Lessons learned from the WWTP benchmarking exercise

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Abstract: This paper summarizes the main results achieved by the Task Group on Benchmarking of Control Strategies for Wastewater Treatment Plants. These results include the Benchmark Simulation Model (BSM) platform, a suite of verified unit process models, and a set of process modelling tools that can generally support wastewater treatment plant modelling studies. More importantly, this paper reflects on the most important lessons learned, both from the BSM platform development and from the use of the BSM platform and its tools: (1) Development of the BSM platform was mostly based on voluntary work and has demonstrated that voluntary work still has a major role to play in the scientific community; (2) Development by a broad and diverse group of experts (e.g. both from industry and academia) has promoted broad acceptance and success of the BSM platform; (3) Model implementation and ringtesting has been one of the most time-consuming development steps, and has to some extent taken the focus away from the original BSM platform purpose, i.e. testing and comparison of control strategies; (4) Modularity and proper documentation of the developed BSM platform tools has contributed substantially to the success of the BSM platform. Finally, the paper also discusses how the BSM platform could form a source of inspiration to other research fields, for example fermentation, biocatalysis and pharmaceutical production.

Keywords: benchmark, BSM, control, modelling, monitoring, simulation, wastewater treatment plant

1. INTRODUCTION

The Scientific and Technical Report (STR) of the IWA Task Group on Benchmarking of Control Strategies for Wastewater Treatment Plants is soon to be published (Gernaey *et al.*, 2013). This Task Group has a long history, as the STR will summarize more than 15 years of work on the Benchmark Simulation Models (BSMs). This paper provides a summary of the results of the Task Group. However, more importantly, the paper is meant as an overview of the most important lessons learned from the work done by the Task Group members and the many other people that have been involved in the BSM development.

As an introduction, it is important to define the term 'Benchmark Simulation Model (BSM)'. In a dictionary, a benchmark is defined as a measure of reference to be used in a test. In computer science a benchmark is a reference performance to which the relative performance of hardware or software can be compared. In process modelling and control, a benchmark is defined as a plant model and associated control strategy that can be used as reference point for the simulation-based comparison of control strategies (Downs and Vogel, 1993). Such a simulation benchmark is not associated with a particular simulation platform. In the case of the BSMs developed by the Task Group, the purpose of the simulation protocol was to generate a tool that could guarantee that different users obtain exactly the same simulation results when running the simulation model of a specific wastewater treatment plant (WWTP).

2. TASK GROUP RESULTS

2.1. THE BSM PLATFORM

The main 'products' of the Task Group are WWTP simulation models, a specific simulation protocol for these simulation models, and a set of evaluation criteria. All these items together form the BSM platform. The platform will be described in detail in the STR (Gernaey *et al.*, 2013).

The first simulation benchmark was the Benchmark Simulation Model No. 1 (BSM1), whose development was initiated two decades ago. The idea to produce a standardized 'simulation benchmark' was first suggested by Bengt Carlsson (Uppsala University, Sweden) at the 1993 ICA Conference in Hamilton, Canada, exactly 20 years and 5 ICA conferences ago. This idea was developed by the first IAWQ Task Group on Respirometry-Based Control of the Activated Sludge Process (Spanjers *et al*., 1998) and subsequently modified by the European Co-operation in the field of Scientific and Technical Research (COST) 682/624 Actions in co-operation with the second IWA Respirometry Task Group (Pons *et al*., 1999; Copp, 2002; Copp *et al*., 2002). The BSM1 plant aims at C/N removal in a series of tanks, and has a simple layout consisting of an activated sludge tank and a secondary clarifier. Although a very flexible tool, BSM1 is not intended for long-term evaluation: performance of control strategies is evaluated based on one week of dynamic input data for three different weather scenarios (Copp, 2002), and the temperature is constant. However, many control actions at a WWTP have an effect on the process over longer time scales than one week.

The Benchmark Simulation Model No. 1 Long Term (BSM1_LT) addresses these BSM1 shortcomings – for example by extending existing BSM1 models to include temperature dependency – but is still focused on control of the activated sludge process using the same plant layout as BSM1. BSM1_LT allows for process monitoring, i.e. tracking measurement variables to detect process deviations, failures and faults, and in order to achieve this in a realistic way, the evaluation period was extended to one year (Corominas *et al*., 2011). The BSM1_LT is the first simulation platform that allows objective comparison of WWTP monitoring methods.

