

Towards an ASM1 - ADM1 State Variable Interface for Plant-Wide Wastewater Treatment Modeling

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Abstract

Plant-wide wastewater treatment modeling that combines the modeling of liquid and solids streams into one overall model is becoming increasingly popular. The idea of whole-plant modeling is complicated by the fact that the models used for each unit process have been for the most part developed in isolation, typically without consideration of the whole treatment process or other unit process models. Hence, each unit process model often uses a different set of state variables. This is especially true if the models were developed to describe fundamentally different biological processes like aerobic and anaerobic treatment. To overcome these differences and facilitate plant-wide modeling, model interfaces are used as a means to convert state variables from one model into state variables of a different model. Recently, there has been significant interest in incorporating a new anaerobic digestion unit process model - ADM1 (Batstone *et al.*, 2002) into the COST and IWA *simulation benchmarks* (Alex *et al.*, 1999; Pons *et al.*, 1999; Copp 2001; Copp *et al.*, 2002) to create a whole-plant simulation benchmark. To do this, an interface is needed to convert the activated sludge state variables to the anaerobic digestion state variables and *visa versa*. Standardised model interfaces are an essential component for allowing objective comparisons of simulation results within the wastewater treatment modeling community. This paper describes such a state variable interface.

Introduction

The availability of faster, more powerful computers has allowed the development of sophisticated mathematical models for the common unit processes used in wastewater treatment systems. Modeling of the wastewater treatment process has traditionally focused on either the liquid stream (i.e. primary sedimentation, the activated sludge process, and secondary clarification) or the sludge stream (i.e. thickening, digestion, dewatering) where assumptions are made with respect to the interaction of these two streams. For instance, a supernatant recycle from a sludge digester to primary sedimentation basins can be crudely modeled as another influent if the characteristics of that supernatant are known or assumed. Similarly, it is possible to model the sludge stream if the composition of the feed sludge streams from the liquid stream are assumed or known. This approach is commonly used, but plant-wide modeling that combines the liquid and sludge streams into one overall model is becoming increasingly popular.

The development of whole-plant modeling in the wastewater treatment field is extremely attractive to many as it provides a more global overview of the process and it allows for a more comprehensive understanding of the interactions of the various unit processes. Further, the impact of dynamic changes in the process can be explored as these changes relate to all the unit processes that may be present in a treatment scheme.

A complicating factor is that some wastewater treatment unit processes are biologically based and others are physically or chemically mediated and each model often has its own set of state variables. Activated sludge and secondary clarification are a case in point. The most commonly used clarification models use total suspended solids (TSS) as a state variable, but the common activated sludge models that are often used in combination with secondary clarification units in a process stream do not explicitly use TSS as a state variable. Total suspended solids can be calculated as a composite variable from the activated sludge state variables, but this requires some additional measurements and or assumptions.

The same holds true for different biological models that may be linked in a process stream. That is, even though the models may have been developed for biologically-mediated wastewater treatment processes, there is no guarantee that the different models will have a consistent set of state variables. A

further complication involves the actual meaning of the state variables and what they are meant to represent. Even if some of the state variables would appear to be the same (i.e. particulate inert COD), the state variable values may be very different in different models depending on the transformations that occur within the models. Also, as in the case of inert COD, material that is biologically inert under aerobic conditions may be degradable under anaerobic conditions so the mapping of seemingly similar state variables may not always be straightforward. Furthermore, care must be taken to ensure that mass balances are maintained in any state variable conversions.

A substantial effort has been directed towards the development of a standardized *simulation benchmark*, which will allow for the unbiased evaluation of different control strategies under realistic conditions (Alex *et al.*, 1999; Pons *et al.*, 1999; Copp 2001; Copp *et al.* 2002). As a continuation of that work, a conceptual plant-wide simulation benchmark has been developed that includes both activated sludge and anaerobic digestion. And so, to facilitate the conversion of state variables in this simulation benchmark specifically and whole-plant models in general an ASM1 (Henze *et al.* 1987) – ADM1 (Batstone *et al.*, 2002) interface has been developed and is presented in this paper.

