	Biomass	Inert (X_I)	Substrate (X_S)
1.6	1.48	1.42	1.58	1.62
1.8	1.48	1.42	1.55	1.90
2.0	1.48	1.42	1.53	2.18
2.2	1.48	1.42	1.50	2.46

The calculation method is based on measured influent and MLSS COD/VSS ratios, assuming that they are a combination of the COD/VSS ratios of the three types of components present (two equations). The biomass and decay product COD/VSS ratio are assumed as fixed at 1.42, and the two unknowns are the COD/VSS ratios for X_I and X_S . In Table 3, a series of COD/VSS ratios have been calculated for the two state variables, from increasing measured influent COD/VSS ratios.

From a practical modeling standpoint, this result seems to point to a) a relatively stable influent inert COD/VSS ratio, and b) a very sensitive COD/VSS ratio for substrates, depending likely on the composition of the sewage (protein/lipid/carbohydrate fractions) This may to a large extent explain the variability found in influent COD/VSS ratios, and points to the usefulness of a more fundamental modelling approach that includes several types of biodegradable organic material, similar to ADM1 (Batstone et al., 2002). Table 4 contains composition data for several typical influent organic materials.

Table 4 Composition of typical influent organic substances

Component	Formula	Reaction	COD/VSS	C/VSS
Lipids/fatty acids (n~14)	$\text{CH}_3\text{-nCH}_2\text{COOH}$	$\text{CH}_3\text{nCH}_2\text{COOH} + (1.5n+2)*\text{O}_2 = (n+2)*\text{CO}_2 + (n+2)*\text{H}_2\text{O}$	2.87	0.87
Mixture of amino acids	Varies, average length is taken as 4 carbons	Varies	1.84	0.63
Biomass	$\text{C}_5\text{H}_7\text{O}_2\text{N}$	$\text{C}_5\text{H}_7\text{O}_2\text{N} + 5\text{O}_2 = 5\text{CO}_2 + 2\text{H}_2\text{O} + \text{NH}_3$	1.42	0.53
Proteins	$\text{C}_{3.5}\text{H}_{7.06}\text{O}_{1.75}\text{N}$	$\text{C}_{3.5}\text{H}_{7.06}\text{O}_{1.75}\text{N} + 3.64\text{O}_2 = 3.5\text{CO}_2 + 2.03\text{H}_2\text{O} + \text{NH}_3$	1.28	0.46
Carbohydrates	CH_2O	$\text{CH}_2\text{O} + \text{O}_2 = \text{CO}_2 + \text{H}_2\text{O}$	1.07	0.47

For the purpose of this paper, for a “typical” influent with a COD/VSS ratio of 1.8, the following state variable COD/VSS ratios were selected: 1.55 for inert X_I and 1.9 for substrate X_S . Carbon contents were used from Henze et al. (2000) as 2.8 COD/TOC ratio for X_I and 3.2 COD/TOC ratio for X_S . Based on the calculation of these combined COD/VSS and COD/TOC ratios from X_I and X_S elemental compositions, and the oxygen and hydrogen balance equations in the $\text{C}_{\alpha_C}\text{H}_{\alpha_H}\text{O} + \gamma_{\text{O}_2}\text{O}_2 = \alpha_C\text{CO}_2 + \gamma_{\text{H}_2\text{O}}\text{H}_2\text{O}$ reaction, four equations can be expressed for the four unknowns (α_C , α_H , γ_{O_2} , $\gamma_{\text{H}_2\text{O}}$), and thus the composition can be calculated. The resulting composition is shown in Table 5. In lack of filtered DOC/VS data, readily biodegradable substrate and soluble inert organics were assigned the same composition as their particulate counterparts. Organic nitrogen forms must be allocated the composition of NH_3 , since all associated carbon and COD is accounted for in the relevant organic state variables.

Table 5. Composition of state variables in ASM1 used in this study

State variable	Unit	Molar composition	Mass fraction of elements
S _I	gCOD/m ³	C _{1.90} H _{2.39} O	C=0.553; H=0.058; O=0.388;
S _S	gCOD/m ³	C _{2.43} H _{3.96} O	C=0.594; H=0.081; O=0.325;
X _I	gCOD/m ³	C _{1.90} H _{2.39} O	C=0.553; H=0.058; O=0.388;
X _S	gCOD/m ³	C _{2.43} H _{3.96} O	C=0.594; H=0.081; O=0.325;
X _H	gCOD/m ³	C ₅ H ₇ O ₂ N	C=0.531; H=0.062; O=0.283; N=0.124;
X _A	gCOD/m ³	C ₅ H ₇ O ₂ N	C=0.531; H=0.062; O=0.283; N=0.124;
X _E	gCOD/m ³	C ₅ H ₇ O ₂ N	C=0.531; H=0.062; O=0.283; N=0.124;
S _O	gO ₂ /m ³	O ₂	O=1.00;
S _{NO}	gN/m ³	HNO ₃	H=0.016; N=0.222; O=0.762;
S _{NH}	gN/m ³	NH ₃	H=0.176; N=0.824;
S _{ND}	gN/m ³	NH ₃	H=0.176; N=0.824
X _{ND}	gN/m ³	NH ₃	H=0.176; N=0.824

