BSM2 Plant-Wide Model construction and comparative analysis with other methodologies for integrated modelling

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Abstract In this paper, a new methodology for integrated modelling of the WWTP has been used for the construction of the Benchmark Simulation Model N°2 (BSM2). The *transformations-approach* proposed in this methodology does not require the development of specific transformers to interface unit process models and allows the construction of tailored models for a particular WWTP guaranteeing the mass and charge continuity for the whole model. The BSM2 PWM constructed as case study, is evaluated by means of simulations under different scenarios and its validity in reproducing water and sludge lines in WWTP is demonstrated. Furthermore the advantages that this methodology presents compared to other approaches for integrated modelling are verified in terms of flexibility and coherence.

Keywords BSM2 integrated model; mass and charge continuity; Plant-Wide Model methodology

Introduction

Mathematical modelling and dynamic simulation of different processes in wastewater treatment plants (WWTPs) is a very useful tool for the study of different operational strategies. It must be taken into account that optimum solutions for the design, operation and control in advanced WWTPs that includes both water and sludge lines must be analyzed as an overall problem in which the unit-process element behaviours are interrelated with each other. For this type of studies, the *Benchmark Simulation Model n°2* BSM2 (Jeppsson *et al.*, 2006) has been proposed as an integrated model that considers water and sludge lines, and in which different operational, control and evaluation procedures can be studied. The BSM2 plant is constituted by a primary treatment with a primary clarifier, a biological treatment equal to the BSM1 plant (Copp *et al.*, 2002), and a sludge treatment line with a thickener, an anaerobic digester and a dewatering unit. Accordingly, the integrated model needed for reproducing the BSM2 plant behaviour should describe the mass transport in each one of these elements, the biological carbon and nitrogen removal in the water line, and the anaerobic digestion of the sludge.

However, to obtain integrated WWTP models that describe the relationships between the unit processes guaranteeing mass and charge continuity is not a straightforward task (Vanrolleghem *et al.*, 2005; Wentzel *et al.*, 2006) because of the differences in model components and transformations among the standard models (varying descriptions of carbonaceous substrates, nitrogen as well as pH and buffer capacity in water or sludge, etc.). Trying to give a solution for this problem, two main approaches have been proposed until now.

The first approach is based on the construction of a *Supermodel* consisting of all the components and transformations needed to reproduce every process within the whole plant (Jones and Tákacs, 2004; Seco *et al.*, 2004). In this kind of model, components and

transformations are common to every unit process model in the WWTP and therefore, specific transformers connecting different process models are not required. However, on the other hand, the use of a unique Supermodel for any WWTP can unnecessarily increase model complexity due to the inclusion of components and transformations not required for a specific study case.

The second approach is based on the construction of *Interfaces* between the existing standard unit-process models. As an example, the ASM1-ADM1 interfaces proposed in Copp *et al.* (2003), converts the origin model components to the destination ones, based on a set of conditional statements. According to the ASM1 and ADM1 requirements, these interfaces have been constructed based on only COD and N mass balances and therefore, elemental mass continuity in terms of C, H, P, or other elements, and charge is not guaranteed. Another example of the *Interfaces* approach is the Continuity-Based Model Interfacing (CBIM) methodology described in Vanrolleghem *et al.* (2005), Volcke *et al.* (2006) and Zaher *et al.* (2007). This methodology provides a general procedure to construct model interfaces between any two standard models in which the elemental mass and charge continuity is guaranteed. The CBIM interfaces are constructed by means of the definition of a set of instantaneous conversions that describe, using Petersen matrices, the translation from the origin model components to the destination model ones. As a methodology requirement, these conversions must guarantee mass and charge continuity.

Combining aspects from both approaches, a new so-called Plant-Wide methodology has recently been proposed in Grau *et al.* (2007) for constructing Plant Wide Models (PWMs) tailored to the case study in which mass and charge is guaranteed and no specific interfaces are required.

