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An ASM/ADM model interface for dynamic plant-wide simulation

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ABSTRACT

Mathematical modelling has proven to be very useful in process design, operation and optimisation. A recent trend in WWTP modelling is to include the different subunits in so-called plant-wide models rather than focusing on parts of the entire process. One example of a typical plant-wide model is the coupling of an upstream activated sludge plant (including primary settler, and secondary clarifier) to an anaerobic digester for sludge digestion. One of the key challenges when coupling these processes has been the definition of an interface between the well accepted activated sludge model (ASM1) and anaerobic digestion model (ADM1). Current characterisation and interface models have key limitations, the most critical of which is the over-use of X_c (or lumped complex) variable as a main input to the ADM1. Over-use of X_c does not allow for variation of degradability, carbon oxidation state or nitrogen content. In addition, achieving a target influent pH through the proper definition of the ionic system can be difficult. In this paper, we define an interface and characterisation model that maps degradable components directly to carbohydrates, proteins and lipids (and their soluble analogues), as well as organic acids, rather than using X_c. While this interface has been designed for use with the Benchmark Simulation Model No. 2 (BSM2), it is widely applicable to ADM1 input characterisation in general. We have demonstrated the model both hypothetically (BSM2), and practically on a full-scale anaerobic digester treating sewage sludge.

1. Introduction

In the last decade, substantial efforts have been directed towards the development of a standardized benchmark simulation model for activated sludge processes (BSM1). It should be stressed that this benchmark model does not aim for a completely accurate description of all unit processes involved. Its purpose is to allow for the unbiased evaluation of different control strategies under realistic conditions (Spanjers et al., 1998; Copp, 2002). However, control strategies that are good practice for the biological process step may well be non-optimal for other process units in the plant.

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To address this limitation of BSM1, a conceptual plant-wide benchmark simulation model (BSM2) has been developed that includes both the biological treatment step (activated sludge) and the sludge train (thickening, anaerobic digestion and dewatering) (Jeppsson et al., 2006, 2007; Vrecko et al., 2006; Nopens et al., 2008). In this way, control strategies can be evaluated on a plant-wide scale. An overview of the BSM2 plant layout is given in Fig. 1.

A complicating factor in plant-wide modelling is the fact that not all wastewater treatment unit processes have a common set of state variables. One example is the coupling of the activated sludge unit and the secondary clarifier. Models for the latter often use total suspended solids (TSS) as a state variable, whereas this state is often not explicitly used in models for the activated sludge unit (e.g. ASM1 (Henze et al., 1987)). TSS can be calculated as a composite variable from the activated sludge state variables, but it is not a state variable. Another example of two biological process models that use different sets of state variables is ASM1 and the anaerobic digester model, ADM1 (Batstone et al., 2002).

There are two common approaches to deal with this: 1) the supermodel approach where a complete set of states applicable in both aerobic and anaerobic environments is defined (Jones et al., 2007); 2) the interface approach which defines the mapping of compounds between established models. The latter approach forms the basis of this paper to interface the ASM1 and ADM1 models. Recent efforts for interfacing these specific biological units have been made by Copp et al. (2003) and Zaher et al. (2007), while more generally applicable methodologies have been suggested by others (Vanrolleghem et al., 2005; Volcke et al., 2006).

Another important issue is the balance between capturing important characteristics of the system and maintaining a reasonable level of complexity. Plant-wide models are typically complex in nature due to the number of unit processes involved. It is, therefore, important to reduce the amount of complexity of these interfaces as much as possible. In that respect, the more generalized and complex Continuity Based Interface Methodology (CBIM) (Vanrolleghem et al., 2005; Volcke et al., 2006), while excellent as a basis for directed models, is not ideal for specific cases.

In addition, the problems of input models in general to ADM1 are well known. ADM1 has, as inputs, a mixture of carbohydrates, proteins, and lipids (as well as their soluble analogues), and organic acids, bicarbonate, and ammonia. In practice, this broad array of components is difficult or even impossible to measure, particularly on a dynamic basis. To overcome this, the ADM1 Task Group proposed a generalized pool of complex material "X_c", which was intended to handle any complex input. In practice, though, this has proven inappropriate as a generalised input because the COD:mass ratio of this component is fixed. With a fixed ratio, the input COD type is also fixed, which can cause incorrect model predictions (especially methane gas composition). This led to theoretical and practical input models, including those of Kleerebezem and van Loosdrecht (2006) and Yasui et al. (2006).

This has led to the need to consolidate the research done with regard to input models for ADM1 with the research concerning generalised CBIM interfaces. The model proposed in this paper provides a highly applicable input/interface model to ADM1, specifically for use with primary and activated sludges (and mixes of the same), but is applicable also more widely. In particular, we propose a new interface/input model, based on Copp et al. (2003), but avoiding the use of X_c, while maintaining general continuity. In addition, an ADM1 to ASM1 interface, based on similar principles, is proposed. As the ADM1 to ASM1 interface involves state simplification, it does not have the degrees of freedom that the ASM1 to ADM1 interface contains, but it is important to define.

2. Characteristics of the Copp interface

The Copp interface for converting a set of ASM1 state variables into a set of ADM states is based on the conservation of both COD and TKN. It uses a lump–delump approach as illustrated

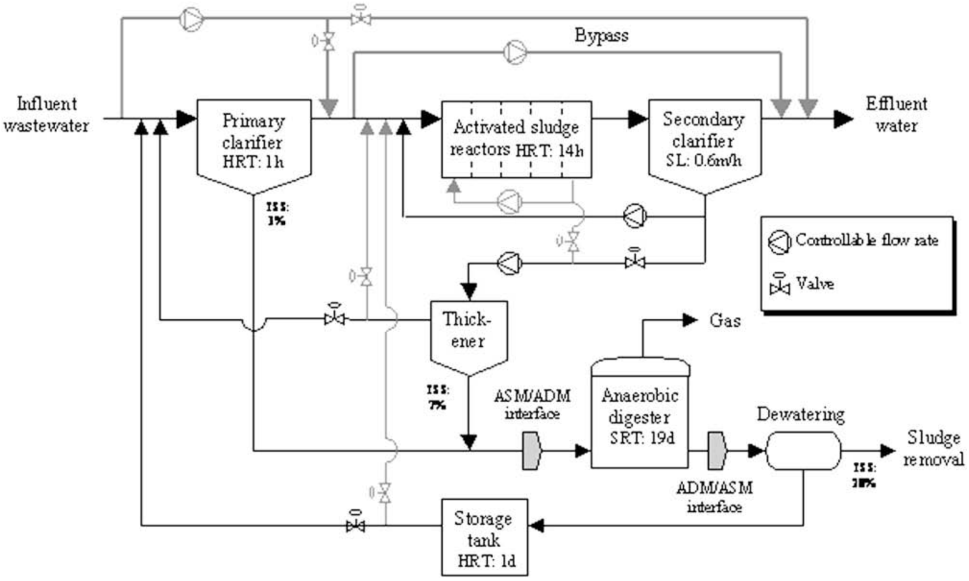

Fig. 1 – Overview of the BSM2 plant layout (Jeppsson et al., 2006).

