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Transformers for interfacing anaerobic digestion models to pre- and post-treatment processes in a plant-wide modelling context

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Abstract

In view of the growing importance of integrated and plant-wide modelling of wastewater treatment plants, this work reviews, applies and compares two transforming/interfacing methods by connecting anaerobic digestion and activated sludge models. The two methods are systematic approaches to transform state variables of one model to another and vice versa. The theory of the first method was presented before (Vanrolleghem et al., 2005. Wat. Sci. Technol., 52(1–2), 493–500.) as a general approach for interfacing any two models presented by Petersen matrices. The present work is the first application and therefore validation of this general approach. The theory of the second method was specifically developed for connecting ASM1 and ADM1, both standard IWA models. As an illustration, in this work a specific simulation example is presented in which the COST/IWA activated sludge benchmark plant is extended by sludge treatment and digestion facilities.

Keywords: ADM1; ASM1; Continuity; Petersen matrix; Plant-wide benchmark; Transformers; Wastewater treatment

1. Introduction

Integrated modelling of wastewater systems comprising the collection network (sewer system), the treatment plant and the receiving water has been growing and advancing since the late 1990s (Butler and Schütze, 2005; Meirlaen et al., 2001). The treatment plant processes too should be dealt with in an integrated manner. Plant-wide modelling including anaerobic sludge digestion which is closely integrated to the activated sludge system has been proposed (Jeppsson et al., 2004; Zaher et al., 2002).

Anaerobic digestion receives a growing attention in the field of wastewater treatment, both in industrial and municipal sectors. For the latter, anaerobic digestion is employed for sludge treatment and stabilization. It considerably reduces the amount of sludge produced. However, the cost of waste sludge treatment constitutes approximately 35% of the capital cost and 55% of the annual operation and maintenance costs of a wastewater treatment plant (Cinar et al., 2004; Knezevic et al., 1995). As a compensation, the lower amounts of sludge reduce the cost of final disposal. The reduction of sludge volumes is turned mainly to biogas that can be used as clean energy source, e.g. generating electrical power for plant operation. For industries, anaerobic treatment could be a good option for wastewater treatment as an alternative to connecting to the sewer and paying higher tariffs. Other loads that can be connected to the digesters are truck loads from decentralised systems or sludge from other treatment plants. To study such scenarios and evaluate plant-wide control systems and operating strategies, integrated modelling of anaerobic digestion and other plant processes is very valuable.

The question tackled in this paper is how to connect models so that control systems, sensors and subsequent treatment

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Nomenclature

ADM1 components:

S_{i}	Inert soluble material
S_{su}	Sugars
S_{aa}	Amino acids
S_{fa}	Total LCFA
S_{va}	Total valerate
S_{bu}	Total butyrate
S_{pro}	Total propionates
S_{ac}	Total acetate
S_{h2}	Hydrogen
S_{ch4}	Methane
X_{i}	Particulate inerts
X_{c}	Composite particulate
X_{ch}	Carbohydrates
X_{pr}	Proteins
X_{li}	Lipids
X_{su}	Sugar degraders
X_{aa}	Amino acids degraders
X_{fa}	Total LCFA degraders
X_{c4}	Valerate and butyrate degraders
X_{pro}	Propionate degraders
X_{ac}	Acetate degraders
X_{h2}	Hydrogen degraders
S_{an}	Anions
S_{cat}	Cations
S_{ic}	Inorganic carbon
S_{in}	Inorganic nitrogen

ASM1 components:

S_{s}	Readily biodegradable material
S_{no3-}	Nitrates
S_{i}	Inert soluble material
X_{s}	Slowly biodegradable substrate
X_{bh}	Heterotrophic biomass
X_{ba}	Autotrophic biomass
X_{i}	Inert particulate material
X_{P}	Inert material from decay
S_{nh4+}	Ammonia
S_{ND}	Soluble organic nitrogen
X_{ND}	Particulate organic nitrogen
S_{alk}	Alkalinity
S_{o}	Dissolved oxygen

ASM1–ADM1 conversions:

S_{nh4+}_S_{in} ASM1 ammonia to ADM1 inorganic nitrogen
S_{ND}, S_{s}_S_{aa}, S_{fa}, S_{su} ASM1 soluble organic nitrogen to ADM1 amino acids, LCFA and sugars
S_{alk}_S_{ic} ASM1 alkalinity to ADM1 inorganic carbon
Hydrolysis X_{ND} Hydrolysis of ASM1 particulate organic nitrogen to soluble organic nitrogen
O_2 depletion Depletion of ASM1 dissolved oxygen
NO_3 depletion Depletion of ASM1 nitrates
S_{i}_S_{i} ASM1 inert soluble material to ADM1 inert soluble material
X_{P}_X_{i} ASM1 inert material from decay to ADM1 particulate inerts
X_{i}_X_{i} ASM1 inert particulate material to ADM1 particulate inerts
X_{s}_X_{c} ASM1 slowly biodegradable substrate to ADM1 composite material
X_{bh}_X_{c}, X_{su} ASM1 heterotrophic biomass to ADM1 composite particulate and sugar degraders
X_{ba}_X_{c} ASM1 autotrophic biomass to ADM1 composite particulate

ADM1–ASM1 conversions:

S_{i}_S_{i}, S_{ND} ADM1 inert soluble material to ASM1 inert soluble material and soluble organic nitrogen
S_{su}_S_{s} ADM1 sugars to ASM1 readily biodegradable material
S_{aa}_S_{ND}, S_{s} ADM1 amino acids to ASM1 soluble organic nitrogen and readily biodegradable material
S_{fa}_S_{s} ADM1 total LCFA to ASM1 readily biodegradable material
S_{va}_S_{s} ADM1 total valerate to ASM1 readily biodegradable material
S_{bu}_S_{s} ADM1 total butyrate to ASM1 readily biodegradable material
S_{pro}_S_{s} ADM1 total propionate to ASM1 readily biodegradable material
S_{ac}_S_{s} ADM1 total acetate to ASM1 readily biodegradable material
X_{i}_X_{i} ADM1 particulate inerts to ASM1 inert particulate material
X_{c}_X_{s} ADM1 composite particulate to ASM1 slowly biodegradable substrate
X_{ch}_X_{s} ADM1 carbohydrates to ASM1 slowly biodegradable substrate
X_{pr}_X_{s} ADM1 proteins to ASM1 slowly biodegradable substrate
X_{li}_X_{s} ADM1 lipids to ASM1 slowly biodegradable substrate
X_{su}_X_{s} ADM1 sugar degraders to ASM1 slowly biodegradable substrate
X_{aa}_X_{s} ADM1 amino acids degraders to ASM1 slowly biodegradable substrate
X_{fa}_X_{s} ADM1 LCFA degraders to ASM1 slowly biodegradable substrate
X_{c4}_X_{s} ADM1 valerate and butyrate degraders to ASM1 slowly biodegradable substrate
X_{pro}_X_{s} ADM1 propionate degraders to ASM1 slowly biodegradable substrate
X_{ac}_X_{s} ADM1 acetate degraders to ASM1 slowly biodegradable substrate
X_{h2}_X_{s} ADM1 hydrogen degraders to ASM1 slowly biodegradable substrate
S_{in}_S_{nh4+} ADM1 inorganic nitrogen to ASM1 ammonia
S_{ic}_S_{alk} ADM1 inorganic carbon to ASM1 inorganic carbon

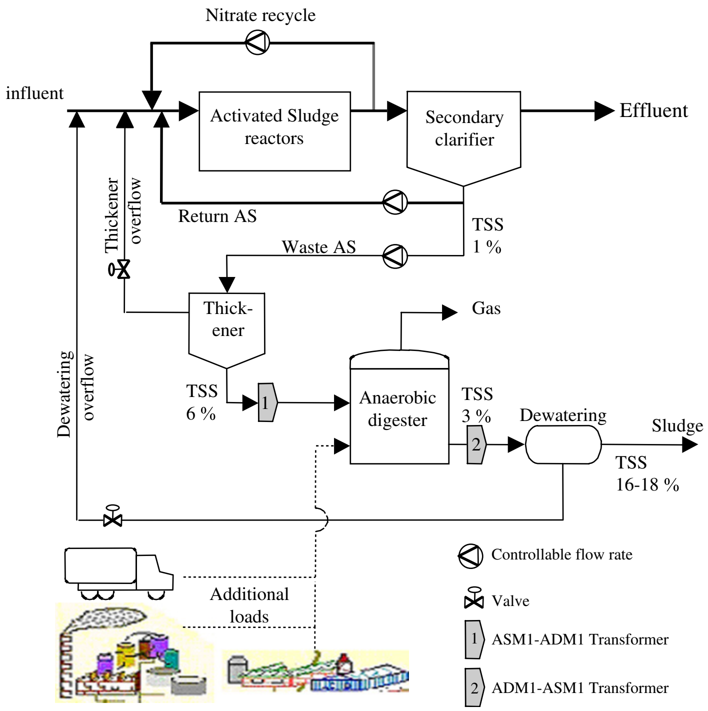

Fig. 1. Extended benchmark plant with sludge treatment including the anaerobic digester, adapted from Jeppsson et al. (2004).

processes can be evaluated at the plant-wide level. Also, the paper aims at enabling both the domestic and industrial sectors to assess the aforementioned possible solutions. For this purpose, a standard benchmark system, the BSM1 developed for activated sludge systems (Spanjers et al., 1998; Copp, 2002), is extended with the sludge treatment line including the anaerobic digester, which is also fed, for instance, with externally supplied truck loads of organic waste (Fig. 1).

The considered models are ASM1 (Henze et al., 2000), the standard model for BSM1, as description of the activated sludge process and ADM1 (Batstone et al., 2002) for the digester. Two transformers are built for each of the two interfacing methodologies that were compared and implemented in this study. The activated sludge plant is considered as a pre-treatment that concentrates the pollutants in the form of thickened secondary sludge to the digester; for this an ASM1−ADM1 transformer is needed. The activated sludge plant is also considered as post-treatment of the return liquors originating from sludge digestion and drying; for this, an ADM1−ASM1 transformer is needed.

In this paper, two methodologies to interface these two different processes (process models) are implemented. The extended benchmark example is used as a case study to compare both methodologies in terms of the overall plant output and simulated dynamics of the components in the digester.