This paper shows the construction of an integrated model for the BSM2 plant according to the PWM methodology. The validity of the obtained BSM2 Plant-Wide Model has been verified by means of simulation studies under different standard scenarios and the main advantages that the utilization of this methodology present against the other approaches have been discussed.

Construction of the BSM2 PWM

In this paper an integrated model for the BSM2 plant has been constructed according to the Plant-Wide model methodology recently proposed in Grau *et al.* (2007). Previous to the construction of the BSM2 PWM, the most important aspects of the PWM methodology are briefly described in the following section.

Fundamentals of the Plant Wide Model methodology

The PWM methodology has been proposed for the systematic construction of the most appropriated mathematical models for describing, in an integrated way, the dynamic behaviour of the entire WWTP under study, including the main unit-process elements of both the water and sludge lines.

This methodology is mainly based on selecting, for a specific WWTP, the set of compatible process transformations needed for modelling the different unit-process elements included in the whole plant. This "*transformation-based*" approach, in comparison with the conventional "*process-based*" approach, does not require specific transformers for interfacing the resulting unit-process models and facilitates the mass and charge continuity throughout the whole plant. Additionally, this modularity facilitates the development of computer applications for simulation.

The construction of any Plant Wide Model must be carried out based on a general *List of Transformations* (LT) which gathers all the most relevant biochemical, chemical and

physico-chemical transformations that can occur in a WWTP. However, it is important to indicate that the construction of a Plant-Wide model does not imply the building of a LT, but the utilization of a standardized one proposed and well accepted by the scientific community. As an example, Figure 1 shows the transformations included in the LT proposed in Grau *et al.* (2007) which is based on the biological processes considered in the ASM1, ASM2 (Henze *et al.*, 2000) and ADM1 (Batstone *et al.*, 2001) standard models. However, in order to obtain a standardized list for plant wide model objectives, some modifications in the transformations or components definition have been introduced (buffer capacity described by means of a set of weak acid-base equilibria, growth of heterotrophic bacteria decoupled depending on the substrate type, etc). According to the methodology requests, kinetic equations include the activation/inhibition terms to reproduce the appropriate bacterial activity under aerobic, anoxic and anaerobic conditions, and the stoichiometry of the transformations has been defined in such a way that mass and charge is well guaranteed in all of them. For this purpose, components involved in the transformations considered have been described in terms of their elemental mass composition (C, H, N, O, P or other additional elements) and charge density, and some components have played the *source-sink* role to accomplish the continuity equation in each transformation (Reichert *et al.*, 2001; De Gracia *et al.*, 2006). Based on the LT, the systematic procedure for constructing Plant Wide Models for any WWTP is carried out by means three consecutive steps detailed in the following paragraphs.

In the first step, the relevant transformations must be selected from the general LT, and the specific *Plant Transformations Model* (PTM) appropriated for the studied plant, must be constructed. The PTM is defined as the biochemical model able to reproduce all the relevant *Biological Processes* that occur in the WWTP under study (carbon, nitrogen or phosphorous removal, anaerobic digestion, etc.). The Plant Transformations Model is constituted by the set of biochemical, chemical and physico-chemical transformations, and all the components involved in them, able to reproduce these *Biological Processes*. The components included in the PTM constitute the Plant Components Vector (PCV) that will be used as the common interface among the different units included in the Plant-Wide Model. To build up the PTM is not a straightforward task because of the inter-relations that exist between different transformations and components. For this reason, a consecutive procedure, which is based on an appropriate identification of the microorganisms populations able to reproduce the *Biological Processes* that take place in the WWTP, has been proposed in Grau *et al.* (2007).

In the second step, the set of compatible *Unit Process Models* (UPMs) describing each unit must be constructed. The set of Unit Process Models is the collection of mathematical models that describe the behaviour of the most relevant elements included in the water and sludge lines of the plant under study. Therefore, each Unit Process Model must incorporate the description of both, the mass transport and the internal transformations, and must use as a common interface, the PCV constituted in the first step. In the elements in which biological activity takes place in a relevant way, internal transformations can be described by the PTM previously constructed.

