

Continuity-based interfacing of models for wastewater systems described by Petersen matrices

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Abstract In this paper the Petersen and composition matrices that modellers are now familiar with are used as a basis to construct interfacing models between subsystems considered in wastewater treatment. Starting from continuity considerations and a set of transformation reactions between components used in the two models of the subsystems to be interfaced, a set of linear algebraic equations needs to be solved. The theoretical development is illustrated using a simplified integrated model of an activated sludge system coupled to an anaerobic digester. Continuity-guaranteed interfacing of subsystems will facilitate optimization studies of the within-the-fence process units of a wastewater treatment plant or of the integrated urban wastewater system.

Keywords Elemental balancing; mathematical modelling; model interfacing; plant-wide modelling; sludge digestion

Introduction

Since the early 1980s there has been an extraordinary increase in the use of models to quantitatively study various aspects of wastewater treatment. Although an extensive range of models has been developed with various levels of detail, the mainstream models in use today are the models prepared by Task Groups under the IWA umbrella. These models constitute a kind of reference set that many researchers and consultants have used to develop their own extensions for particular applications. As of 2002 the set consists of models for the following water systems:

- (1) Activated sludge unit processes (aerobic COD oxidation, nitrification, denitrification, decay, biological/chemical phosphorus removal), i.e. ASM1, ASM2(d), ASM3 (Henze *et al.*, 2000).
- (2) River systems (COD oxidation, nitrification, denitrification, algae growth, predation, decay, hydrolysis, sorption/desorption, chemical equilibria), i.e. RWQM1 (Reichert *et al.*, 2001).
- (3) Anaerobic digestion unit process (acidogenesis, acetogenesis, hydrogenotrophic and aceticlastic methanogenesis, disintegration, hydrolysis, chemical equilibria), i.e. ADM1 (Batstone *et al.*, 2002).

The conversion processes considered in these “standard” models differ significantly. While each particular selection of conversions is essential for the unit process under consideration, the differences become problematic for the integrated model applications

studied in this contribution. Until the mid-1990s, most model-based studies related to water issues focused on a single system, be it an anaerobic digester, a river, or some other system. Computational limitations and specialisation of the engineering society were obvious reasons for the delineation of the work. In other words, the system boundaries were put around a relatively coherent (or similarly behaving) system.

Things have gradually changed, however. Increasing pressure for optimisation of treatment systems has led to a growing awareness that synergies can be found (and should be exploited) by enlarging the boundaries to include other systems, e.g. the sludge train may be an important component when optimising nitrogen removal in an activated sludge process (Vanrolleghem *et al.*, 1996). A fundamental change occurred in the 1990s concerning the way the wastewater system was looked upon and this new vision has translated into new legislation (EU Water Framework Directive): traditionally, an emission point of view was adhered to, in which attention focused on the individual emitting systems (treatment plant, sewer system, etc.), but legislation is now imposing an integrated view in which the receiving water (quality) is defining the system boundaries. Consequently, the treatment plant can no longer be considered in isolation (Lijklema *et al.*, 1993).

This widening of system boundaries has led to the necessity for integrated models that can support the quantitative analysis of the overall system under study (Rauch *et al.*, 1998, 2002). While several attempts have been made in the last few years to develop and work with such integrated models (Benedetti *et al.*, 2003; Copp *et al.*, 2003; Wett and Alex, 2003; Zaher *et al.*, 2002), *ad hoc* solutions were typically derived to circumvent the following three problems that occur when one tries to link existing, state-of-the-art models (that were originally developed in isolation):

1. Some state variables used in one model do not exist in the connected model.
2. The “meaning” of a state variable in one system may not hold for the other system (e.g. components can be considered as inert in one system but may be biodegradable in another).
3. The elemental composition of a component in one model may not be identical for the connected model and in some instances, the elements considered are not the same (e.g. in ASM3 COD, N and charge are considered whereas in ADM1 COD, C and N are taken in account).

The objective of the paper is to provide a general framework for tackling these problems in a consistent way. First, the basic idea of the algebraic equations that constitute interfaces between models is presented. Subsequently, a simple illustrative example is developed for an activated sludge/sludge digestion interface. Concluding remarks and perspectives complete this contribution.

Principle of the continuity-based model interface

The interface concept described here is based on the development of a set of algebraic transformation equations based on a Petersen matrix description of the two models to be interfaced. Table 1 presents the basic concept. The P “origin” model components and their elemental composition are shown in the left pane, and the Q “destination” model components and composition reside in the right pane. The inputs to the interface are the fluxes of the “origin” components and the outputs of the interface are the fluxes of the “destination” components.

