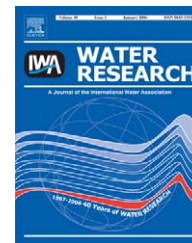


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Continuity-based model interfacing for plant-wide simulation: A general approach

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ABSTRACT

In plant-wide simulation studies of wastewater treatment facilities, often existing models from different origin need to be coupled. However, as these submodels are likely to contain different state variables, their coupling is not straightforward. The continuity-based interfacing method (CBIM) provides a general framework to construct model interfaces for models of wastewater systems, taking into account conservation principles. In this contribution, the CBIM approach is applied to study the effect of sludge digestion reject water treatment with a SHARON–Anammox process on a plant-wide scale. Separate models were available for the SHARON process and for the Anammox process. The Benchmark simulation model no. 2 (BSM2) is used to simulate the behaviour of the complete WWTP including sludge digestion. The CBIM approach is followed to develop three different model interfaces. At the same time, the generally applicable CBIM approach was further refined and particular issues when coupling models in which pH is considered as a state variable, are pointed out.

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1. Introduction

The usefulness of modelling and simulation to gain insight into and evaluate the behaviour of wastewater treatment facilities is nowadays widely acknowledged. The activated sludge models (ASM, Henze et al., 2000), the river water quality model no. 1 (RWQM1, Reichert et al., 2001) and the anaerobic digestion model no. 1 (ADM1, Batstone et al., 2002), developed by the respective IWA task groups, are generally accepted. Although these different types of models are very suitable to evaluate the behaviour of the processes for which they have been developed, the coupling of these models to evaluate the behaviour of a wastewater treatment plant (WWTP) in a plant-wide context is often a source of problems. Typically, each model contains its own state variables with their own meanings and their own elemental composition,

which makes their coupling not straightforward, as mass conservation needs to be maintained. One solution is to adapt and extend the individual models to create a ‘supermodel’ that comprises all state variables of all submodels, as has been done by Jones and Takacs (2004). However, this is often not desirable because it increases model complexity as the behaviour of all state variables must be described in each subsystem and it results in the addition of unused state variables to submodels. Alternatively, model interfaces can be developed to link the state variables of one submodel to the state variables of another submodel. These model interfaces are placed between the two models considered, leaving the individual models unchanged. As a result, differences in model state variables, composition and units are accounted for in the model interfaces and not in the models themselves. Fig. 1 illustrates the two approaches.

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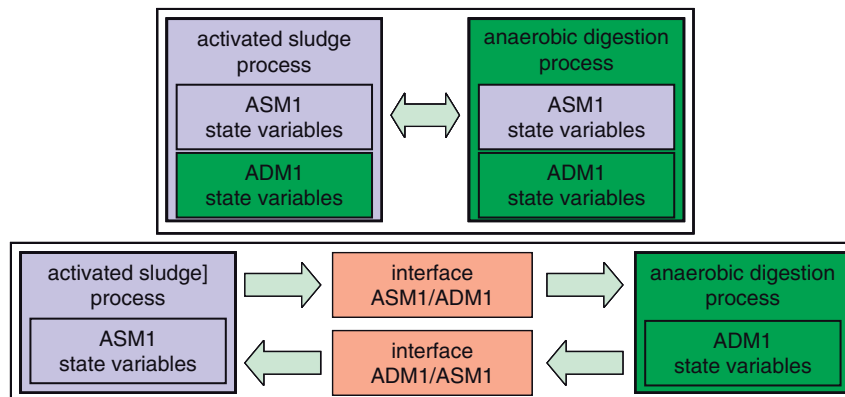


Fig. 1 – Supermodel approach (top) versus model interfacing (bottom) for the coupling of ASM1 and ADM1.

In the last few years, the issue of model interfacing has already been addressed in several specific cases, e.g. the coupling of ASM1 with RWQM1 (Meirlaen et al., 2001; Benedetti et al. 2004) and the coupling of ASM1 to ADM1 and vice versa (Copp et al., 2003; Zaher et al., 2006). A more generally applicable framework for constructing model interfaces has been proposed by Vanrolleghem et al. (2005) in the form of the continuity-based interfacing method (CBIM), a further development of the method proposed by Meirlaen et al. (2001). The CBIM approach is a way to construct model interfaces between subsystems considered in wastewater treatment, maintaining continuity of e.g. C, H, O, N, P, charge and COD.

In this contribution, the CBIM approach is applied to three different interfacing cases. The CBIM approach is further refined and particular points of attention when dealing with one or more submodels with varying pH, are pointed out. Although the interfaces are developed for a specific case, the followed methodology is generally applicable and should be easily extrapolated to other cases.

2. Case study: implementation of a SHARON and Anammox model in BSM2

The model interfaces developed in this study serve to evaluate the effect of treatment of sludge digestion reject water with a SHARON–Anammox process on a plant-wide scale. Although the reject water stream only represents a small volume fraction of the influent wastewater stream, it contributes significantly to the influent nitrogen load of the main plant, to which it is typically recycled. In order to relieve the main plant, it can be decided to treat the reject water stream before recirculation, e.g. through a SHARON–Anammox process (van Dongen et al., 2001). To evaluate the influence of reject water with SHARON–Anammox on the performance of the activated sludge tanks, it was decided to implement the existing SHARON and Anammox models in the Benchmark simulation model no. 2 (BSM2, Jeppsson et al., 2006), developed by the IWA task group on Benchmarking (Fig. 2). The BSM2 itself already contains submodels: besides primary and secondary clarifier models, the activated sludge plant is modelled according to the activated sludge model no. 1 (ASM1, Henze et al., 2000), while the anaerobic digester is

modelled following the ADM1 of Batstone et al. (2002). Consequently, the BSM2 also contains model interfaces between ASM1 and ADM1, as indicated in Fig. 2. Note that the current interfaces (Copp et al., 2003) are not CBIM-based but only ensure conservation of COD and N. As the treatment of reject water with the SHARON and Anammox processes is located behind the dewatering facility, additional interfaces will be required

- (1) from ASM1 to the SHARON model,
- (2) between the SHARON and the Anammox model, and
- (3) from the Anammox model to the ASM1 model.

The ASM1/SHARON interface is applied to the stream that comes from the sludge dewatering, in order to connect it to the SHARON process (see Fig. 2). This approach was preferred over the removal of the existing ADM1/ASM1 interface before sludge dewatering in the BSM2 and replacing it by an ADM1/SHARON interface. The latter would also require rewriting the dewatering model and is not in accordance with the starting-point of not changing the models, as stated above. Leaving the existing ADM1/ASM1 interface in the BSM2 unchanged, also allows a more fair comparison with operating strategies in which the reject water is not treated with a SHARON–Anammox process.