2. Interfacing methodologies

Two methodologies are implemented in this work to interface the anaerobic model ADM1 to the activated sludge model ASM1 and vice versa. The first method is the general *C*ontinuity-*B*ased *I*nterfacing *M*ethod (CBIM) for models of wastewater systems described by Petersen matrices (Vanrolleghem et al., 2005). Since it is the first time the CBIM is applied and validated, the CBIM itself and its results will be illustrated in detail. The second method was specifically developed for ASM1−ADM1−ASM1 interfacing. It operates by *M*aximising some components with respect to the total *C*OD and *N*itrogen contents. In this paper the method is further referred as MCN. The complete theory of MCN is described in detail in Copp et al. (2003) but no examples or results are given there. Therefore, the MCN will be introduced briefly in Section 2.2 and results of its application will be presented. It will also be compared with the general CBIM method.

2.1. CBIM transformer

2.1.1. Step 1: elemental mass fractions and charge density

The fundamental formulation of elemental mass fractions is based on the hypothesis that the mass of each component in a model is made up of constant mass fractions of the elements C, H, O, N and P according to Reichert et al. (2001). Note that no other elements are considered here (e.g. S, K,...), but an extension would be straight forward. Furthermore, each component may have an associated charge per unit of mass (De Gracia et al., 2004; Reichert et al., 2001). The elemental mass fractions ($\alpha_{C,k}$, $\alpha_{H,k}$, $\alpha_{O,k}$, $\alpha_{N,k}$, $\alpha_{P,k}$) for a generic model component X_k are defined as the mass of elements: C, H, O, N or P per unit of mass of this component (X_k). The calculation of these mass fractions is immediate for all those model components that have a known composition formula. A proper estimation must be carried out for the elemental mass fractions of the components that do not have a known composition. According to the hypothesis above, the sum of all elemental mass fractions of each component X_k must be unity (Eq. (1)):

$$\alpha_{C,k} + \alpha_{H,k} + \alpha_{O,k} + \alpha_{N,k} + \alpha_{P,k} = 1. \tag{1}$$

The charge density ($\alpha_{Ch,k}$) for a generic model component X_k is defined as the electric charge associated to its unit of mass. For each component X_k, it is calculated as the quotient of its molecular charge and its molecular weight. Normally, not all the components X_k can be defined by a molecular formula, i.e. their molecular weight is unknown. However, once the elemental mass fractions and the charge density have been assigned, one unit of mass of any model component X_k can be expressed with a general formula (Eq. (2)):

$$\left[C_{(\alpha_{C,k}/12)}H_{(\alpha_{H,k})}O_{(\alpha_{O,k}/16)}N_{(\alpha_{N,k}/14)}P_{(\alpha_{P,k}/31)}\right]^{\alpha_{Ch,k}}. \tag{2}$$

2.1.2. Step 2: composition matrix

A composition matrix can be defined as in Table 1. For a model component X_k that has an elemental mass fraction α_k of a certain element (mass unit of element/mass unit of model component), a composition matrix element i_k (mass unit of element/stoichiometric unit of model component) can be defined from Eq. (3):

$$i_k = \alpha_k m_k, \tag{3}$$

where m_k is the mass of the component per stoichiometric unit. For all model components, corresponding composition matrix elements ($i_{ThoD,k}$, $i_{C,k}$, $i_{N,k}$, $i_{O,k}$, $i_{H,k}$, $i_{P,k}$) are evaluated in unit of mass per stoichiometric unit. As the models to be interfaced can express their components in different units, a certain unit of mass is chosen in common for all composition matrix elements except for charge. As a result, the unit conversions between both models are considered during transformation. In the presented case study, the composition matrix elements have been expressed as grams of C, H, N, O, P and charge per stoichiometric unit. The charge of the ionised portion of the component, $i_{e,k}$ is calculated as positive or negative charge unit per stoichiometric unit of component. The composition matrix elements are easily calculated when the stoichiometric formulae of the components are well-known. However, for the components with unknown stoichiometric formulae and measured in COD units, a relationship between the mass fractions and COD must be established to calculate the corresponding composition matrix elements. Once the elemental mass fraction and charge density have been defined for these model components, their Theoretical Oxygen Demand (ThOD) can be calculated. ThOD has been introduced to characterise organic as well as inorganic compounds (Gujer et al., 1999).

2.1.3. Step 3: transformation matrix

The CBIM aims to construct a set of algebraic transformation equations on the basis of a Petersen matrix description of

Table 1
Matrix description of interface between Peterson matrix based models, adapted from Vanrolleghem et al. (2005)

Peterson matrix section Model 1 ("origin")					Peterson matrix section Model 2 ("destination")				
$\xrightarrow{k}$ $\downarrow j$	X_1	X_2	…	X_P	X_{P+1}	X_{P+2}	…	X_{P+Q}	Rate
Conv. 1	$\nu_{1,1}$	$\nu_{1,2}$	…	$\nu_{1,P}$	$\nu_{1,P+1}$	$\nu_{1,P+2}$	…	$\nu_{1,P+Q}$	ρ_1
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
Conv. n	$\nu_{n,1}$	$\nu_{n,2}$	…	$\nu_{n,P}$	$\nu_{n,P+1}$	$\nu_{n,P+2}$	…	$\nu_{n,P+Q}$	ρ_n
Composition matrix section Model 1					Composition matrix section Model 2				
ThOD	$i_{ThOD,1}$	$i_{ThOD,2}$	…	$i_{ThOD,P}$	$i_{ThOD,P+1}$	$i_{ThOD,P+2}$	…	$i_{ThOD,P+Q}$	
C	$i_{C,1}$	$i_{C,2}$	…	$i_{C,P}$	$i_{C,P+1}$	$i_{C,P+2}$	…	$i_{C,P+Q}$	
N	$i_{N,1}$	$i_{N,2}$	…	$i_{N,P}$	$i_{N,P+1}$	$i_{N,P+2}$	…	$i_{N,P+Q}$	
H	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	
O	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	
P	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	
Charge	$i_{e,1}$	$i_{e,2}$	…	$i_{e,P}$	$i_{e,P+1}$	$i_{e,P+2}$	…	$i_{e,P+Q}$	

the two models to be interfaced. In this methodology, the matrix description is somewhat different from the original models' Petersen matrices. The new matrix has the components of the two models to be interfaced, sorted into two panes: P components of the "origin" model and Q components of the "destination" model (see Table 1). A set of transformations (conversions) are left to the CBIM user to be defined on the basis of expert knowledge concerning the two model systems. Yet, before starting to generate the algebraic transformation equations, the elemental mass fractions of the models' components need to be defined. The mass fractions of all the components are determined and subsequently the composition matrix elements are defined.

The next step is to define the conversion processes from the origin to the destination components. All proposed conversions must guarantee the continuity of C, H, O, N, P and charge. For this purpose a set of components taken either from the origin or the destination model should act as source–sink. These components are also called compensation terms (Benedetti et al., 2004) and are needed to accomplish the next equations that are written for each conversion j:

$$\sum_k \nu_{j,k} i_{j,\mathrm{Comp}} = 0_{\text{with Comp=Thod, C, N, H, O, }e}. \tag{4}$$

Eq. (4) generates a set of algebraic equations as constraints on the stoichiometry terms $\nu_{j,k}$ to achieve the mass and charge conservation of a conversion j. If the number of non-zero $\nu_{j,k}$ is less than the number of rows in the composition matrix, the set of equations will be over-determined. The approach in this situation is to add other "source–sink" components in order to have a single solution of the equations that maintains the continuity. For other conversions, the number of non-zero $\nu_{j,k}$ may be larger than the number of rows in the composition matrix and the solution of the linear equation to calculate the stoichiometric parameters is under-determined.

Guiding Transformation Principles (GTPs) that will lead to a feasible solution of the linear system of equations produced by Eq. (4) (stoichiometry calculation) are as follows:

- Try different choices of source–sink components.
- Some conversions can be split and some other can be combined.
- More knowledge (assumptions) can be incorporated in the conversions, e.g. fractions of "origin" components to "destination" components.

In a first step of calculating the stoichiometric parameters, the GTPs are applied to guide the user to select proper conversions. These principles are also to be applied in two other steps when setting up the transformation algebraic equations.

The introduction of the sourcing components turns the problem of defining the stoichiometry from an algebraic solution of linear equations to a minimisation problem. In general, the value of $\nu_{j,k}$ related to the "sourcing" components should be kept to a minimum, e.g. just to compensate for the difference in the elemental composition between origin and destination components. One component, in the presented case study it is only oxygen, can be chosen to be minimised by tuning the other $\nu_{j,k}$ in each conversion to maintain the continuity within an acceptable tolerance.

A constraint needs to be added on the sign of some stoichiometric parameters. First, an exception is that the sign of a stoichiometric parameter related to the sourcing components is allowed to be positive or negative. Second, for conversions that are assumed to happen immediately in the "origin" model only, e.g. oxygen and nitrate depletion and immediate hydrolysis of slowly degradable substrate, the sign of the corresponding stoichiometric parameters should be assigned logically to maintain the assumed conversion direction. Third, the sign of the remaining stoichiometry is such that the "origin" stoichiometry is negative while the destination stoichiometry is positive to maintain the conversion in the right direction.

A spreadsheet can be used to easily evaluate the stoichiometry. Minimisation can be done using the spreadsheet. Also, the evaluation of the stoichiometry can be automated by building the transformer in a simulation platform and implementing a simple constrained minimisation algorithm.

2.1.4. Step 4: transformation equations

Once the stoichiometric parameters have been defined, a set of algebraic equations is generated (Eq. (5)) to determine the unknown conversion rates of all conversions ρ_j by using the influxes of the transformer that are coming from the "Origin" model:

$$\sum_{j=1}^{n} \nu_{j,k}\rho_j = \mathrm{influx}_k \quad \text{for } k = 1, P. \tag{5}$$

Transformer outfluxes can then be calculated as function of the calculated conversion rates according to Eq. (6):

$$\mathrm{outflux}_k = \sum_{j=1}^{n} \nu_{j,k}\rho_j \quad \text{for } k = P+1, P+Q. \tag{6}$$

Two conditions need to be fulfilled to make the solution of Eq. (5) for values of ρ_j feasible and practical. First, to make it feasible, the number of suggested conversions should not exceed the number of the "origin model" components. The use of fraction parameters can help in combining conversions and therefore reduce the total number of conversions. Reducing the number of conversions solves the problem of an under-determined solution of linear equations needed to calculate the conversion rates. This is the second step in which the GTPs can be applied to help in designing the right conversions. Second, to make the solution of Eq. (5) practical, all rates should lead to obligatory negative outfluxes, i.e. the transformation should be carried out in the right direction. This can be tested by applying a practical range of influxes and check the sign of the outfluxes. If some outfluxes are not negative, i.e. the conversion is not in the right direction, the conversions should be modified. In addition to the change of conversions, the mass fractions and fraction parameters should be checked. This is the third step in which the GTPs can be applied to guide the user to find the right conversions and maintain the transformation in the right direction.