Mass Balances

Crucial to any interface is the maintenance of mass balances after conversion. Because ASM1 and ADM1 are fundamentally different, it was decided that the mass balance emphasis in the conversions should be placed on COD and TKN and, where possible, on particular state variables but this was deemed to be less important due to these fundamental differences in the models. Listings of the state variables in each model are shown below in Table 1 (ASM1) and Table 2 (ADM1).

Table 1: State variables in ASM1.

State Variable Description	State Symbol	Units
Soluble inert organic matter	S_i	g COD m^{-3}
Readily biodegradable substrate	S_s	g COD m^{-3}
Particulate inert organic matter	X_i	g COD m^{-3}
Slowly biodegradable substrate	X_s	g COD m^{-3}
Active heterotrophic biomass	X_{bh}	g COD m^{-3}
Active autotrophic biomass	X_{ba}	g COD m^{-3}
Particulate products arising from biomass decay	X_p	g COD m^{-3}
Oxygen	S_o	g COD m^{-3}
Nitrate and nitrite nitrogen	S_{no}	g N m^{-3}
$\text{NH}_4^+ + \text{NH}_3$ nitrogen	S_{nh}	g N m^{-3}
Soluble biodegradable organic nitrogen	S_{nd}	g N m^{-3}
Particulate biodegradable organic nitrogen	X_{nd}	g N m^{-3}
Alkalinity	S_{alk}	mol L^{-1}

Table 2: State variables in ADM1.

State Variable Description	State Symbol	Units
Soluble inerts	S_i	kg COD m ⁻³
Monosaccharides	S_{su}	kg COD m ⁻³
Amino acids	S_{aa}	kg COD m ⁻³
Long chain fatty acids (LCFA)	S_{fa}	kg COD m ⁻³
Total valerate	S_{va}	kg COD m ⁻³
Total butyrate	S_{bu}	kg COD m ⁻³
Total propionate	S_{pro}	kg COD m ⁻³
Total acetate	S_{ac}	kg COD m ⁻³
Hydrogen gas	S_{h2}	kg COD m ⁻³
Methane gas	S_{ch4}	kg COD m ⁻³
Particulate inerts	X_i	kg COD m ⁻³
Composites	X_c	kg COD m ⁻³
Carbohydrates	X_{ch}	kg COD m ⁻³
Proteins	X_{pr}	kg COD m ⁻³
Lipids	X_{li}	kg COD m ⁻³
Sugar degraders	X_{su}	kg COD m ⁻³
Amino acid degraders	X_{aa}	kg COD m ⁻³
LCFA degraders	X_{fa}	kg COD m ⁻³
Valerate and butyrate degraders	X_{c4}	kg COD m ⁻³
Propionate degraders	X_{pro}	kg COD m ⁻³
Acetate degraders	X_{ac}	kg COD m ⁻³
Hydrogen degraders	X_{h2}	kg COD m ⁻³
Inorganic nitrogen	S_{in}	kmole N m ⁻³
Inorganic carbon	S_{ic}	kmole C m ⁻³
Anions	S_{an}	kmole m ⁻³
Cations	S_{cat}	kmole m ⁻³

From Table 1 and Table 2 it is clear that the default set of units are somewhat different in ASM1 and ADM1. Consequently care must be taken to avoid unit conversion errors when implementing the model interfaces. These simple, but common, implementation errors are not further discussed in this paper.

In each model, total COD (COD_t) is a composite variable calculated through the addition of the organic state variables while total Kjeldahl nitrogen (TKN) is a composite measure of organic nitrogen including ammonia. The following equations show how COD and TKN are calculated for the two models.

ASM1

$$\begin{aligned} \text{COD}_s &= S_i + S_s \\ \text{COD}_p &= X_i + X_s + X_{bh} + X_{ba} + X_p \\ \text{COD}_t &= \text{COD}_s + \text{COD}_p \end{aligned}$$

$$\text{TKN} = S_{nh} + S_{nd} + X_{nd} + i_{xb} (X_{bh} + X_{ba}) + i_{xe} (X_i + X_p)$$

where: COD_s = soluble COD
 COD_p = particulate COD
 COD_t = total COD
 TKN = total Kjeldahl nitrogen

Note: The equation listed above for the calculation of TKN_t is consistent with the COST and IWA simulation benchmark definitions. However, it should be recognized that there is some confusion related to organic nitrogen as described in the original ASM1 publication (comp. pgs 8 and 14 in Henze *et al.*, 1987). Because of this confusion, some implementations of ASM1 include a soluble inert organic nitrogen component that would be included in this TKN calculation. Nevertheless, for the purposes of this paper and for the simulation benchmarks, this soluble inert organic nitrogen has been left out of the calculation. Inclusion of this soluble nitrogen, will require minor changes to the algorithms presented here to maintain the applicable mass balances.

