A comparative analysis of different approaches for integrated WWTP modelling

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ABSTRACT

In this paper a comparative analysis of the most important approaches for integrated WWTP modelling is presented. After an introductory presentation of the most important drawbacks and challenges for plant wide modelling, the fundamentals of three different approaches to construct integrated models are presented: "Interfaces" "Standard Supermodel" and "Tailored Supermodel". Afterwards, a comparative analysis of these approaches from different points of view (difficulties for the model end user, characterization of the process in the plant, flexibility or adaptability for each case of study, simulation platform requirements and computational costs) is carried out. From this comparison, some important conclusions about the suitability of each alternative depending on the simulation case study are extracted.

Key words | interfaces, plant-wide mathematical modelling, supermodels, WWTP

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INTRODUCTION

Since the beginning of the seventies, dynamic mathematical modelling of WasteWater Treatment Plants (WWTPs) has evolved significantly. Some of the first work in this field of mathematical modelling of the activated sludge process was carried out by the University of Cape Town (Ekama & Marais, 1977; Dold *et al.* 1980). In 1987, the Activated Sludge Model n 1 (ASM1) which described carbon (C) and nitrogen (N) removal in activated sludge systems was published (Henze *et al.* 1987). But the publication of the ASM1 model also initiated a standardization for wastewater characterization and computational code development that made communication among different research groups easier. Furthermore, this publication also marked the start of some crucial discussions in biochemical modelling and was the basis for the development of more complex models (Henze *et al.* 2000). According to its aim, ASM1 describes the biochemical activity of two bacteria populations: a heterotrophic population consuming the biodegradable organic matter and an autotrophic population (the nitrifiers) able to oxidize ammonia. The organic matter is characterized by means of four lumped components expressed in Chemical Oxygen Demand (COD) units: the easily and slowly biodegradable material and the soluble and particulate unbiodegradable material. On the other hand, the nitrogen is characterized as nitrogen content in the readily and slowly biodegradable matter, ammonia and nitrates.

The ASM2/ASM2d models arose due to the need for a mathematical model that could represent the behaviour of phosphorus (P) removal in activated sludge processes (Henze *et al.* 1995). With respect to ASM1, ASM2 presented

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additional transformations and some differences in the components description and characterization. In ASM2–ASM2d the organic substrate, expressed in COD units, is divided into fermentable, fermented and slowly biodegradable components and there are no specific components for the nitrogen and phosphorus substrate content. An important aspect introduced by ASM2 was the definition of the continuity equation that was proposed as a general tool for the elemental mass and charge continuity evaluation in the transformations.

Subsequent to ASM2, ASM3 was published (Gujer *et al.* 1999) with the aim to correct some limitations detected in the ASM1, describing in more detail the processes of substrate storage and endogenous respiration by the bacteria populations. As a way to evaluate the Theoretical Oxygen Demand (ThOD), N and charge continuity, ASM3 established a procedure to calculate the ThOD (for organic and inorganic compounds) based on the elements oxidation states. In ASM3, like in the previous ASM models, the buffer capacity of the wastewater was reproduced by means of a component that represented the alkalinity and indicated, implicitly, drops in the pH of the media.

An important contribution to the wastewater treatment modelling has come from the IWA Task Group on River Water Quality Modelling that went a step further in the complete definition of the elemental composition of the model components (Reichert *et al.* 2001). Also, two ways (equilibrium and dynamic) were proposed for explicitly calculating pH using acid-base equilibria functions, rather than relying on the ASM's alkalinity balance to monitor acid/base effects.

In the field of anaerobic digestion, standardization in mathematical models started later than in the wastewater field. The Anaerobic Digestion Model n° 1 (ADM1), summarizing work carried out on this subject until the moment, was published by Batstone *et al.* (2002). ADM1 describes the anaerobic degradation of organic matter requiring a more detailed description of the active bacterial populations and organic substrates (sugars, amino acids, Volatile Fatty Acids (VFAs), carbohydrates, proteins, etc.). Because anaerobic bacteria populations tend to be highly sensitive to pH, ADM1 includes the buffer capacity of the media by means of a set of acid-base equilibria and solves the pH dynamically.

An analysis of the existing standard models proposed until now shows that they have been developed focused on reproducing individual unit process behaviour. As such, the models have significant inconsistencies in their initial hypothesis, elemental mass continuities and description of components and transformations (inert compounds, COD fractionation, organic N, pH and alkalinity, etc.). Because of this, the development of procedures for plant-wide modelling and the creation of methodologies for constructing unit process models for new technologies (lagoons, ozonation, two-step nitrification, etc.) in a coherent and compatible way are important challenges that should be overcome in the future.

