Towards BSM2-GPS-X: A plant-wide benchmark simulation model not only for carbon and nitrogen, but also for greenhouse gases (G), phosphorus (P), sulphur (S) and micropollutants (X), all within the fence of WWTPs/WRRFs

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INTRODUCTION

Benchmarking WWTP/WRRF control strategies has turned out to be a very successful vehicle for development of consolidated models of whole facilities (Gernaey et al., 2014). Over the last year, a comprehensive think tank of researchers involved in this development has put together a wish list of future developments in WWTP/WRRF modelling. They want these ideas to be exposed to the modelling community gathered at WWTmod2014. Starting from a summary ongoing work on extending the Benchmark Simulation Model No.2 (BSM2) and the wish to extend the current BSM2 to include phosphorus aspects, the think tank presents this abstract to outline the options lying ahead. The lecture will present arguments for choosing among the identified modelling options, in order to get informed feedback from the WWTmod2014 audience and define a roadmap for future modelling efforts. It is believed that this way of guiding the combined (voluntary) efforts of model development will be beneficial to the WWTP/WRRF modelling community at large.

The developments in the benchmarking area this paper will discuss relate to:

G. <u>Greenhouse gases (GHG):</u> Next to methane and CO_2 that are intrinsically part of the plant-wide benchmark simulation model, recent work has focused significantly on N_2O emissions, leading to considerable extensions to the details of the N-removal sub-model of the BSM2;

P. <u>Phosphorus:</u> P-removal has been a focus of WWTP/WRRF design and operation, but its inclusion in whole plant models is lagging behind that of N-removal, due to the difficulties in modelling the precipitation processes that P is involved in, especially in the sludge train.

S. Sulphur: This element is receiving increased attention not only because of its role as a competitor for P and the related impact on P-complexation and release, but also because new processes in seawater-based systems (e.g. the SANI-process) take advantage of sulphur as a reactive element. Efforts to control H_2S emissions and induced corrosion in sewer systems will benefit from such S-focused modelling efforts as well.

X. Micropollutants: Recent interest in micropollutants has led to a diversity of model developments that would benefit from consensus-building and inclusion in the benchmark simulation platform. The diversity of micropollutants remains a challenge, but consensus can probably be found regarding models of the overall fate-determining mechanisms (sorption, biodegradation, volatilization, hydrolysis, photolysis …).

With these four themes combined, the name to be given to this extension of the plant-wide Benchmark Simulation Model No.2 coincidentally turns out to be BSM2-GPS-X, a nice wink to one of the important WWTP/WRRF simulators.

To reach this goal, the following topics will have to be addressed: 1) new evaluation criteria; 2) new chemical and biochemical processes that should be taken into account; 3) new components involved in these processes that thus need to be modelled; 4) new influent wastewater characteristics; 5) modifications to the original BSM2 physical plant layout and new unit process models; 6) model integration; and, 7) new control handles and opportunities. These are shortly presented below.

The intention at the WWTmod2014 seminar is to select a number of the more clear-cut topics developed below, and get the opinion from the audience by presenting them with a clear choice and a way to directly provide feedback (colored cards or a SurveyMonkey on-line voting system).

DISCUSSION TOPICS

1. New evaluation criteria

With the ambition to use benchmark simulation models to evaluate the control and monitoring performance of WWTP/WRRFs that go beyond what could be achieved with BSM1/2 (COD/N-removal) a new set of evaluation criteria needs to be put forth:

- ✓ Is the approach for GHG-emission evaluation appropriate (Flores-Alsina et al., 2014)?
- ✓ P-related criteria should be added, such as its contribution to the effluent quality index.
- ✓ Given the interest in nutrient recovery, should evaluation criteria be developed that highlight production of (high quality) recovered nutrients from WWTPs/WRRFs?
- ✓ Should sulphur compounds be considered in performance evaluation and in what way?
- ✓ Do we consider ecotoxicity to evaluate micropollutant removal (Clouzot et al., 2013)?