ADM1

$$\text{COD}_s = S_i + S_{su} + S_{aa} + S_{fa} + S_{va} + S_{bu} + S_{pro} + S_{ac} + S_{h2} + S_{ch4}$$

$$\text{COD}_p = X_i + X_{su} + X_{aa} + X_{fa} + X_{c4} + X_{pro} + X_{ac} + X_{h2} + X_c + X_{ch} + X_{pr} + X_{li}$$

$$\text{COD}_t = \text{COD}_s + \text{COD}_p$$

$$\text{TKN}_t = S_{in} + N_{xc} X_c + N_i (S_i + X_i) + N_{aa} (X_{pr} + S_{aa}) + N_{bac} * (X_{su} + X_{aa} + X_{fa} + X_{c4} + X_{pro} + X_{ac} + X_{h2})$$

As would be expected, these composite variable calculations are different in each model. It should also be noted that whereas the COD calculations are simply the sum of various state variables, the TKN is calculated as a sum of nitrogenous state variables plus the nitrogenous fraction of some organic state variables. For instance, ADM1 assumes that the composite state variable (i.e. X_c) contains organic nitrogen. The nitrogenous fraction is defined by N_{xc} such that the concentration of organic nitrogen associated with X_c is given by N_{xc} times X_c . Similar calculations are made for the other state variables assumed to contain a nitrogenous fraction. The need to account for this organically bound nitrogen stems from the fact that this organic nitrogen would be measured in a TKN measurement and so if the modeled TKN is to agree with the measured data then it must be included in the calculation. This, in and of itself, is not difficult or complicated, but it does pose unique problems when transforming one set of state variables into another because both the COD and TKN balances must be done simultaneously to ensure that both balances hold.

ASM1 → ADM1

The basic idea behind the conversion to ADM1 state variables is to maximize X_c (composites) S_{aa} (amino acids), S_i (soluble inert COD) and X_i (particulate inert COD) with respect to the available incoming nitrogen and COD. The approach described here makes use of state variable *degrees of freedom* to force the balances. In each case the degrees of freedom refer to state variables that are solely carbon (without nitrogenous fraction) or solely nitrogen (without carbon) and are used to close the balances when necessary. In this conversion, S_{su} (monosaccharides), X_{ch} (carbohydrates) and X_{li} (lipids) are used as the carbonaceous degrees of freedom as ADM1 assumes that none of these state variables has any associated nitrogen. Similarly, S_{in} (inorganic nitrogen) is used as the nitrogenous degree of freedom as it has no associated carbon. The following sections outline the proposed conversion algorithms. Schematic representations of the COD and TKN conversions are shown in Figure 1 and Figure 2. In this case, only the state variables shown in these figures are given values (if applicable) and all others are assumed to be zero at the point of conversion to anaerobic conditions.

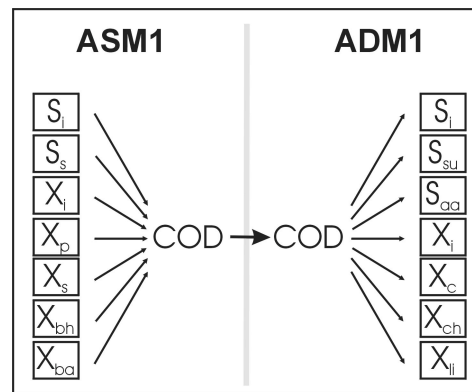


Figure 1: ASM1 to ADM1 state variable conversions for COD.