Within the interface a number of transformations need to be considered to ensure that the P origin components are transformed *completely* into the Q destination components. Each of these transformations converts a number of origin components into a number of destination components.

Table 1 Matrix description of interface between Petersen matrix-based model

Petersen matrix section model 1 ("origin")					Petersen matrix section model 2 ("destination")				
	X_1	X_2	...	X_P	X_{P+1}	X_{P+2}	...	X_{P+Q}	Rate
Conv. 1	$\nu_{1,1}$	$\nu_{1,2}$...	$\nu_{1,P}$	$\nu_{1,P+1}$	$\nu_{1,P+2}$...	$\nu_{1,P+Q}$	ρ_1
...
Conv. n	$\nu_{n,1}$	$\nu_{n,2}$...	$\nu_{n,P}$	$\nu_{n,P+1}$	$\nu_{n,P+2}$...	$\nu_{n,P+Q}$	ρ_n
Composition matrix section model 1					Composition matrix section model 2				
COD	$i_{COD,1}$	$i_{COD,2}$...	$i_{COD,P}$	$i_{COD,P+1}$	$i_{COD,P+2}$...	$i_{COD,P+Q}$	
Carbon	$i_{C,1}$	$i_{C,2}$...	$i_{C,P}$	$i_{C,P+1}$	$i_{C,P+2}$...	$i_{C,P+Q}$	
Nitrogen	$i_{N,1}$	$i_{N,2}$...	$i_{N,P}$	$i_{N,P+1}$	$i_{N,P+2}$...	$i_{N,P+Q}$	
Charge	$i_{e,1}$	$i_{e,2}$...	$i_{e,P}$	$i_{e,P+1}$	$i_{e,P+2}$...	$i_{e,P+Q}$	

Quantitatively, each transformation j is characterised by its "stoichiometry" $\nu_{j,k}$, i.e. the ratio of the amounts of components used and produced in a particular transformation. For instance, readily biodegradable substrate (in ASM1) could be transformed into two VFA fractions (in ADM1). In this transformation, all but three $\nu_{j,k}$ terms would be zero. Each transformation j is also characterized by its transformation rate ρ_j , which, together with the stoichiometry, specifies the amount of component k transformed per unit of time ($= \nu_{j,k} \cdot \rho_j$).

To this point, the approach is consistent with the Petersen matrix representation of the process models used to describe wastewater treatment systems. However, for the use intended here, the process rates ρ_j are not specified in terms of process kinetics (typically functions of the component concentrations), but rather are the outcome of the solution of a set of equations resulting from continuity considerations.

The definition of the transformations is user-specified on the basis of process knowledge and insight. One of the guiding principles is that for each of the elements considered (COD, C, N, charge, etc.) one specific model component should be selected as the source-sink component in order to facilitate mass and charge compensations. Essentially, building the transformation equations boils down to the selection of non-zero stoichiometric parameters among the components of the interfaced models. They are subsequently quantified as follows. For each of the n transformations, elemental continuity (COD, C, N, charge, etc.) must be guaranteed. This leads to a number of linear constraints on the parameters $\nu_{j,k}$. The elemental continuity check for each transformation j is easily accomplished by using the elemental composition matrix that is also specified for the two models (see lower panels of Table 1):

$$\sum_{k=1}^{P+Q} \nu_{j,k} i_{k,Comp} = 0 \quad \text{with } Comp = N, C, COD, e \quad (1)$$

It should be noted that the elemental composition of similar state variables – with the same "meaning" – might be different for the two models (e.g. biomass compositions may differ because of different growth conditions). In general, the set of linear algebraic equations (1) must be solved for all $\nu_{j,k}$.

The set of interface unknowns consists of the stoichiometric coefficients $\nu_{j,k}$ and the transformation rates ρ_j . Together they enable the calculation of the outflux of the Q destination components:

$$\text{Outflux}_k = \sum_{j=1}^n \nu_{j,k} \rho_j \quad \text{for } k = P + 1, P + Q \quad (2)$$

The transformation rates ρ_j that remain unknown in the above equation can be obtained from a similar equation that holds for the influxes to the interface:

$$\sum_{j=1}^n v_{j,k} \rho_j = \text{Influx}_k \quad \text{for } k = 1, P \quad (3)$$

Indeed, what is known is the influx of each P “origin” component into the interface. The structure of the interface (and resulting mass balances) ensures that the influx of these components is completely accounted for in the transformations. The resulting set of equations (3) provides constraints on $v_{k,j}$ and enables the calculation of the unknown transformation rates ρ_j through each of the n proposed transformation processes. When the set of linear equations is solved, all information is available to calculate the outflux of each Q “destination” components, using the above set of equations (2).