After initial studies with BSM1 were published, it was quickly realized that it does not allow for the evaluation of control strategies on a plant-wide basis. In recent years, the importance of integrated and plant-wide control has been emphasized by the research community. The wastewater industry is starting to realize the benefits of such an approach, and it is the intent of the Benchmark Simulation Model No. 2 (BSM2) to take these issues into account. The BSM2 extends the BSM1 layout by adding wastewater pre-treatment and a sludge treatment train including anaerobic digestion. Similar to BSM1_LT, the benchmark evaluation period is extended to one year for the BSM2, which allows for the inclusion of seasonal effects on the WWTP in terms of temperature variations for example.

2.2. VERIFIED UNIT PROCESS MODELS

A second major result of the work of the Task Group is a set of verified unit process models that are essential when performing WWTP simulation studies, also for other WWTP configurations. The Activated Sludge Model No. 1 (ASM1) (Henze *et al*., 2000), Takács secondary clarifier model (Takács *et al*., 1991), and Anaerobic Digestion Model No. 1 (ADM1) (Batstone *et al*., 2002) etc. were all verified and ringtested extensively across software platforms before including those unit process models in the BSM platform. The implementation and validation of the Anaerobic Digestion Model No. 1 (ADM1, Batstone *et al*., 2002; Rosen *et al*., 2006), to avoid excessively long simulation times for the BSM2, is one example of a major milestone in the BSM2 development. The Matlab implementation of ADM1 is one of the stand-alone models that are freely – and frequently – distributed by the Task Group.

2.3. PROCESS MODELLING TOOLS

The work of the Task Group has also resulted in a set of generic tools that can support the modelling of activated sludge WWTPs in general including but not limited to: (1) A set of evaluation criteria with focus on effluent quality and plant operating cost which can be used – often without any modification at all – independent of any BSM (e.g. Abusam *et al*., 2002); (2) The influent disturbance generator model (Gernaey *et al*., 2011) was originally developed as a phenomenological influent model specifically designed for the model-based generation of the influent sequence of the BSM2, but has now been calibrated and extended on the basis of full-scale plant data as well (Flores-Alsina *et al*., 2013); (3) A set of sensor models that adopted the principles and models described by Rieger *et al*. (2003) were implemented as part of the BSM platform; (4) Models for sensor and actuator faults (Rosen *et al*., 2008) were developed and incorporated; (5) ASM1→ADM1 and ADM1→ASM1 model interfaces

(Nopens *et al*., 2009) which allow coupling both models together in a plant-wide simulation model; and, (6) A risk assessment module for microbiology related settling problems which is the direct result of Task Group work (Comas *et al*., 2008).

3. LESSONS LEARNED

3.1. GENERAL – THE BSM PLATFORM DEVELOPMENT

It is important to emphasize that the development of the BSM platform was mostly based on voluntary work. Considering the large number of papers that have appeared on the development and the use of the BSM platform, one important lesson learned is that voluntary work still has a major role to play in the scientific community. Of course, there has been some financial support, for example to arrange regular meetings of the benchmark developers, through the COST actions 682 and 624, and later IWA. Clearly, the BSM platform development has demonstrated that such COST actions are important in promoting frequent contacts between researchers working in similar areas. It is difficult to imagine that the BSM platform development would have been possible without the support of both COST actions. Regular face-to-face discussion meetings are indeed essential when embarking on a journey such as the development of the BSM platform. Still, most of the work was conducted through "home-work", performed in large part by MSc and PhD students whose projects were modulated to fit into the benchmark development project.

Another lesson learned from the BSM platform development is that collaboration between industry and academia, software developers, simulation software end-users and consultants/practitioners is very important for a system like the BSM platform to be successful. Indeed, the fact that the development of the BSM platform has been an effort supported by a broad and diverse group of people is probably one of the most important keys to its success in the wastewater modelling and simulation community, and this has been assisted of course by the fact that the BSM platform development, from the outset, has been developed to be simulation platform independent. However, it is also important to issue a warning here. The main purpose of the BSM platform has been to create tools for the objective evaluation of control strategies through simulation. It was never the plan to solve problems on a real plant with the BSM platform. The BSM user must be aware of the fact that the BSM platform does not include all-encompassing tools, nor are they 'best-practice' tools to be interpreted as showcasing the best models for specific unit processes. Many of the published models used in the BSM platform were chosen based on compatibility and international acceptability at the time. The Task Group is not advocating the use of these models for purposes unrelated to benchmark studies as it is fully recognized that some of the benchmark models have specific short-comings. Likewise, the user should be careful with respect to parameter values of the models used in the BSM platform. The model parameters defined in the BSM platform are for benchmarking control and monitoring evaluation purposes only. The chosen parameters are believed to be reasonable for all of the unit processes, but the Task Group is not suggesting that these parameters be used for any other modelling purposes.