2. New chemical and biochemical transformations

Upgrading the BSM WWTP with the GPS-X related transformations inevitably leads to a wide range of processes that need to be added. The level of complexity remains an open question though:

- ✓ GHG-modelling has matured significantly over the last two years, but finalization is still required (e.g. Ni et al., 2013);
- ✓ In GHG-models temperature dependency of reaction kinetics has been modelled using the Ratkowsky equation instead of Arrhenius, enabling to model decreasing rates at high temperatures. Is this to be applied to all kinetics?
- ✓ Is ASM2d still adequate for modelling enhanced biological P-removal or do we need modifications, e.g. electron acceptor dependent decay, denitrification by specific

substrates with special kinetics (methanol, glycerol, methane, …), role of the ions Mg^{2+}, Ca^{2+}, K^{+};

- ✓ Is it important to model the behaviour of PAO's when they enter the anaerobic digester with a consequent P-release, VFA uptake, storage? How must ADM1 be upgraded to account for phosphorus and treatment of Bio-P sludge? Is ADM1 the proper model (Ikumi et al., 2011)?
- ✓ Is it important to include anoxic-aerobic digestion of Bio-P wastage sludge with lime or Mg dosing for P-precipitation (to achieve low N and P dewatering liquors) for sludge treatment and how must ASM2/2d be modified to also model this (Vogts and Ekama, 2012)?
- ✓ Which precipitation reactions to model and which numerical approach to use?
- ✓ How will the physico-chemical model look like (precipitation, acid-base reactions, pH, ion-pairing, ion activity, etc.) in terms of level of detail, equation structure and solver requirements, etc. (Batstone et al., 2012);
- ✓ If S-containing components are considered important for P-modelling (e.g. competition for iron), which of the (bio)chemical S-related oxido-reduction processes need to be included and how is the competition with methanogens to be modelled?
- ✓ Do the traditional micropollutant fate models (volatilization, sorption, photolysis, biodegradation) that only require standard chemical properties (Henry coefficients, Kow, …) suffice or are dedicated models necessary for each micropollutant (Clouzot et al., 2013)?

3. New components

If the above list of processes is all considered important, a wide range of new components will have to be added to the current set of components considered in the next generation of BSM models:

- ✓ Inert inorganic suspended solids need to be added for proper TSS accounting;
- ✓ P-related components (phosphate, PAO's, poly-P, PHA) and the components related to precipitation and PAO hydrolysis (calcium, magnesium, potassium, iron, struvite, K-struvite, newberyite, calcium phosphate, iron phosphate, iron hydroxide, calcite, magnesite);
- ✓ S-related components (sulphate, sulphite, sulphur, H_2S, poly-S, iron and other sulphides);
- ✓ A multitude of micropollutants (and their transformation products);
- ✓ Components related to GHG emissions (methane, CO_2, NO, N_2O, NH_2OH).

4. New influent wastewater characteristics

Evidently, when the set of state variables is extended, the inputs to the system will have to be extended too, including methane (G), phosphorus (P), sulphur (S), micropollutants (X). Are colloids important for the proposed configuration? Multiple approaches could be proposed:

- ✓ Can we just use correlations with the traditional wastewater components in the influent files used so far (using TSS, COD and N-fractions as independent variables to correlate with)?
- ✓ Do we need to develop new influent generation models that include, for instance, methane formation in the sewer (Guisasola et al., 2009), micropollutant release patterns (De Keyser et al., 2010), sulphur conversions, etc.?
- ✓ Do we need to provide detailed information on influent pH-dynamics and acid-base / ion composition to support the physico-chemical model that is required?

5. New physical layout and unit process models

The suggested layout of the BSM2-GPS-X WWTP is shown in Figure 1. The activated sludge section has been modified by including an anaerobic section for Bio-P removal. The actual volumes are still open for discussion and will be obtained through application of standard design guidelines, just as for BSM2 (Gernaey et al., 2014). Some proposals have been made to extend the layout that this paper will put to the floor for feedback:

- ✓ Should we include a P-recovery unit process in the sludge train and how do we model it? Evidently, including such a process in the layout would attract a lot of attention to the BSM work, and in principle the physico-chemical model contains the necessary processes, but is there a "typical" P-recovery process that industry would accept as being representative?
- ✓ Sludge reject water treatment was already tried out in the BSM2 process layout (Volcke et al., 2006). Is it time to make this an integral part of a whole plant model?
- ✓ Should we also model the pumping station, screens and grit chamber so as to really model all processes within the fence? A storage tank prior to the digester could allow for more control options and the addition of external organic material input to the system.
- ✓ The primary clarifier is receiving increased attention due to its potential role in separating organics for energy recovery by anaerobic digestion (Flores-Alsina et al., 2014). Should chemical enhancing of primary treatment (CEPT) be added to the BSMs (Tik et al., 2013)?
- ✓ Is a "fermenter" that generates VFA's out of primary sludge a unit process to be included in the whole plant configuration to be studied in the future? It certainly would provide an interesting possibility for control.
- ✓ Should the secondary settler model be upgraded to include compression and dispersion and to make its numerical solution consistent (Bürger et al., 2011)?
- ✓ Is it now time to explicitly consider the reactions in the secondary clarifier, in particular denitrification, and how would that best be done (fully reactive settler, separate reactor, etc. (Gernaey et al., 2006))? Must the same hold for thickeners and storage tanks?
- ✓ Should we add effluent polishing systems for nutrients (denitrifying filters) and TSS (disk filters) and can consensus on a representative technology and appropriate models be found?