in Fig. 2. Hence, all ASM1 COD states are pooled and stepwise distributed to ADM1 COD states. A similar approach is used for TKN. The approach consists of different steps and has built-in safety features in order to handle abnormal situations:

(1) All negative COD (i.e. oxygen and nitrate) is subtracted from the COD pool with an associated loss of substrate (S_S, X_S, X_{BH}, X_{BA} in that order).
(2) Readily biodegradable COD and organic nitrogen (S_S and S_{ND}) are converted into amino acids (S_{aa}). Indeed, the latter can be considered as a readily biodegradable fraction containing both COD and nitrogen.
(3) Any remaining S_S is mapped to sugars (S_{su}) that can be considered a readily degradable COD substrate in ADM1, not containing any nitrogen.
(4) Soluble inerts are mapped to soluble inerts considering the possibility of different nitrogen fractions in ASM1 and ADM1 associated with this material.
(5) Particulate inerts (both X_I and X_P) are mapped in a similar fashion to ADM1-X_I while checking to ensure there is sufficient organic nitrogen for this transition. Any unmapped inerts are added to the COD pool.
(6) The COD pool is then mapped to the composite material (X_c) state (taking into consideration the available organic nitrogen). If nitrogen is limiting, then the COD is mapped to carbohydrates and lipids. Any remaining nitrogen at this point is mapped to the ADM1 inorganic nitrogen state. The interface conserves both COD and TKN balances.

Results of the ASM1 to ADM1 transition for both primary and secondary sludges as calculated by the Copp interface are shown in Fig. 3. It can be seen that in both cases the major ADM1 fractions present are composites and particulate inerts (X_c and X_I). These ADM1 state variables were subsequently fed to the anaerobic digester and some differences are observed. Primary sludge led to a pH of 7.07 and secondary sludge led to a digester pH of 7.16 (steady state results for a mesophilic reactor (35 °C) and a retention time of 20 days). This is in agreement with values observed in practice. No major differences in state composition could be observed, and the pH-difference is likely due to increased inorganic nitrogen (S_{IN}) concentration from secondary sludge. Another criterion to verify the realistic performance of the interface is the methane production (MP). This can be obtained from the gas flow rate and the methane partial pressure in the gas phase through the general gas law as

$$MP = \frac{16}{RT} p_{gas,CH_4} Q_{gas}$$

where $\rho_{gas,\ CH_4}$ is the partial pressure of methane in the gas phase and Q_{gas} the total gas flow rate. When MP is normalized according to VSS content of the respective sludge loads it is observed that only 27% more methane production (per kg VSS) is achieved from the primary sludge compared to the secondary sludge (from activated sludge system with nutrient removal and long sludge age) using the Copp interface. This difference is considered unrealistically low compared to results observed in research (Svärd, 2003) and practice (Gossett and Belser, 1982; Siegrist et al., 2002). However, it is clear that more realistic results can be achieved if different

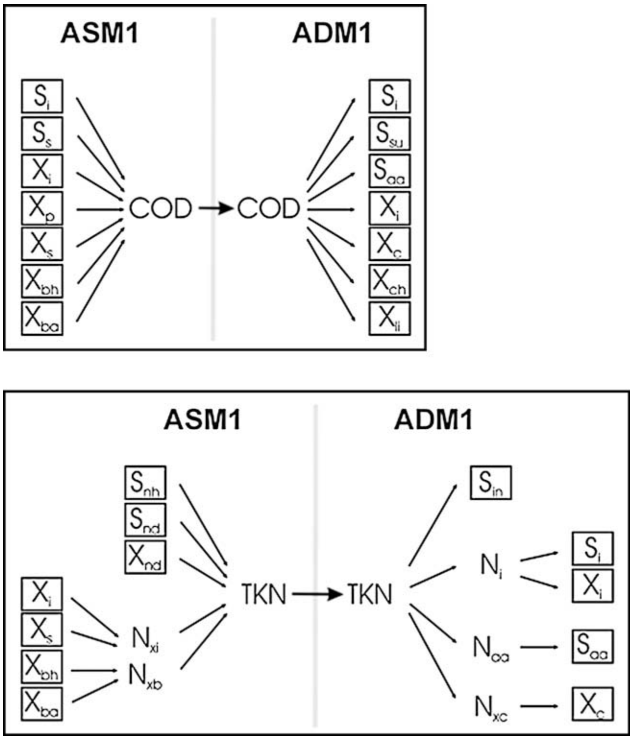

Fig. 2 – Illustration of the lump–delump approach of the Copp interface (after Copp et al., 2003).

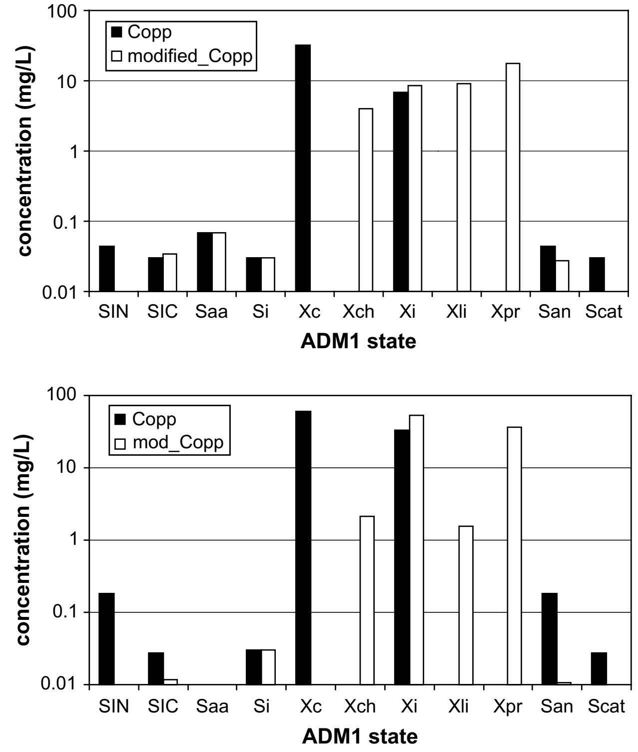

Fig. 3 – Comparison of the ADM1 states after passing the ASM1–ADM1 interface for both the Copp and modified Copp interface: primary sludge (top) and secondary sludge (bottom). Note: logarithmic scale.