Specifically, the construction of plant-wide models that consider the mutual relationships among the different unit processes guaranteeing mass and charge continuity throughout the model plant is not a straightforward task (Vanrolleghem *et al.* 2005; Wentzel *et al.* 2006). One of the most controversial subjects in this area revolves around the different approaches used to model in an integrated way the different processes in an advanced WWTP. Several different approaches have been developed with the most popular addressed here:

1. Direct connection among standard unit-process models ("Interfaces" approach)
2. Modelling of the whole plant based on a common components vector
    (a) Using standard biochemical models ("Standard Supermodel" approach)
    (b) Constructing biochemical models adapted to the plant under study ("Tailored Supermodel" approach)

In this paper, the most important fundamentals of these approaches are presented and a discussion analyzing the advantages and disadvantages of each one is carried out.

DIFFERENT APPROACHES FOR PLANT-WIDE MODELLING

In this section a brief description of the fundamentals of each approach is presented to put the discussion in context so that a meaningful comparison can be made.

Direct connection among Standard Unit-process models ("Interfaces" approach)

The Interfaces approach is based on connecting existing standard well known models by means of specific interfaces that appropriately convert components between the different unit-process models. The principles involved in model interfaces can be explained as: what is the best way to transform the state variables of one unit-process model into the state variables of another. However, not only are the model components not the same, but they are often not even compatible with respect to meaning. Some typical examples of incompatibilities between models are the differences in COD fractionation or in the description of organic nitrogen, the description of pH versus alkalinity or the definition of inert materials in aerobic or anaerobic models. It is clear that the issue becomes more complex when the models being interfaced are becoming more complicated but the principle remains the same: how can this be done while maintaining a mass balance on the quantities of interest.

Some examples of the simplest WWTP model interfaces were developed nearly a quarter century ago to link the biological activated sludge models to the settling models used for secondary clarification: all particulate fractions in the bioreactor are lumped into a variable "X" representing the Total Suspended Solids (TSS) concentrations in the settler, and after the settler the TSS is fractionated ("delumped") again into the bioreactor model components.

An illustrative example of interfaces connecting the ASM1 activated sludge unit and the anaerobic digestion model ADM1 was proposed by Copp *et al.* (2003) for the simulation of a standard WWTP in the benchmark study (BSM2) (Jeppsson *et al.* 2006). Vanrolleghem *et al.* (2005) proposed the general Continuity-Based Interfacing Methodology (CBIM) to connect any two standard models (Volcke *et al.* 2006; Zaher *et al.* 2007; Benedetti *et al.* 2008). 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 by means of a set of instantaneous conversions from the origin model components to the destination model ones.

The main advantages of the Interfaces approach are the use of all knowledge previously acquired about the practical implementation of well known standard models and their simplicity. However, the development of the interfaces between new advanced models is becoming more and more complex. Additionally, it is not always simple to guarantee a total elemental mass continuity among standard models for any process under dynamic conditions without a revision and, sometimes, a re-definition of the mass composition of the components to be converted is needed. It is important to point out that, although the main advantage of this approach is the use of well known models, most of the difficulties to construct the interfaces could be easily solved by defining new component vectors, equally valid for describing each particular unit-process, but more compatible for connection with the rest of the unit-process models (pH calculation in activated sludge units and anaerobic digesters, the same organic nitrogen characterization in all standard models, etc.).

Modelling of the whole plant based on a common components vector

This approach is based on a unique model for describing the most relevant biochemical, chemical and physico-chemical processes in all unit-processes of the plant. Therefore, all of the transformations are active in all of the streams regardless of the type of stream or unit process. That is, in this approach, all of the aerobic transformations are active in all streams including those that are anaerobic as are the anaerobic transformations in the aerobic streams. They might be zero, but they are still being solved and integrated within the model.

With this approach, there is a unique common vector for the description of the state of the process at each point of the whole plant. From this vector definition, two approaches can be used for constructing models, the "Standard Supermodel" and the "Tailored Supermodel" approach.