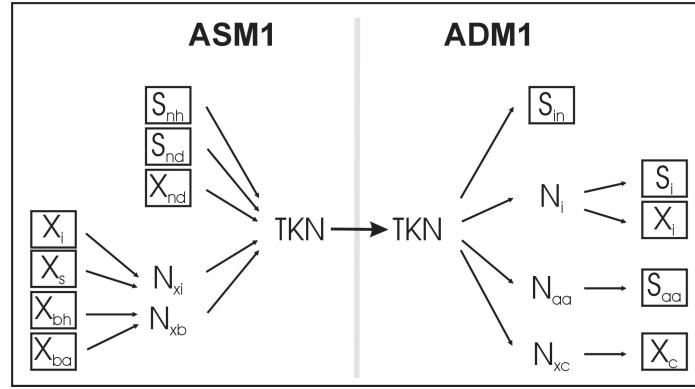


Figure 2: ASM1 to ADM1 state variable conversions for TKN.

COD Demand

The first step in the proposed conversion algorithm is to calculate the equivalent COD demand needed to reduce the electron acceptors present in the incoming stream. The COD demand is calculated as follows:

$$\text{COD}_{\text{demand}} = S_o + 2.86 S_{no}$$

where: $\text{COD}_{\text{demand}}$ = the COD required to reduce the incoming electron acceptors
 S_o = incoming dissolved oxygen (mg/L)
 S_{no} = incoming nitrate-nitrogen (mgN/L)

It is assumed that both oxygen and nitrate will be reduced instantaneously upon entering the anaerobic environment, so the total incoming COD is reduced by this incoming COD demand to compensate for the reduction of the electron acceptors present in the incoming stream. The total incoming COD is reduced in a step-wise manner until the COD demand has been satisfied. The reduction is based on a hierarchy of ASM1 state variables such that S_s is reduced by the $\text{COD}_{\text{demand}}$ first. If there is insufficient S_s present, then S_s is reduced to zero and the remaining demand is subtracted from X_s . If necessary, X_{bh} and X_{ba} may also need to be reduced. The hierarchy is shown in Figure 3.

Example: If the DO entering the digester is 5 mg/L and the nitrate is 10 mgN/L, then the $\text{COD}_{\text{demand}}$ is 33.6. If S_s entering the digester is 40 mg/L, then it is reduced to 6.4 mg/L and all other state variables are left unchanged. If S_s entering the digester is 10 mg/L, then S_s is reduced to zero and X_s is reduced by 23.6 mg/L.

$$S_s \rightarrow X_s \rightarrow X_{bh} \rightarrow X_{ba}$$

Figure 3: ASM1 state variable hierarchy for reducing the incoming total COD to compensate for the reduction of incoming oxygen and nitrate.

In the extreme case when not enough COD is available for the reduction of oxygen and nitrate, special actions must be taken (i.e. when $\text{COD}_{\text{demand}} > S_s + X_s + X_{bh} + X_{ba}$). The reduction of oxygen is first carried out and then as much nitrate as possible is reduced. Any excess nitrate is either stored as a special variable and allowed to pass through the digester unchanged or it is added to the pool of inorganic nitrogen. If there is excess oxygen, then this should simply be allowed to pass through the digester. In either case, a warning message should be presented to the user so that the influent characterization may be evaluated. Note that in this special case no biological reactions will take place in the anaerobic digester as there will be no biologically available COD in the influent.

Soluble Organic Nitrogen

The next step in the conversion involves calculating the appropriate allocation of soluble COD and nitrogen to the ADM1 amino acid state variable (S_{aa}). Soluble biodegradable organic nitrogen in ASM1 is represented by S_{nd} . In ADM1, soluble biodegradable organic nitrogen is not a state variable but rather is calculated as a fraction of S_{aa} . The equivalent S_{aa} needed in ADM1 to give a soluble biodegradable organic nitrogen equal to S_{nd} is given by:

$$\text{ReqCOD}_s = \frac{S_{nd}}{N_{aa}}$$

where: ReqCOD_s = required S_{aa} in ADM1

N_{aa} = nitrogen fraction of the amino acid state variable, S_{aa}

The calculated ReqCOD_s is compared to the available incoming readily biodegradable COD ($S_{s,in}$) and if sufficient $S_{s,in}$ is present, then:

$$S_{aa} = \text{ReqCOD}_s$$

and the remaining S_s (i.e. $S_{s,in} - \text{ReqCOD}_s$) is assigned to S_{su} . If there is insufficient $S_{s,in}$ present in the incoming stream then:

$$S_{aa} = S_{s,in}$$

and the remaining S_{nd} (i.e. $S_{nd} - S_{aa} * N_{aa}$) is added to the organic nitrogen pool. A schematic illustration of this step is shown in Figure 4.

