The Benchmark Simulation Modelling Platform – Areas of Recent Development and Extension

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Abstract. As the formal work of the IWA Task Group on Benchmarking of Control Strategies for Wastewater treatment Plants (WWTPs) has come to an end, it is essential to continue to disseminate the intense research in this field that is still carried out. In 2013 and 2014, all authors of the IWA Scientific and Technical Report on benchmarking came together to provide their insights, highlighting areas where knowledge was still deficient and where new opportunities were emerging, as well as to propose potential avenues for future development and application of the general benchmarking framework and its associated tools. The focus was on the topics of temporal and spatial extensions, process modifications within the WWTP, improved realism of models, control strategy extensions, the potential for new evaluation tools within the existing benchmark system and the need for full-scale validation. Four years later, it is clear that many of these goals have already been accomplished and the toolbox of Benchmark Simulations Models has been greatly extended and enhanced. The focus of this paper is to provide a number of examples of these recent extensions. As always, the different BSM softwares are freely available for the benefit of the global research community.

Keywords: Benchmark \cdot BSM \cdot Control \cdot Modelling \cdot Simulation \cdot Wastewater treatment

1 Introduction

Over the past 20 years, considerable investments have been made in acquiring knowledge as how to best perform objective benchmarking of control and monitoring strategies for wastewater treatment plants (WWTPs) and how to evaluate the results using a detailed simulation protocol. The success of the COST/IWA benchmark sim-ulation models BSM1, BSM1_LT and BSM2 (e.g. Spanjers et al. [1998;](#page-10-0) Copp [2002;](#page-8-0) Rosen et al. [2004](#page-9-0); Jeppsson et al. [2007;](#page-9-0) Nopens et al. [2010;](#page-9-0) Corominas et al. [2011;](#page-8-0) Gernaey et al. [2014;](#page-9-0) <http://www.benchmarkwwpt.org>) for control strategy and monitoring system development and evaluation clearly illustrates the usefulness of such tools for the wastewater research community. More than 500 papers, conference presentations and theses on work based on/related to the benchmark systems have been

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published to date. The freely available simulation models are used by numerous research groups around the world for various purposes and are available as predefined software tools in several commercial WWTP simulator packages (e.g. GPS- X^{TM} , $SIMBA^{\circledR}$, $WEST^{\circledR})$ – as well as in a stand-alone FORTRAN implementation and for the general MATLAB®/SIMULINK® platform. Implementations (and ring-testing) with varying success have also been achieved in $STOAT^{TM}$, $Biowin^{TM}$, $AQUASIM$, JASS, SciLab and EFORTM.

Efforts have focussed on providing tools for analysing and solving real problems for real WWTPs and establishing a general platform and simulation protocol that can be further extended in the future. As the IWA Task Group on Benchmarking of Control Strategies published the official Scientific and Technical Report (STR) in 2014 (Gernaey et al. [2014](#page-9-0)), it is important to take advantage of the experience gained by the researchers that have been involved in the BSM development over the years. The focus of this paper is to provide a number of examples of the main areas for recent extensions and enhancements of the BSM family.

Jeppsson et al. [\(2013](#page-9-0)); Vanrolleghem et al. [\(2014](#page-10-0)) discuss a number of potential avenues for extensions of the BSMs. Based on those defined needs, recent developments related to five areas: (1) Spatial extensions; (2) Process extensions within the WWTP; (3) Improved realism of the models used in the BSMs; (4) Control strategy extensions; and (5) Extended evaluation tools, are presented and discussed.

2 Area 1: Spatial Extensions

The family of benchmark systems were traditionally defined as 'within-the-fence' systems, *i.e.* model descriptions and simulations did not extend outside the borders of the WWTP. However, the catchment, sewer system, WWTP and receiving water body are strongly interlinked and therefore it is essential to understand the interactions between the sub-systems in order to improve the performance of both the individual sub-systems but also the system as a whole as well as to protect the receiving waters in a holistic manner. Modelling is a valuable tool for not only understanding the sub-systems and their interactions but also serves as an engineering tool to explore the potential for improvement in the performance using different approaches (e.g. process control, upgrading of the existing infrastructure).