2.2. Case study

In this section, the CBIM is applied to build ASM1–ADM1 and ADM1–ASM1 transformers. A brief description is also provided for implementing the alternative methodology to build the transformers, MCN of Copp et al. (2003). A plant-wide model is used to compare both CBIM and MCN methods in Section 3.

2.2.1. CBIM ASM1–ADM1 transformer

2.2.1.1. Step 1: elemental mass fractions and charge density. A list of mass fractions suggested for ASM1 and ADM1 is given in Tables 2 and 3, respectively. The mass fractions of the models' components are estimated according to their stoichiometric formulae. For components that do not have stoichiometric formulae, some assumptions are made as indicated in Tables 2 and 3.

For example, empirical formula $C_5H_7O_2N$ is used to represent biomass, as in the ASM series (Henze et al., 1987) and as suggested in the IWA ADM1 report (Batstone et al., 2002) but adjusted with addition of a phosphorous fraction. Note, however, that phosphorous is not considered in the original models. A 3% phosphorous mass fraction has been considered for the biomass to ensure a complete implementation of the elemental mass balances.

Note that model parameters should agree with the applied assumptions. For example, the fractions of nitrogen, hydrogen and oxygen are maintained similar to the empirical formula so that they agree with the nitrogen content given in ASM1. Accordingly, the biomass carbon and nitrogen fractions in ADM1 should be 0.0305 kmol C/kg COD and 0.0061 kmol N/kg COD.

In another example, the carbon and nitrogen fractions are considered first to agree with the ADM1 parameters, i.e. the fractions of X_c leading to carbohydrates, proteins, lipids and inerts. Consequently, the oxygen mass fraction is assumed similar to biomass (secondary sludge), but a lower phosphorous fraction of 1% is assumed (release of phosphorous under anaerobic conditions).

It is also assumed that the pH will be in the optimum range for both processes, e.g. pH from 7 to 8. Hence, alkalinity and inorganic carbon will be mainly bicarbonate, inorganic nitrogen is mainly ammonium and VFAs are mainly in the ionised form. The charge density for those components is calculated accordingly.

In addition to the elemental mass fractions of the components of both models, three source–sink components are needed. Their mass fractions are defined in Table 4. Also, a component S_{n2} is considered for stripping of nitrogen when S_{no3-} is denitrified.

2.2.1.2. Step 2: composition matrix. The mass fractions α are calculated as g element/g component. The composition matrices i of both models are calculated by multiplying the elemental mass fractions and charge density by the number of grams in each component's stoichiometric unit. The unit of the composition matrix is g element/stoichiometric unit. Therefore, differences in stoichiometric units between components of both models are reflected in the composition matrices and unit conversions need to be considered during transformation. Composition matrices are given as the bottom panes of the transformation matrices in Tables A1 and A2.

2.2.1.3. Step 3: transformation matrix. The Petersen matrix suggested in Table 1 is built and presented in Tables A1 and A2. From the "origin" model ASM1 S_o is taken as a "sourcing sink" component for oxygen. Accordingly, $\nu_{j,14}$ was kept minimal during the calculation of the other stoichiometric parameters. On the other side, two sourcing components S_{ic} and S_{in} are taken from the "destination" model ADM1 as sourcing components for carbon and nitrogen. Three other components S_{ip}, S_{H+} and S_{H2O} (inorganic phosphorus, protons and water) are introduced to the destination matrix. These components are used as source–sink for phosphorous, charge and hydrogen, respectively. If these components and the corresponding continuity of phosphorus, charge and hydrogen are eliminated, the other stoichiometry values and the COD, C and O continuity will remain unaffected. However, these components are

Table 2
Elemental mass fractions and charge density of ASM1 components

Mass fractions	Components													
	S_s	S_{no3-}	S_i	X_s	X_{bh}	X_{ba}	X_i	X_P	S_{nh4+}	S_{ND}	X_{ND}	S_{alk}	S_{n2}	S_o
α_C (g C/g component)[a]	0.62		0.65	0.62	0.51	0.51	0.56	0.51				0.20		
α_N (g N/g component)		0.23			0.12[d]	0.12[d]	0.09[e]	0.12[d]	0.78	1.00	1.00		1.00	
α_O (g O/g component)	0.28[b]	0.77	0.28[b]	0.28[b]	0.28[d]	0.28[d]	0.28[e]	0.28[d]				0.79		1.00
α_H (g H/g component)	0.08[b]		0.07[b]	0.08[b]	0.06[d]	0.06[d]	0.06[e]	0.06[d]				0.02		
α_P (g P/g component)	0.02[c]			0.02[c]	0.03[c]	0.03[c]	0.01[c]	0.03[c]						
α_Ch (Ch/g component)		−0.02							0.06			−0.02		

[a] Calculated as the remaining mass fraction after the assignment of other elements fractions.

[b] Taken from RWQMI (Reichert et al., 2001).

[c] Assumed phosphorous content.

[d] Biomass stoichiometric formula (Batstone et al., 2002; Henze et al., 1987).

[e] Similar to ADM1.

Table 3
Elemental mass fractions and charge density of ADM1 components

Mass fractions	Components																	
	S_i	S_{su}	S_{aa}	S_{fa}	S_{va}	S_{bu}	S_{pro}	S_{ac}	S_{h2}	S_{ch4}	X_i	X_c	X_{ch}	X_{pr}	X_{li}	$X_{su..h2}$	S_{in} [f]	S_{ic} [g]
α_C (g C/g component)[a]	0.56[b]	0.40	0.47[b]	0.75	0.59	0.55	0.49	0.41		0.75	0.56[b]	0.57[b]	0.40	0.47[b]	0.76	0.51[a]		0.20
α_N (g N/g component)	0.09[b]		0.15[b]								0.09[b]	0.06[b]		0.15[b]		0.12[d]	0.78	
α_O (g O/g component)	0.28[e]	0.53	0.28[b]	0.12	0.32	0.37	0.44	0.54			0.28[e]	0.28[e,d]	0.53	0.28	0.11	0.28[d]		0.79
α_H (g H/g component)	0.06[a]	0.07	0.10[a,b]	0.13	0.09	0.08	0.07	0.05	1.00	0.25	0.06[a]	0.09[a]	0.06	0.10	0.12	0.06[d]	0.02	0.02
α_P (g P/g component)	0.01[c]										0.01[c]	0.01[c]	0.01[c]		0.01[c]	0.03[c]		
α_Ch (Ch/g component)					−0.01	−0.01	−0.01	−0.02									0.06	−0.02

[a] Calculated as the remaining mass fraction after the assignment of other elements fractions.

[b] Satisfy ADM1 fraction parameters.

[c] Assumed phosphorous content.

[d] Biomass stoichiometric formula (Batstone et al., 2002; Henze et al., 1987).

[e] Similar to ASM1.

[f] $S_{in} = NH_4^+$.

[g] $S_{ic} = HCO_3^-$.

Table 4
Elemental mass fractions and charge density of the additional sourcing components

Mass fractions	Components		
	S_{ip}	S_{H+}	S_{H2O}
α_C (g C/g component)			
α_N (g N/g component)			
α_O (g O/g component)	0.67		0.89
α_H (g H/g component)	0.01	1.00	0.11
α_P (g P/g component)	0.32		
α_Ch (Ch/g component)	−0.02	1.00	

still mentioned in both transformers' matrices for the sake of completeness of the method illustrated. They could be used in future for interfacing extended models but their stoichiometry will not be considered in the present implementation and simulation.

The number of suggested conversions is 12. In conversions 1 and 3, S_{nh4+} and S_{alk} are assigned directly to the sourcing components S_{in} and S_{ic}. The conversions 4, 5 and 6 are held internally in the "origin" model pan assuming the immediate hydrolysis of X_{ND} to S_{ND} and the depletion of S_o and S_{no3-}. The depletion is accompanied by formation of X_{bh} and a minimal increase of S_{ic} and a decrease of S_{in}.

Conversion 2 represents transformations of S_{ND} and S_s to S_{su}, S_{aa} and S_{fa}. Note that this is the most complex conversion. For $\nu_{2,1} = -1$ (under S_s) the assumed COD fractions to S_{su} and S_{fa} are 0.3 and 0.2, respectively. So, the $\nu_{2,16}$ (under S_{su}) and $\nu_{2,18}$ (under S_{fa}) are then calculated straightforwardly. The $\nu_{2,17}$ (under S_{aa}) has been assigned a formula to close the nitrogen balance of this conversion. The $\nu_{j,10}$ is assigned a value of -1 (under S_{ND}). The $\nu_{2,4}$ (under X_s) is then determined by minimising $\nu_{2,14}$ (under S_o), i.e. by closing the COD balance properly.

The main reason for the complexity of this conversion is the simultaneous transformation of S_{ND} and S_s with the instantaneous hydrolysis of X_s. Efforts have been made to split this conversion into two independent conversions, one for each component, but it was not feasible because the conversion of S_{ND} alone to S_{aa} will need a big sourcing of COD for which the S_s influxes are normally not sufficient. It would lead to a reverse outflux, i.e. immediate COD consumption from the digester. Of course, this is not acceptable. That is why conversion 8 that was originally meant for the direct conversion of S_s has been eliminated and combined with conversion 2. Further needs of COD can now be provided from X_s, in two steps. The first compensates the COD deficiency in the transformation to S_{aa}. The second step will be described in the next section as part of the calculation of the conversion rates. The design of conversion 2 highlights the insight required when designing the conversions.