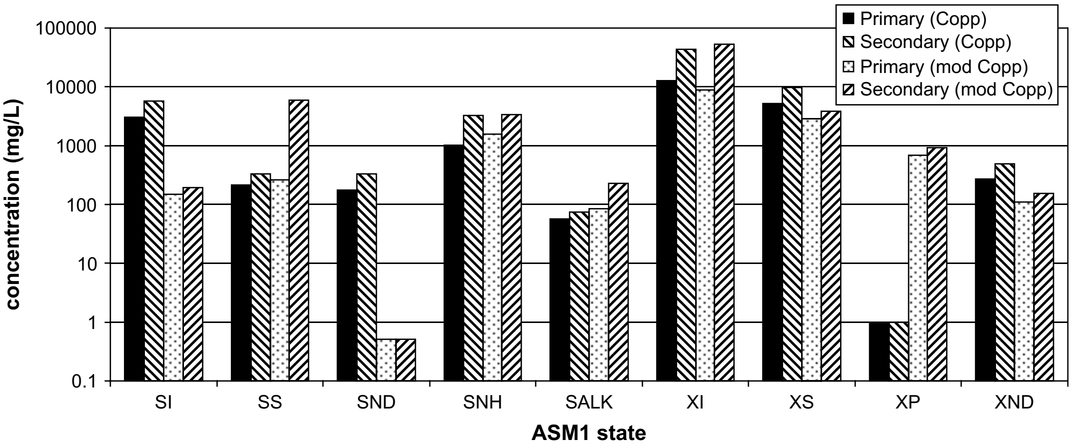

Fig. 4 – Comparison of the ASM1 states after passing the ADM1–ASM1 interface for both the Copp and modified Copp interface and for both primary and secondary sludges. Note: logarithmic scale.

parameter sets would be used for primary and secondary sludges in the Copp interface.

The effluent of the digester needs to be reconverted into ASM1 state variables prior to being recycled back to the plant (reject water). Copp et al. (2003) also proposed an interface to establish this transformation. Results for the primary and secondary sludges expressed as ASM1 variables using this interface are shown in Fig. 4. The outcome in terms of composition is similar in both cases: (1) particulate and soluble inert material were major constituents, (2) a reasonable amount of slowly biodegradable material (X_S) was present and (3) a large ammonia fraction was calculated. The latter is to be expected in reject water, but the predicted soluble inert fraction could result in unrealistically large concentrations (see Fig. 4) in the biological system.

In order to overcome the problems described above, Copp interfaces were analysed in an attempt to identify which steps were responsible for the large amount of soluble inerts and the poor gas production from primary sludge compared to secondary sludge. The maximization of composite material in the influent to the digester has two drawbacks: (1) it decreases the overall transformation rates as the disintegration process is the slowest and (2) it allows for direct production of particulate inerts from the influent sludge. Another important issue is the fact that the default decomposition of X_c in ADM1 is based on a secondary sludge. As all ASM1 COD is lumped and converted to X_c, primary sludge will be lumped with secondary sludge, unless the internal structure is modified to represent complex fractions, with two parallel disintegration processes. The use of composite material as a general input variable as defined in ADM1 also leads to a more general problem. It links the disintegration of influent particulate materials (e.g. from primary and secondary sludges) with different characteristics to the disintegration of products from biomass decay created within the digestion process. The creation of such correlations between materials with very different characteristics represents a fundamental problem (Wett et al., 2006).

The preceding discussion explains the source of the problems encountered with the Copp interface. Two possible solutions can be adopted:

- The Copp interface approach is maintained and the COD pool is only partly converted to composites to lower the inert fraction, with the remaining COD distributed over lipids, carbohydrates and proteins, in different fractions for primary and secondary sludges, resulting in a need for separate interfaces to handle different sludges;
- The Copp interface approach is modified at the incoming state variable level to consistently convert both primary and secondary sludges. In this way one single interface could deal with different sludges.

The latter was adopted as the more general and elegant solution.

3. Conversion requirements for ASM–ADM and ADM–ASM interfaces

While the interface we propose here can be used in a number of applications, its principal application is wastewater treatment systems. Typical influents received by an anaerobic digester in wastewater treatment systems are sludges from the underflow of the primary clarifier (primary sludge) and sludges from the underflow of the secondary clarifier further thickened in a thickener unit (secondary sludge). The interface behaviour can be judged at several points: (1) ADM1 state variables prior to the digester, (2) ADM1 state variables after the digester and (3) ASM1 state variables after the digester.

The composition of primary and secondary sludges used for interface testing was obtained through simulation of the well-described BSM1 plant extended with a primary clarifier and a thickener. The characteristics describing the influent wastewater were taken from Gernaey et al. (2006) and resulted in the sludge compositions shown in Table 1. As expected, the simulated primary sludge mainly consists of slowly biodegradable particulate material (X_S), with a significant inert particulate and heterotrophic biomass fraction (X_I and X_{BH}). It has a TSS content of about 3%, determined by the primary clarifier model. The primary clarifier was assumed to have a TSS removal efficiency of 50% at this influent loading rate. In contrast, the secondary sludge is mainly biomass (X_{BH} and

X_{BA}) and inert particulate material (X_I) together with inert particulates resulting from biomass decay (X_P). The thickener model had a fixed underflow concentration of 7% TSS.