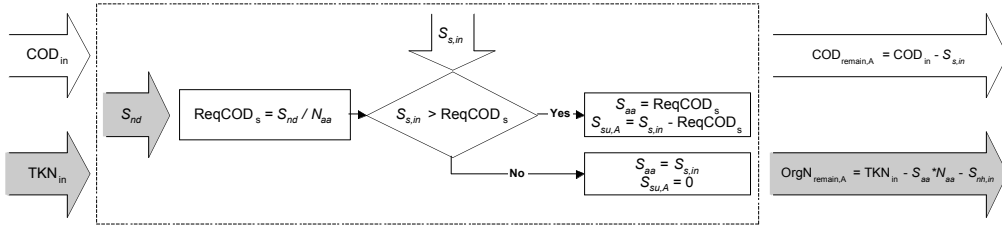


Figure 4: Schematic illustration of S_{nd} and S_s mapping.

Inert Organic Material

The next step involves mapping the soluble and particulate inert material. In this step, S_i (ASM1) is mapped to $S_{i,ADM1}$ and $f_{xi} * (X_p + X_i)$ from ASM1 is mapped to $X_{i,ADM1}$. Note that this assumes that some fraction ($1-f_{xi}$) of the aerobically inert COD in ASM1 is degradable anaerobically (otherwise f_{xi} should be set to 1 making all incoming inert COD also anaerobically inert). In this mapping of state variables, the available organic nitrogen is checked to ensure that sufficient nitrogen is available to satisfy the mass balances. That is, in ADM1 the required soluble inert organic nitrogen is given by:

$$\text{ReqOrgN}_s = S_i * N_i$$

If the pool of organic nitrogen is larger than ReqOrgN_s :

$$S_{i,ADM1} = S_i$$

If the pool of organic nitrogen is smaller than ReqOrgN_s :

$$S_{i,ADM1} = \frac{\text{OrgN}_{\text{remain,A}}}{N_i}$$

and the remaining S_i (i.e. $S_i - \text{OrgN}_{\text{remain,A}} / N_i$) is added to S_{su} .

The remaining pool of organic nitrogen is reduced by $S_{i,ADM1} * N_i$. A schematic illustration of this step is shown in Figure 5.

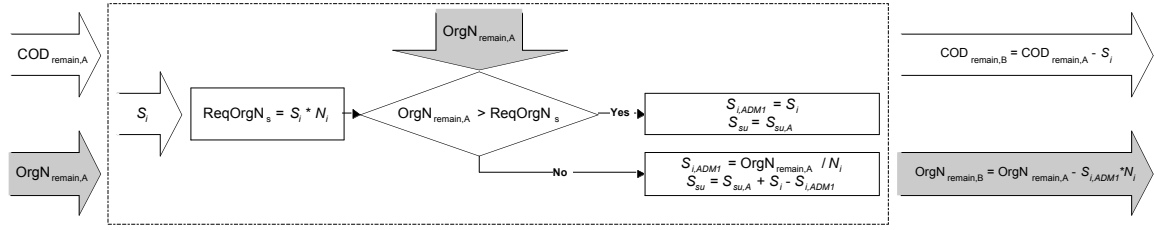


Figure 5: Schematic illustration of soluble inert COD mapping.

This approach is somewhat of a paradox. As the soluble inert material in ASM1 does not have an associated nitrogen component whereas the soluble inert material in ADM1 has, nitrogen must be taken from the pool of other available nitrogen in ASM1 in order to complete this transformation (to maintain the mass balances).