"Standard Supermodel" approach

This approach is based on the utilization of a set of standard supermodels that describe the most relevant processes within the whole WWTP. Theses models have been developed recently and are briefly described. The BNRM1

model proposed by Seco *et al.* (2004) reproduces the activated sludge units for biological C, N and P removal and anaerobic digestion. The ASMD model includes, in addition to C, N and P biological removal and anaerobic digestion, some chemical precipitation processes and additional calculations (DO, pH, pH inhibitions, etc.) that can be switched on or off depending on the case study (Jones & Takacs 2004). Recently, Jones *et al.* (2007) developed a new Standard Supermodel that includes important reactions in side-stream processes.

Because all state variables are consistent and integrated in all streams, the main advantage of this approach is that the need for model interfaces is eliminated and any applicable transformations are simply turned on or off depending on the environmental condition. However, as weak points, the use of the Supermodels implies a lack of flexibility for describing simpler or more complex plants. For example, with the Supermodels previously mentioned, a plant with only C and N removal will include the PAO activity (or lack thereof) with all their related transformations. Furthermore, plants with new processes for sludge or side-stream treatment (ozonation, autothermical aerobic digestion, etc.) would require the development of new Supermodels. Because Supermodels are not normally described in the literature and their use is restricted to specific simulation platforms, adaptation of one of these models might be difficult.

"Tailored Supermodel" approach

This approach is based on the construction of a global biochemical model specific for the plant under study, only including the most relevant biochemical, chemical and physico-chemical processes within the specific plant. Therefore, the descriptive capacity of the resulting models and, consequently, the complexity of its mathematical formulation and the number of components are adapted to the specific requirements and objectives of the plant under study.

Although some versions of the Standard Supermodels are already able to activated or deactivate some blocks of transformations, the construction of a Tailored Supermodel is based on the user selecting, from a well known list, the set of compatible transformations strictly required to reproduce the activity of the relevant bacteria populations in the WWTP under study. Therefore, a crucial aspect of this approach is the availability of a common and consensual list of transformations including all relevant process transformations in a WWTP, described by their balanced stoichiometry and kinetics under all possible environmental conditions within the plant. This general list should also be expandable, in order to incorporate new transformations in the future.

The main advantage of this approach is the flexibility it includes to construct supermodels that are specifically adapted to the requirements of the plant under study. However, as weak point, this flexibility can be easily misused when there is no rigorous and systematic procedure available to select the transformations and to construct the most appropriate model for each specific case. For this reason, it would be interesting to define some rules to come up with an extensive list of potential groups of reactions that in principle could be disabled or enabled (C-removal, flocculation, fermentation, methanogenesis, sulphur oxidation/reduction, water chemistry, precipitates of calcium/magnesium etc.).

According to this, a systematic approach totally oriented to construct Tailored Supermodels called PWM methodology has been recently proposed by Grau *et al.* (2007). The PWM methodology is based on a complete definition of the elemental mass fractions of the model components and the selection of the strictly required mass-balanced transformations to describe the relevant processes occurring in the studied plant. The systematic and rigorous procedure to select the appropriate transformations in each case is based on the user selection of the relevant biological processes that take place in the whole plant (biological C, N, P removal, anaerobic digestion, Sharon, etc). Depending on theses processes, a set of bacterial populations is identified and transformations describing their growth, decay and enzymatic hydrolysis are automatically selected (see Table 2 and Fig. 2 in Grau *et al.* 2007). This procedure was recently used to model C and N removal at a wastewater treatment plant (Grau *et al.* 2007b), in a model that combines aerobic and anaerobic sludge digesters (De Gracia *et al.* 2008) and in a model that incorporated ozone treatment in the sludge line of a conventional activated sludge plant (Manterola *et al.* 2007).

DISCUSSION

All the modelling approaches presented above can be used to construct dynamic models for whole WWTPs. Therefore, their suitability depends on the specific requirements and objectives of the case under study. However, a comparative analysis from the point of view of model users and model developers can help to show the weakest and strongest points of each alternative.

A very relevant topic for discussion is the difficulties that model end users are faced with when creating and simulating a plant model. It is very clear that using the Interfaces approach, all the experience previously gained with Standard models can be easily used but, in contrast, differences in the model components used at different points of the plant can lead to misunderstandings. The Standard Supermodel approach eliminates this problem but the simulation of transformations and components that are not relevant for the plant under study can also be confusing, especially when models are not well known by the users. On the other hand, to work with a complete model even for simple plants can help to identify unexpected processes that with simpler models could not be detected. For example, a model that considers C and N removal could be able to detect unexpected nitrification under unusual conditions (higher temperature, lower load or changes in sludge wastage) in plants only designed for C removal. Finally, the Tailored Supermodel approach only includes transformations that are relevant for the plant under study but, the procedure to properly select the required transformations for each specific plant, can be difficult for model end users, unless a very systematic, rigorous and automatic procedure is available. Moreover, the fact that each plant model could be unique will handicap end users that are not familiar with the specific transformations in isolation.

