

From WWTP to WRRF: A new modelling framework

Izaro Lizarralde¹, Tamara Fernández-Arévalo^{1,2}, Eduardo Ayesa¹, Xavier Flores-Alsina³, Ulf Jeppsson⁴, Kimberly Solon⁵, Peter A. Vanrolleghem⁶, Celine Vaneekhaute⁷, David Ikumi⁸, Christian Kazadi Mbamba⁹, Damien Batstone⁹ and Paloma Grau¹

¹Tecnum and Ceit-IK4, Paseo Manuel Lardizábal 15, 20018 San Sebastián, Spain. (Email: ilizarralde@ceit.es; tfernandez@ceit.es; eayesa@ceit.es; pgrau@ceit.es)

²Conaqua, Paseo Manuel Lardizábal 15, 20018 San Sebastián, Spain. (Email: tfernandez@conaqua.es)

³PROSYS Research Center, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Building 229, DK-2800 Kgs. Lyngby, Denmark. (Email: xfa@kt.dtu.dk)

⁴Division of Industrial Electrical Engineering and Automation (IEA), Department of Biomedical Engineering, Lund University, Box 118, SE-221 00 Lund, Sweden. (Email: ulf.jeppsson@iea.lth.se)

⁵Department of Biosystems Engineering, Ghent University, Coupure links 653, B-9000 Gent, Belgium. (Email: kimberly.solon@ugent.be)

⁶modelEAU, Département de génie civil et de génie des eaux, Université Laval, 1065 Avenue de la Médecine, Québec, QC, G1V 0A6, Canada. (Email: peter.vanrolleghem@gci.ulaval.ca)

⁷BioEngine, Research Team on Green Process Engineering and Biorefineries, Chemical Engineering Department, Université Laval, 1065 Avenue de la Médecine, Québec, QC, G1V 0A6, Canada. (Email: celine.vaneekhaute@gch.ulaval.ca)

⁸Water Research Group, Department of Civil Engineering, University of Cape Town, Rodenbosh, 7700, South Africa. (Email: david.ikumi@uct.ac.za)

⁹Advanced Water Management Centre, The University of Queensland, St Lucia, Brisbane, Queensland, Australia, 4072. (Email: d.batstone@awmc.uq.edu.au)

Abstract

Resource recovery is a rapidly emerging research area, which promotes the development of several technologies that have the potential to extract different type of organics, nutrients and/or energy from wastewater. However, along with such development, there is a need for a new generation of (plant-wide) engineering tools to simulate resource recovery options before/after implementation. Indeed, state-of-the-art mathematical models used nowadays in wastewater engineering are mainly focused on improving water quality and not on extraction of valuable compounds. In this paper, different groups discuss what research issues should be addressed to support the model-based analysis during the transition of wastewater treatment plants to water resource recovery facilities.

Keywords

Plant-wide modelling, ASM, ADM, Physico-chemistry, WRRF, Benchmark scenarios, Model building

INTRODUCTION

Due to the shift from the concept of WWTP to the one of WRRF, the scope and structure of the WRRF models of the XXIst century need to be defined. In addition to conventional IWA models, mainly developed for describing biological processes (nutrient removal, aeration needs, sludge production), the new models need to consider jointly biochemical transformations, physico-chemical processes (for example precipitation-redissolution, gas-liquid transfers), chemical reactions (acid-base reactions, effects of ion strength, ion pairing reactions, etc.) and energy needs/production and all this, in a plant-wide context.

During the last years, different approaches in the WWT modelling field have been proposed presenting new solutions for fulfilling these new requirements (Grau *et al.*, 2007; Ekama 2009; Gernaey *et al.*, 2014; Lizarralde *et al.*, 2015; Solon *et al.*, 2017). However, simplicity (given by the well-known and validated IWA ASM and ADM models) vs complexity (proposed in new models with great numbers of components, processes and insufficiently

validated parameters), is a question for which there is no clear agreement among scientists and practitioners. Proof of this is the final vote about the question that arose in the model complexity debate at WWTmod2016 in Annecy, France, in which 56% agreed that we need more detailed models to adequately describe the complexity of wastewater treatment systems against the 44% that disagreed.