In the third step, and once the set of UPMs have been constructed, the *Plant-Wide Model* (PWM) can be easily created by means of the direct connection of the mass fluxes between these Unit Process Models.

Construction of the BSM2 Plant Wide Model (BSM2 PWM)

The BSM2 PWM construction has been carried out based on the List of Transformations detailed in Figure 1 and following the procedure previously proposed.
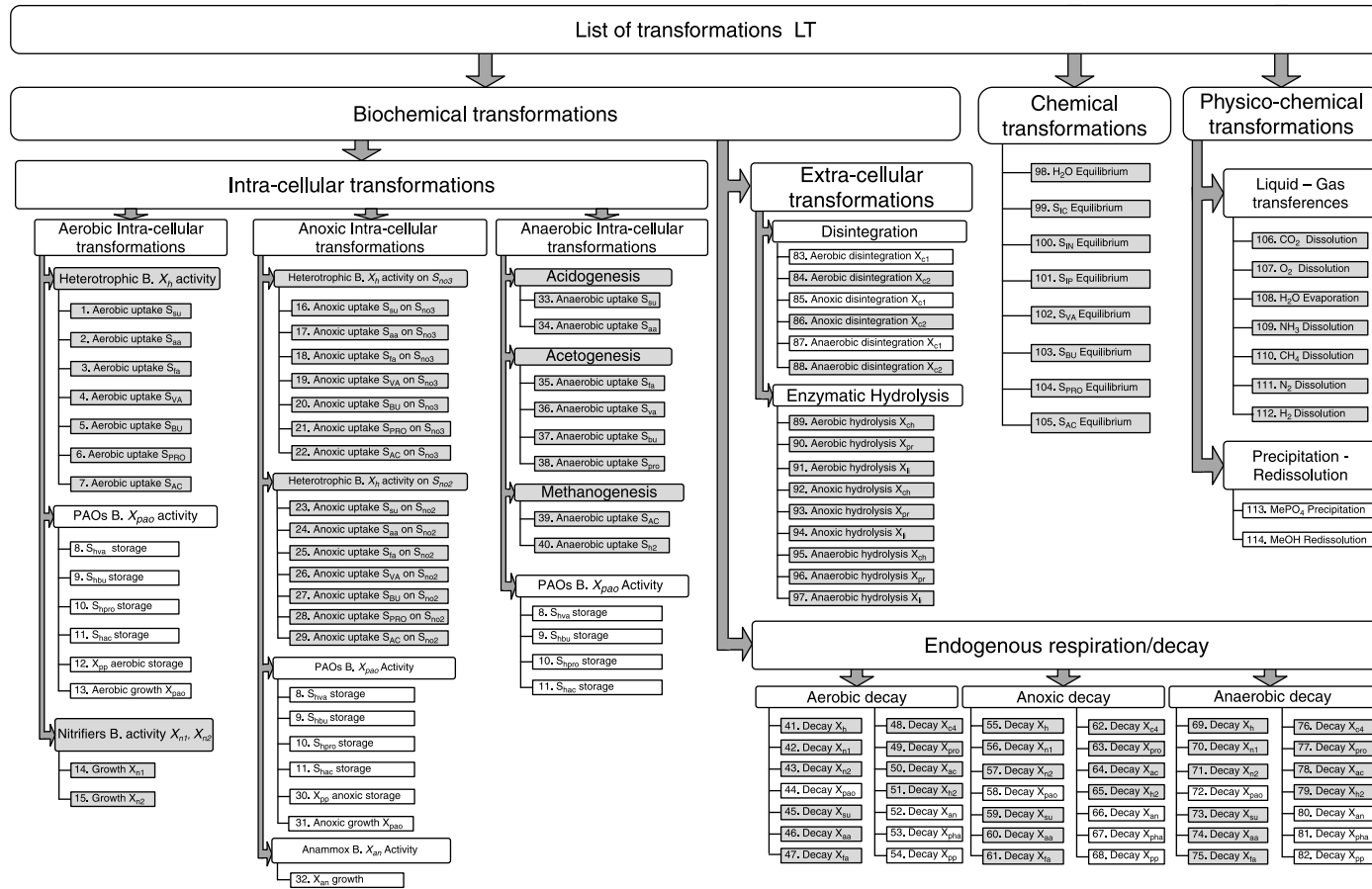
List of transformations LT