3. Application of the CBIM approach

The CBIM approach, proposed by Vanrolleghem et al. (2005), comprises the development of a set of algebraic transformation equations based on a description of the two models to be interfaced through their Petersen and composition matrices that modellers are familiar with. The methodology is followed step by step.

3.1. Step 1: formulation of elemental mass fractions and charge density

The coupling of the ASM1, SHARON and Anammox models, is not straightforward, as each model has its own state variables, only partly overlapping with the ones of the other models (see Table 1) For state variables that have the same

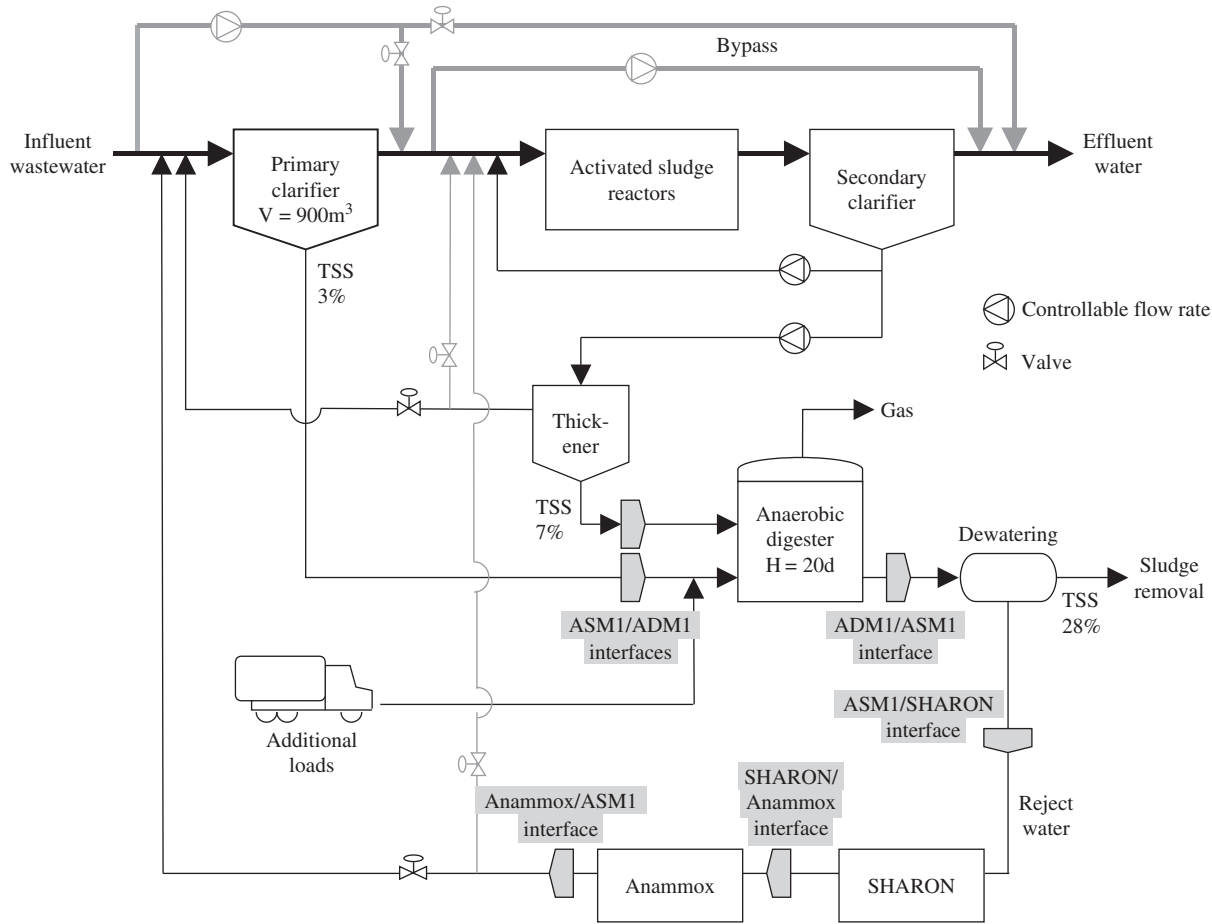


Fig. 2 – Extended benchmark plant with anaerobic sludge digestion and reject water recirculation, adapted from Jeppsson et al. (2006). The location for inclusion of the SHARON and Anammox process is indicated, as well as the model interfaces.

meaning, their dimensions and even the elemental composition can differ between the models. Besides, in the SHARON model (Hellings et al., 1999; Volcke, 2006) the pH is a state variable, as the pH is highly influenced by the conversion of high ammonium concentrations, as well as by CO_2 stripping, while the conversion processes themselves depend on pH. In the Anammox and in the ASM models, on the other hand, pH is considered constant and the model parameter values are valid for a pH of 7–8.

Elemental mass fractions (in gram element per gram component) are formulated for all state variables, relying on the hypothesis that the mass of each component is made up of constant mass fractions of the elements C, H, O, N, and P:

$$\alpha_k^C + \alpha_k^H + \alpha_k^O + \alpha_k^N + \alpha_k^P = 1. \quad (1)$$

Note that no other elements (e.g. S) are considered here, but an extension would be straightforward. Besides, also the charge density (α_k^{ch} , expressed in equivalents per gram component) and the COD content (α_k^{COD} , expressed in gCOD per g component) of each state variable are identified. One gram of any model component k is thus represented by the following molecular formula:

$$\left[\text{C}_{(\alpha_k^C/12)} \text{H}_{(\alpha_k^H/1)} \text{O}_{(\alpha_k^O/16)} \text{N}_{(\alpha_k^N/14)} \text{P}_{(\alpha_k^P/31)} \right]^{\alpha_k^{\text{ch}}}. \quad (2)$$

From the composition of a component, also its molecular weight is known. The COD content of a component is defined here as the amount of oxygen (expressed in g) that is consumed during oxidation of a mass unit of this component to NH_4^+ , CO_2 , H_2O , H^+ and PO_4^{3-} . It is the conservative quantity that effectively accounts for the electrons involved in the biological redox processes, denoted as theoretical oxygen demand (ThOD) in Henze et al. (2000). One finds:

$$\alpha_k^{\text{COD}} = 32 \frac{\alpha_k^C}{12} + 8 \alpha_k^H - 16 \frac{\alpha_k^O}{16} - 24 \frac{\alpha_k^N}{14} + 40 \frac{\alpha_k^P}{31} - 8 \alpha_k^{\text{ch}}. \quad (3)$$