The three model-linking problems presented in the introduction are in this way reduced to a single problem: the user (or, preferably, the scientific community) must provide the n transformations between “ins” and “outs” of the two models in question. Then the problem is reduced to a linear algebraic problem that may be solvable or not. The example below illustrates some of the issues that need to be dealt with during the selection of the transformation reactions. For instance, there are constraints on the unknowns that must be satisfied (e.g. transformation rates ρ and outfluxes must be positive at all times) and if these constraints are not satisfied, it may be necessary to question the selected transformation reactions or even the elemental compositions used in the original models.

Illustrative example

Connected models

For this illustrative example, a simple wastewater treatment system is considered. The system is composed of a carbon removing activated sludge system with anaerobic waste sludge digestion. The models used to describe the two subsystems are the so-called ASM0 and AM2 models.

The first model is the activated sludge process model that is used in the ASM1 description (Henze *et al.*, 2000) to introduce the Petersen matrix representation, here conveniently termed ASM0. The model describes growth and decay processes using biodegradable substrate S_S , oxygen S_O and biomass X_B . For illustrative purposes the model is extended with a nitrogen-containing component, ammonium S_{NH} , as this allows a better illustration of the usefulness of a nitrogen balance.

The second subsystem is modelled using the recently presented, rather simple, two-step anaerobic digestion model of Bernard *et al.* (2001), termed AM2. It describes the anaerobic digestion process using (only) two processes: (i) acidogenesis, by which organic matter S_1 is converted into volatile fatty acids S_2 with the concomitant growth of acidogenic bacteria X_1 and (ii) methanisation of S_2 into methane and carbon dioxide P_1 with the concomitant growth of methanogens X_2 . Again, for nitrogen balancing, the model was extended to include ammonium, S_{NH} .

Interface development

Table 2 summarises the proposed interface, containing one possible set of transformation processes between ASM0 and AM2. It is useful to explain the construction of this interface as it shows the underlying reasoning. The development started by assuming that methanogens do not grow in aerobic activated sludge systems. Next, it was assumed that

Table 2 Matrix description of interface between ASM0 activated sludge and AM2 anaerobic digestion model

Component transformation process	Influx ASM0					Outflux AM2				
	S_s [gCOD]	S_o [gCOD]	X_B [gCOD]	S_{NH} [gN]	S_1 [gCOD]	S_2 [gCOD]	X_1 [gCOD]	X_2 [gCOD]	P_1 [gC]	S_{NH} [gN]
ρ_1				-1						1
ρ_2		$\nu_{2,O}$	-1		1		1		$\nu_{2,P}$	$\nu_{2,N}$
ρ_3	-1	$\nu_{3,O}$							$\nu_{3,P}$	$\nu_{3,N}$
ρ_4	-1	$\nu_{4,O}$			1				$\nu_{4,P}$	
ρ_5		$\nu_{5,O}$	-1		1				$\nu_{5,P}$	$\nu_{5,N}$
Composition										
C [gC]	$i_{C,SS}$	0	$i_{C,XB}$	0	$i_{C,S1}$	$i_{C,S2}$	$i_{C,X1}$	$i_{C,X2}$	1	0
N [gN]	0	0	$i_{N,XB}$	1	$i_{N,S1}$	0	$i_{N,X1}$	$i_{N,X2}$	0	1
O [gO]	$i_{O,SS}$	1	$i_{O,XB}$	0	$i_{O,S1}$	$i_{O,S2}$	$i_{O,X1}$	$i_{O,X2}$	32/12	0
COD[gCOD]	1	-1	1	0	1	1	1	1	0	0

ammonium entering the interface would automatically be propagated into the AM2-ammonium (reaction ρ_1).