The urban wastewater system (UWS) consists of different sub-systems that are interconnected. These sub-systems include: (1) catchment – generating the wastewater during dry weather and rain events; (2) sewer system – transporting the generated wastewater for treatment; (3) WWTP – where physico-chemical and biological processes are used to remove pollutants from the wastewater; and finally, (4) receiving water system – where all the treated wastewater as well as excess flow from the sewer network (overflows) are discharged.

Traditionally, these sub-systems are operated and optimized individually. For example, sewer systems are optimized to reduce the overflow volumes and pollutant discharges to the receiving water whereas WWTPs are optimized to reduce the concentration of pollutants that are released as effluent. However, it is well established that strong interactions exist and all the sub-systems in the UWS should be operated in a holistic manner in order to improve the receiving water quality.

For the above reasons the BSM–UWS has been developed. It is an integrated model library that can be used to simulate the dynamics of flow rate and pollutant loads in all the sub-systems of an UWS on a single simulation platform. It defines a hypothetical UWS using the model library, so that future users can use the pre-defined layout to study multiple control strategies and system modifications. In order to facilitate an objective evaluation of the results, evaluation criteria for river water quality as well as sewer system and WWTP performance have been added.

The existing dynamic influent pollutant disturbance generator (DIPDSG) presented by Gernaey et al. ([2011\)](#page-8-0) is extended with several new model blocks to describe the catchment (Flores-Alsina et al. [2014b\)](#page-8-0). An upgraded BSM2 WWTP is used (currently only the water line) with minor modifications is used to simulate the WWTP. Model blocks for the sewer network (includes transportation and storage) have been developed (Saagi et al. [2016\)](#page-9-0) and the river water system model is based on the River Water Quality Model no. 1 (Reichert et al. [2001\)](#page-9-0). In addition, extensions to the sewer models to describe the transport and transformation of micropollutants have been developed (Lindblom [2009;](#page-9-0) Snip et al. [2014\)](#page-9-0). New evaluation criteria for sewer performance and river water quality are included.

Using the model library, a hypothetical UWS for an urban catchment with 80 000 population equivalents and an area of 540 hectares is available (Saagi et al. [2017\)](#page-9-0). The developed UWS layout can be used to develop different integrated control strategies and analyse system modifications.

3 Area 2: Process Extensions

Apart from the necessary new process modules to describe the UWS (see above), much focus has been directed towards recovery processes. As problems associated with shortage in resource supply arise, wastewater treatment plants turn to innovation to transform themselves into resource recovery facilities. Water groups worldwide recognize that wastewater treatment plants are no longer disposal facilities but rather sources of clean water, energy and nutrients. Process models for stripping units, crystallisers and biogas upgrading units (to vehicle gas quality) have been included in some BSM versions (Arnell [2016;](#page-7-0) Solon et al. [2017\)](#page-10-0). However, more process extensions are needed to fully describe the different possibilities for nutrient recovery.

To better describe and analyse the aeration system and how to best control it, the BSM has been extended with a blower module and an adequate description of the oxygen transfer efficiency for different membrane diffuser discs (Arnell [2016\)](#page-7-0).

Currently, additional process extensions related to fixed-film and integrated fixed-film activated sludge (IFAS) processes, granular sludge (Feldman et al. [2016](#page-8-0), [2017\)](#page-8-0) and membrane bioreactor systems are also being developed.

4 Area 3: Improved Realism of Existing Models

As the traditional BSMs were based on the Activated Sludge Model no. 1 (Henze et al. [1987\)](#page-9-0) and the Anaerobic Digestion model no. 1 (Batstone et al. [2002\)](#page-8-0), they only allowed for detailed analysis and evaluation of COD and nitrogen removal systems. This was a major drawback and significant work has been devoted to enhance the BSMs in this respect.

One of the most important resources that can be recovered from wastewater treatment plants is phosphorus. Mathematical modelling can be utilised to analyse various operational strategies to recover phosphorus from the wastewater. However, incorporating phosphorus transformation processes in plant-wide models is complex. Firstly, the tri-valence of phosphates suggests non-ideality which requires the use of a physico-chemical model to account for this non-ideality. Secondly, phosphorus has strong interlinks with sulfur and iron which necessitates inclusion of their transformations into biological and physico-chemical models. Lastly, consolidating a plant-wide model aimed at describing phosphorus removal and/or recovery requires interfacing, modifications to the plant layout, addition of recovery unit processes and development of new control and operational strategies.