This general CBIM-procedure has been followed straightforwardly to define the composition of the state variables for the ASM1 and Anammox model, as well as for the state variables of the SHARON model that are not involved in chemical equilibria and correspond with a known molecular formula. State variables that participate in chemical equilibria, exchanging protons, require special attention. The state variables total ammonium (TNH), total nitrite (TNO₂), total inorganic carbon (TIC) and total inorganic phosphorus (TIP) of the SHARON model represent lumped components of which the total concentrations equal the sum of concentrations of the corresponding equilibrium forms, e.g. TNH represents the sum of ionized ammonium (NH_4^+) and uncharged ammonia (NH_3), of which the proportions vary

Table 1 – Composition matrices for the models under study

ASM1 (as used in BSM2)								
Description	Symbol	Unit	Composition (mass fractions in g/g component)					
			α^C	α^N	α^H	α^O	α^P	α^{ch}
Soluble inert organic matter	S_I	gCOD m^{-3}	0.65 ^a	0 ^c	0.07 ^b	0.28 ^b	0 ^c	0
Readily biogradable substrate	S_S	gCOD m^{-3}	0.62 ^a	0 ^c	0.08 ^b	0.28 ^b	0.02 ^c	0
Particulate inert organic matter	X_I	gCOD m^{-3}	0.56 ^a	0.09 ^e	0.06 ^e	0.28 ^e	0.01 ^c	0
Slowly biodegradable substrate	X_S	gCOD m^{-3}	0.62 ^a	0	0.08 ^b	0.28 ^b	0.02 ^c	0
Heterotrophic biomass	X_{BH}	gCOD m^{-3}	0.516 ^a	0.114 ^f	0.06 ^d	0.28 ^d	0.03 ^c	0
Autotrophic biomass	X_{BA}	gCOD m^{-3}	0.516 ^a	0.114 ^f	0.06 ^d	0.28 ^d	0.03 ^c	0
Particulate products from biomass decay	X_P	gCOD m^{-3}	0.5575 ^a	0.0925 ^d	0.06 ^d	0.28 ^d	0.01 ^c	0
Oxygen (O ₂)	S_O	g m^{-3}	0	0	0	1	0	0
Nitrate+total nitrite (NO ₃ ^{-*})	S_{NO}	gN m^{-3}	0	0.2258	0	0.7742	0	−0.0161
Total ammonium (NH ₄ ⁺ *)	S_{NH}	gN m^{-3}	0	0.7778	0.2222	0	0	0.0556
Soluble biodegradable organic nitrogen (NH ₃ [*])	S_{ND}	gN m^{-3}	0	0.8235	0.1765	0	0	0
Particulate biodegradable organic nitrogen (NH ₃ [*])	X_{ND}	gN m^{-3}	0	0.8235	0.1765	0	0	0
Alkalinity (HCO ₃ [*])	S_{alk}	mole m^{-3}	0.1967	0	0.0164	0.7869	0	−0.0164
SHARON model								
Description	Symbol	Unit	Composition					
Total ammonium	TNH	mole m^{-3}	NH ₃ (pH)+NH ₄ ⁺ (pH)					
Total nitrite	TNO ₂	mole m^{-3}	HNO ₂ (pH)+NO ₂ ⁻ (pH)					
Total inorganic carbon	TIC	mole m^{-3}	CO ₂ (pH)+HCO ₃ ⁻ (pH)+CO ₃ ²⁻ (pH)					
Total inorganic phosphorus	TIP	mole m^{-3}	H ₂ PO ₄ ⁻ (pH)+HPO ₄ ²⁻ (pH)					
Nitrate	NO ₃ ⁻	mole m^{-3}	NO ₃ ⁻					
Oxygen	O ₂	mole m^{-3}	O ₂					
Nitrogen gas	N ₂	mole m^{-3}	N ₂					
Ammonium oxidizing biomass	X _{amm}	mole m^{-3}	CH _{1.8} O _{0.5} N _{0.2} P _p ^{**}					
Nitrite oxidizing biomass	X _{nit}	mole m^{-3}	CH _{1.8} O _{0.5} N _{0.2} P _p ^{**}					
Heterotrophic biomass	X _{het}	mole m^{-3}	CH _{1.8} O _{0.5} N _{0.2} P _p ^{**}					
Methanol	CH ₃ OH	mole m^{-3}	CH ₃ OH					
Protons	H ⁺	mole m^{-3}	H ⁺					
Anammox model								
Description	Symbol	Unit	Composition (mass fractions in g/g component)					
			α^C	α^N	α^H	α^O	α^P	α^{ch}
Oxygen	S_O	$\text{gO}_2 \text{ m}^{-3}$	0	0	0	1	0	0
Readily biodegradable substrate	S_S	gCOD m^{-3}	0.62 ^a	0 ^c	0.08 ^b	0.28 ^b	0.02 ^c	0
Total ammonium (NH ₄ ⁺ *)	S_{NH}	gN m^{-3}	0	0.7778	0.2222	0	0	0.0556
Total nitrite (NO ₂ ^{-*})	S_{NO2}	gN m^{-3}	0	0.3043	0	0.6957	0	−0.0217
Nitrate (NO ₃ ⁻)	S_{NO3}	gN m^{-3}	0	0.2258	0	0.7742	0	−0.0161
Nitrogen gas (N ₂)	S_{NO4}	gN m^{-3}	0	1	0	0	0	0
Heterotrophic biomass	X_H	gCOD m^{-3}	0.516 ^a	0.114 ^f	0.06 ^d	0.28 ^d	0.03 ^c	0
Ammonium oxidizing biomass	X_{NH}	gCOD m^{-3}	0.516 ^a	0.114 ^f	0.06 ^d	0.28 ^d	0.03 ^c	0
Nitrite oxidizing biomass	X_{NO}	gCOD m^{-3}	0.516 ^a	0.114 ^f	0.06 ^d	0.28 ^d	0.03 ^c	0
Anammox biomass	X_{AN}	gCOD m^{-3}	0.4830 ^g	0.0845 ^g	0.0805 ^g	0.3220 ^g	0.03 ^g	0
Slowly biodegradable substrate	X_S	gCOD m^{-3}	0.62 ^a	0	0.08 ^b	0.28 ^b	0.02 ^c	0
Particulate products	X_P	gCOD m^{-3}	0.5575 ^a	0.092 ^d	0.06 ^d	0.28 ^d	0.01 ^c	0
Alkalinity	S_{alk}	mole m^{-3}	0.1967	0	0.0164	0.7869	0	−0.0164

* In agreement with the model stoichiometry and the (major) form in which the state variable occurs.