A similar procedure is followed for particulate inert material. In ADM1 the required particulate inert organic nitrogen is given by:

$$\text{ReqOrgN}_X = f_{xi} * (X_p + X_i) * N_i$$

If the pool of organic nitrogen is larger than ReqOrgN_X :

$$X_{i,ADM1} = f_{xi} * (X_p + X_i)$$

If the pool of organic nitrogen is smaller than ReqOrgN_X :

$$X_{i,ADM1} = \frac{\text{OrgN}_{\text{remain},B}}{N_i}$$

and the remaining X_i (i.e. $f_{xi} * (X_p + X_i) - \text{OrgN}_{\text{remain},A} / N_i$) is added to the incoming pool of remaining COD. In both cases, the pool of organic nitrogen is reduced by $X_{i,ADM1} * N_i$. A schematic illustration of this step is shown in Figure 6.

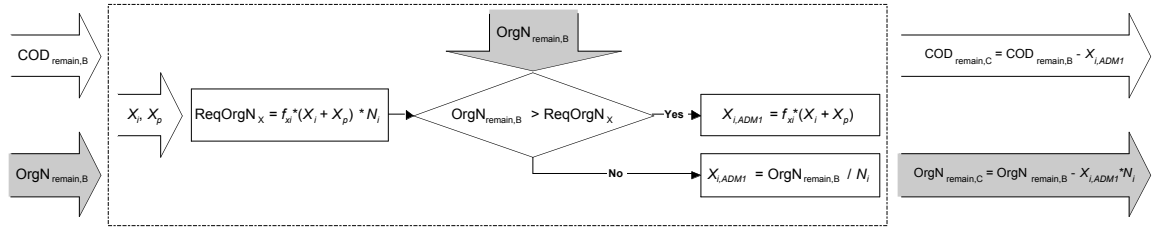


Figure 6: Schematic illustration of particulate inert COD mapping.

Partitioning of Remaining COD and TKN

The final step in the algorithm is the mapping of the remaining particulate COD and TKN. The goal here is to maximize the mapping of the remaining COD into X_c . In ADM1, X_c has an associated nitrogen component given by N_{xc} . Hence, the required COD to map all of the remaining organic nitrogen into X_c is given by:

$$\text{ReqCOD}_{Xc} = \frac{\text{OrgN}_{\text{remain},C}}{N_{xc}}$$

If the remaining pool of COD is larger than ReqCOD_{Xc} :

$$X_c = \text{ReqCOD}_{X_c}$$

and the remaining COD is mapped to X_{ch} and X_{li} in accordance with the proportions used for X_c disintegration in ADM1; that is:

$$X_{ch} = \left(\frac{f_{ch,x_c}}{f_{ch,x_c} + f_{li,x_c}} \right) (\text{COD}_{\text{remain,C}} - X_c), \text{ and};$$

$$X_{li} = \left(\frac{f_{li,x_c}}{f_{ch,x_c} + f_{li,x_c}} \right) (\text{COD}_{\text{remain,C}} - X_c)$$

If the remaining pool of COD is smaller than ReqCOD_{X_c} :

$$X_c = \text{COD}_{\text{remain,C}}$$

In each case, the ADM1 input inorganic nitrogen (S_{in}) is calculated as

$$S_{in} = S_{nh,in} + (\text{OrgN}_{\text{remain,C}} - X_c * N_{x_c})$$

If the remaining pool of COD is larger than ReqCOD_{X_c} , $\text{OrgN}_{\text{remain,C}} - X_c * N_{x_c}$ reduces to zero and the input inorganic nitrogen equals the ammonia coming from ASM1, but if the remaining pool of COD is smaller than necessary to use up all the remaining organic nitrogen, then this nitrogen is added to the input inorganic nitrogen to close the TKN balance. Setting all the remaining ADM1 state variables to zero will result in TKN and COD mass balances. A schematic illustration of this step is shown in Figure 7.