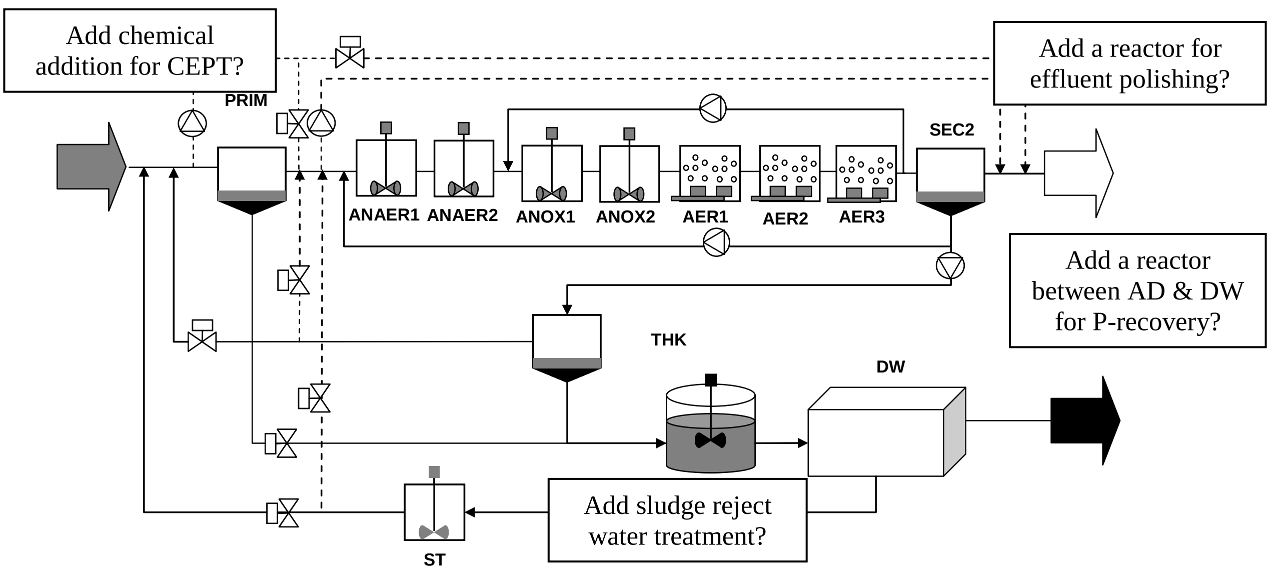

Figure 1. Plant layout of the proposed BSM2-GPS-X. Some questions remain to be answered.

6. Model integration

So far, BSMs have used interfaces to integrate the submodels. As complexity increases, the following questions can be asked:

- ✓ Do we stick to the approach with submodels with individual component sets and mass continuity interfaces to connect them or do we move towards the plant-wide modelling concept or the Supermodel approach (Grau et al., 2009)?
- ✓ If we stick to interfaces, do we extend the existing ad hoc interface or do we rigorously apply the continuity-based-interfacing-of-models (CBIM) approach (Vanrolleghem et al., 2005)?

7. New sensors and control handles

Control of WWTP/WRRFs will require a new set of sensor models to measure, for example, phosphate concentrations. Also, more control handles will become available compared to BSM2.

- ✓ Models for P-analysers and nitrite measurement devices need to be established;
- ✓ Will off-gas analysis (methane, H_2S, O_2, N_2O, CO_2…) break through and how will we model these measuring systems with gas sample preparation?
- ✓ Models for actuators needed for CEPT may have to be developed, given their particularities;
- ✓ Which sensors and control handles can be modelled for nutrient recovery systems? For instance one could imagine on-line particle size distribution measurement combined with seeding as a control handle for struvite formation.

CONCLUSION

This contribution intends to allow the control benchmarking community to get feedback from the wastewater modelling community regarding the requirements for the next generation benchmark simulation model. Given the many spin-offs that the benchmark modelling efforts have generated for the wastewater modelling community at large (Gernaey et al., 2013), it is believed that streamlining the work that is planned to occur in this benchmarking framework should be guided by the specialists in the discipline.

Efforts have and will be deployed to make the interaction with the audience as efficient as possible by presenting only a selected number of key topics presented above and providing clear choices that can be answered during the time allocated for the presentation.