** A value of $p = 0.02454$ is found for an assumed phosphorus content of $\alpha^P = 0.03 \text{ gP/g biomass}$.

*** The equilibrium forms H_3PO_4 and PO_4^{3-} are negligible in a pH operating range of 5–9.

^a Calculated as the remaining mass fraction after the assignment of other element fractions.

^b Taken from RWQM1 (Reichert et al., 2001).

^c Assumed fraction.

^d According to stoichiometric formula $\text{C}_5\text{H}_7\text{O}_2\text{N}$, also used by Henze et al. (2000) and Batstone et al. (2002).

^e Similar to ADM1.

^f In agreement with the ASM1 nitrogen fraction used in BSM2.

^g Corresponding with stoichiometric formula determined by Strous et al. (1998), and an phosphorus content of $\alpha^P = 0.03 \text{ gP/g biomass}$, i.e. $\text{CH}_2\text{O}_{0.5}\text{N}_{0.5}\text{P}_p$ with $p = 0.0240$.

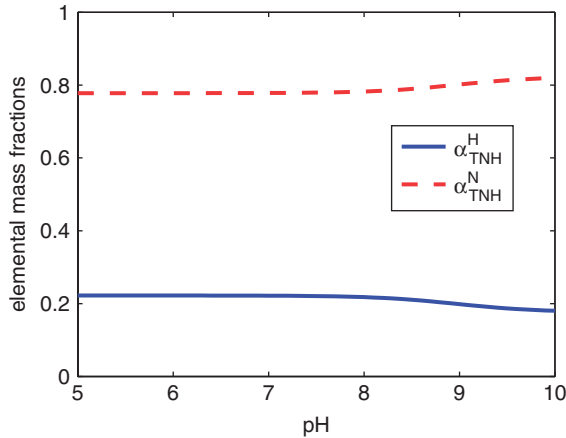


Fig. 3 – Elemental hydrogen and nitrogen mass fractions of total ammonium as a function of pH.

with varying pH. As the pH varies with time, the composition of these lumped state variables is also time-varying (Fig. 3). For this reason, no fixed composition can be written down for these state variables.

The inclusion of P-balances in the model interfaces is not self-evident in the given case study. The ASM1, SHARON and Anammox models do not consider any biological conversion reactions involving phosphorus. Only the effect of the phosphorus dissociation reactions on the pH is considered in the SHARON model. However, P-balances have been incorporated in the interfaces to anticipate for future inclusion of conversion reactions involving phosphorus. One could indeed decide to use ASM2 instead of ASM1 and in this way consider biological P-removal and P-uptake during biomass growth. Another incentive to take up P-balances is the ongoing development of anaerobic digestion models involving the fate of phosphorus (Jones and Takacs, 2004; Ekama et al., 2005). For this purpose, all components have been assigned a certain phosphorus content (that of course can be zero). Note that in case it would be decided not to include the P-balances, the formulation of elemental mass fractions should be done without considering P (as it is done now, for instance, by not considering S). In particular, the COD content of each component should then also be calculated without considering phosphorus.

3.2. Step 2: set-up of composition matrices

A composition matrix is set up for each model. A composition matrix element i_k^E represents the elemental, charge or COD fraction of a component (expressed in gram for $E = C, H, O, N, P$, in equivalents for $E = \text{charge}$ and in gCOD for $E = \text{COD}$) per stoichiometric mass unit of this component. It is related to α_k^E through

$$i_k^E = \alpha_k^E M_k, \quad (4)$$

where M_k stands for the mass of components expressed in g per stoichiometric mass unit (e.g. gCOD, gN or mole). The calculation of the composition is straightforward.

3.3. Step 3: definition of transformation matrices

3.3.1. General procedure

Transformation processes have to be defined from the state variables of the origin model to those of the destination model. The definition of these transformations is done by the user, who takes a decision based on process knowledge and insight. The number of transformations is typically equal to the number of state variables of the origin model, that need to be transformed (see step 4). All proposed transformations must guarantee continuity:

$$\sum_k v_{jk} i_k^E = 0 \quad (5)$$

for each $E = C, H, O, N, P$, charge and COD. Note that one of these seven equations can be omitted because of the relationship given by Eq. (3), resulting in six linear constraints that need to be fulfilled for each transformation process. v_{jk} represents the ‘stoichiometric’ coefficient of component k for transformation j . The summation is made over all components k of both the source and destination model. The stoichiometric coefficients should be negative for components of the origin model, that are ‘consumed’ in the interface and positive for components of the destination model, that are ‘produced’. In this way the transformation is maintained in the right direction.

In this contribution the following general procedure is followed to determine the stoichiometric coefficients for each transformation j :

1. Each transformation reaction j corresponds with the transformation of a component of the origin model. The stoichiometric coefficient of this component is set to an arbitrary value, e.g. -1 , with a negative sign to express that this component is consumed in the interface. The coefficients of the destination component(s), to which the source component is mapped on the basis of process insight, are set in such a way that the transformation conserves the COD content. For components with COD content zero (i.e. NH_4^+ , CO_2 , H_2O , H^+ and PO_4^{3-}), transformation is usually straightforward (based on N-, C-, O-, H- and P-content, respectively).
2. So-called compensation components (Meirlaen et al., 2001) are used to close the remaining balances, in case they are not fulfilled yet. The user is free to choose which of the seven balances (COD, C, H, O, N, P, charge) will be omitted (as one balance is linearly dependent on the others, see Eq. (3)) and to choose which components will be used for compensation. After closing the COD-balance, the following choice was made:
 - 2.1. The C-balance is closed with HCO_3^- .
 - 2.2. The N-balance is closed with NH_4^+ .
 - 2.3. The P-balance is closed with HPO_4^{2-} .
 - 2.4. The charge balance is closed with H^+ .
 - 2.5. The O-balance is closed with H_2O .
 - 2.6. The H-balance is then automatically fulfilled, since the balances are linearly dependent on each other (see Eq. (3)).

Noteworthy is that if this procedure is followed in the order as described, every step is independent of the previous ones.