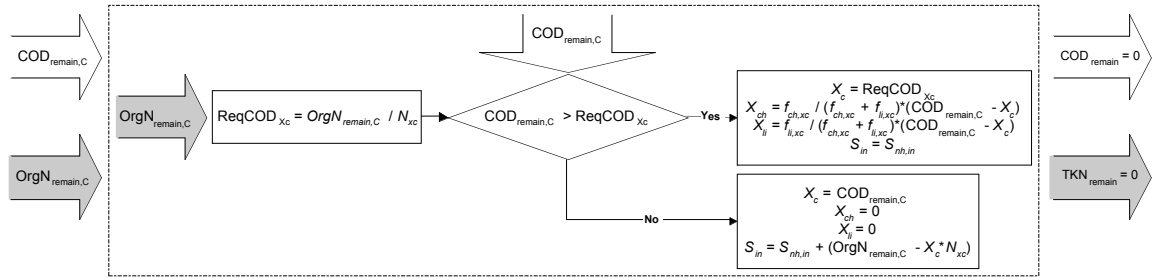


Figure 7: Schematic illustration of final COD and TKN mapping.

Finally, the state variables describing cations and anions in ADM1 do not have any equivalent variables in ASM1. Ideally they should be estimated from measurements on the actual wastewater. If no information is available then the variables may be estimated from S_{ic} and S_{in} .

$$\begin{aligned} S_{cat} &= S_{ic} \\ S_{an} &= S_{in} \end{aligned}$$

ADM1 \rightarrow ASM1

The conversion to ASM1 is somewhat simpler. In this conversion, the goal is to maximize X_s (slowly biodegradable substrate), S_s (readily biodegradable substrate), S_i (soluble inert COD) and X_i (particulate inert COD) with respect to the available COD and, S_{nh} (ammonia), X_{nd} (particulate organic nitrogen) and S_{nd} (soluble organic nitrogen) with respect to nitrogen. Figure 8 shows a schematic representation of the COD conversions and Figure 9 shows the TKN conversions.

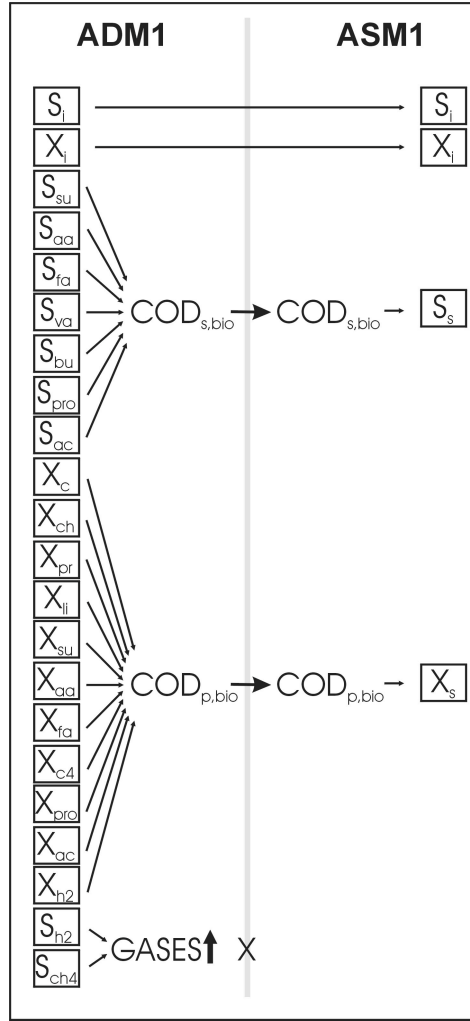


Figure 8: ADM1 to ASM1 state variable conversions for COD.

Dissolved Gaseous COD

From Figure 8, it is possible to see that a COD mass balance is maintained in the conversion to ASM1 with the exception of the dissolved gases; namely, hydrogen (S_{h2}) and methane (S_{ch4}). In the case of these gases it is assumed that they will be stripped to the atmosphere from the liquid upon entering an aerobic environment. As such, the mass of COD conserved in the transition is the total anaerobic COD minus the COD of the gases dissolved in the liquid.

$$\text{COD}_{\text{conserved}} = \text{COD}_{\text{t,anaerobic}} - S_{h2} - S_{ch4}$$

As neither S_{h2} nor S_{ch4} has associated nitrogen, this reduction in COD has no impact on the TKN converted.