Understanding conversion 2 makes the rest of the conversions straightforward and self-explanatory from the matrix. Some points should be noted, however. In conversion 7, $\nu_{7,10}$ was calculated from the nitrogen balance. $\nu_{7,15}$ was determined by minimising $\nu_{7,14}$, i.e. by closing the COD balance without oxygen leaks. In conversions 9 and 10 a 10% fraction of the inerts in ASM1 was assumed to be anaerobically biodegradable. A 10% fraction of the aerobic heterotrophic biomass is considered capable of sugar fermentation. These fractions are examples of the degrees of freedom that one can add to reflect some actual phenomena occurring in the system. However, with such assumptions, the continuity should still be carefully checked to prevent any leaks of mass.

2.2.1.4. Step 4: transformation equations. Once all $\nu_{j,k}$ have been evaluated, a set of algebraic equations is generated to evaluate the conversion rates ρ_i using Eq. (5). During simulation, these equations are evaluated at every time step as functions of the influxes, i.e. incoming fluxes of components of the "origin" model. According to Table A1, the equations are as follows:

$$\rho_1 = \text{influx}_9/\nu_{1,9}, \tag{7}$$

$$\rho_2 = (\text{influx}_{10} - \nu_{4,10}\rho_4 - \nu_{7,10}\rho_7)/\nu_{2,10}, \tag{8}$$

$$\rho_3 = \text{influx}_{12}/\nu_{3,12}, \tag{9}$$

$$\rho_4 = \text{influx}_{11}/\nu_{4,11}, \tag{10}$$

$$\rho_5 = (\text{influx}_{14} - \nu_{6,14}\rho_6 - \nu_{7,14}\rho_7)/\nu_{5,14}, \tag{11}$$

$$\rho_6 = \text{influx}_2/\nu_{6,2}, \tag{12}$$

$$\rho_7 = \text{influx}_3/\nu_{7,3}, \tag{13}$$

$$\rho_9 = \text{influx}_8/\nu_{9,8}, \tag{14}$$

$$\rho_{10} = \text{influx}_7/\nu_{10,7}, \tag{15}$$

$$\rho_{11} = (\text{influx}_4 - \nu_{2,4}\rho_2)/\nu_{11,4}, \tag{16}$$

$$\rho_{12} = (\text{influx}_5 - \nu_{5,5}\rho_5 - \nu_{6,5}\rho_6)/\nu_{12,14}, \tag{17}$$

$$\rho_{13} = \text{influx}_6/\nu_{13,6}. \tag{18}$$

Eqs. (7)–(18) calculate the conversion rates in terms of the influxes. The influx of S_s is not used since conversion 8 is cancelled for the above stated reasons. Instead of estimating ρ_8, Eq. (19) is used to determine the theoretical S_s influx required to satisfy the COD required for conversions 2, 5 and 6 as a second step for sourcing a COD deficiency, e.g. to accomplish O_2 and NO_3 depletion, the difference between the theoretically needed and actual influx of S_s is deducted from the X_s influx. If the influx of X_s is not sufficient for the removal of O_2 and NO_3, an update to the plant design is probably needed to avoid O_2 and NO_3 effects on the digester:

$$\text{influx}_{1,\text{theoretical}} = \nu_{2,1}\rho_2 + \nu_{5,1}\rho_5 + \nu_{6,1}\rho_6. \tag{19}$$

Note that in Eq. (11) for the evaluation of ρ_5 some terms were ignored since the stoichiometry values were too small (<1E−15); the oxygen sourcing was kept to a minimum for all other conversions.

Last, calculate the outfluxes using Eq. (6) and check that all outfluxes are oriented outwards.

2.2.2. CBIM ADM1–ASM1 transformer

For the reverse transformation, the elemental mass fractions and charge density are of course the same as defined for the first transformer. Also, the composition matrix is the same but its two panes are switched according to the new direction of transformation, as shown in Tables A3 and A4. Accordingly, *Step 1 and 2* are similar to the first transformer. Note that the sourcing components are replaced as illustrated below.

2.2.2.1. Step 3: transformation matrix. The Petersen matrix suggested in Table 1 is built and presented in Tables A3 and A4. In a similar way to the previous transformer, source–sink components are designated. From the "destination" model ASM1 S_o, S_{alk} and S_{nh4+} are chosen as source–sink components for oxygen, carbon and nitrogen, respectively. Also, the three other source–sink components S_{ip}, S_{H+} and S_{H2O} (inorganic phosphorus, protons and water) are introduced to the destination matrix.

The number of suggested conversions is 22. The evaluation of the stoichiometry for this transformer is straightforward since ADM1 is based on more specific components that are likely to be assigned directly to ASM1 lumped components. In conversion 1, ADM1 S_i is assigned to ASM1 S_i on the basis of the ThOD continuity and to ASM1 S_{nd} on the basis of the nitrogen balance. ADM1 soluble components 2–8 are converted by conversions 2–8. They are converted to S_s on the basis of the ThOD continuity and only ADM1 S_{aa} produced ASM1 S_{nd} on the basis of the nitrogen continuity. In a similar way, the transformations of the particulate components are defined. In conversion 9, ADM1 X_i is mapped to ASM1 X_i. ADM1 particulate components 12–22 are transformed by conversions 10–20. In these conversions the transformations to ASM1 X_{nd} are evaluated on the basis of nitrogen continuity. Transformations to ASM1 X_s are calculated by minimising $\nu_{j,43}$ (stoichiometry under S_o). In the remaining two conversions S_{in} and S_{ic} are mapped to ASM1 S_{nh4+} and S_{alk}, respectively. Note that in both transformers, gas components are not considered in the transformations because they are assumed to be stripped to the gas phase and transformations are only considered for components in the liquid phase.

2.2.2.2. Step 4: transformation equations. Setting up the transformation conversions is also straightforward because of the detailed structure of ADM1 compared to ASM1. In the "origin" model pan Table A3 the stoichiometry is a diagonal matrix and therefore each conversion rate is presented explicitly as a function of the influx of one component of the "origin" model components (Eq. (20)):

$$\rho_j = \text{influx}_k/\nu_{j,k}. \tag{20}$$

Last, the outfluxes are calculated using Eq. (6).

2.2.3. MCN transformers

Copp et al. (2003) developed ad hoc transformers to connect ASM1 and ADM1. Their transformation concept is twofold. First, the total COD and TKN are determined for the components of the "origin" model and then distributed to the other model components. Second, the distribution is done step-wisely with the aim to maximise certain components in a predefined order. The distribution is done so that the COD continuity is maintained. If there is remaining TKN, it is mainly assigned to ammonia that is a component in both models.

For the transformation from ASM1 to ADM1, the COD of all ASM1 soluble components is summed and subsequently reduced to compensate for ASM1 nitrate and oxygen concentrations that need to be removed before entering ADM1. The reduction is done in sequence to ASM1 components S_s, X_s, X_{bh} and X_{ba}. Based on the ASM1 S_{nd}, ADM1 S_{aa} is maximised as far as the soluble COD allows. ASM1 S_i is mapped to ADM1 S_i. If there is soluble COD left from the assignment to ADM1 S_{aa} and S_i, the remaining is assigned to sugars, ADM1 S_{su}. In a similar way, starting from ASM1 particulate COD and X_{nd}, ADM1 X_c is maximised first and X_i is mapped according the available ASM1 X_{nd}. If there is COD remaining after assignment of ASM1 X_{nd}, it will be assigned to X_{ch} and X_{li} according to predefined fractions. In the assignment of ASM1 TKN, if the ASM1 COD is insufficient to source the assignments, the remaining nitrogen is added to the inorganic nitrogen pool of ADM1, i.e. S_{in}.

For the transformation ADM1–ASM1, a similar procedure is followed with the goal to maximise X_s, S_s, S_i and X_i with respect to the available COD and maximise S_{nh}, X_{nd} and S_{nd} with respect to nitrogen.

In a last step of both of the above transformations direct assignment is done between S_{nh} and S_{in}. Direct mapping is also done between S_{alk} and S_{ic}. In ADM1, S_{cat} is considered equal to S_{ic} and S_{an} is considered equal to S_{in}.

2.2.4. Plant-wide modelling

All modelling and simulation were performed in the WEST software (Hemmis nv, Kortrijk, Belgium) (Vanhooren et al., 2003). An extended benchmark plant is implemented according to the configuration of Fig. 1. The added units are dimensioned to achieve the average Total Suspended Solids (TSS) indicated in the figure. The plant is extended for receiving additional loads to the digester. However, during the comparison of the transformation methodologies, no external flows were assigned. Two similar configurations were built: one is using the CBIM transformers and the other is using the MCN transformers. The 14-day dynamic influent of BSM1 is simulated by both configurations starting from initial conditions obtained with a 1000 days constant influent load.

3. Results and discussions

The simulation results are discussed in two parts. In the first part, using the practical plant-wide example, the CBIM transformers are designed and the standard MCN transformers are applied. The first part aims to study the practical issues related to the use of the CBIM transformers and presents the ad hoc assumptions implemented in the first CBIM transformer to produce additional fluxes of S_{fa}, S_{su} and X_{su}. The second part of the results discusses the main differences between the two transformer types by using identical inputs and without additional fluxes of the S_{fa}, S_{su} and X_{su} as originally designed for the MCN.

3.1. Plant-wide simulation

In this section, the designed CBIM and MCN transformers are simulated with the plant-wide model. The dynamic simulation results are shown and discussed at 5 locations in the treatment system presented in Fig. 1 (components before and after the two transformers and the digester pH and biogas flow).

3.1.1. Inflow to ASM1–ADM1 transformers

Although the model initialisation is done separately for each transformation method and there is recycle after the sludge dewatering, the input concentrations from the thickener to the ASM1–ADM1 transformer are identical using both methods. For example, ammonia and alkalinity were expected to be the most different when comparing both methods but the influent to the first transformer is almost the same as shown in Fig. 2. Therefore, using any of the transformation methods has the same effect on the 14 days simulation of the activated sludge plant final effluent.

3.1.2. Outflow from ASM1–ADM1 transformers

The effluent from the transformers is different due to the differences between the two methods and their assumptions. Fig. 3 shows the main differences in effluent concentrations from the ASM1–ADM1 transformers. The S_{in} from the CBIM transformer is slightly higher than the MCN. However, when all components are considered the nitrogen balance is closed with both methods, i.e. the difference in S_{in} is compensated by the nitrogen content of other components. The CBIM S_{ic} is much higher compared to the MCN one. CBIM achieves the carbon balance using S_{ic} as a source–sink component for carbon while MCN is not considering the carbon balance and its S_{ic} is only mapped from ASM1 S_{alk}.