The stoichiometric coefficients $v_{j,m}$ (for all components m involved in point 1), v_{j,HCO_3^-} , v_{j,NH_4^+} , $v_{j,\text{HPO}_4^{2-}}$, v_{j,H^+} and $v_{j,\text{H}_2\text{O}}$ are calculated by solving the matrix equation

$$\begin{bmatrix} i_{\text{HCO}_3^-}^{\text{C}} & 0 & 0 & 0 & 0 \\ 0 & i_{\text{NH}_4^+}^{\text{N}} & 0 & 0 & 0 \\ 0 & 0 & i_{\text{HPO}_4^{2-}}^{\text{P}} & 0 & 0 \\ i_{\text{HCO}_3^-}^{\text{charge}} & i_{\text{NH}_4^+}^{\text{charge}} & i_{\text{HPO}_4^{2-}}^{\text{charge}} & i_{\text{H}^+}^{\text{charge}} & 0 \\ i_{\text{HCO}_3^-}^{\text{O}} & 0 & i_{\text{HPO}_4^{2-}}^{\text{O}} & 0 & i_{\text{H}_2\text{O}}^{\text{O}} \end{bmatrix} \begin{bmatrix} v_{j,\text{HCO}_3^-} \\ v_{j,\text{NH}_4^+} \\ v_{j,\text{HPO}_4^{2-}} \\ v_{j,\text{H}^+} \\ v_{j,\text{H}_2\text{O}} \end{bmatrix} = \begin{bmatrix} -\sum_m i_m^{\text{C}} v_{j,m} \\ -\sum_m i_m^{\text{N}} v_{j,m} \\ -\sum_m i_m^{\text{P}} v_{j,m} \\ -\sum_m i_m^{\text{charge}} v_{j,m} \\ -\sum_m i_m^{\text{O}} v_{j,m} \end{bmatrix},$$

where the summations are made over all components m for which stoichiometric coefficients have been determined under point 1. Of course this yields the same result as when calculating the stoichiometric coefficients v_{j,HCO_3^-} , v_{j,NH_4^+} , $v_{j,\text{HPO}_4^{2-}}$, v_{j,H^+} and $v_{j,\text{H}_2\text{O}}$ one by one. Following this procedure, the number of compensation components is minimized, as well as the resulting values of their stoichiometric coefficients. Note that taking up the elemental H-balance in addition to the other balances, aiming to determine the stoichiometric coefficient of an additional component, would result in a matrix of stoichiometric coefficients in Eq. (6) that is singular (i.e. with determinant zero), which would make matrix inversion, necessary to obtain the values of the stoichiometric coefficients, impossible, indicating that the system is overdetermined. It is advisable to check the accuracy of the performed calculations by calculating the H-balance, that should be fulfilled.

The number of balances to be considered can be reduced when certain components are not considered in the destination model. For instance, the O-balance can be omitted when H_2O is not considered in the destination model, without influencing the stoichiometric coefficients of the remaining components. In the same way, the charge balance can be omitted when H^+ is not taken up in the destination model. Even if the destination model would consider H_2O but not H^+ , the charge balance can still be omitted since the order of (d) and (e) may be switched, so the stoichiometric coefficient of H^+ determined by the charge balance does not influence the stoichiometric coefficient of H_2O . In this contribution however, all balances are considered in every case to illustrate the principle of maintaining continuity of all elements, charge and COD.

3.4. Application to the model interfaces

During the definition of the transformation matrices, different types of transformation processes can be distinguished:

Type 1: Direct transformation of state variables, e.g. O_2 , that have the same composition in the origin model and in the destination model, possibly after unit conversion.

Type 2: Transformation of state variables that have the same meaning in the two models to be connected, while their composition differs (slightly). An example is heterotrophic biomass, of which the composition slightly differs between the ASM1 and Anammox model on the one hand and the SHARON model on the other hand. The state variables representing heterotrophic biomass are mapped to each other on a COD-basis and the compensation state variables are used to close the remaining balances (see Tables 2 and 3).

Type 3: Splitting up or merging lumped state variables. For instance, in the ASM1/SHARON interface (Table 2), the ASM1 state variable S_{NH} , expressed as if it were all NH_4^+ , is mapped to the lumped state variable TNH . Upon entering the SHARON reactor, the latter is split up into NH_4^+ and NH_3 , in proportions that depend on the incoming pH. To ensure continuity, protons are released in the interface, equivalent with the amount of NH_3 that corresponds with the given amount of S_{NH} transformed and the incoming pH. It is important to note that the resulting coefficient v_{j,H^+} varies with the incoming pH and thus with time. Secondly, also in the ASM1/SHARON interface, the state variable representing total autotrophic biomass in ASM1 is split into ammonium oxidizing and nitrite oxidizing biomass on a COD-basis, proportional with the biomass yield coefficients (Table 2). A third example is the transformation of nitrite in the Anammox-ASM1 interface: nitrite (NO_2^-) is lumped with nitrate (NO_3^-) into the state variable S_{NO} , that is expressed as if it were all nitrate. This transformation is performed on COD-basis while N_2 is released, so the overall biomass and N_2 production (by denitrification) remains the same (see Fig. 4 and Table 4).

Type 4: Transformation of state variables of the origin model that are not included in the destination model, or exhibit a different behaviour. For instance, the state variables S_{S} of the ASM1 and CH_3OH of the SHARON model both represent readily biodegradable components, but with different composition and yield coefficient. The lower biomass production associated with growth on CH_3OH is compensated by adding heterotrophic biomass (Fig. 4, Table 2). Another example is the transformation of the ASM1 state variable S_{alk} , representing alkalinity ($\text{HCO}_3^- + 2\text{CO}_3^{2-}$), into the SHARON state variable TIC , representing total inorganic carbon ($\text{CO}_2 + \text{HCO}_3^- + \text{CO}_3^{2-}$). This transformation depends on the incoming pH, so the associated coefficient v_{TIC} is time-dependent (Table 2).

Type 5: Incoming values for state variables of the destination model that are not included in the origin model. For instance, the SHARON model requires an incoming pH value, that in this study has been taken from the anaerobic digester effluent, thus bypassing the existing ADM1/ASM1 interface, in which this information had been lost. Further, since the ASM1 does not contain inorganic phosphorus, a realistic concentration of inorganic phosphorus (TIP , 1.5 mole m^{-3}) has been 'added' to the SHARON influent to include its effect on the chemical equilibria. This amount of TIP is again 'removed' from the SHARON effluent (Fig. 5).