Biochemical transformations

Chemical transformations

Physico-chemical transformations

Intra-cellular transformations

Aerobic Intra-cellular transformations

Heterotrophic B. X_h activity

1. Aerobic uptake S_{su}
2. Aerobic uptake S_{aa}
3. Aerobic uptake S_{fa}
4. Aerobic uptake S_{VA}
5. Aerobic uptake S_{BU}
6. Aerobic uptake S_{PRO}
7. Aerobic uptake S_{AC}

PAOs B. X_{pao} activity

8. S_{hva} storage
9. S_{hbu} storage
10. S_{hpro} storage
11. S_{hac} storage
12. X_{pp} aerobic storage
13. Aerobic growth X_{pao}

Nitrifiers B. activity X_{n1}, X_{n2}

14. Growth X_{n1}
15. Growth X_{n2}

Anoxic Intra-cellular transformations

Heterotrophic B. X_h activity on S_{no3}

16. Anoxic uptake S_{su} on S_{no3}
17. Anoxic uptake S_{aa} on S_{no3}
18. Anoxic uptake S_{fa} on S_{no3}
19. Anoxic uptake S_{VA} on S_{no3}
20. Anoxic uptake S_{BU} on S_{no3}
21. Anoxic uptake S_{PRO} on S_{no3}
22. Anoxic uptake S_{AC} on S_{no3}

Heterotrophic B. X_h activity on S_{no2}

23. Anoxic uptake S_{su} on S_{no2}
24. Anoxic uptake S_{aa} on S_{no2}
25. Anoxic uptake S_{fa} on S_{no2}
26. Anoxic uptake S_{VA} on S_{no2}
27. Anoxic uptake S_{BU} on S_{no2}
28. Anoxic uptake S_{PRO} on S_{no2}
29. Anoxic uptake S_{AC} on S_{no2}

PAOs B. X_{pao} Activity

8. S_{hva} storage
9. S_{hbu} storage
10. S_{hpro} storage
11. S_{hac} storage
30. X_{pp} anoxic storage
31. Anoxic growth X_{pao}

Anammox B. X_{an} Activity

32. X_{an} growth

Anaerobic Intra-cellular transformations

Acidogenesis

33. Anaerobic uptake S_{su}
34. Anaerobic uptake S_{aa}

Acetogenesis

35. Anaerobic uptake S_{fa}
36. Anaerobic uptake S_{va}
37. Anaerobic uptake S_{bu}
38. Anaerobic uptake S_{pro}

Methanogenesis

39. Anaerobic uptake S_{AC}
40. Anaerobic uptake S_{h2}

PAOs B. X_{pao} Activity

8. S_{hva} storage
9. S_{hbu} storage
10. S_{hpro} storage
11. S_{hac} storage

Extra-cellular transformations

Disintegration

83. Aerobic disintegration X_{c1}
84. Aerobic disintegration X_{c2}
85. Anoxic disintegration X_{c1}
86. Anoxic disintegration X_{c2}
87. Anaerobic disintegration X_{c1}
88. Anaerobic disintegration X_{c2}

Enzymatic Hydrolysis

89. Aerobic hydrolysis X_{ch}
90. Aerobic hydrolysis X_{pr}
91. Aerobic hydrolysis X_{li}
92. Anoxic hydrolysis X_{ch}
93. Anoxic hydrolysis X_{pr}
94. Anoxic hydrolysis X_{li}
95. Anaerobic hydrolysis X_{ch}
96. Anaerobic hydrolysis X_{pr}
97. Anaerobic hydrolysis X_{li}