Although MCN aims to maximise S_{aa}, MCN does not produce S_{aa} and only produces S_i as soluble substrate. Thus, MCN produces slightly higher S_i compared to CBIM. S_{aa} is produced by CBIM. Also, sugars and fatty acids are produced (results not shown). The MCN COD source required for S_{aa} is S_s only. Normally in the effluent of activated sludge plant, S_s is very low compared to the COD required to deplete the effluent oxygen and nitrate and, therefore, no COD is left to produce S_{aa} as originally proposed in the MCN. In CBIM, both S_s and X_s are used to source the conversion to S_{aa}, S_{su} and S_{fa}. Also, the COD deficiency for the depletion of oxygen and nitrate is balanced by utilising the X_s influx. The use of X_s to source COD for the transformation to S_{aa}, S_{su} and S_{fa} can be supported by the fact that a fraction of X_s (aerobically: slowly biodegradable substrate) is quickly hydrolysed to easily biodegradable substrates when confronted with the anaerobic enzymes.

For particulates, MCN produces only X_i and X_c while CBIM produces X_{su} too. Both methods result in the same X_i

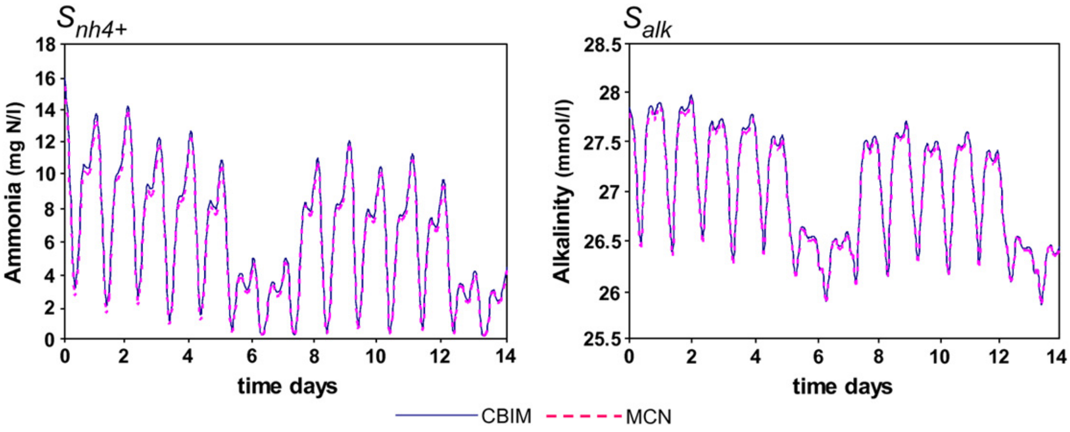

Fig. 2. Ammonia and alkalinity concentrations in the influents to ASM1–ADM1 transformers.

(results not shown). X_{su} is produced only by the CBIM approach since it is assumed that a part of the heterotrophic biomass is capable of fermenting. The assigned value to X_{su} is reflected as a difference between the X_c values estimated by both methods.

3.1.3. Inflow to ADM1–ASM1 transformers

Concentrations at this location are equal to the concentrations in the ideally mixed digester. Noticeable differences between both methods are shown in Fig. 4. In the case of CBIM, S_{in} and S_{ic} are higher since they were also higher in the digester influent. The dynamics of soluble substrates, e.g. S_{aa} and S_{bu}, are more pronounced when using the CBIM because of the distribution of the soluble substrates in the digester influent. In CBIM, S_{ac} is higher and S_{su} is lower than in MCN since CBIM estimated the sugar fermenters input to the digester. Also, the fermenters influent results in a lower X_c and a higher X_{su} values by the CBIM approach. This is due to the conversion of some X_{bh} into X_{su}. Also, the conversion S_s to S_{su} in the CBIM ASM1–ADM1 transformer will support the rapid growth of X_{su} in the anaerobic digester.

3.1.4. Outflow from ADM1–ASM1 transformers

Results at this location are shown in Fig. 5. S_{nh4+} and S_{alk} are calculated to be higher when using the CBIM transformer. Alkalinity is higher due to the conservation of carbon. The slight difference in ammonia is due to the compensation needed for other components in terms of the nitrogen balance. For instance, the non-nitrogen components of ASM1 S_s and X_s are calculated to be higher when CBIM transformation is used. On the other side, the nitrogen components of ASM1 S_{ND} and X_{ND} are estimated to be higher by the MCN transformer. For all model components the nitrogen continuity is maintained by both methods. X_s is estimated higher by CBIM since with the CBIM the X_{su} in the digester effluent is higher and X_s sums all anaerobic particulates. This is counteracted by the X_i results. In other words, MCN leads to a more stabilised sludge from the digester. However, the difference in X_i is only about 2% of its total concentration. Note that X_i is the largest particulate product from the digester and it is the most significant component in terms of stabilised sludge.

3.1.5. Digester biogas flow and pH

As shown in Fig. 6, both transformation methods lead to almost the same pH in the digester and the same gas output from the digester. Also, the difference in gas composition is very small (data not shown).

3.2. Main differences between transformer types

In order to compare the two transformers on a completely equal basis, another simulation study was performed with the following settings for the two transformer approaches.

Similar to the MCN ASM1–ADM1 transformer, the ASM1–ADM1 CBIM transformer was updated to have zero fractions from S_s to S_{su} and S_{fa} and a zero fraction from X_{bh} to X_{su}. Accordingly, some values of the stoichiometric parameters were changed in Tables A1 and A2 to maintain the continuity of the elemental mass and COD. The values of $\nu_{2,4}$, $\nu_{2,16}$, $\nu_{2,18}$, $\nu_{2,40}$, $\nu_{12,26}$, $\nu_{12,30}$, $\nu_{12,39}$ and $\nu_{12,40}$ were changed to −10.822, 0, 0, 3.9E−05, 0.001, 3.94E−06 and 4.73E−06, respectively. Transformation to S_{aa} was maintained in both the MCN and CBIM ASM1–ADM1 transformers.

Three configurations were created from the plant-wide example (Fig. 1) to compare the transformer types using identical inputs. Fig. 7 shows the arrangement of the transformers in the three configurations. Three changes were necessary. First, the recycle from the dewatering unit was cancelled to prevent propagation of the differences in the transformer outputs back into their inputs. Hence, the three configurations in Fig. 7 have exactly the same influent of thickened secondary sludge. Second, simulations of the three configurations were started from the same initial conditions. Third, when comparing the ADM1–ASM1 transformers (configurations 2 and 3) the ASM1–ADM1 transformer was of the MCN type. The results from the three configurations confirm the main differences of the transformer types and agree with the detected differences using the plant-wide model.

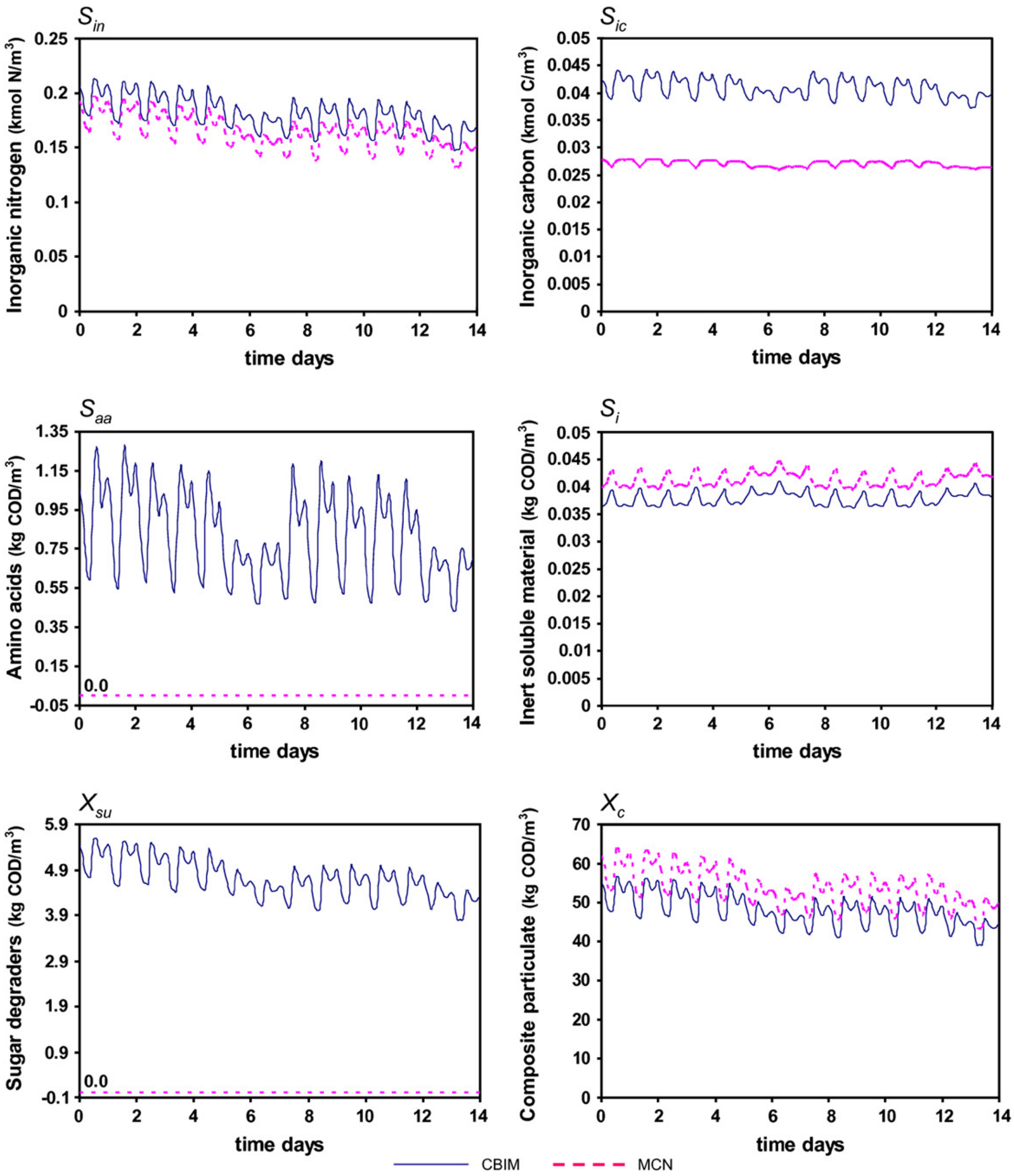

Fig. 3. Comparison of effluent concentrations from the ASM1–ADM1 transformers using the CBIM and the MCN methodologies.