COD Conversions

Inert soluble and inert particulate COD are mapped directly to the corresponding ASM1 state variables.

$$\begin{aligned} S_{i,ASM1} &= S_{i,ADM1} \\ X_{i,ASM1} &= X_{i,ADM1} \end{aligned}$$

The soluble biodegradable COD is summed and mapped to readily biodegradable COD (S_s) and the particulate biodegradable COD is summed mapped to slowly biodegradable COD (X_s).

$$S_s = S_{su} + S_{aa} + S_{fa} + S_{va} + S_{bu} + S_{pro} + S_{ac}$$

$$X_s = X_c + X_{ch} + X_{pr} + X_{li} + X_{su} + X_{aa} + X_{fa} + X_{c4} + X_{pro} + X_{ac} + X_{h2}$$

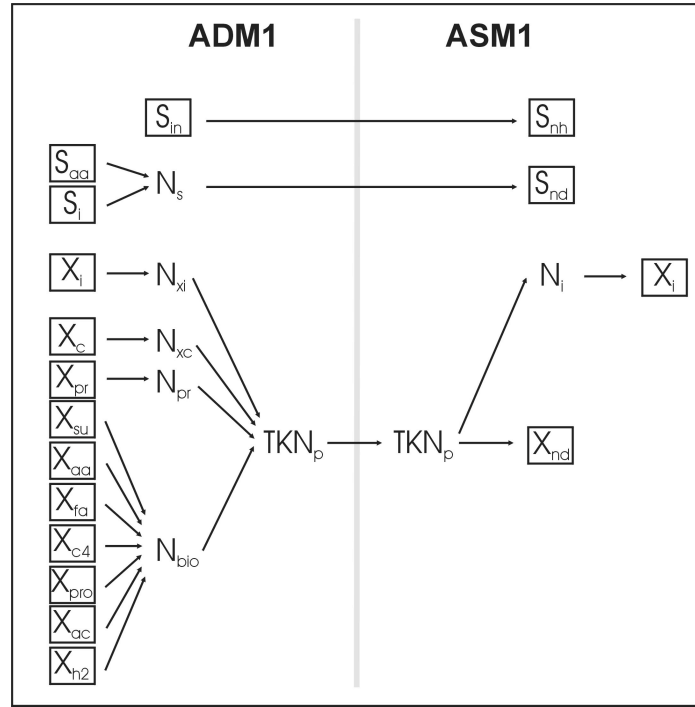


Figure 9: ADM1 to ASM1 state variable conversions for TKN.

TKN Conversions

The TKN conversion is equally straightforward. Inorganic nitrogen is mapped directly to ammonia (S_{nh}).

$$S_{nh} = S_{in}$$

Organic nitrogen is mapped to soluble biodegradable nitrogen (S_{nd}) and particulate organic nitrogen (X_{nd}) depending on its form in ADM1. Note that the nitrogen fraction of the inert soluble material in ADM1 is mapped into S_{nd} as the inert soluble material in ASM1 has no nitrogen associated with it. As the fraction of nitrogen in the inert particulate COD (X_i) may be different in ASM1 and ADM1, the calculated X_{nd} is the total particulate nitrogen (including that associated with the ADM1 inert material) minus the nitrogen being partitioned to the ASM1 inert particulate material.

$$S_{nd} = (S_{i,ADM1} * N_i) + (S_{aa} * N_{aa})$$

$$X_{nd} = N_{bac} * (X_{su} + X_{aa} + X_{fa} + X_{c4} + X_{pro} + X_{ac} + X_{h2}) + N_i * X_i + N_{xc} * X_c + N_{aa} * X_{pr} - i_{xe} * X_i$$

Setting the ASM1 biomass state variables (i.e. X_{ba} and X_{bh}) and the unbiodegradable products state variable (X_p) to zero completes the conversion and results in both COD and TKN mass balances across the interface.

Alkalinity

Finally, alkalinity may be estimated from S_{ic} .

$$S_{alk} = S_{ic}$$

Conclusion

To facilitate plant-wide wastewater treatment modeling model, state variable interfaces are necessary to convert state variables from one model into state variables of a different model. For objective comparisons of simulation results from different groups, it is important to describe how different model interfaces are implemented in the same way as the models themselves are described. This paper has described two conversion algorithms that convert ASM1 state variables to ADM1 state variables and

visa versa. The algorithms are based on maintaining COD and TKN mass balances while at the same time converting the input variables to the most accurate variables in the output model. These algorithms will help the development of plant-wide models that include activated sludge and anaerobic digestion.

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