Note: Atomic weights used are: C = 12.011, H = 1.0079, O = 15.9994 and N = 14.007

Extended Gujer matrix

It is proposed that the Gujer (Petersen) matrix be extended with the necessary state variables (N₂, CO₂, H₂O and others for more detailed models) to allow the continuity check on conservation of elements. Table 6 contains the extended ASM1 stoichiometry matrix. Stoichiometric constants and their values are listed in Table 7.

Table 6. Extended ASM1 stoichiometry matrix

Process	S _I	S _S	X _I	X _S	X _H	X _A	X _P	S _O	S _{NO}	S _{NH}	S _{ND}	X _{ND}	S _{N2}	S _{CO2}	S _{H2O}
	gCOD.m ⁻³							gO ₂ .m ⁻³	gN.m ⁻³				mole.m ⁻³		
1		$\frac{1}{Y_H}$			I			$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$				$\frac{\gamma_{CO_2,1}}{160}$	$\frac{\gamma_{H_2O,1}}{160}$
2		$\frac{1}{Y_H}$			I			$-\frac{1-Y_H}{2.86Y_H}$		$-i_{XB}$			$\frac{1-Y_H}{2.86Y_H}$	$\frac{\gamma_{CO_2,2}}{160}$	$\frac{\gamma_{H_2O,2}}{160}$
3						I		$-\frac{4.57-Y_A}{Y_A}$	$\frac{1}{Y_A}$	$-\frac{1}{Y_A}-i_{XB}$				$\frac{\gamma_{CO_2,3}}{160}$	$\frac{\gamma_{H_2O,3}}{160}$
4				$I-f_P$	$-I$		f_P							$\frac{\gamma_{CO_2,4}}{160}$	$-\frac{\gamma_{H_2O,4}}{160}$
5				$I-f_P$	$-I$		f_P							$\frac{\gamma_{CO_2,5}}{160}$	$-\frac{\gamma_{H_2O,5}}{160}$
6										I	$-I$				
7		I		$-I$											
8											I	$-I$			

Note: 160 gCOD.m⁻³ is the COD of one mole of biomass. Processes: 1. Aerobic growth of heterotrophs 2. Anoxic growth of heterotrophs 3. Aerobic growth of autotrophs 4. 'Decay' of heterotrophs 5. 'Decay' of autotrophs 6. Ammonification 7. Hydrolysis of slowly biodegradable substrate 8. Hydrolysis of particulate biodegradable organic nitrogen

Table 7 Extended ASM1 stoichiometric parameters

Stoichiometric parameter	Unit	Value
Y_H	gCOD/gCOD	0.667
Y_A	gCOD/gN	0.24
f_P	gCOD/gCOD	0.08
i_{XB}	gN/gCOD	0.088
i_{XP}	gN/gCOD	0.088
$\gamma_{CO_2,i}$ and $\gamma_{H_2O,i}$	Mole	From the relevant process in Table 9

For clarity, a column with the chemical reactions should be added after the process rates to describe the specific process as a reaction, according to accepted chemical principles. This information can be expressed in three different ways:

1. Generally (for any composition of state variables and any value of stoichiometric constants)
2. For a chosen fixed composition of state variables and any value of stoichiometric constants
3. For fixed composition of state variables and selected stoichiometric constants.

Table 8 shows the three ways of expressing the reactions (example for the aerobic growth process in ASM1). In order to present a complete example of the simplest presentation mode of ASM1 reactions, with fixed constants, Table 9 is given. Since reactions are expressed for one mole of biomass, and the stoichiometry matrix (Table 6) is expressed in gCOD.m⁻³ units, it is necessary to convert reaction coefficients using the COD content of one mole of biomass (e.g. 160 gCOD.m⁻³).