Two main differences were detected in the outflow of the two types of ASM1–ADM1 transformers (by comparing configurations 1 and 2). First, the CBIM transformer produces more S_{ic} than the MCN transformer. The CBIM transformers maintain the continuity of carbon through all transformations, whereas the MCN transformers only consider the continuity of COD and nitrogen. Second, the CBIM transformer produces S_{aa} whereas the MCN transformer does not. However, it should be noted that the input sludge in this case is secondary sludge only and in case of transforming primary sludge, the S_s will be sufficient to source the required COD for the MCN transformer so as to produce the required amino acids. The transformation to S_{aa} induced more dynamics of VFAs of the digester outflow in configuration 1 than in configuration 2. Indeed, the uptake of S_{aa} in the ADM1 model yields all types of VFAs.

Comparing the ADM1–ASM1 transformers by using configurations 2 and 3, the main difference was found in the produced S_{alk}. Again, the CBIM transformer maintains the continuity of carbon and, therefore, produces more S_{alk} compared to the MCN transformer. An appropriate estimate of bicarbonate alkalinity (S_{ic} and S_{alk}) by maintaining the carbon balance is important since alkalinity is important in both models. Alkalinity is connecting heterotrophic and autotrophic

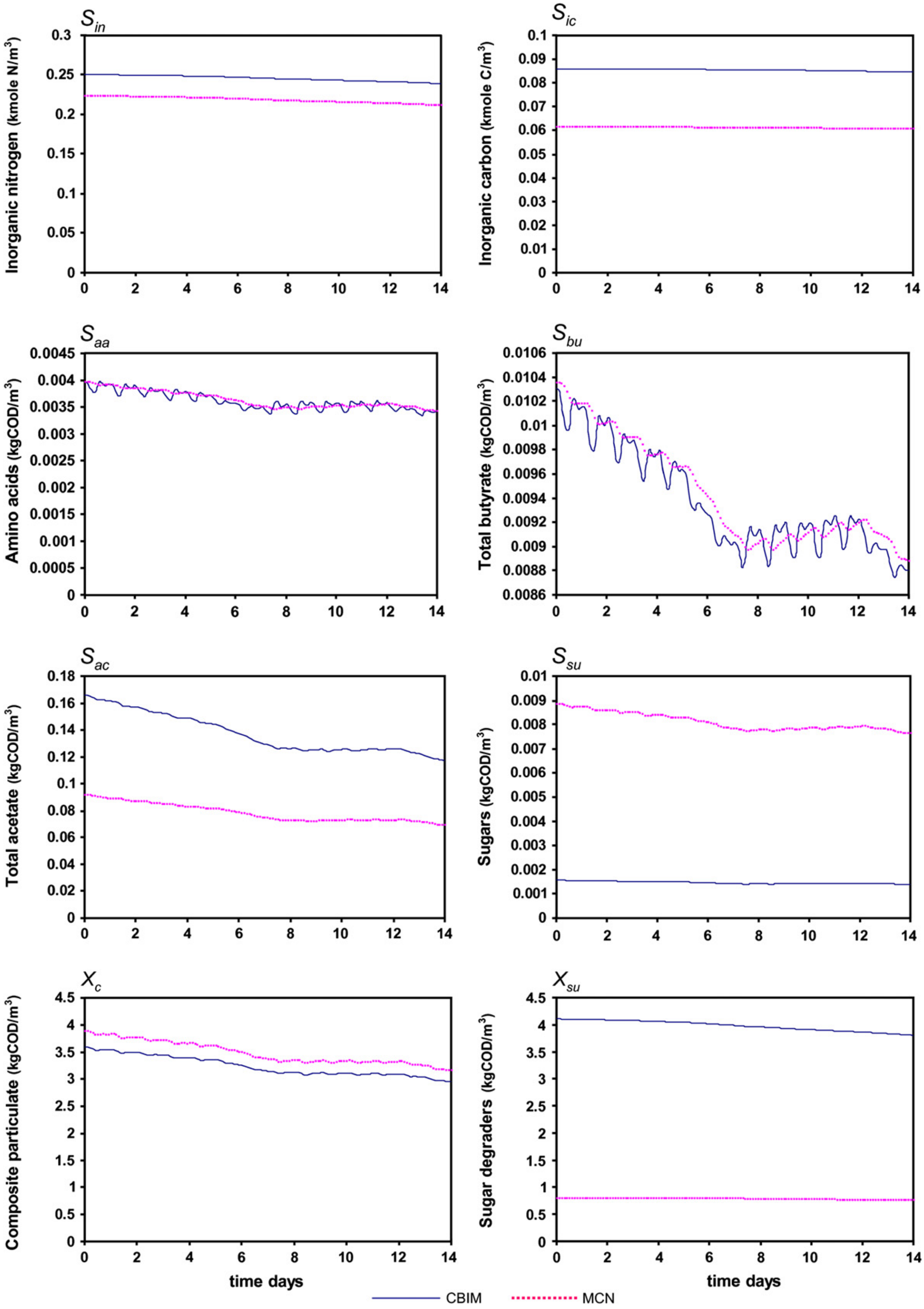

Fig. 4. Comparison of influent concentrations to the ADM1–ASM1 transformers using the CBIM and the MCN methodologies.

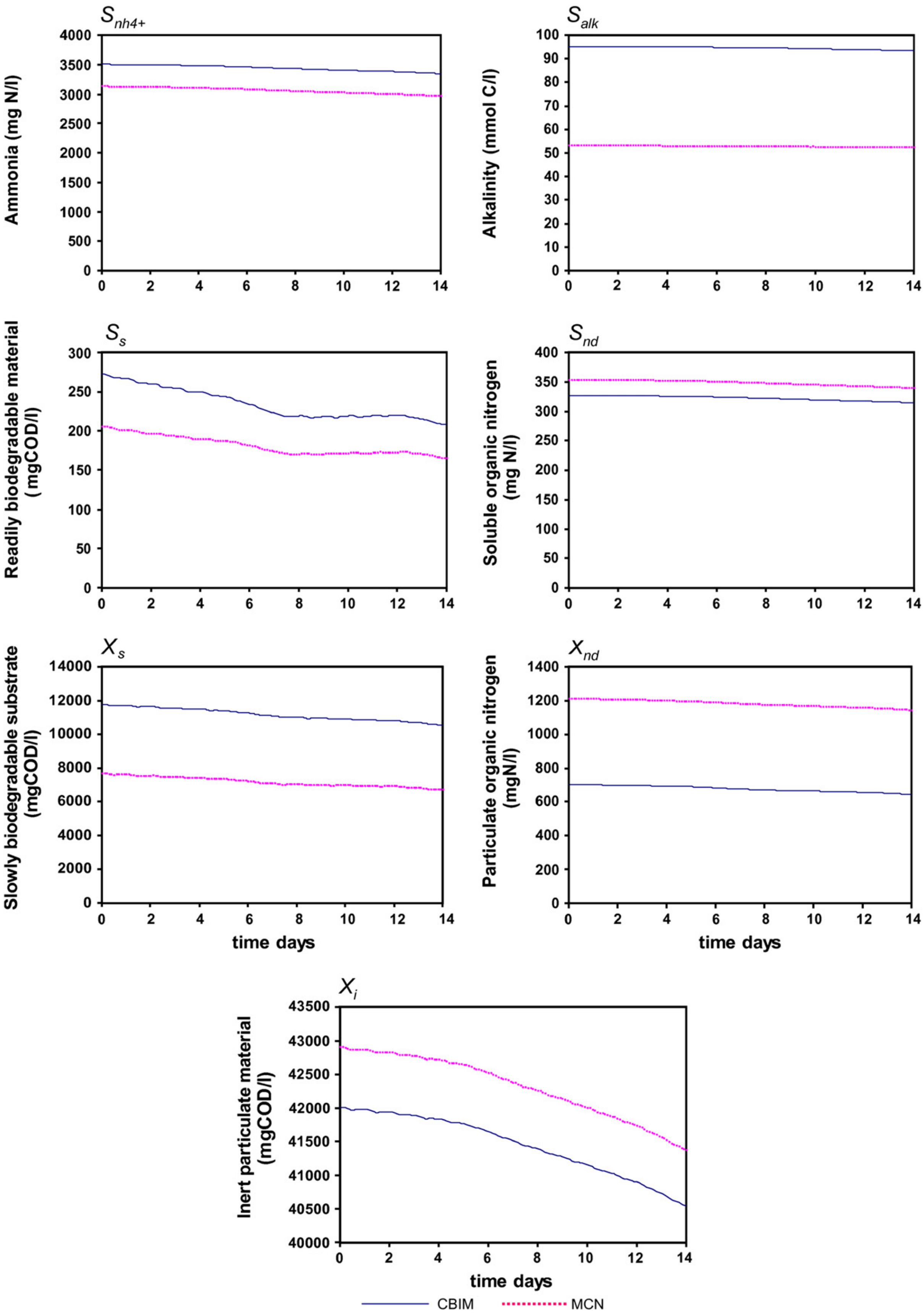

Fig. 5. Comparison of effluent concentrations from the ADM1–ASM1 transformers using the CBIM and the MCN methodologies.