4. Modified Copp interface

4.1. *ASM1 to ADM1 conversion*

The steps of the modified Copp interface to convert state variables from ASM1 to ADM1 are depicted in Fig. 5 (top). Unlike the lump–delump approach used in the Copp interface, it was decided to convert the different ASM1 sludge fractions independently. The first two steps are identical to the Copp interface, i.e. remove any remaining COD-demand and convert readily biodegradable COD and TKN into amino acids and sugars (see previous section). In step 3, a similar principle as used in step 2 is adopted for the particulate biodegradable fractions of both COD and nitrogen (X_S and X_{ND}). The required amount of X_S needed to convert all X_{ND} into proteins can be calculated. If there is excess X_S, the remainder is allocated to lipids (70%) and carbohydrates (30%). These percentages are currently an arbitrary choice of values, based on comparative fractions of lipids and carbohydrates in primary sludge (Siegrist et al., 2002). As stated below (step 4), the mix for secondary sludge is 40% lipids and 60% carbohydrates. If there

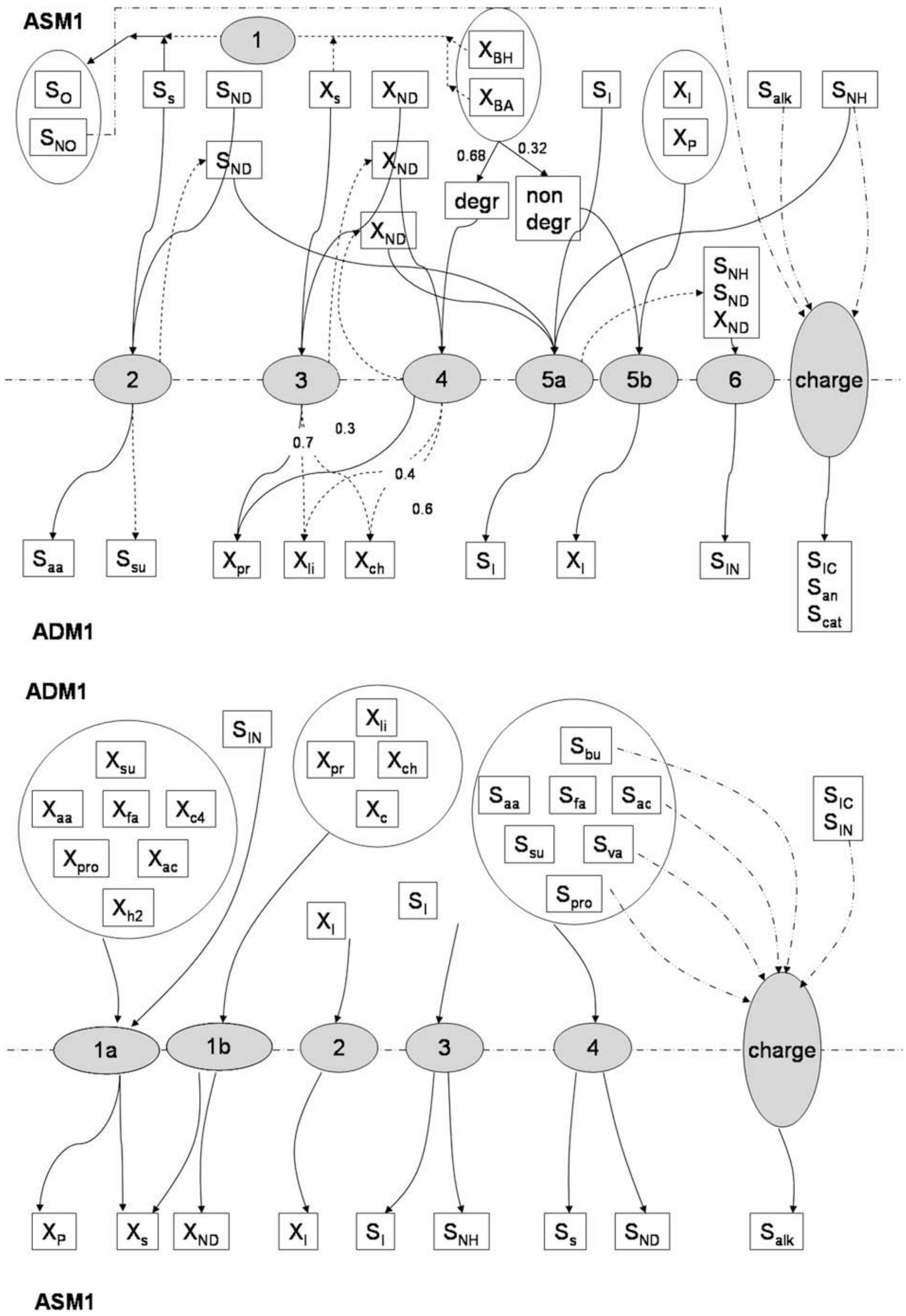

Fig. 5 – Approach of the modified Copp interface. ASM1 to ADM1 (top), ADM1 to ASM1 (bottom).

is excess X_{ND}, it is used in the biomass allocation step below. Step 3 allows for the distinction between primary and secondary sludges as the X_S content is very different in the two sludges (Table 1). Another major difference compared to the Copp interface is the fact that the conversion is made directly into lipids, carbohydrates and proteins. Hence, the disintegration step for influent sludge is bypassed and thereby reduces the immediate production of inert material inside ADM1. This will avoid secondary kinetics and the direct formation of particulate inerts imposed by the disintegration step. The disintegration step of ADM1 remains active for the biomass decay products produced within the digester. In step 4, biomass is directly converted into proteins, lipids, carbohydrates and inerts. The proteins formed use the nitrogen present in the sludge and, if necessary, any remaining X_{ND}. Any remaining anaerobically biodegradable biomass COD-fraction is mapped to lipids (40%) and carbohydrates (60%). These values were chosen in order to maintain a COD:mass ratio of 1.42 g COD/g VS (based on the assumed biomass composition ($C_5H_7O_2N$) in both the ASM and ADM models). This COD:mass ratio can be varied in situations where the COD:mass ratio of activated sludge varies significantly from the norm. Step 5 directly maps the ASM1 particulate inerts (X_I, X_P and the non-biodegradable biomass COD-fraction) into ADM1 particulate inerts. This is possible provided the inert N-content is the same in both ASM1 and ADM1, otherwise some special rules have to be applied to ensure mass balances for both COD and N. Furthermore, it is assumed that aerobically inert material is also anaerobically inert (Ekama et al., 2007). The soluble inert fraction cannot be mapped directly due to the higher soluble N-content in ADM1 compared to ASM1 (6% vs 0% using default values). For this mapping, nitrogen is taken from any remaining S_{ND}, X_{ND} and S_{NH} (in that sequence). In the case when not enough nitrogen is available, the remaining soluble inert COD is mapped to carbohydrates (no N-content) and a warning is issued to the user. However, the interface is written in a general form allowing the user to modify the parameters representing the nitrogen content of the various inert fractions of the ASM and ADM variables. Step 6 maps any remaining nitrogen (S_{ND}, X_{ND} and S_{NH}) to the inorganic nitrogen fraction of ADM1. At this point the proposed interface conserves both COD and TKN balances.