Table 2 – ASM1-SHARON transformation matrices

components → transformations ↓	comp. N													comp. C			
	S_I	S_S	X_I	X_S	X_BH	X_BA	X_P	S_O	S_NO	S_NH	S_ND	X_ND	S_alk				
1. S_O to O2	0	0	0	0	0	0	0	-32	0	0	0	0	0				
2. S_NH to TNH	0	0	0	0	0	0	0	0	0	-14	0	0	0				
3. S_NO to NO3	0	0	0	0	0	0	0	0	-14	0	0	0	0				
4. X_BH to Xhet	0	0	0	0	-34.5817	0	0	0	0	-0.0223	0	0	0.0477				
5. X_BA to Xamm/Xnit	0	0	0	0	0	-34.5817	0	0	0	-0.0223	0	0	0.0477				
6. S_S to CH3OH/Xhet	0	-1	0	0	0	0	0	0	0	-0.0476	0	0	-0.0002				
7. X_S to CH3OH/Xhet	0	0	0	-1	0	0	0	0	0	-0.0476	0	0	-0.0002				
8. S_ND to TNH	0	0	0	0	0	0	0	0	0	0	-14	0	0				
9. X_ND to TNH	0	0	0	0	0	0	0	0	0	0	0	-14	0				
10. Direct pass S_I	-1	0	0	0	0	0	0	0	0	0	0	0	0				
11 Direct pass X_I	0	0	-1	0	0	0	0	0	0	0	0	0	0				
12. Direct pass X_P	0	0	0	0	0	0	-1	0	0	0	0	0	0				
13. S_alk to TIC	0	0	0	0	0	0	0	0	0	0	0	0	-1				

components → transformations ↓	TNH	TNO2	TIC	TIP	NO3-	O2	N2	Xamm	Xnitr	Xhet	CH3OH	S_I	X_I	X_P	HPO4(2-)	H+	H2O
	mole/m3	mole/m3	mole/m3	mole/m3	mole/m3	mole/m3	mole/m3	mole/m3	mole/m3	mole/m3	mole/m3	gCOD/m3	gCOD/m3	gCOD/m3	mole/m3	mole/m3	mole/m3
1. S_O to O2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
2. S_NH to TNH	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3. S_NO to NO3	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
4. X_BH to Xhet	0	0	0	0	0	0	0	0	0	1	0	0	0	0	-9.63E-04	0.0474	-0.2129
5. X_BA to Xamm/Xnit	0	0	0	0	0	0	0	0.75	0.25	0	0	0	0	0	-9.63E-04	0.0474	-0.2129
6. S_S to CH3OH/Xhet	0	0	0	0	0	0	0	0	0	0.0170	0.0086	0	0	0	-1.31E-04	0.0029	-0.0074
7. X_S to CH3OH/Xhet	0	0	0	0	0	0	0	0	0	0.0170	0.0086	0	0	0	-1.31E-04	0.0029	-0.0074
8. S_ND to TNH	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1+v2,++ ^{AS}	0
9. X_ND to TNH	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1+v2,++ ^{AS}	0
10. Direct pass S_I	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
11 Direct pass X_I	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
12. Direct pass X_P	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
13. S_alk to TIC	0	0	v13,TIC ^{AS}	0	0	0	0	0	0	0	0	0	0	0	0	0	0

$$\text{in which } v_{13,TIC}^{AS} = \frac{H_{SH,in}^{+2} + H_{SH,in}^{+} \cdot K_{eCO_2} + K_{eCO_2} \cdot K_{eHCO_3^-} \cdot v_{2,H}^{AS}}{H_{SH,in}^{+} \cdot K_{eCO_2} + 2K_{eCO_2} \cdot K_{eHCO_3^-}}$$

$$= \frac{K_{e,NH_4^+}}{H_{SH,in}^{+} + K_{e,NH_4^+}}$$

Top: Petersen section ASM1 model ('origin'). Bottom: Petersen section SHARON model ('destination'). Important note: the pH from the anaerobic digester effluent is directly passed to the SHARON model but is not taken up here as it is no ASM1 state variable. Columns in *italics* correspond with compensation state variables that are not passed on in the interface.

Table 3 – SHARON–Anammox interface

components →	TNH	TNO2	TIC	NO3-	O2	Xamm	Xnltr	Xhet	CH3OH	S_I	X_I	X_P	S_alk	S_I	X_I	H2O	HPO4(2-)	CO2	H+
transformations ↓	mole/m3	mole/m3	mole/m3	mole/m3	mole/m3	mole/m3	mole/m3	mole/m3	mole/m3	gCOD/m3	gCOD/m3	gCOD/m3	mole/m3	gCOD/m3	gCOD/m3	mole/m3	mole/m3	mole/m3	mole/m3
1. TNH to S_NH	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2. TNO2 to S_NO2	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3. NO3- to S_NO3	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4. O2 to S_O	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5. Xamm to X_NH	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0
6. Xnit to X_NO	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0
7. Xhet to X_H	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0
8. CH3OH to S_S	0	0	0	0	0	0	0	-0.0170	-0.0086	0	0	0	0	0	0	0	0	0	0
9. Direct pass S_I	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0
10. Direct pass X_I	0	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0
11. Direct pass X_P	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
12. TIC to S_alk	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

components →	S_O	S_S	S_NH	S_NO2	S_NO3	S_N2	X_H	X_NH	X_NO	X_AN	X_S	X_P	S_alk	S_I	X_I	H2O	HPO4(2-)	CO2	H+
transformations ↓	gO2/m3	gCOD/m3	gN/m3	gN/m3	gN/m3	gN/m3	gCOD/m3	gCOD/m3	gCOD/m3	gCOD/m3	gCOD/m3	gCOD/m3	mole/m3	gCOD/m3	gCOD/m3	mole/m3	mole/m3	mole/m3	mole/m3
1. TNH to S_NH	0	0	14	0	0	0	0	0	0	0	0	0	-V1,H+ ^{SA}	0	0	V1,H+ ^{SA}	0	V1,H+ ^{SA}	V1,H+ ^{SA}
2. TNO2 to S_NO2	0	0	0	14	0	0	0	0	0	0	0	0	-V2,H+ ^{SA}	0	0	V2,H+ ^{SA}	0	V2,H+ ^{SA}	V2,H+ ^{SA}
3. NO3- to S_NO3	0	0	0	0	14	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4. O2 to S_O	32	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5. Xamm to X_NH	0	0	0.0223	0	0	0	0	34.5817	0	0	0	0	-0.0003	0	0	0.1655	9.63E-04	-0.04739	-0.0474
6. Xnit to X_NO	0	0	0.0223	0	0	0	0	0	34.5817	0	0	0	-0.0003	0	0	0.1655	9.63E-04	-0.04739	-0.0474
7. Xhet to X_H	0	0	0.0223	0	0	0	34.5817	0	0	0	0	0	-0.0003	0	0	0.1655	9.63E-04	-0.04739	-0.0474
8. CH3OH to S_S	0	1	0.0476	0	0	0	0	0	0	0	0	0	0.0031	0	0	0.0045	1.31E-04	-0.00294	-0.0039
9. Direct pass S_I	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
10. Direct pass X_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
11. Direct pass X_P	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
12. TIC to S_alk	0	0	0	0	0	0	0	0	0	0	0	0	V12,Salk	0	0	0	0	0	0

with

$$V_{1,H+}^{SA} = -\frac{K_{e,NH_4^+}}{H_{SH,out}^+ + K_{e,NH_4^+}} ; v_{2,H+}^{SA} (pH_{SH,out}) = \frac{H_{SH,out}^+}{H_{SH,out}^+ + K_{eHNO_2}} ;$$

$$V_{12,Salk}^{SA} = \frac{H_{SH,out}^+ \cdot K_{eCO_2} + 2K_{eCO_2} \cdot K_{eHCO_3^-}}{H_{SH,out}^+ + H_{SH,out}^+ \cdot K_{eCO_2} + K_{eCO_2} \cdot K_{eHCO_3^-}}$$