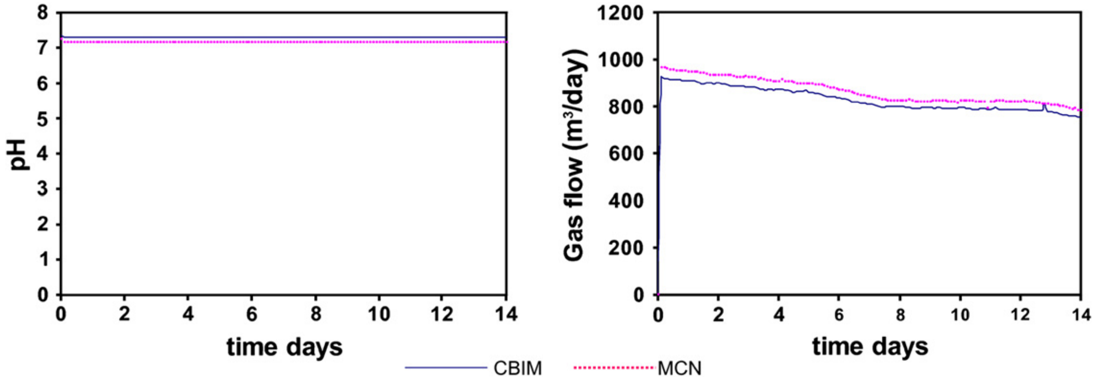

Fig. 6. pH in and gas flow from the digester.

processes in the ASM1 model whereas it is important for pH simulation in the ADM1 model that is connected to all substrate uptake processes through inhibition terms.

The eliminated ad hoc assumptions and fraction parameters from the ASM1–ADM1 CBIM transformer helped the fair comparison with the MCN transformer. However, the selection of these fractions can lead to significant differences in the related digester output components, e.g. S_{su} and X_{su} (Fig. 4). Therefore, it is recommended to also include these fractions in the MCN transformers with the advantage that they can be estimated from real measurements, whereas in the CBIM transformer they need to be determined first by wastewater characterisation and need then to be considered in the transformation matrix to update the continuity check.

4. Conclusions

Two methods recently proposed to interface ASM1 and ADM1 models were compared in a case study of a plant-wide model of a treatment works. Both lead to similar results in terms of the plant-wide output. Both interfacing methods lead to almost the same output of the activated sludge plant, biogas from the digester and sludge production. However, with the additional flexibility of the CBIM approach, the transformation of ‘‘origin’’ components can be distributed over a larger number of components on the ‘‘destination’’ side. This will lead to better simulations of dynamics which are needed for better parameter estimation, control strategy benchmarking and implementation of advanced treatment processes, e.g. for high rate nitrogen removal. The CBIM approach is general and it can be applied to any model conversion and it, therefore, allows to incorporate more knowledge about the process, e.g. the amino acids and sugar fermenters estimation in the influent to the digester.

The CBIM interface is somewhat more complex to develop and is more meant for model developers that define consistent interfaces between any combination of Petersen-based models. The MCN interface is possibly easier to understand and makes it possible to create a reasonable interface between ASM1–ADM1 and extend it for particular needs. An example of such particular need stems from the aim of the MCN approach to maximise the conversion from the soluble organic nitrogen and COD to amino acids. This maximisation is possible when implementing the MCN transformer for primary sludge treatment. In case of secondary sludge treatment, however, the MCN transformer should be extended to allow the conversion to amino acids, i.e. by utilising part of the ASM1 slowly biodegradable substrate. The conversion to amino acids is important in order to

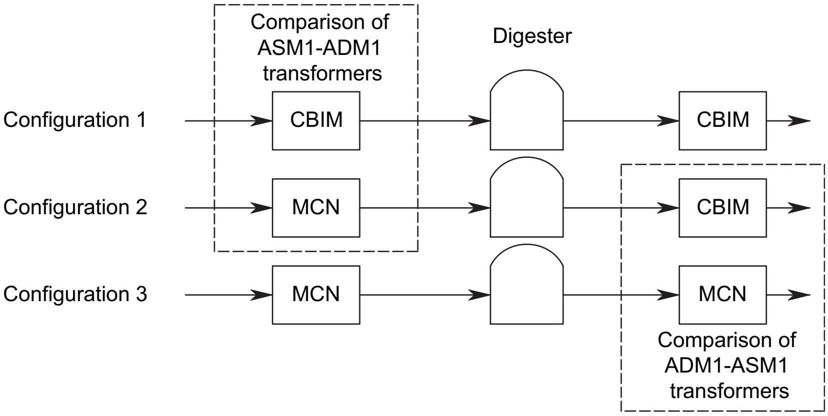

Fig. 7. Transformers arrangements for their comparisons using identical inputs.

represent observed VFA dynamics. Also, other fraction parameters can be added to the MCN for better simulation of the digester components. These parameters can be estimated from measurements in the digester.

An important advantage of the CBIM approach is maintaining the continuity of all elements and COD. For instance, the CBIM transformers maintained the continuity of carbon when interfacing ASM1 and ADM1 whereas the MCN approach did not consider the carbon balance. The carbon balance is important in this case since alkalinity is connected to the main processes considered by both models.

For both applied methods, the transformation from ADM1 to ASM1 is easier to set up compared to the one from ASM1 to ADM1. This is due to the fact that ADM1 is based on a more detailed and more specific set of components. Application of the CBIM approach needs a careful design of the conversions requiring deep insight in the two models to be connected. However, there are three Guiding Transformation Principles (GTPs) to help the user to refine the conversions. The GTPs are suggested to solve the under-determination problems found in the definition of the transformer stoichiometry and conversions. Also, the GTPs are useful to update the designed conversions and guarantee that transformation occurs in the right direction.

The introduction of the source−sink components is necessary since, so far in the field of wastewater treatment, the developed models do not consider all elemental balances. Therefore, the CBIM transformation approach provides a good opportunity to close this gap in terms of integrated modelling.

The general steps for applying the CBIM transformation are:

1. to define the mass fractions of all the components from both models;
2. to design the composition matrix;
3. to design the transformation matrix assigning the right source−sink components;
4. to obtain outfluxes by means of a set of algebraic equation.

Acknowledgement

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Appendix

Table A1
ASM1−ADM1 transformer: “origin” model pan

J ↓	K → components / Conversions	1	2	3	4	5	6	7	8	9	10	11	12	13	14
		S_s	S_{no3-}	S_i	X_s	X_{bh}	X_{ba}	X_i	X_P	S_{nh4+}	S_{ND}	X_{ND}	S_{alk}	S_{n2}	S_o
		(gCOD m^{-3})	(gN m^{-3})	(gCOD m^{-3})	(gCOD m^{-3})	(gCOD m^{-3})	(gCOD m^{-3})	(gCOD m^{-3})	(gCOD m^{-3})	(gN m^{-3})	(gN m^{-3})	(gN m^{-3})	(molHCO$_3^-$ m^{-3})	(gN m^{-3})	(-gCOD m^{-3})
1	$S_{nh4+}\_S_{in}$									**−1**					**3.331E−16**
2	$S_{ND},S_{s}\_S_{aa},S_{fa},S_{su}$	**−1**			**−11.32222**						**−1**				**−2.22E−15**
3	$S_{alk}\_S_{ic}$												**−1**		
4	**Hydrolysis** X_{ND}										**1**	**−1**			
5	**O_2 depletion**	**−1.492537**				**1**									**−0.492537**
6	**NO_3 depletion**	**−1.492537**	**−0.172216**			**1**								**0.1722158**	**−0.000492**
7	$S_{i}\_S_{i}$			**−1**							**−0.052754**				**−1E−06**
9	$X_P\_X_I$								**−1**						**1.318E−16**
10	$X_i\_X_i$							**−1**							**−4.86E−17**
11	$X_s\_X_c$				**−1**										**−2.78E−16**
12	$X_{bh}\_X_c,X_{su}$					**−1**									**−8.33E−17**
13	$X_{ba}\_X_c$						**−1**								**−8.33E−17**
composition matrix	i_ThOD (g ThOD/stoich.unit)	1.000	−4.571	1.00	1.000	1.00	1.00	1.00	1.00		−1.714	−1.714		−1.714	−1.000
	i_C (g C/stoich.unit)	0.305		0.32	0.305	0.37	0.37	0.36	0.37				12.000		
	i_N (g N/stoich.unit)		1.000			0.09	0.09	0.06	0.09	1.00	1.000	1.000		1.000	
	i_O (g O/stoich.unit)	0.137	3.429	0.14	0.137	0.20	0.20	0.18	0.20				48.000		1.000
	i_H (g H/stoich.unit)	0.039		0.03	0.039	0.04	0.04	0.04	0.04	0.29			1.000		
	i_P (g P/stoich.unit)	0.009			0.009	0.02	0.02	0.01	0.02						
	i_Ch (g Ch/stoich.unit)		−0.0714286							0.07			−1.000		