98. H_2O Equilibrium
99. S_{IC} Equilibrium
100. S_{IN} Equilibrium
101. S_{IP} Equilibrium
102. S_{VA} Equilibrium
103. S_{BU} Equilibrium
104. S_{PRO} Equilibrium
105. S_{AC} Equilibrium

Liquid – Gas transferences

106. CO_2 Dissolution
107. O_2 Dissolution
108. H_2O Evaporation
109. NH_3 Dissolution
110. CH_4 Dissolution
111. N_2 Dissolution
112. H_2 Dissolution

Precipitation - Redissolution

113. $MePO_4$ Precipitation
114. MeOH Redissolution

Endogenous respiration/decay

Aerobic decay

41. Decay X_h
42. Decay X_{n1}
43. Decay X_{n2}
44. Decay X_{pao}
45. Decay X_{su}
46. Decay X_{aa}
47. Decay X_{fa}

48. Decay X_{c4}
49. Decay X_{pro}
50. Decay X_{ac}
51. Decay X_{h2}
52. Decay X_{an}
53. Decay X_{pha}
54. Decay X_{pp}

Anoxic decay

55. Decay X_h
56. Decay X_{n1}
57. Decay X_{n2}
58. Decay X_{pao}
59. Decay X_{su}
60. Decay X_{aa}
61. Decay X_{fa}

62. Decay X_{c4}
63. Decay X_{pro}
64. Decay X_{ac}
65. Decay X_{h2}
66. Decay X_{an}
67. Decay X_{pha}
68. Decay X_{pp}

Anaerobic decay

69. Decay X_h
70. Decay X_{n1}
71. Decay X_{n2}
72. Decay X_{pao}
73. Decay X_{su}
74. Decay X_{aa}
75. Decay X_{fa}

76. Decay X_{c4}
77. Decay X_{pro}
78. Decay X_{ac}
79. Decay X_{h2}
80. Decay X_{an}
81. Decay X_{pha}
82. Decay X_{pp}

Figure 1 General Scheme of the transformations included in the LT

Construction of the Plant Transformation Model (PTM). In this case, according to the BSM2 Plant configuration and model aims, the Biological Processes considered have been the *Carbon and Nitrogen removal* and *Anaerobic Digestion*. Consequently, the active microorganisms populations considered to construct the PTM must be the *Heterotrophic*, the nitrifiers (*Nitrosomonas* and *Nitrobacter*) and the set of anaerobic microorganisms that carry out the acidogenesis, acetogenesis and methanogenesis processes. Once these microorganism populations have been selected, biochemical transformations describing their growth, decay and enzymatic hydrolysis under aerobic, anoxic and anaerobic conditions have been selected from the general LT. In accordance with these transformations, components representing the soluble substrate (monomers and VFAs), the selected microorganisms populations, the decay products, the particulate substrate, and the *source-sink* components, that assume the mass imbalances in the transformations, have been included in the PTM. Finally, according to the components previously selected, the required acid-base equilibria, the liquid-gas transfers and the additional acid/base and gaseous components needed to reproduce these transformations have been incorporated to the PTM.

Once these steps have been completed the set of transformations selected (highlighted in Figure 1) and the list of model components involved in them, comprise the Plant Transformations Model (PTM) and the Plant Components Vector (PCV).