In a final step, the inorganic carbon fraction (S_{IC}), which will be fed to ADM1, is calculated. This is done as part of the charge interface. To adopt the expression for calculation of S_{IC} in the interface, a charge balance needs to be defined on both sides of the interface. The following components in ASM1 and ADM1 are assumed to exhibit a charge (all other components have zero charge):

- ASM1: S_{alk}, S_{NH}, S_{NO} check in rebuttal
- ADM1: S_{AC}, S_{PRO}, S_{BU}, S_{VA}, S_{IN}, S_{IC}.

For the ASM1/ADM1/ASM1 interface, the charge balance can be written as

$$\left[S_{alk}\alpha_{alk}^{ch} + S_{NH}\alpha_{NH}^{ch} + S_{NO}\alpha_{NO}^{ch}\right]_{ASM1} = \left[S_{AC}\alpha_{AC}^{ch} + S_{PRO}\alpha_{PRO}^{ch} + S_{BU}\alpha_{BU}^{ch} + S_{VA}\alpha_{VA}^{E} + S_{IN}\alpha_{IN}^{ch} + S_{IC}\alpha_{IC}^{ch}\right]_{ADM1}$$

The α_i^{ch}-terms refer to the charge per unit of component. For components comprising different equilibrium forms (ratio determined by the pH) (e.g. S_{AC} comprises both Ac^- and HAc), their charge calculation is also pH-dependent. Calculation of α_i^{ch} will be developed later for all charged ADM-components (the charged ASM-components have a fixed charge as no pH calculation is performed). Note that H^+ and OH^- are, therefore, implicitly present in the above charge balance.

When using this balance for the ASM1/ADM1 interface, the concentrations on the left-hand-side are all known. The ones on the right-hand-side (RHS), except for the inorganic carbon (S_{IC}), are all known as a result of the interface calculations. The fact that S_{IC} is not defined yet provides the necessary degree of freedom to ensure the charge continuity of the interface. Rearranging the charge balance yields the following expression for S_{IC}:

$$S_{IC} = \frac{\left[S_{alk}\alpha_{alk}^{ch} + S_{NH}\alpha_{NH}^{ch} + S_{NO}\alpha_{NO}^{ch}\right]_{ASM1} - \left[S_{AC}\alpha_{AC}^{ch} + S_{PRO}\alpha_{PRO}^{ch} + S_{BU}\alpha_{BU}^{ch} + S_{VA}\alpha_{VA}^{ch} + S_{IN}\alpha_{IN}^{ch}\right]_{ADM1}}{\alpha_{IC}^{ch}}$$

As mentioned before, all species concentrations on the RHS are known (they were derived in the previous steps). However, the values of α_i^{ch} need to be determined. The latter is not straightforward as some of these factors are pH-dependent because of their chemical equilibria (e.g. $NH_4^+ \leftrightarrow NH_3 + H^+$).

In the ASM1/ADM1 realm, only nitrate and alkalinity have a fixed charge of −1 per mole (i.e. in case of nitrate −1 for 14 g of nitrogen). VFAs are almost completely (negatively) charged at normal pH (at pH = 6.8 about 99% of the VFAs are negatively charged). In contrast, at pH = 5.8, only 90% of the VFAs are negatively charged. Equations to calculate the charge of a VFA-component are quite straightforward:

$$\alpha_{AC}^{ch} = \alpha_{PRO}^{ch} = \alpha_{BU}^{ch} = \alpha_{VA}^{ch} = \frac{-1/C_i}{1 + 10^{pK_a - pH}}$$

where $pK_a = 4.76$, 4.88, 4.82, 4.86, respectively at 25 °C and $C_i = 64$, 112, 160, 208.

Similarly, the charge for ammonia is essentially +1 per - mole (or +1/14 per g N) at neutral pH, or mathematically:

$$\alpha_{IN}^{ch} = \frac{10^{pKa - pH}}{1 + 10^{pK_a - pH}}$$

where $pK_a = 9.25$ at 25 °C.

The charge balance is therefore as follows, including the OH^- and H^+ ions:

$$0 = \left[S_{AC}\alpha_{AC}^{ch} + S_{PRO}\alpha_{PRO}^{ch} + S_{BU}\alpha_{BU}^{ch} + S_{VA}\alpha_{VA}^{ch} + S_{IN}\alpha_{IN}^{ch} + S_{IC}\alpha_{IC}^{ch} + OH^- - H^+ + S_{AN} - S_{CAT}\right]_{ADM1}$$

where $H^+ = 10^{-pH}$, $OH^- = 10^{(-pK_w + pH)}$ and $pK_w = 14$

or

$$S_{CAT} - S_{AN} = S_{AC}\alpha_{AC}^{ch} + S_{PRO}\alpha_{PRO}^{ch} + S_{BU}\alpha_{BU}^{ch} + S_{VA}\alpha_{VA}^{ch} + S_{IN}\alpha_{IN}^{ch} + S_{IC}\alpha_{IC}^{ch} + OH^- - H^+$$

This problem has two degrees of freedom, with the unknown variables being S_{CAT}, S_{AN}, and pH (which effectively set all α-values, as well as OH^-, and H^+), and a single equation (thus removing a degree of freedom). To remove the other degree of freedom, the pH of the influent to the digester can be set. In our case, we set it to a nominal pH of 7.0 (as no pH calculation is included in ASM), but actual pH values can be used, if available. The remaining degree of freedom can be removed by setting either S_{CAT} or S_{AN} to zero.