Next, it was reasoned that a fraction of the heterotrophic biomass would be a source of acidogens, while the remaining portion would enter the anaerobic digester as biodegradable organic matter. These two destinations for the biomass were accounted for in the interface through two transformation processes, ρ_2 and ρ_5 . The first transformation of biomass-COD leads to an equivalent COD-amount of acidogens. The second transformation leads to the production of organic matter-COD. The fact that both processes are defined within a COD-balance context automatically results in a COD mass balance. The stoichiometric entries for the two components are set to -1 and $+1$ indicating the origin and destination of the considered component. In addition to the COD-continuity, nitrogen, oxygen and carbon continuity must also be imposed. For each process three additional linear equations as given in Eq. (1) can be constructed, enabling the determination of the three unknown stoichiometric parameters for S_O , S_{NH} and P_1 . Note that the fluxes in these 3 components can be considered to be compensation terms (Benedetti *et al.*, 2003) that account for the differences between the elemental compositions of the components considered in the transformation process. For instance, if the acidogens have a lower N-to-COD ratio than the heterotrophic biomass, a positive stoichiometric term in S_{NH} , $\nu_{2,N}$ would result. On the contrary, a negative $\nu_{2,N}$ could also occur, indicating that some of the ammonium-N provided by the activated sludge waste stream (or other transformations processes) is used to fill the needs for “acidogens creation” in the interface.

Related to the latter situation, it is essential that the total outflux in AM2-ammonium is not negative as this would mean that more ammonia is needed for the compensation terms than can be provided by the ammonia originating from the activated sludge system. If such conditions are encountered, a possible approach consists of modifying the assumed elemental compositions of the components. Obviously the interface is then assisting the user to validate the compatibility of the models.

The two remaining transformation processes (ρ_3 and ρ_4) deal with the biodegradable substrate remaining in the activated sludge waste stream. Here it is assumed that part of this substrate may already be volatile fatty acids S_2 . So, again two processes were constructed to describe two transformations, one towards organic matter S_1 and the other towards S_2 . In this case too compensation terms are needed, because S_1 contains nitrogen whereas S_2 does not. Similarly, the oxygen content of the volatile fatty acids may be quite different from the biodegradable substrate considered in ASM0, and oxygen usage may have to be considered to fill this mass balancing gap. This oxygen may be available in the waste sludge stream as dissolved oxygen, but if not, a problem may surface if overall there is a need for oxygen in the interface. To account for this, it may be necessary to virtually “aerate” the interface and supply the necessary oxygen. However, by explicitly accounting for this oxygen supply, one maintains the requirement of elemental balancing, and provides the user with the overall fluxes in the plant-wide treatment system.

In case an “origin” component is transformed via two transformation reactions, one should realise that in fact a degree of freedom is created in the interface, in this particular case the fraction of the component following one or the other transformation reaction. This degree of freedom can be used to deal with the above oxygen requirement problem in case one transformation requires less of the compensating term than the other. In case this degree of freedom is not needed for elemental balancing, the user can set it at a particular value on the basis of, for instance, collected data.

The CO_2 component (P_1) is illustrative of another aspect of the interfaces. In case an “origin” model does not include a certain component that is included in the “destination” model, a source term should be added to the interface. In the illustrative example, CO_2 is

not explicitly considered in ASM0, but the bicarbonate system is essential for the anaerobic digestion process. So, in addition to the compensation rates of CO₂ in the previously defined transformation processes, a source of CO₂ could be added to the interface, e.g. as a constant flux of CO₂ or by using pH as a parameter of the interface from which the out-flux-CO₂ is calculated.

Finally, the fate of volatile components such as O₂, CO₂ or methane should be considered when mixed liquor is moving between process units. Indeed, this transfer can lead to actual stripping of components. Moreover, to fulfil the required mass balancing at the interface, transformation reactions can be used as a sink for these components, e.g. by using “virtual stripping” as a mechanism. While this gives the user the ability to solve a number of continuity problems that may surface, it is essential that these sinks be considered explicitly, as complete mass balancing of the integrated system must remain guaranteed.

Conclusions

Using the Petersen and composition matrices that modellers are now familiar with, interfaces can be defined and described with the general methodology presented in this contribution. It is expected that the scientific community will shortly define “standard” interfaces between the “standard” IWA models by specifying the set of transformations likely to occur between subsystems of the urban wastewater system. Such continuity-guaranteed interfacing of subsystems will facilitate optimisation studies of within-the-fence process units of a wastewater treatment plant (Jeppsson *et al.*, 2004; Vanrolleghem *et al.*, 1996; Wett and Alex 2003; Zaher *et al.*, 2002) and of the integrated urban wastewater system (Benedetti *et al.*, 2004).

Acknowledgements

This research was undertaken with the support of the IST and EESD Programmes of the European Union (TELEMAC, project no. IST-2000-28156, CD4WC, project no. EVK1-CT-2002-00118 and Harmoni-CA, project no. EVK1-CT-2002-20003).

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