To the surprise of the Task Group members, the BSM platform development has resulted in far more spin-off benefits than actual results regarding its core ambition (benchmarking control and monitoring strategies). During the BSM2 development, for example, most of the efforts have been spent on model development (e.g. ADM1 implementation, influent disturbance generator model, ASM1→ADM1 and ADM1→ASM1 model interfaces, etc.) and ringtesting of models. Ringtesting of models – the confirmation of results using different software platforms and different developers – has in general been a very time-consuming exercise, and has been one of the most challenging tasks during the BSM development due to the large number of data (steady-state, dynamic). Furthermore, during ringtesting of the models it was in general observed that the differences between platforms became larger with increasing complexity of the models and under more dynamic conditions. For example, the deviations were somewhat larger in BSM2 than with BSM1.

The extension of the BSM1 layout (only activated sludge tanks and secondary clarifier) to the BSM2 layout (including primary clarifier and sludge treatment with anaerobic digestion) resulted in some interesting developments as well, from a control point of view. The first BSM2 version was presented at the WaterMatex2007 conference (Jeppsson *et al*., 2007), with the activated sludge tank volumes identical to the BSM1 volumes. The paper included 15 simple demonstration cases, both with and without active controllers, and was aimed at investigating how the evaluation criteria captured differences caused by various operational conditions. It was however revealed that: (1) the evaluation criteria were not very sensitive to the different cases tested; and, (2) the very highly loaded system, which was deliberately adopted for BSM1, limited what could be accomplished by control. Indeed, it was shown that control has its limitations and control authority is insufficient to significantly improve the performance of a highly overloaded plant. Interestingly, the high nitrogen (N) load that was causing some of the issues was associated with the reject water, which was not present or accounted for in the BSM1 case. The activated sludge tanks in BSM2 were redesigned and the final layout was presented by Nopens *et al*. (2010). This layout (compared to the earlier versions) included: (1) a reduced N load to compensate for the contribution of the reject water; (2) increased activated sludge tank volumes, compared to BSM1, in order to obtain a WWTP that can benefit from process control; and, (3) modifications to the evaluation criteria. The new criteria made a distinction between nitrate and ammonium nitrogen and reduced the dominating effect of aeration that was observed in earlier versions of BSM2.

3.2. THE BSM PLATFORM MODELS AND TOOLS, AND THEIR USE

The BSM platform has been well-received by the research community, and especially the BSM1 and the BSM2 are used frequently for their original purpose, i.e. benchmarking of control strategies (e.g. Vrecko *et al*., 2002; Stare *et al*., 2007). The main reasons for this frequent use of the BSM platform are believed to be that the BSM platform is addressing a real need, and that the use of the BSM platform is relatively easy because the different parts (e.g. unit process models, control strategies, evaluation criteria, etc.) are well documented. The concept of benchmarking monitoring strategies, as introduced in the BSM1_LT, has hardly been used thus far, probably also because there are not that many monitoring strategies implemented on full-scale WWTPs. The Task Group hopes of course that this will change in the future and that the availability of the BSM1_LT can be a source of inspiration and training material.

<u>Modularity</u>

The modular construction of the BSM platform is probably one of the main reasons for its success as well. As a consequence of the modular construction, it has been relatively easy for the user to pick out one or several of the tools provided as part of the BSM platform, or to add on one or several extra functions to the BSM platform without the need to implement a lot of computer code. This is illustrated with some examples below.

Starting with a rather recent example, Sin *et al*. (2009; 2011) used the BSM1 plant layout to demonstrate the application of sensitivity and uncertainty analysis methods. This forms a nice illustration of how the plant layouts defined in the BSM platform have indeed been used often as a convenient vehicle for the demonstration of new ideas or tools, as most people active within modelling and control of WWTPs will know the BSM1 and the BSM2.