When S_{CAT} exceeds S_{AN}, S_{AN} is set to zero and the charge balance can be closed through:

$$S_{CAT} = S_{AC}\alpha_{AC}^{ch} + S_{PRO}\alpha_{PRO}^{ch} + S_{BU}\alpha_{BU}^{ch} + S_{VA}\alpha_{VA}^{ch} + S_{IN}\alpha_{IN}^{ch} + S_{IC}\alpha_{IC}^{ch} + OH^- - H^+$$

When S_{AN} exceeds S_{CAT}, S_{CAT} is set to zero and the charge balance can be closed through:

$$S_{AN} = -1\left(S_{AC}\alpha_{AC}^{ch} + S_{PRO}\alpha_{PRO}^{ch} + S_{BU}\alpha_{BU}^{ch} + S_{VA}\alpha_{VA}^{ch} + S_{IN}\alpha_{IN}^{ch} + S_{IC}\alpha_{IC}^{ch} + OH^- - H^+\right)$$

All parameters used in the modified Copp interface are summarised in Table 2.

4.2. *ADM1 to ASM1 conversion*

For reasons of consistency, the existing ADM1 to ASM1 interface of Copp et al. (2003) was modified using similar reasoning. The different steps are depicted in Fig. 5 (bottom). In a first step, biomass is converted to X_P and X_S taking into account the corresponding nitrogen fractions (6 and 3.76%, respectively). The biomass itself serves as a nitrogen source. If insufficient nitrogen is available from this source, inorganic nitrogen can be used. The remainder of the particulate COD (X_c, X_{pr}, X_{li}, X_{ch}) is directly mapped to X_S. The nitrogen associated with proteins is mapped to X_{ND}. In a second step, the particulate inerts are directly mapped (again assuming the same nitrogen content in ADM1 and ASM1). Step 3 maps soluble inerts taking into account the different nitrogen fractions. Any remaining inorganic nitrogen is mapped to ammonia. In step 4, all soluble COD states (S_{su}, S_{aa}, S_{fa}, S_{va}, S_{bu}, S_{pro} and S_{ac}) are mapped to soluble COD (S_S). The nitrogen associated with the amino acids is mapped to S_{ND}. As a final step the charge balance is used to calculate the alkalinity in a similar fashion as in the ASM1 to ADM1 interface:

$$S_{alk} = \frac{\left[S_{AC}\alpha_{AC}^{ch} + S_{PRO}\alpha_{PRO}^{ch} + S_{BU}\alpha_{BU}^{ch} + S_{VA}\alpha_{VA}^{ch} + S_{IN}\alpha_{IN}^{ch} + S_{IC}\alpha_{IC}^{ch}\right]_{ADM1} - \left[S_{NH}\alpha_{NH}^{ch}\right]_{ASM1}}{-1}$$

5. Behaviour of the modified Copp interfaces

5.1. *ASM1–ADM1 – ASM1: BSM case*

The behaviour of the modified Copp interface was tested in exactly the same way as the Copp interface. Results of the ADM1 composition prior to the digester are shown in Fig. 3 for the primary and secondary sludges. It can be seen clearly that a difference in composition is calculated with the two sludges using the modified Copp interface. X_c is no longer present as it is no longer "produced" in the interface definition. Primary sludge mainly consists of proteins, lipids, particulate inerts and carbohydrates, whereas secondary sludge contains large fractions of inerts and proteins and relatively small amounts of lipids and carbohydrates.

Differences in the composition of the anaerobic digester effluent based on the digester influent produced by the Copp and modified Copp interfaces are shown in Fig. 6 for primary

Table 1 – Composition of primary and secondary sludges entering the interface.

Variable	Description	Primary clarifier underflow	Thickener underflow	Unit
S_I	Soluble inert matter	30	30	g COD/m^3
S_S	Ready biodegradable matter	68.22	0.89	g COD/m^3
S_O	Dissolved oxygen	0.01	0.49	g COD/m^3
S_{NO}	Nitrate	0.19	10.17	g N/m^3
S_{NH}	Ammonia	31	1.74	g N/m^3
S_{ND}	Soluble organic nitrogen	6.83	0.69	g N/m^3
X_I	Particulate inert material	7148.21	24708.71	g COD/m^3
X_S	Slowly degradable matter	27987.36	1058.18	g COD/m^3
X_{BH}	Heterotrophic biomass	4043.27	54710.72	g COD/m^3
X_{BA}	Autotrophic biomass	8.49	3162.07	g COD/m^3
X_P	Biomass decay products	26.02	9693.65	g COD/m^3
X_{ND}	Particulate organic nitrogen	1464.99	75.66	g N/m^3
S_{ALK}	Alkalinity	29.95	27.14	kmol HCO_3^-/m^3

Table 2 – Parameters used in the Copp and modified Copp interfaces.

Parameter	Description (unit)	Values
Copp interface		
N_aa	Nitrogen content of amino acids (mole N/g COD)	0.007
N_I	Nitrogen content of inerts in ADM1 (mole N/g COD)	0.06/14
N_xc	Nitrogen content of ADM1 composites (mole N/g COD)	0.0376/14
f_xi	Anaerobic degradable fraction of X_I and X_P	0.05
f_chxc	Fraction carbohydrates formed from composites	0.2
f_lixc	Fraction lipids formed from composites	0.3
Modified Copp interface		
N_aa	Nitrogen content of amino acids (mole N/g COD)	0.007
f_rlixs	Lipid fraction of non-nitrogenous Xs	0.7
f_rxi	Anaerobic degradable fraction of biomass	0.68
i_nx	Biomass nitrogen content (mole N/g COD)	0.08
f_rlixb	Lipid fraction of non-nitrogenous biomass	0.4
nsi	Nitrogen content of soluble inerts in ASM1 (mole N/g COD)	0
nsi_adm	Nitrogen content of soluble inerts in ADM1 (mole N/g COD)	0.06

and secondary sludges, respectively (positive values indicate higher values for the Copp interface). For primary sludge, it can be seen that both soluble and particulate inert fractions have decreased significantly when using the modified Copp interface. Also, the level of composites decreased, while more biomass is produced. The latter is the result of the difference in the COD-division in the modified interface compared to the X_C default division present in ADM1. In the case of secondary sludge, a decrease in soluble inerts is observed for the modified Copp interface and an increase in particulate inerts is calculated. This is the result of the biomass mapping in the two interfaces. In the Copp interface, biomass is mapped to X_c, but in the modified version, a portion of the biomass (the non-biodegradable fraction) is mapped to X_I (this can be observed in Fig. 3 as well).