A physico-chemical model has been developed to take into account ion activity corrections, ion pairing effects, aqueous phase chemical equilibria, multiple mineral precipitation and gas stripping/adsorption allowing also for full pH prediction (Solon et al. [2015a,](#page-10-0) [b](#page-10-0); Flores-Alsina et al. [2015\)](#page-8-0). This model is then linked with standard approaches used in wastewater engineering, such as the Activated Sludge Models no. 1, 2d and 3 (ASM1, 2d, 3) and Anaerobic Digestion Model no. 1 (ADM1) (Solon et al. [2015b\)](#page-10-0). The extension of the ASM2d and the ADM1 with phosphorus, sulfur and iron-related conversions followed (Flores-Alsina et al. [2016](#page-8-0)). Finally, the extended models and the physico-chemical model have been consolidated into a plant-wide model provided by the Benchmark Simulation Model No. 2 (Solon et al. [2017\)](#page-10-0). The resulting model is used for simulation-based scenario analysis aiming at finding ways to improve the operation of a wastewater treatment plant aimed at phosphorus removal and recovery. For users not requiring the high complexity of the above model, special versions of BSM1 and BSM2 exist, which are based on the traditional ASM2d, ASM3 and ASM3-bioP (Rieger et al. [2001\)](#page-9-0) models.

The Takács secondary settler model (Takács et al. [1991\)](#page-10-0) has previously been the standard choice in the BSM systems. It uses a modified Vesilind settling function (Vesilind [1968](#page-10-0)) to describe the hindered settling. Although widely used, the approach has issues related to numerical robustness and also limitations in its ability to predict wet weather operation of the settler. The Bürger-Diehl settler model (Bürger et al. [2011,](#page-8-0) [2012,](#page-8-0) [2013](#page-8-0)) overcomes many of these limitations. Three principal processes included in the BD-model are: (1) bulk flow; (2) hindered settling; and (3) compression. Without a significant increase in simulation time, the model has been able to improve the description of the secondary settler behaviour. Gradually, the Bürger-Diehl model is becoming the standard settler model used in the BSMs. In many cases, the settler is now also modelled as a reactive settler based on any of the standard ASM models. The inclusion of inorganic dissolved and particulate fractions in all models are

becoming standard as well as applying different settling efficiencies for different particulate fractions in the primary clarifier.

It has been shown in numerous studies that aeration is one of the most energy consuming processes at WWTPs, commonly accounting for 40–60% of the total electrical power demand (Olsson [2012](#page-9-0); Lingsten et al. [2013\)](#page-9-0). Therefore, aeration comprises one of the major operational costs for any WWTP with secondary biological treatment facilitating nitrification. Because of its importance, the aeration system models in BSM have been improved in terms of oxygen transfer and blower models rather than applying the BSM default volumetric mass transfer coefficient of oxygen supply.

The importance of predicting greenhouse gas emissions has increased dramatically since the BSMs were first conceived. For this reason a special version of the BSM2 named Benchmark Simulation Model no. 2 Greenhouse gas (BSM2G) has been developed. The principles described by Hiatt and Grady [\(2008](#page-9-0)) with two-step nitrification and four-step denitrification have been included, featuring heterotrophic N_2O production. As a complement, denitrification by ammonia oxidizing bacteria (AOB) has been included following Mampaey et al. [\(2013](#page-9-0)) where AOB have the capability of reducing $NO₂⁻$ to NO and N₂O. Fundamental contributions to this development was done by Flores-Alsina et al. ([2011\)](#page-8-0) and Guo and Vanrolleghem [\(2014](#page-9-0)) and finalised by Arnell [\(2016](#page-7-0)). Apart from the $CO₂$ from biological respiration of COD in the activated sludge unit, anaerobic digester and biological side-stream treatment and N2O from nitrogen conversion processes in activated sludge and side-stream reactors, several direct and indirect emissions are also included:

- fugitive emissions of $CO₂$ and $CH₄$ from the anaerobic digester and co-generation unit. Dissolved CH₄ in the digester effluent is stripped and a $CO₂$ credit is included for power production from biomethane;
- $CO₂$, N₂O and CH₄ from sludge storage;
- $CO₂$ from off-site heat and power generation;
- $CO₂$ from production of external carbon source;
- N_2 O from conversion of effluent nitrogen in recipient;
- $CO₂$ for transport of sludge for disposal;
- $CO₂$, N₂O and CH₄ from disposal of sludge.