In other cases, the benchmark users have not used the standard BSM plant layouts, and have instead used part of the benchmark tools (e.g. the evaluation criteria) to compare control strategy performance on models of other plants. Abusam *et al*. (2002) were one of the first to apply the BSM1 evaluation criteria to another plant model, in this case an oxidation ditch WWTP. Many similar applications of the evaluation criteria can be found in the literature. Others have only used the BSM1 influent data files (dry, storm and rain weather data) or transformations thereof in order to have a reasonable input data set to perform simulations under dynamic conditions.

The Task Group is of course supportive to the idea that users take parts of the BSM platform, and use these parts in their research projects. One critical issue, though, is documentation, or better, the lack of sufficient documentation. It is important that the users, when documenting their work, specify precisely which parts of the BSM platform have been used, and then add a detailed description about new things that have been added to it. This, we think, is essential to ensure that other users understand what has been done.

Extensions

With the extension of the BSM1 to the plant-wide BSM2, the number of potential extensions of the plant layout has exploded. Volcke *et al.* (2006) were the first to modify the BSM2 layout by addition of the reject water treatment. In this context, the Task Group has also observed that there have been quite a number of recent publications where the BSM2 plant layout was used as a basis, and was extended with extra functionality. One known limitation of the BSM2 is for example that the activated sludge part of the plant relies on one-step nitrification and denitrification models, as described in ASM1 (Henze *et al*., 2000). Recently there has been a growing interest in predicting greenhouse gas formation in the WWTP, and N_2O – an important nitrification and denitrification intermediate with a high greenhouse gas (GHG) potential produced in WWTPs – is one of the compounds that are studied extensively. Multi-step nitrification/denitrification models including N_2O production have already been implemented in the BSM2 benchmark framework (Flores-Alsina *et al*., 2011; Corominas *et al*., 2012; Guo *et al*., 2012; Guo and Vanrolleghem, 2013). Several other potential extensions have been described by Jeppsson *et al*. (2013). Also here, the Task Group supports such extensions. But in order to be really useful for the entire research community, documentation of such extensions is again a critical issue. Moreover, the Task Group also recommends that model extensions are ringtested (e.g. by comparison of two or three independent implementations by different users) before being distributed. Ringtested model examples should indeed get a quality stamp, such that the user receiving such an implementation can be reasonably sure about the quality of the computer code received. Here, the Task Group could support the effort by defining a suitable protocol that needs to be followed in order to earn the quality stamp.

3.3. THE BSM PLATFORM – INSPIRATION SOURCE TO OTHER FIELDS?

It is also important to reflect on the question: "Can the efforts put into the BSM platform development be a source of inspiration to other research fields?" The answer to that question is: Yes, undoubtedly. We will illustrate that with a few examples.

Fermentation and biocatalysis

The whole BSM platform concept has been inspired by similar work in the chemical engineering field (Downs and Vogel, 1993). Undoubtedly, many of the basic concepts incorporated in the BSM platform could again be transferred to other research fields, such as fermentation or biocatalysis, in which interest is growing in applying process modelling and simulation due to the fact that it is prohibitively expensive to perform experiments in full-scale fermentation tanks. One could easily imagine a fermentation benchmark platform – of course with different biological unit process models – reusing BSM platform tools such as the sensor models (Rieger *et al.*, 2003), or the sensor fault and actuator fault models (Rosen *et al.*, 2008) without any need for modifications. In fact, several fermentation models – with varying degrees of detail, but typically unstructured models – are available and could be excellent candidate models to set up a fermentation benchmark platform, e.g. the models presented by Sonnleitner and Käppeli (1986) for *Saccharomyces cerevisiae* (baker's yeast), or by Birol *et al*. (2002) for penicillin production. The evaluation criteria would of course need modification for application to a fermentation process. However, the current set of BSM2 evaluation criteria could form a good source of inspiration to start defining a set of fermentation process evaluation criteria with focus on operating cost – including for example aeration cost and raw material costs of the fermentation – and replacing effluent pollutant concentration thresholds by thresholds on impurities, or undesired by-products that could yield problems later on in the downstream processing train. Of course, inspired by the plant-wide BSM2, a fermentation benchmark platform could also go beyond the fermentation process itself, and include a number of downstream process steps as needed.