Construction of the set of Unit Process Models (UPMs). Firstly, in the UPM developed for the activated sludge reactors and for the anaerobic digester, the PTM previously constructed has been used to describe the internal transformations. On the other hand, the mass transport description has been based on mass balances applied, for all the components included in the PCV, including transport between the liquid and gaseous phases. Secondly, the mass transport description in the Primary settler has been based on the Otterpohl and Freud (1992) model for each component included in the PCV. As it has been considered that no relevant biological activity takes place in the primary settler, the description of the internal transformations has not been considered in this UPM. Thirdly, the mass transport description in the Secondary settler has been based on the layered model described in Tákacs *et al.* (1991). As previously, the internal transformations description has been avoided and mass transport description has been based on the lumped variable *TSS* (Total Suspended Solids). In this way, and according to the methodology requirements, specific transformers converting the components included in the PCV to the *TSS* variable and vice-versa have been constructed and incorporated to the UPM.

Construction of the BSM2 Plant Wide Model (BSM2 PWM). Finally, the BSM2 PWM has been obtained by means of the direct connection between the different UPM previously developed.

Results

Validation of the BSM2 PWM to reproduce the ASM1 and ADM1 models

The BSM2 PWM obtained has been implemented in the simulation platform WEST (http://www.mostforwater.com) and the easy connection between the different unit process models has been verified. Also, the BSM2 PWM capability for reproducing the most relevant biological processes that take place in the BSM2 plant has been validated.

On the one hand, nitrification and denitrification processes have been checked under the BSM1 scenario (Copp *et al.*, 2002) and the results obtained with the BSM2 PWM and ASM1 have been compared. Figures 2 and 3 show the particulate substrate in the first anoxic reactor and the ammonia in the effluent obtained with the two models for five days of dynamic simulation.
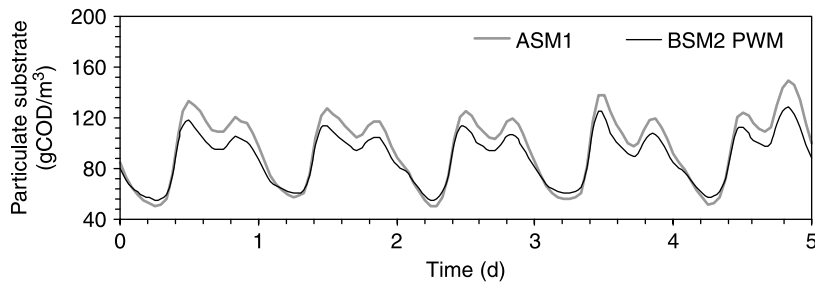
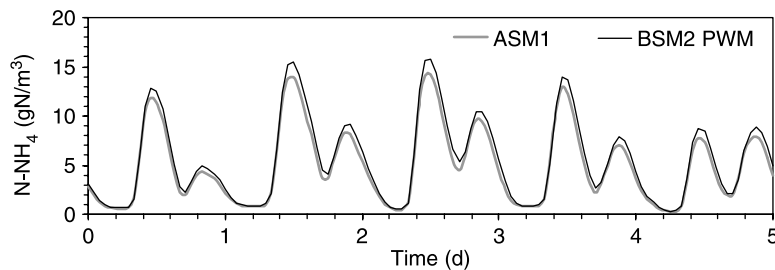**Figure 2** Particulate substrate in the first anoxic tank

Figure 3 Ammonia (N—NH$_4$) in the effluent

These Figures show that the BSM2 PWM is able to reasonably reproduce the carbon and nitrogen removal predicted by the ASM1. Specifically, differences shown in Figure 2 for the particulate substrate are caused by the consideration of the hydrolysis transformation with a first order kinetics against the *Contois* kinetic equation used in the ASM1 model. On the other hand, small differences obtained for the N—NH$_4$ in the effluent (Figure 3) can be caused by the different description of the organic nitrogen in both models. In this way, against the S_{nd} component considered in the ASM1 model, the soluble organic nitrogen in the BSM2 PWM has been considered as the nitrogen content in the aminoacids substrate. Consequently, differences between S_{nd} and nitrogen content in the aminoacids in the aeration reactors lead to slight differences in the nitrification process. Finally, the BSM2 PWM capability for reproducing anaerobic processes has been validated under the Anaerobic Cost Benchmark proposed in Rosen *et al.* (2002). In this case, the obtained results are equal to those obtained with the standard ADM1 model (Grau, 2007).