Top: Petersen section SHARON model ('origin'). Bottom: Petersen section Anammox model ('destination'). Columns in grey correspond with (compensation) state variables that are not passed on in the interface.

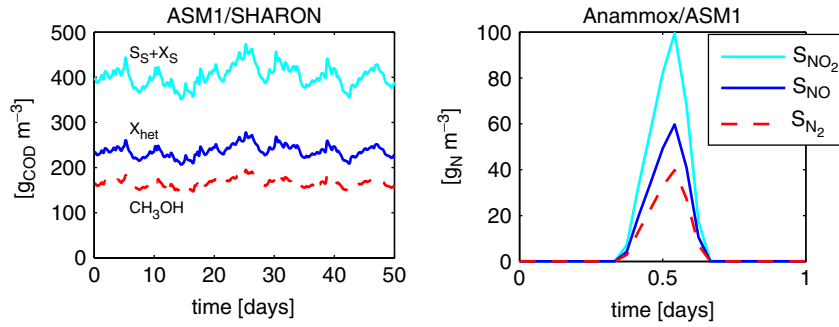
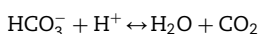


Fig. 4 – Transformation of S_S and X_S to CH_3OH and X_{het} in ASM1/SHARON interface (left); transformation of S_{NO_2} (nitrite) to S_{NO} (nitrite+nitrate) and S_{N_2} in Anammox/ASM1 interface (right).

Type 6: Direct pass-through of state variables of the origin model that are not included in the destination model and do not influence the behaviour of the destination model (see Fig. 5). This is the case for S_I , X_I and X_P , that are state variables of the ASM1 and Anammox models, but are bypassed from the SHARON models, in which they are not considered.

Type 7: Some state variables are not passed on. For example, nitrogen gas (N_2) is not passed on between the SHARON and Anammox models, even if it is a state variable in both. However, N_2 from the SHARON reactor does not influence the biological conversions in the Anammox reactor. By not passing this state variable, the nitrogen in the Anammox reactor effluent equals the nitrogen produced in the latter reactor, making interpretation easy.

The protons that are produced or consumed in the model interfaces and are modelled by the compensation state variable H^+ , require special attention. As these protons do not represent ‘free’ protons but will immediately take part in the water equilibrium and other chemical equilibria, they cannot be passed on by summing up like the other state variables. For this reason, the pH of the anaerobic digester effluent (assumed to remain unchanged by the dewatering process) is passed on unaltered as the SHARON model influent pH, while the protons produced in the ASM1/SHARON interface (Table 2) are passed on separately to the SHARON model, where they take part in the chemical equilibria and in this way influence the pH (see Fig. 5). Protons produced in the SHARON/Anammox and Anammox/ASM1 interfaces (Tables 3 and 4) should also be accounted for. However, since the destination models (Anammox and ASM1, respectively) do not consider pH as a state variable, protons that are produced or consumed in these model interfaces should be accounted for in their pH-related state variable S_{alk} , representing alkalinity. As S_{alk} is represented as bicarbonate, continuity of elemental and charge balances is ensured by considering the reaction



in the interface. In this way, the protons that are produced/consumed are transformed into an equivalent amount of

HCO_3^- , H_2O and CO_2 . HCO_3^- is then passed on as S_{alk} , while H_2O and CO_2 are not passed on.

Tables 2–4 give the transformation matrices for the three model interfaces constructed in this case study. More details on these transformations are given by Volcke (2006).

3.5. Step 4: transformation equations

Besides the stoichiometric coefficients v_{jk} , defined in the previous step, also transformation ‘rates’ ρ_j need to be identified for full definition of the interfaces. These transformation rates must fulfill the following equations (Vanrolleghem et al., 2005):

$$\phi_k^{in} = - \sum_{j=1}^N v_{jk} \rho_j, \quad k = 1, \dots, P, \quad (6)$$

$$\phi_k^{out} = \sum_{j=1}^N v_{jk} \rho_j, \quad k = P+1, \dots, P+Q \quad (7)$$

in which ϕ_k^{in} represents the known (positive) influx of a component $k = 1, \dots, P$ of the source model, while ϕ_k^{out} stands for the unknown outflux of component $k = P+1, \dots, P+Q$ of the destination model. Eq. (6) enables the calculation of the transformation rates ρ_j in terms of the known stoichiometric components and influxes, the latter being time-varying. These expressions are subsequently substituted in Eq. (7) to calculate the outflux of destination components at every time step:

$$\begin{aligned} \begin{bmatrix} \phi_{P+1}^{out} \\ \vdots \\ \phi_{P+Q}^{out} \end{bmatrix} &= - \begin{bmatrix} v_{1,P+1} & \cdots & v_{N,P+1} \\ \vdots & \ddots & \vdots \\ v_{1,P+Q} & \cdots & v_{N,P+Q} \end{bmatrix} \begin{bmatrix} v_{1,1} & \cdots & v_{N,1} \\ \vdots & \ddots & \vdots \\ v_{1,P} & \cdots & v_{N,P} \end{bmatrix}^{-1} \begin{bmatrix} \phi_1^{in} \\ \vdots \\ \phi_P^{in} \end{bmatrix} \\ &\equiv -T_{dest} T_{orig}^{-1} \cdot \begin{bmatrix} \phi_1^{in} \\ \vdots \\ \phi_P^{in} \end{bmatrix}. \end{aligned} \quad (8)$$

Note that inversion of the second matrix is only possible unambiguously when $N = P$, i.e. if the number of transformation reactions defined is equal to the number of components of the origin model, as long as the matrix does not contain any rows or columns only containing zeros and if these transformation reactions are linearly independent of each