Table A2
ASM1−ADM1 transformer: "destination" model

→	K	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43
↓	**components**	S_I	S_{su}	S_{aa}	S_{fa}	S_{va}	S_{bu}	S_{pro}	S_{ac}	S_{h2}	S_{ch4}	X_I	X_c	X_{ch}	X_{pr}	X_{li}	X_{su}	X_{aa}	X_{fa}	X_{c4}	X_{pro}	X_{ac}	X_{h2}	S_{an}	S_{cat}	S_{in}	S_{ic}	S_{ip}	S_{H+}	S_{H2O}
J	**Conversions**	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kmole m^{-3})	(kmole m^{-3})	(kmoleN m^{-3})	(kmoleC m^{-3})	(kmoleP m^{-3})	(kmole m^{-3})	kmole
1	**$S_{nh4+}\_S_{in}$**																									**7.143E−05**			**−1.39E−20**	**−2.08E−20**
2	**$S_{ND},S_{s}\_S_{aa},S_{fa},S_{su}$**		**0.0003**	**0.0101079**	**0.0002**																						**3.806E−05**	**3.468E−06**	**4.5E−05**	**−0.000149**
3	**$S_{alk}\_S_{ic}$**																										**0.001**			
4	**Hydrolysis X_{ND}**																													
5	**O_2 depletion**																									**−6.16E−06**	**7.368E−06**	**−2.64E−07**	**1.3E−05**	**9.961E−06**
6	**NO_3 depletion**																									**−6.16E−06**	**7.368E−06**	**−2.64E−07**	**6.951E−07**	**1.611E−05**
7	**$S_i\_S_I$**	**0.0009096**																									**−4.5E−07**	**−1.86E−07**	**−8.22E−07**	**5.285E−07**
9	**$X_P\_X_I$**											**0.0009**	**0.0001**													**2.206E−06**	**8.775E−07**	**4.861E−07**	**−3.57E−07**	**−3.11E−06**
10	**$X_i\_X_I$**											**0.0009**	**0.0001**													**1.932E−07**	**4.279E−07**	**6.666E−09**	**2.48E−07**	**−1.13E−06**
11	**$X_s\_X_c$**												**0.001**													**−2.21E−06**	**−4.08E−07**	**1.436E−07**	**2.09E−06**	**−2.48E−07**
12	**$X_{bh}\_X_c,X_{su}$**												**0.0009**				**0.0001**									**3.55E−06**	**4.255E−06**	**4.915E−07**	**1.688E−06**	**−1.19E−05**
13	**$X_{ba}\_X_c$**												**0.001**													**3.945E−06**	**4.728E−06**	**5.461E−07**	**1.875E−06**	**−1.33E−05**
composition matrix	*i*_ThOD (g ThOD/stoich.unit)	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000							
	*i*_C (g C/stoich.unit)	360.883797	375	309.987437	256.849315	288.5	300	321.4	375		187.5	360.883797	309.539613	388.6	310	263	366.27907	366.3	366.3	366.3	366.3	366.3	366.3				12000			
	*i*_N (g N/stoich.unit)	57.9991817		98.9321608								57.9991817	30.9539613		98.93		86.1833105	86.18	86.18	86.18	86.18	86.18	86.18			14000				
	*i*_O (g O/stoich.unit)	180.441899	500	184.673367	41.0958904	153.8	200	285.7	500			180.441899	151.511495	514.9	184.7	38.07	201.094391	201.1	201.1	201.1	201.1	201.1	201.1				48000	64000		16000
	*i*_H (g H/stoich.unit)	38.6661211	62.5	65.9547739	44.5205479	43.27	43.75	44.64	46.88	125	62.5	38.6661211	46.7024679	58.29	65.95	41.53	43.0916553	43.09	43.09	43.09	43.09	43.09	43.09			4000	1000	1000	1000	2000
	*i*_P (g P/stoich.unit)	6.44435352										6.44435352	4.34441562	9.715		3.461	21.5458276	21.55	21.55	21.55	21.55	21.55	21.55					31500		
	*i*_Ch (Ch/stoich.unit)					−4.81	−6.25	−8.93	−15.6																	1000	−1000	−2000	1000	

Table A3
ADM1−ASM1 transformer: “origin” model pan

j	Conversions / components K	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26
		S_I	S_{su}	S_{aa}	S_{fa}	S_{va}	S_{bu}	S_{pro}	S_{ac}	S_{h2}	S_{ch4}	X_I	X_c	X_{ch}	X_{pr}	X_{li}	X_{su}	X_{aa}	X_{fa}	X_{c4}	X_{pro}	X_{ac}	X_{h2}	S_{an}	S_{cat}	S_{in}	S_{ic}
		(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kgCOD m^{-3})	(kmole m^{-3})	(kmole m^{-3})	(kmoleN m^{-3})	(kmoleC m^{-3})
1	S_I_S_I,S_{ND}	−1																									
2	S_{su}_S_s		−1																								
3	S_{aa}_S_{ND},S_s			−1																							
4	S_{fa}_S_s				−1																						
5	S_{va}_S_s					−1																					
6	S_{bu}_S_s						−1																				
7	S_{pro}_S_s							−1																			
8	S_{ac}_S_s								−1																		
9	X_I_X_I											−1															
10	X_c_X_s												−1														
11	X_{ch}_X_s													−1													
12	X_{pr}_X_s														−1												
13	X_{li}_X_s															−1											
14	X_{su}_X_s																−1										
15	X_{aa}_X_s																	−1									
16	X_{fa}_X_s																		−1								
17	X_{c4}_X_s																			−1							
18	X_{pro}_X_s																				−1						
19	X_{ac}_X_s																					−1					
20	X_{h2}_X_s																						−1				
21	S_{in} _S_{nh4+}																									−1	
22	S_{ic}_S_{alk}																										−1
composition matrix	i_ThOD (g ThOD/stoich.unit)	#####	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000				
	i_C (g C/stoich.unit)	360.9	375	310	256.8	288.5	300	321.4	375		187.5	360.9	309.5	388.6	310	263	366.3	366.3	366.3	366.3	366.3	366.3	366.3				12000
	i_N (g N/stoich.unit)	58.0		98.93								58	30.95		98.93		86.18	86.18	86.18	86.18	86.18	86.18	86.18			14000	
	i_O (g O/stoich.unit)	180.4	500	184.7	41.1	153.8	200	285.7	500			180.4	151.5	514.9	184.7	38.07	201.1	201.1	201.1	201.1	201.1	201.1	201.1				48000
	i_H (g H/stoich.unit)	38.7	62.5	65.95	44.52	43.27	43.75	44.64	46.88	125	62.5	38.67	46.7	58.29	65.95	41.53	43.09	43.09	43.09	43.09	43.09	43.09	43.09			4000	1000
	i_P (g P/stoich.unit)	6.4										6.444	4.344	9.715		3.461	21.55	21.55	21.55	21.55	21.55	21.55	21.55				
	i_Ch (Ch/stoich.unit)					−4.81	−6.25	−8.93	−15.6																	1000	−1000

Table A4
ADM1–ASM1 transformer: "destination" model pan

	K	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43
	components	S_s	S_{no3}	S_i	X_s	X_{bh}	X_{ba}	X_i	X_P	S_{ND}	X_{ND}	S_{n2}	S_{nh4+}	S_{alk}	$S_{ip\ (HPO4-)}$	S_{H+}	S_{H2O}	S_o
j	Conversions	(gCOD m^{-3})	(gN m^{-3})	(gCOD m^{-3})	(gCOD m^{-3})	(gCOD m^{-3})	(gCOD m^{-3})	(gCOD m^{-3})	(gCOD m^{-3})	(gN m^{-3})	(gN m^{-3})	(gN m^{-3})	(gN m^{-3})	(molHCO$_3^-$ m^{-3})	(gP m^{-3})	(gH m^{-3})	(gH m^{-3})	(-gCOD m^{-3})
1	**S_I_S_I,S_{ND}**			**1099.4272**						**57.999182**				**0.4946903**	**6.4443535**	**0.9038556**	**−1.162124**	**3.02E−13**
2	**S_{su}_S_s**	**1000**												**5.8628133**	**−8.866533**	**5.2998588**	**12.429708**	**3.268E−13**
3	**S_{aa}_S_{ND},S_s**	**1169.598**								**98.932161**				**−3.860516**	**−10.37028**	**−4.518947**	**28.827963**	**1.99E−13**
4	**S_{fa}_S_s**	**1000**												**−3.983077**	**−8.866533**	**−4.546032**	**14.142037**	**−8.53E−14**
5	**S_{va}_S_s**	**1000**												**−1.348725**	**−8.866533**	**−6.719372**	**12.429708**	**5.684E−14**
6	**S_{bu}_S_s**	**1000**												**−0.387187**	**−8.866533**	**−7.200141**	**12.429708**	**5.684E−14**
7	**S_{pro}_S_s**	**1000**												**1.3985276**	**−8.866533**	**−8.092998**	**12.429708**	**1.137E−13**
8	**S_{ac}_S_s**	**1000**												**5.8628133**	**−8.866533**	**−10.32514**	**12.429708**	**1.99E−13**
9	**X_i_X_i**							**1000**										
10	**X_C_X_s**				**1053.0639**						**30.953961**			**−0.939363**	**−4.992611**	**−1.256354**	**7.7880562**	**7.105E-15**
11	**X_{ch}_X_s**				**1000**									**6.9952343**	**0.8481932**	**7.0490878**	**5.0280122**	**4.974E-14**
12	**X_{pr}_X_s**				**1169.598**						**98.932161**			**−3.860516**	**−10.37028**	**−4.518947**	**28.827963**	**−2.84E-14**
13	**X_{li}_X_s**				**1000**									**−3.467723**	**−5.405565**	**−3.810933**	**9.7927805**	**3.126E-13**
14	**X_{su}_X_s**				**1147.7428**						**86.183311**			**1.3852946**	**11.369328**	**2.1071567**	**−5.740731**	**8.527E-14**
15	**X_{aa}_X_s**				**1147.7428**						**86.183311**			**1.3852946**	**11.369328**	**2.1071567**	**−5.740731**	**8.527E-14**
16	**X_{fa}_X_s**				**1147.7428**						**86.183311**			**1.3852946**	**11.369328**	**2.1071567**	**−5.740731**	**8.527E-14**
17	**X_{c4}_X_s**				**1147.7428**						**86.183311**			**1.3852946**	**11.369328**	**2.1071567**	**−5.740731**	**8.527E-14**
18	**X_{pro}_X_s**				**1147.7428**						**86.183311**			**1.3852946**	**11.369328**	**2.1071567**	**−5.740731**	**8.527E-14**
19	**X_{ac}_X_s**				**1147.7428**						**86.183311**			**1.3852946**	**11.369328**	**2.1071567**	**−5.740731**	**8.527E-14**
20	**X_{h2}_X_s**				**1147.7428**						**86.183311**			**1.3852946**	**11.369328**	**2.1071567**	**−5.740731**	**8.527E-14**
21	**S_{in} _S_{nh4+}**												**14000**					
22	**S_{ic}_S_{alk}**													**1000**				
composition matrix	*i*_ThOD (g ThOD/stoich.unit)	1.000	−4.571	1.000	1.000	1.000	1.000	1.000	1.000	−1.714	−1.714	−1.714						−1.000
	*i*_C (g C/stoich.unit)	0.305		0.323	0.305	0.366	0.366	0.361	0.366					12.000				
	*i*_N (g N/stoich.unit)		1.000			0.086	0.086	0.058	0.086	1.000	1.000	1.000	1.000					
	*i*_O (g O/stoich.unit)	0.137	3.429	0.139	0.137	0.201	0.201	0.180	0.201					48.000	2.032		8.000	1.000
	*i*_H (g H/stoich.unit)	0.039		0.035	0.039	0.043	0.043	0.039	0.043				0.286	1.000	0.032	1.000	1.000	
	*i*_P (g P/stoich.unit)	0.009			0.009	0.022	0.022	0.006	0.022						1.000			
	*i*_Ch (Ch/stoich.unit)		−0.07										0.071	−1.000	−0.063	1.000		

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