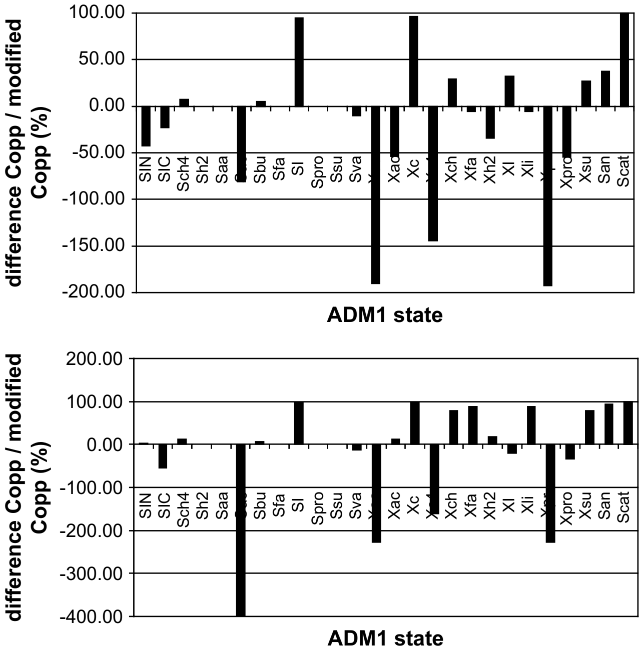

Fig. 6 – Differences between the digester effluents resulting from Copp and modified Copp digester influents for primary sludge (top) and secondary sludge (bottom) (positive values indicate higher values for the Copp interface).

Another indicator of the improved degree of realism with the modified Copp interface is the gas production. No significant differences in partial methane pressure in the headspace were observed compared to the Copp interface for both sludges. However, for the primary sludge a significantly larger gas flow rate was observed (2986 vs 1886 m^3/d). For the secondary sludge, a smaller gas flow rate was predicted (3200 vs 3470 m^3/d). Both of these results are consistent with the general interface characteristics – the original Copp interface simply utilized a component (X_c) that is inconsistent with primary sludge as defined by ADM1 which resulted in lower than expected performance (gas production) on primary sludge. Both interfaces produce similar results when mapping secondary sludge. Comparing methane yield, an increased amount is found for primary sludge (from 0.155 to 0.233 $kg\,CH_4\,kg\,VSS^{-1}$ and 0.233 to 0.344 $Nm^3\,CH_4\,kg\,VSS^{-1}$) and a decreased amount was calculated for secondary sludge (0.122–0.107 $kg\,CH_4\,kg\,VSS^{-1}$ and 0.178–0.158 $Nm^3\,CH_4\,kg\,VSS^{-1}$). In this example the primary sludge produced 117% more methane than the secondary sludge did which is in better agreement with literature values. For a general case this value will obviously vary somewhat depending on the sludge characteristics.

To evaluate the performance of the ADM1 to ASM1 interface only, the digester steady states obtained by using primary and secondary sludges, respectively, in combination with the modified ASM1 to ADM1 Copp interface were used as input. Results can be found in Fig. 7 and show a slight increase in ammonia (8 and 5% for primary and secondary sludge, respectively) and alkalinity for the modified interface. A more pronounced increase is observed for X_P and decreases for S_{ND}, X_{ND} and X_S were calculated.

5.2. ASM1 to ADM1: practical validation

To further validate the modified Copp interface, a practical test case was adopted. Data were obtained from a full-scale digester in Brisbane, Australia. The feed consisted of a mixture of primary and secondary sludge. The flow rate and volatile solids concentration in both streams were separately

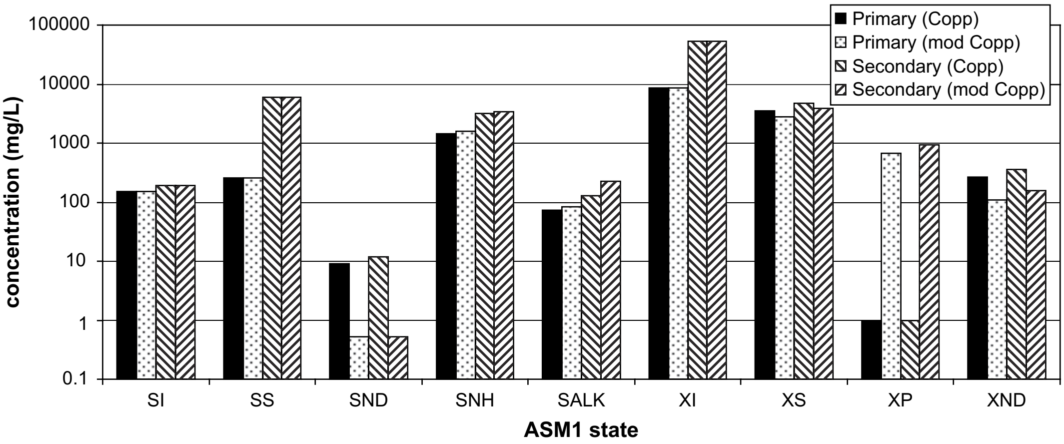

Fig. 7 – Comparison of the original and modified Copp ADM1 to ASM1 interface for both primary and secondary sludges. Note: logarithmic scale.

measured at least weekly (daily totals for flow rate), and COD was also measured, although less frequently. Primary sludge volatile and total solids concentrations were occasionally measured and the secondary sludge solids concentrations were intermittently measured. Primary sludge was converted from volatiles to COD by multiplying by 1.5 (from COD and volatiles measurements), and fractionated into 53% degradable (X_S) and 47% non-degradable (X_I), based on modeller experience of Australian primary sludge. The secondary sludge was converted from volatiles to COD by multiplying by 1.42, based on Henze et al. (1987), and fractionated to 72% heterotrophs/autotrophs and 28% inerts, based on an upstream model of the activated sludge process (7 day sludge age at 20–25 °C). In general, gas flow rate, gas composition, pH and effluent solids were well predicted, but only the gas flow rate showed substantial dynamics. A diagram showing the last 200 days of simulated and measured gas flow rates is given in Fig. 8a. As can be seen, the model predictions are in good agreement with the dynamic measurements.