Comparative analysis of the different approaches for integrated BSM2 plant modelling

Comparison with the interfaces proposed in Copp et al. (2003). The behaviour of the BSM2 PWM has been evaluated for one year simulation according to indications given in Vreko *et al.* (2006) and Rosen *et al.* (2006). As an example, the results obtained for the soluble nitrogen in the effluent and the methane flow rate in the anaerobic digester are presented in Figures 4 and 5, compared with those obtained with the Copp *et al.* (2003) interfaces.

These figures show the capability of the BSM2 PWM for reproducing the results obtained with the Copp interfaces. Differences observed in Figure 4 have been previously discussed and differences in methane gas flow rate are mainly based on the different stoichiometry description of the biomass decay with respect to the ADM1 model proposed in Rosen *et al.* (2006). However, the Plant-Wide methodology used for the BSM2 PWM construction provides a general procedure for constructing tailored models
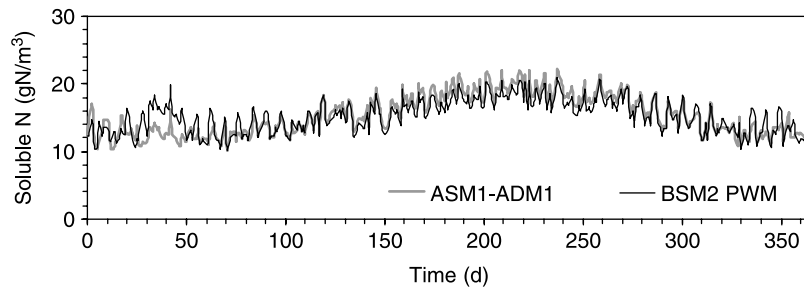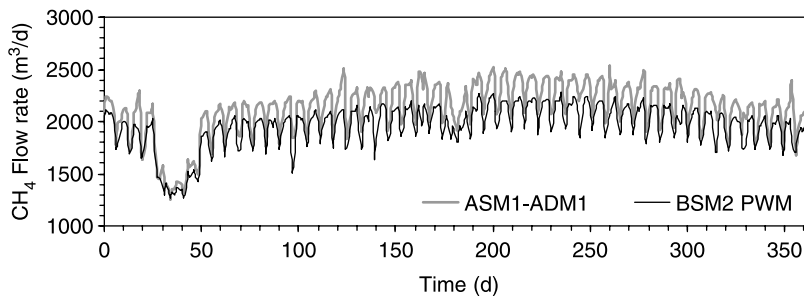
Figure 4 Soluble Nitrogen in the effluent

Figure 5 Methane gas flow rate in the AD

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guaranteeing elemental mass and charge continuity throughout the plant. It must be taken into account that, although the Copp interfaces allows the specific connection between the ASM1 and ADM1 models, these interfaces should be modified adding mass restrictions, if models requiring more mass continuities than N and COD were going to be interfaced (for example, if both models to be interfaced should guarantee C or P mass continuity).