5 Area 4: Control Strategy Extensions

Due to the spatial extension, new processes and enhanced models a large number of new control possibilities have become possible and have therefore been added to the BSM family. Many of these are directly related to system-wide control strategies, i.e. including the sewer system and (limited number) the receiving water body. However, also the addition of a complete physico-chemical description and phosphorus, sulfur and iron-related conversions implies new control possibilities within the WWTP itself, especially related to addition of different chemicals. Examples can be found in Flores-Alsina et al. ([2014a](#page-8-0)); Saagi et al. [\(2016](#page-9-0)); Saagi et al. ([2017\)](#page-9-0); Solon et al. ([2017\)](#page-10-0). More details related to this area will be provided in the final paper.

6 Area 5: Extension of Evaluation Tools

The basic premise on which benchmarking is based are the metrics used in the evaluation phase. The availability and reliability of the evaluation tools to effectively 'score' the process under study is essential for the success of any benchmark system. Hence, the evaluation criteria (the metrics) must efficiently simplify a complex comparison into a few meaningful index values that capture the relative strengths and weaknesses of the items being compared.

The standard BSM platform was, and still is, based on three main types of evaluation criteria (effluent quality, operational cost issues and risk). Effluent quality is considered through an Effluent Quality Index (EQI) , which has been defined to quantify into a single term the effluent pollution load to a receiving water body. This combined with an effluent violation metric gives a reasonable overview of the ability of the benchmarked system to meet a particular effluent requirement whatever that might be. Energy 'costs' are considered through pumping, mixing and aeration energy calculations. Sludge 'costs' are considered through sludge production and disposal calculations and costs related to chemical additions are also included (external carbon source). Together these 'costs' form an Operational Cost Index (OCI) using empirical factors. Finally, process risk is considered through a fuzzy logic calculation of microbiology-related operational problems to create a Risk Index (has not been modified).

To assess the performance of the now possible combined C, N and P control strategies, an updated set of evaluation criteria is necessary. The EQI has been updated to include the additional P load, both organic and inorganic. Because of the modifications to the plant layout and operation, additional costs are also considered, such as those relating to the additional recycles (anoxic, anaerobic), aerators $(CO₂$ stripping) and several chemicals (for chemical P precipitation and/or recovery) (Solon et al. [2017](#page-10-0)).

Sewer system performance during rain events is generally assessed by the amount of flow rate and pollution that is discharged into the river system (the lower, the better). As part of the new BSM–UWS the following new set of evaluation criteria are computed:

- 1. Overflow duration $(d.yr^{-1})$: the total overflow duration for a given year/evaluation period.
- 2. Overflow frequency (events.yr⁻¹): represents the number of overflow events annually. Two overflow events are separated if there is at least one hour difference in time between these events.
- 3. Overflow volume $(m^3.yr^{-1})$: the total volume of overflow from all overflow locations that reaches the receiving water system in a year.
- 4. Overflow quality index (*OQI*, kg pollutant units.d⁻¹): an aggregated pollution index similar to the EQI used for the wastewater treatment plant. It considers the pollutant load from different pollutants (chemical oxygen demand (COD), biological oxygen demand (BOD), total suspended solids (TSS), total Kjeldahl nitrogen (TKN), nitrate $(NO₃⁻)$ and phosphate $(PO₄³⁻)$) and assigns weights to each one. The *OQI* is the sum of the total load for each pollutant multiplied with its individual weight. The weights for individual pollutants are similar to those used in the BSM1 and BSM2 models.
- 5. Hourly maximum concentration $(g.m^{-3})$: the concentration that is continuously exceeded for a period of at least 1 h. Calculated for TSS, TKN and PO_4^{3-} .
- 6. Exceedance duration $(d.yr^{-1})$: the total duration for which the pollutant concentration exceeds a pre-defined threshold limit. It represents the duration of acute pollutant discharge to the receiving water system. Pollutants considered are TSS, TKN and PO_4^{3-} .