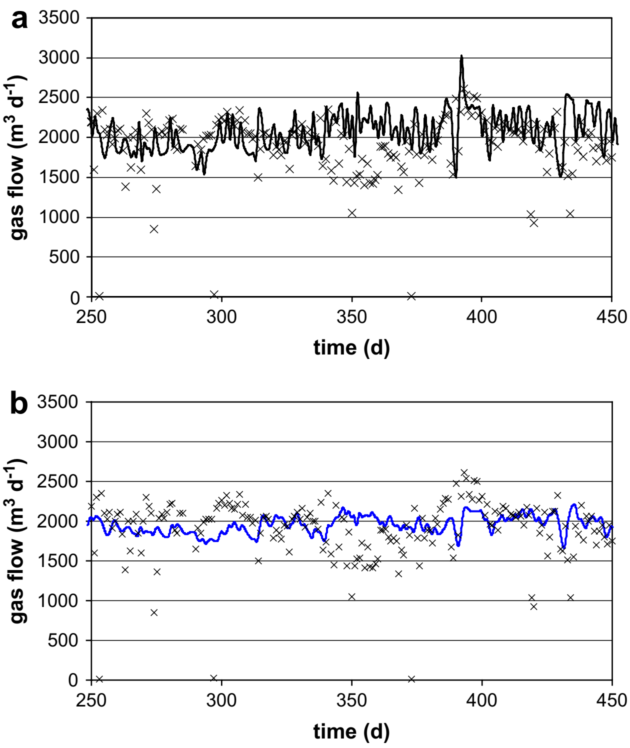

Fig. 8 – Model predictions (–) and measurements (x) of gas flow rate from a full-scale digester fed with mixed primary and activated sludges over 200 days using (a) the modified Copp interface and (b) the original Copp interface.

For comparison, the original Copp interface was also tested on this data set. However, significant additional fitting was required to increase disintegration rates (k_{dis} rate increased to 0.45 day^{-1}). The latter is too high for secondary sludge, but too low for primary sludge. Moreover, the X_C/X_I mix was set to 0.82 for secondary sludge (based on sludge age) and 0.80 for primary sludge (based on overall gas yield and effluent solids), respectively. After fitting, reasonable results were found, but still dynamics were slower in comparison to the currently proposed interface (Fig. 8b). The latter is clearly caused by the lumping of primary and secondary sludges in X_C. In addition, the physicochemical inputs needed to be set separately, requiring a higher level of user expertise. Therefore, the newly proposed interface can be considered superior as it needs much less effort.

6. Discussion

Interfacing activated sludge and anaerobic digestion and addressing the general problem of the composite material in ADM1 have been some of the most intensively addressed topics since publication of ADM1 (e.g. Copp et al., 2003; Huete et al., 2006; Kleerebezem and van Loosdrecht, 2006; Vanrolleghem et al., 2005; Wett et al., 2006). There are several important issues that have been partially addressed here:

6.1. *Primary sludge to ADM1*

The original ADM1 publication recommended use of the X_c variable for mapping of secondary sludge. As found by the

IWA Benchmarking Task Group, this is not adequate for mapping primary sludge, as it:

(a) results in two-step hydrolysis kinetics. In addition, in mixed primary and secondary sludge systems, the kinetics of hydrolysis of primary sludge are set to the kinetics of X_c hydrolysis, thereby imposing the slower secondary sludge kinetics on the hydrolysis of primary sludge;
(b) results in the excessive production of inerts during the "disintegration" of X_c; and
(c) fixes the COD:mass ratio to that of X_c. As primary sludge tends to be more energy rich than secondary sludge (e.g. due to higher lipids content), fixing this ratio limits the ability of the model to predict varying gas flow rates and compositions with different sludges.

The best alternative method, as proposed and demonstrated in this paper, is to map the organic compounds directly to total and soluble proteins, carbohydrates and lipids (amino acids, sugars and VFA), by explicitly using the ASM1 states.

6.2. *Secondary sludge to ADM1*

Using X_c as a mapping variable for secondary sludge is also not recommended in most circumstances. Secondary sludge composition can vary depending on upstream parameters, including sludge age. When the lumped parameter X_c is used, the impact that these upstream operational items might have, is masked and the true degradability of the influent might be misinterpreted. Using the interface proposed in this paper it should be possible (at a minimum) to obtain more realistic estimates of the sludge degradability.

6.3. *Preserving charge information*

Calculating a balanced ionic input set to the ADM1 can be a challenge, given variable bicarbonate, ammonia, organic acids and other buffers. The interface model proposed here removes much of this difficulty, as it can account for this, given a target input pH. The cases addressed here assumed a neutral ASM1-side pH but the interface can be easily adapted to allow for variable pH levels in other systems.

6.4. *Utility of a practical input/interface model*

It is accepted that to use ADM1, it is not necessary to measure all possible inputs present in the model, but instead, define inputs such as organic nitrogen, electrons (or COD), carbon (or mass) and particulate/soluble fractions. It is also accepted that this requires a limited subset of available measurements. Translation of measurements to ASM1 states is also widely done, and can facilitate subsequent translation to ADM1 states. However, translating from these measurements (or ASM1 state set) to ADM1 inputs in a consistent manner, using repeatable and documented assumptions is more difficult. Use of an interface model, such as the one proposed here can allow others to transparently and consistently translate inputs to ADM1. To further promote this interface, we have made the source code available as supplementary material. Although designed for primary and secondary sludges, the methodology is applicable to any feed where the COD:mass:N ratio is known.

7. Conclusions

As determined in this work, the drawbacks of the Copp interface model (and other interfaces, which utilise X_c) are; (1) production of excess inerts, (2) lumped characteristics of primary and secondary sludges and (3) low methane production from primary sludge. These issues can be addressed by sequential mapping to secondary components (carbohydrates, proteins and lipids) rather than the less flexible X_c state. Applying this concept in a modified interface model has shown that the digester performance on two different feed sludges (primary and secondary sludges) will be different using one single interface. A new approach to charge balancing also removes much of the guess work in equalising charges across the interface. States such as S_{IC}, S_{an} and S_{cat} can be consistently set. The modified interface results in a more widely applicable interface/input model and addresses most of the limitations in the X_C-based approach. Furthermore, this new interface allows the use of one interface for a range of input sludges, resulting in realistic gas production without the need for extensive parameter calibration. Validation was performed and showed that realistic behaviour was obtained.

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