Table 4 – Anammox–ASM1 interface

components →	S_O	S_S	S_NH	S_NO2	S_NO3	S_N2	X_H	X_NH	X_NO	X_AN	X_S	X_P	S_alk	S_I	X_I
transformations ↓	gO ₂ /m ³	gCOD/m ³	gN/m ³	gN/m ³	gN/m ³	gN/m ³	gCOD/m ³	gCOD/m ³	gCOD/m ³	gCOD/m ³	gCOD/m ³	gCOD/m ³	gCOD/m ³	gCOD/m ³	gCOD/m ³
1. S_O	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2. S_S	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0
3. S_NH	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0
4. S_N2	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0
5. X_H to X_BH	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0
6. X_S	0	0	0	0	0	0	0	0	0	0	-1	0	0	0	0
7. X_P	0	0	0	0	0	0	0	0	0	0	0	-1	0	0	0
8. S_NO3 to S_NO	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0
9. S_NO2 to S_NO	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0
10. X_NH to X_S/P	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0
11. X_NO to X_S/P	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0
12. X_AN to X_S/P	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0
13. Direct pass S_I	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	0
14. Direct pass X_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
15. S_alk	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	0

components →	S_I	S_S	X_I	X_S	X_BH	X_BA	X_P	S_O	S_NO	S_NH	S_NO2	X_ND	S_alk	S_H2O	S_HPO ₄ ²⁻	S_N2	CO ₂	H+
transformations ↓	gCOD/m ³	gCOD/m ³	gCOD/m ³	gCOD/m ³	gCOD/m ³	gCOD/m ³	gCOD/m ³	gO ₂ /m ³	gN/m ³	gN/m ³	gN/m ³	gN/m ³	mole/m ³	mole/m ³	gP/m ³	gN/m ³	mole/m ³	mole/m ³
1. S_O	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
2. S_S	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3. S_NH	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
4. S_N2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
5. X_H to X_BH	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
6. X_S	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7. X_P	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
8. S_NO3 to S_NO	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
9. S_NO2 to S_NO	0	0	0	0	0	0	0	0	0.6	0	0	0	0.028571	-0.0143	0	0.4	-0.029	-0.03
10. X_NH to X_S	0	0	0	0.92	0	0	0.08	0	0	0	0	0.0755	-0.0008	-0.0063	0.012	0	0.0053	0.005
11. X_NO to X_S/P	0	0	0	0.92	0	0	0.08	0	0	0	0	0.0755	-0.0008	-0.0063	0.012	0	0.0053	0.005
12. X_AN to X_S/P	0	0	0	0.92	0	0	0.08	0	0	0	0	0.0514	-0.00073	0.0019	0.011	0	0.0017	0.002
13. Direct pass S_I	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14. Direct pass X_I	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15. S_alk	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0

Top: Petersen section Anammox model ('origin'). Bottom: Petersen section ASM1 model ('destination'). Columns in grey correspond with (compensation) state variables that are not passed on in the interface.

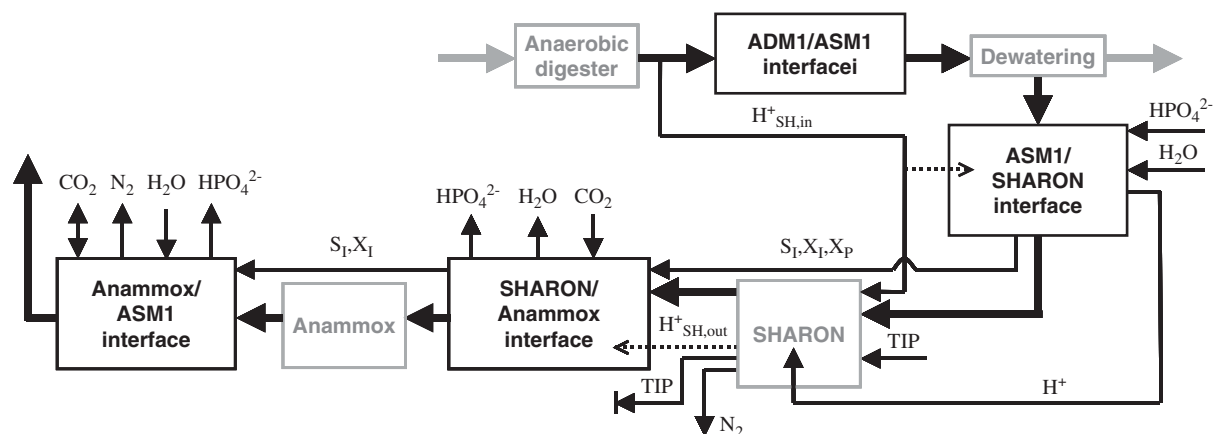


Fig. 5 – Construction of the ASM1/SHARON, SHARON/Anammox and Anammox/ASM1 model interfaces: direct pass-through of variables and fate of compensation state variables.

other. So, care must be taken to define independent transformation reactions for all components of the origin model (step 1).

By implementing the transformation matrices between in fluxes and out fluxes, coupling of the resulting models maintaining continuity is realized at every time step. During the interfacing, it is important to check that all transformation rates ρ_j are positive, to ensure that the transformation is carried out in the right direction, i.e. from the source to the destination model (Vanrolleghem et al., 2005).

4. Conclusions

This paper discusses the use of the general CBIM for the construction of model interfaces, taking into account conservation principles. The approach is illustrated for a plant-wide simulation case study, in which the effect of sludge digestion reject water treatment by means of the combined SHARON-Anammox process is evaluated on plant-wide scale, using the BSM2 to simulate the behaviour of a complete WWTP including sludge digestion. For this case study, model interfaces have been constructed between the models ASM1/SHARON, SHARON/Anammox and Anammox/ASM1, in such a way that the continuity of COD, C, N, H, O, P and charge is maintained. Avoiding leaks of elements is indeed essential in model coupling. In this respect, the authors also want to stress the desirability to check the existing BSM2 model interfaces and revise them where necessary, so that not only continuity of COD and N, but also of all other elements is guaranteed.

Special points of attention during the construction of model interfaces in general and more specifically when using the CBIM approach were pointed out, e.g. how the order in which the elemental balances are closed and the choice of sink/source components can minimize the number of compensation components required, as well as the values of their stoichiometric coefficients. Besides, special attention was given to the construction of interfaces between models in which pH is considered as a state variable and lumped state variables are used to represent the sum of concentrations of

different equilibrium components. Although the method was illustrated for a specific case, it was described in such way that it can easily be generalized and used in other applications.

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