Comparison with the ASM1-ADM1 CBIM interfaces. On the other hand, the interfaces for ASM1 and ADM1 models have been constructed according to the CBIM methodology. Following this methodology requests, mass fractions of the origin and destination model components have been defined as proposed in Zaher *et al.* (2007), and the conversions have been defined based on the transformations proposed in Copp *et al.* (2003), but accomplishing the continuity equation for each element and charge. Nevertheless, although the mass and charge can be well guaranteed with these interfaces, their construction and later utilization in different simulation scenarios under dynamic conditions, is a task which is not straightforward and presents some weak points. Firstly, as in this case the ASM1 and ADM1 models do not guarantee a complete elemental mass and charge continuity in their internal transformations, some additional model components assuming the mass of P, H, or charge imbalances in the conversions should be considered at the interface, and also in the models, if the complete mass and charge balance needs to be guaranteed. Secondly, as these interfaces do not include conditional restrictions as Copp interfaces does, the CBIM interfaces can lead to negative values for the destination model components when the mass requirement of a component at any simulation time, is higher than its mass entering to the interface. For example, in the ASM1 → ADM1 interface, Figure 6 shows, compared with the Copp interfaces, how the mass flux of sugars take negative values at times in which soluble substrate required for the nitrates, oxygen and organic nitrogen depletion is higher than the soluble substrate at the entrance.
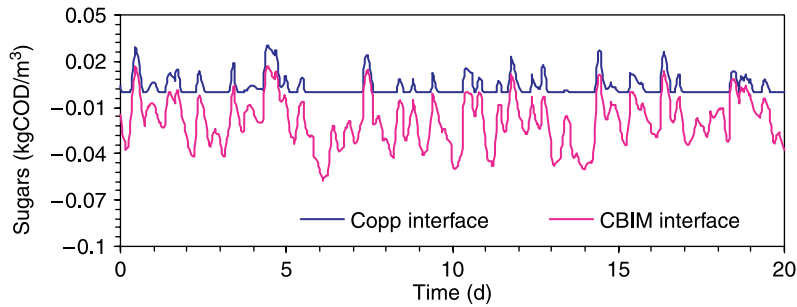
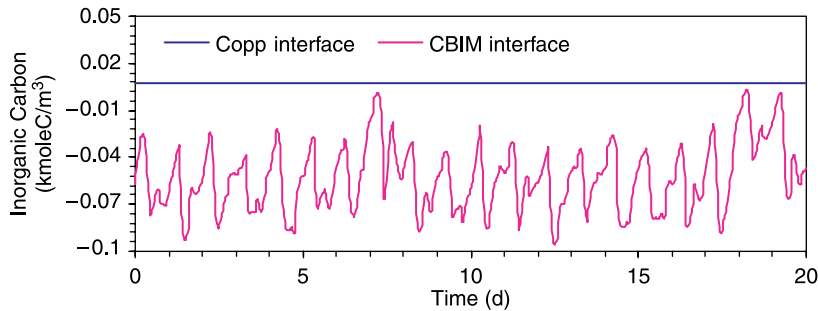**Figure 6** Sugars at the output of the interface

Figure 7 C at the output of the interface

Other example related to this are the negative mass fluxes obtained for inorganic carbon that assume the carbon imbalances in each conversion (Figure 7). Similar problems have been obtained for protons mass fluxes that assume charge imbalances in the conversions, causing large pH fluctuation. Therefore, the utilization of the CBIM interface requires, for each study case, a continuous evaluation of the destination model components mass fluxes, and the rewriting of the mass fractions components or conversions until the correct behaviour of the interface is ensured. Logically, this restriction is very difficult to guarantee under any possible dynamic scenario. This limitation is overcome by the PWM approach proposed in this paper. Additionally and thanks to methodology flexibility, further extensions of the BSM2 PWM with, for example, *Sharon-Anammox* processes (Volcke *et al.*, 2006), can be easily carried out following the procedure proposed for PWMs construction.

Conclusions

The BSM2 PWM has been successfully constructed based on the plant-wide modelling methodology and the advantages that this methodology presents for interfacing the different unit process models included in the plant have been visualized. The obtained model has been evaluated under different standard scenarios and its validity for reproducing the most common biological processes in WWTPs that include water and sludge lines has been verified.

From the comparative analysis with other integrated modelling approaches it can be concluded that, with respect to the *Interfaces* approach, the BSM2 PWM guarantees the mass and charge continuity at any stationary or dynamic condition without the need of specific transformers. With respect to the *Supermodel* approach, the PWM methodology allows the construction of tailored models for each case study and has the capacity of

future extensions for new processes. Further research is focused on optimizing numerical properties and improving the speed of the simulations achieved with the BSM2 PWM.

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