Pharmaceutical production

In the pharmaceutical industry, production has traditionally been based on batch processes that are operated according to a standard recipe without much control or reaction on input disturbances. Such 'frozen' batch processing is then followed by extensive off-line lab testing to ensure that all quality criteria have been met. As a consequence, traditional pharmaceutical production is not very efficient and often leads to a considerable number of batches that have to be wasted when they do not meet all quality criteria. Some of the main reasons for industry to maintain batch processes are the flexibility of batch equipment – many different production processes can be operated using the same equipment, taking organic synthesis as an example – and regulatory uncertainty. Indeed, for a long time industry has been reluctant to make any changes in order to optimize their production processes due to the large amount of paperwork required to get such changes approved, and due to the fact that industry was uncertain about the attitude of the regulators with respect to establishing more efficient production processes.

The US Food and Drug Administration (FDA) has tried to change this, and it has certainly managed to do so with the publication of the Process Analytical Technology (PAT) guidance (FDA, 2004). PAT is one of the most influential new trends in pharmaceutical manufacturing. Interestingly, seen from a modelling and control perspective, PAT does not really bring much new to consider, as the concepts described in the PAT guidance (continuous production, mechanistic process understanding, establishment of product quality based on on-line measurements, process adjustment as a reaction to disturbances, etc.) have been applied for quite a long time by other industries (e.g. petrochemical, polymer and chemical sectors) (Kourti, 2006), including the wastewater industry. The focus on the introduction of PAT has led to a significant increase in the use of Process Systems Engineering (PSE) methods and tools (modelling, optimization, plant design, control), as demonstrated in a recent review paper (Gernaey *et al*., 2012).

Obviously, there must be quite a number of methods and tools, which are frequently used in other industries that can be used in pharmaceutical production in a PAT context, and the BSM platform is certainly one of them. Taking the methodology of Singh *et al*. (2009) for design of PAT systems as an example, one of the essential supporting tools is a database with information on the properties of different types of sensors. The information contained in this database is then used to select the sensors that are best suited for a specific monitoring task, but these sensor properties (e.g. drift, accuracy, etc.) are not used actively in any simulations. One could imagine coupling such a database with sensor properties to the BSM platform sensor models (Rieger *et al*., 2003), such that the effect of selecting a specific sensor on a proposed control strategy could be evaluated in a more realistic way.

Simulations are also increasingly used to study new or improved control strategies of pharmaceutical production processes, both for specific unit operations such as crystallization (Fujiwara *et al*., 2005; Nagy and Braatz, 2012) and in a plant-wide context (Lakerveld *et al*., 2013). Typically, each published control strategy has been described for one specific case study, and it is difficult to compare the performance of different control strategies across systems. This was exactly the reason for the development of the wastewater treatment control benchmark. Thus, an effort similar to the wastewater BSM platform could be extremely useful, as it would allow objective comparison of different control strategies on one well-defined case study. Also, the simulated control strategies of a pharmaceutical process typically assume ideal measured variables, and here the sensor models (Rieger *et al*., 2003) could again be useful to add additional realism to simulation results. This would fit perfectly in the 'first time right' approach, i.e. where one attempts to design production processes such that they operate within specifications right away, without extensive testing and fine-tuning on the production process itself. In this respect, models of sensor and actuator faults (Rosen *et al*., 2008) could also be useful to evaluate the impact of such faults on the process performance, and to support simulation-based development of suitable monitoring strategies to detect such faults. Likewise, simulation-based development of fault-tolerant control strategies would also come one step closer.

4. CONCLUSIONS AND PERSPECTIVES

The BSM platform development has been an international collaborative effort that has resulted in a number of new modelling initiatives. This effort has provided significant insights into the modelling of wastewater treatment from a mathematical and numerical point of view. It has produced a number of new process modelling tools (for influent, sensors, error, interfacing and evaluation), important modifications to published models (ADM1), and has provided standardized simulation

protocols for the objective comparison of control and monitoring strategies. It is critically important to realize that none of these models have been calibrated to real data from a full-scale facility and that the processes being modelled are not based on a real plant. However, it is equally important to point out that the BSMs represent years of discussions, debates and compromises by a comprehensive, global expert team and although not perfect they have identified and focused attention on numerous modelling issues that did not have standardized solutions prior to this work.
It is also quite clear that the work of the Task Group on the BSM platform will not be finished with the publication of the STR. This is probably best illustrated by consulting the recent paper of Jeppsson *et al*. (2013) titled “Benchmark simulation models, quo vadis?”, where potential future developments of the BSM platform are discussed. The BSM platform, or at least essential parts of it, might also be useful for other research fields, as illustrated with fermentation and pharmaceutical production examples.

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