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REFERENCES

Batstone D.J., Amerlinck Y., Ekama G., Goel R., Grau P., Johnson B., Kaya I., Steyer J.-P., Tait S., Takács I., Vanrolleghem P.A., Brouckaert C.J. and Volcke E. (2012) Towards a generalized physicochemical framework. *Wat. Sci. Tech.*, 66(6), 1147-1161.

Bürger R., Diehl S. and Nopens I. (2011) A consistent modelling methodology for secondary settling tanks in wastewater treatment. *Water Res.*, 45, 2247-2260.

Clouzot L., Choubert J.-M., Cloutier F., Goel R., Love N.G., Melcer H., Ort C., Patureau D., Plósz B.G., Pomiès M. and Vanrolleghem P.A. (2013) Perspectives on modelling micropollutants in wastewater treatment plants. *Wat. Sci. Tech.*, 68(2), 448-461.

De Keyser W., Gevaert V., Verdonck F., De Baets B. and Benedetti L. (2010) An emission time series generator for pollutant release modelling in urban areas. *Environ. Modell. Softw.*, 25, 554-561.

Flores-Alsina X., Arnell M., Amerlinck Y., Corominas Ll., Gernaey K.V., Guo L., Lindblom E., Nopens I., Porro J., Shaw A., Snip L., Vanrolleghem P.A. and Jeppsson U. (2014) Balancing effluent quality, economic cost and greenhouse gas emissions during the evaluation of (plant-wide) control/operational strategies in WWTPs. *Sci. Total Environ*. 466-467, 616-624.

Gernaey K.V., Jeppsson U., Batstone D.J. and Ingildsen P. (2006) Impact of reactive settler models on simulated

WWTP performance. *Wat. Sci. Tech.*, 53(1), 159-167.

Gernaey K.V., Jeppsson U., Vanrolleghem P.A. and Copp J.B. (2014) *Benchmarking of Control Strategies for Wastewater Treatment Plants*. IWA Scientific and Technical Report, IWA Publishing, London, UK.

Gernaey K.V., Copp J.B., Vanrolleghem P.A. and Jeppsson U. (2013) Lessons learned from the WWTP benchmarking exercise. In: *Proceedings 11th IWA Conference on Instrumentation, Control and Automation (ICA2013)*, Narbonne, France, September 18-20 2013.

Grau P., Copp J., Vanrolleghem P.A., Takács I. and Ayesa E. (2009) A comparative analysis of different approaches for integrated WWTP modelling. *Wat. Sci. Tech.*, 59(1), 141-147.

Guisasola A., Sharma K.R., de Haas D., Keller J. and Yuan Z. (2009) Development of a model for assessing methane formation in rising main sewers. *Water Res.*, 43, 2874-2884.

Ikumi D.S., Brouckaert C.J. and Ekama G.A. (2011) A 3 phase anaerobic digestion model. In: *Proceedings 8th IWA International Symposium on Systems Analysis and Integrated Assessment in Water Management (Watermatex2011)*. San Sebastian, Spain, June 20-22 2011.

Ni B.-J., Yuan Z., Chandran K., Vanrolleghem P.A. and Murthy S. (2013) Evaluating four mathematical models for nitrous oxide production by autotrophic ammonia-oxidizing bacteria. *Biotechnol. Bioeng.*, 110, 153-163.

Tik S., Langlois S. and Vanrolleghem P.A. (2013) Establishment of control strategies for chemically enhanced primary treatment based on online turbidity data. In: *Proceedings 11th IWA Conference on Instrumentation, Control and Automation (ICA2013)*. Narbonne, France, September 18-20 2013.

Vanrolleghem P.A., Rosen C., Zaher U., Copp J., Benedetti L., Ayesa E. and Jeppsson U. (2005) Continuity-based interfacing of models for wastewater systems described by Petersen matrices. *Wat. Sci. Tech.*, 52(1-2), 493-500.

Vogts M. and Ekama G.A. (2012) Anoxic-aerobic digestion of waste activated sludge from biological nitrogen and phosphorus removal systems. In: *Proceedings 12th biennial WISA conference and exhibition*, Cape Town, South Africa, May 7-10 2012. Paper 1154-164.

Volcke E.I.P., Gernaey K.V., Vrecko D., Jeppsson U., van Loosdrecht M.C.M. and Vanrolleghem P.A. (2006) Plant-wide (BSM2) evaluation of reject water treatment with a SHARON-Anammox process. *Wat. Sci. Tech.*, 54(8), 93-100.