Table 8. Different ways of expressing process rates (example: aerobic heterotrophic growth)

For variable Y_H and any component composition
$\frac{A}{Y_H B} C_{\alpha_{C,S}} H_{\alpha_{H,S}} O + \frac{A(Y_H - \alpha_{C,S})}{4Y_H} O_2 + NH_3 \rightarrow C_{\alpha_{C,B}} H_{\alpha_{H,B}} O_{\alpha_{O,B}} N + \frac{Y_H \alpha_{C,B} B - \alpha_{C,S} A}{Y_H B} CO_2$ $+ \frac{\alpha_{H,S}(4\alpha_{C,S} - 2\alpha_{O,B} - Y_H \alpha_{H,B}) - Y_H \alpha_{H,B} B + 3Y_H B}{2Y_H B} H_2O$
where
$A = 4\alpha_{C,B} + \alpha_{H,B} - 2\alpha_{O,B}$
$B = 4\alpha_{C,S} + \alpha_{H,S} - 2$
Notation for number of atoms in formula (α) = $\alpha_{\text{element, state}}$ element is C, H or O, state is Biomass or Substrate
For variable Y_H and component composition listed in Table 5:
$\frac{1.71}{Y_H} C_{2.43} H_{3.96} O + 5 \frac{1 - Y_H}{Y_H} O_2 + NH_3 \rightarrow C_3 H_7 O_2 N + \frac{4.16 - 5Y_H}{Y_H} CO_2 + \frac{3.39 - 2Y_H}{Y_H} H_2O$
For $Y_H=0.667$ and component composition listed in Table 5:
$2.57 C_{2.43} H_{3.96} O + 2.50 O_2 + NH_3 \rightarrow C_3 H_7 O_2 N + 1.24 CO_2 + 3.09 H_2O$

Table 9. ASM1 reaction column

Process	Reaction
Aerobic growth of heterotrophs	$2.57 C_{2.43}H_{3.96}O + 2.50 O_2 + NH_3 \rightarrow$ $C_5H_7O_2N + 1.24 CO_2 + 3.09 H_2O$
Anoxic growth of heterotrophs	$2.57 C_{2.43}H_{3.96}O + 2.0 HNO_3 + NH_3 \rightarrow$ $1.24 CO_2 + C_5H_7O_2N + N_2 + 4.09 H_2O$
Growth of autotrophs	$48.59 NH_3 + 5 CO_2 + 90.19 O_2 \rightarrow$ $C_5H_7O_2N + 47.59 HNO_3 + 45.59 H_2O$
Decay of heterotrophs	$C_5H_7O_2N + 1.28 H_2O \rightarrow$ $1.58 C_{2.43}H_{3.96}O + 0.08 C_5H_7O_2N + 0.92 NH_3 + 0.77 CO_2$
Decay of autotrophs	$C_5H_7O_2N + 1.28 H_2O \rightarrow$ $1.58 C_{2.43}H_{3.96}O + 0.08 C_5H_7O_2N + 0.92 NH_3 + 0.77 CO_2$
Hydrolysis of particulate substrate	$C_{2.43}H_{3.96}O \rightarrow C_{2.43}H_{3.96}O$
Hydrolysis of particulate nitrogen	$NH_3 \rightarrow NH_3$
Ammonification	$NH_3 \rightarrow NH_3$

Concluding remarks

The proposed methods will increase the information contained in wastewater process models used today, enable modellers to construct models that preserve elements, will make reading of the models more informative, and will make constructing CBIM-based transformers between submodels more rigorous, by reducing significantly the number of degrees of freedom from estimating state variable elemental compositions.

It was found that not all data are readily available for elemental balancing of municipal wastewater components. TOCs, as well as DOC and VS on filtrates would help to establish typical state variable compositions. Direct chemical component measurement (e.g. protein extraction, ether extractable lipids) would be useful as well.

The composition of certain state variables (e.g. biomass, inerts) seems to be stable. Others (influent substrate) vary significantly. Proper handling of this may lead to models based on more fundamental components like proteins, lipids and carbohydrates (similar to ADM1, Batstone et al., 2002). This should lead to more stable stoichiometric constants and more predictive power for the models.

There is evidence (e.g. Pramanik and Keasling, 1997) that elemental composition changes even for variables that are considered stable. For example biomass can have different N content in high-loaded, low-loaded or nutrient-limited conditions. Current modelling methodology does not deal with this in an elegant way and is in need of more research and development. Hence, in today's models, composition parameters have to be considered for calibration as well.

Elemental balancing increases the complexity and data requirements of models, while at the same time increasing the amount of information contained in models. On a process model basis, this is not always required. For example, O₂ uptake and sludge production predictions do not change in the proposed extended ASM1 matrix. However, elemental balancing provides a rigorous integrity check for models, leads to new insights into the behaviour of wastewater treatment systems, and facilitates the use of the continuity-based interfacing method to link different models.

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