A logical requirement for a plant-wide model should be the definition of a common characterization of the state of the process at any point of the plant. With the Supermodel approaches, this state vector is logically associated to the model components vector and it includes a very detailed characterization of compounds in order to be usable to describe all the transformations within the plant. The use of such a descriptive list of components allows a more realistic characterization of their elemental mass fractions with constant values (constant stoichiometric formula) and, consequently, facilitates the rigorous calculation of the relationship between mass and ThOD or the additional measurable variables at each point of the plant. This contrasts the Interfaces approach, in which the characterization of the state of the process and the mass flux is described differently at each point of the plant as unit process models frequently describe the same compounds with different components (readily biodegradable substrate is described by S_S in ASM1 or S_{su}, S_{aa}, S_{fa}, and VFAs in ADM1 model, organic nitrogen is S_{ND} with ASM1 or a fraction of S_{aa}, etc.). The advantage of this difference, however, is that the characterization methods for the components have typically been developed in the context of the behaviour in these unit processes (e.g. definition of readily biodegradable substrate in ASM1), and this can be taken advantage of.

Another important aspect that has to be considered in the analysis is the flexibility and adaptability of each approach to further developments in WWTP modelling. The Interfaces approach is based on standard model components and, therefore, any change in the components of these models or the development of new ones will require the construction of new interfaces for all the models to be connected. Similarly, any modification in the Standard Supermodel would require re-writing the complete model, and the progressive increase in size as new processes are incorporated could become a serious handicap for this holistic approach. The Tailored Supermodel approach has advantages from the point of view of flexibility and expandability because the mathematical description of new processes will only require the addition of the appropriate set of new transformations to the standard list, although the incorporation of new elements (for example sulphur) would imply a re-calculation in the mass balances. In this sense, discussion and consensus about the most appropriate mathematical description of each biochemical transformation at each possible environmental condition seems to be easier than the possibility to agree about the "best model" for plant-wide modelling.

Simulation platform requirements are also different for each plant-wide modelling alternative. The Interfaces approach is based on well known standard models completely described in the literature and normally available in all

the existing simulation platforms. However, standardization in the recommended interfacing approach, e.g. asking for complete elemental mass continuity (CBIM) or only for partial mass continuity (Copp *et al.* 2003), would make easy the development of simulation codes. In constrast, most of the Standard Supermodels have been developed in specific simulation platforms so the knowledge and expertise in this case can not be utilized in a general way for adapting the models to specific case studies with other simulation platforms. Therefore, their adaptation to other potential users and platforms within the modelling community is not so straightforward at this moment.

Computational cost is another point of concern, especially when long-term simulation or multiple runs are required (for example for statistical analysis or Monte Carlo simulation). In this aspect, the Interfaces approach seems to be the most efficient solution, although the presence of "if" functions can cause problems when using implicit differential equation (stiff) solvers. In general, the Supermodel approaches will require more time to solve. However, although one might think that these approaches are computationally inefficient since all transformations are to be calculated under all environmental conditions, it must be pointed out that the integration step size is not controlled by these "unused", slow variables, but rather by the fast kinetic transformations. Unused variables will only slow the execution in proportion to their weight in the code (i.e. the number of differential equations). On a side note, the time for the compilation of each model constructed according the "Tailored Supermodel" approach should also be taken into account.

CONCLUSIONS

In this paper, three different approaches have been proposed for plant wide modelling purposes. All three are capable of describing the behaviour of the entire WWTP, but their suitability will depend on the requirements and objectives of the study at hand.

From the analysis of the three approaches, it can be concluded that a change is required in the way WWTPs are modelled: to a plant wide perspective rather than from the point of view of individual units.

This plant-wide perspective is implicitly considered when a single definition of the model components vector is used, facilitating coherency, clarity and the direct characterization of the state of the process at each point of the plant. However, it must be taken into account that the optimum solution in plant-wide modelling can depend on several factors such as the aim of the study, user profile, the available simulation platform, etc. Hence, the use of interfaces constructed to the developers best knowledge and experience can sometimes be the simplest and most practical solution. In other cases, a hybrid solution based on supermodels constructed with a standard method and complemented, if required, by model interfaces such as settlers, thickeners, separation systems or very specific biochemical processes may be the best approach.

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