All the above criteria are described for the entire sewer system but can also be computed for each overflow location individually.

Three new evaluation criteria have been defined to assess the chemical quality of the river in BSM–UWS, mainly in terms of un-ionized ammonia $(NH₃)$ and dissolved oxygen (DO). They are:

- 1. Exceedance duration $(d.yr^{-1})$: represent the total duration in a year for which the concentrations of DO and NH3 exceed threshold values. The threshold values used are: NH₃ – 0.018 g.m⁻³ and DO – 6 g.m⁻³.
- 2. Hourly minimum oxygen concentration (g.m⁻³): minimum dissolved oxygen concentration that is continuously reached for a duration of at least 1 h.
- 3. Hourly maximum ammonia concentration $(g.m^{-3})$: un-ionized ammonia concentration that is continuously exceeded for a period of at least 1 h.

More information on BSM–UWS evaluation criteria is available in Saagi et al. [\(2016](#page-9-0), [2017\)](#page-9-0).

As the BSM platform has been extended with greenhouse gas emissions (in BSM1G and BSM2G), a criterion to evaluate the impact of control strategies on this has also been added, offering more knowledge about the overall "sustainability" of the plant (Flores-Alsina et al. [2011](#page-8-0), [2014a](#page-8-0); Arnell [2016](#page-7-0)). The calculated greenhouse gas emissions are converted to $CO₂$ equivalents using GWP factors for a 100-year time horizon from IPCC ([2013\)](#page-9-0): 34 for methane and 298 for nitrous oxide, including climate-carbon feedbacks. The various emissions are reported separately and a selection of which emissions to report can be made case-by-case (for example in total or excluding biogenic emissions).

However, along with on-site effects the plant operations at the same time have global environmental impacts due to production of input goods, discharge of residues and discarding of wastes. These impacts are only covered to a limited extent in the dynamic process models. Greenhouse gas emissions from production of power and some chemicals, residual effluent nitrogen and disposal of sludge are for example included in the BSM2G. Other impacts are not considered but may very well be crucial for the overall environmental impact of the operations. Global environmental impacts of products and processes are commonly assessed by life cycle analysis (LCA). In LCA, the object under study is evaluated for the environmental impacts that the inputs and outputs give rise to over the course of the entire life cycle. For these reasons, an LCA model was constructed following ISO 14040 ([2006\)](#page-9-0) using the Gabi software tool (Gabi software 6.3, Thinkstep, Leinfelden-Echterdingen, Germany, 2013) for the BSM2G describing the same unit operations but extended with up-stream processes for production of input goods and downstream impact of residuals and wastes. The exported results from the BSM2G were imported to the LCA model.

When combining the BSM2G with the LCA model two exceptions from the default evaluation procedure were made. The offsite processes, production of power and chemicals, together with the downstream ones in recipient and from sludge disposal, are excluded from the evaluation procedure of BSM2G. Instead the impacts from these processes are included in the LCA. The six most important impact categories were selected based on previous studies (Corominas et al. [2013\)](#page-8-0) for which impacts were calculated: abiotic depletion potential of elemental and fossil resources, eutrophication potential, acidification potential, global warming potential and ozone depletion potential.

The above extension of combining BSM and LCA for a more holistic evaluation has been successful and more information is available in Arnell (2016) and Arnell et al. ([2017\)](#page-8-0). However, it cannot be considered as a standard way of evaluating BSM systems as it requires access to special LCA software. But for cases when an extra thorough evaluation is required, it has been shown that the principle works well.

7 Conclusions

The BSM systems serve as a highly useful and freely available software platform and simulation protocol for research groups all over the world. Whether used for their initially intended purpose of objective benchmarking of control strategies and monitoring algorithms or as a starting point for other types of investigations, is of minor importance. As the IWA Task Group has come to an end, it is the group's obligation and responsibility to promote potential avenues for future development and disseminate information about the latest developments. A significant number of the extensions and improvements suggested in 2013/2014 have now been accomplished and were briefly described in this paper. It is the sincere hope of the Task Group that this will inspire other research groups to continue the development of the BSM platform, thereby allowing it to flourish and remain a state-of-the-art tool for research, development and practical application within the fascinating field of modelling, control, monitoring and simulation of urban wastewater systems.

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