Questions that may arise when discussing the best solution for XXIst century WRR mathematical models and how these new models should be constructed are:

- How complex should our models be?
- After almost 30 years using well-known IWA models, should we move to other nomenclature, components and processes?
- How much more information do we gain by the new models? How can this potentially 'increased' knowledge be put into practical use?
- Can the increase of complexity make our models impracticable? How can we make complex models practicable?
- Can the new data sources; e.g. sensor data, chemical and molecular analyses, new analytical techniques, off-gas analysis; keep up with the increasing model complexity?
- How does the new generation of models affect the needs for sensors and laboratory measurements?
- Can we guarantee an increase of complexity without decreasing model identifiability?
- Can the increasingly advanced WRRF processes be described by the old ASMs? If not, which extensions are felt essential (2-step nitrification, 4-step denitrification, Anammox, Glycogen Accumulating Organisms (GAO), anaerobic digestion extended for description of sulphur oxidation/reduction or phosphorus accumulation/release, etc.)?
- Can the models be calibrated for practical applications?
- Have the modelling tools improved in proportion with the increased model complexity (sensitivity analysis, uncertainty analysis, (Bayesian?) parameter estimation, etc.)?
- Have the simulator platforms kept up with model complexity in terms of model building capacity (editing, calibrating) and numerical methods?

Having the above questions in mind and with the objective of providing some answers, this paper proposes a general approach, based on a consensus among different research groups, for constructing such new models based on the experience and approaches proposed during the last 10 years. In order to promote deeper discussions and solutions of these issues, the paper also aims to be a proposal for the creation of an IWA Working Group on plant-wide modelling.

NEW MODEL BUILDING

Considering the discussion at WWTmod2016 about model complexity vs simplicity, this paper proposes a new way of building and using WRRF models based on a common framework that allows the user to build tailored models for a practical study as complex as required. This requires two main tasks: (1) the set-up of a new modelling framework to build WRRF models and (2) the development of procedures and tools that guide the building and use of such models.

New modelling framework for WRRF models

The proposed new framework gathers the most relevant biochemical, physico-chemical (liquid-gas transfer and precipitation-redissolution) and chemical equilibrium processes (acid-base reactions, ion pairing reactions, etc.) that can occur in a WRRF. These three types of processes are defined in two different modules according to their scope, nature of process being described and numerical solution.

The *first module* is constituted by slow processes and these will be described by means of ordinary differential equations (ODEs), defined as proposed in standard IWA models, with stoichiometry and kinetics formulation. This module will usually account for biochemical and physico-chemical reactions:

- Stoichiometry will guarantee elemental mass, charge and energy continuity in all reactions. On the one hand elemental mass description of all components (Ikumi *et al.*, 2014; Ekama *et al.*, 2017; Grau *et al.*, 2007) will allow closing elemental mass balances in all reactions. On the other hand, definition of formation enthalpy of each component according to its mass composition will allow the calculation of heat of reaction in each transformation (Fernández-Arévalo *et al.*, 2014).
- Biochemical and physico-chemical processes considered in this framework will describe:
 - o Organic matter biodegradation under aerobic, anoxic and anaerobic conditions and removal of N and P according to the well-accepted IWA models (ASM1, 2 and ADM1) but re-written according to the premises mentioned above (Grau *et al.*, 2007). Provided that the models are constructed by re-formulation of traditional models, the parameters used in this new framework are the same as in the traditional models. This allows for continued use of validated values for the kinetic and stoichiometric parameters.
 - o Aerobic/anaerobic sulphur reduction (Flores-Alsina *et al.*, 2016; Solon *et al.*, 2017; Feldman *et al.*, 2017; Vaneekhaute *et al.*, 2017).
 - o Precipitation-redissolution (Kazadi Mbamba *et al.*, 2015; Vaneekhaute *et al.*, 2017; Barat *et al.*, 2013; Van Rensburg *et al.*, 2003).
 - o Stripping-dissolution of gaseous components (Lizarralde *et al.*, 2015; Vaneekhaute *et al.*, 2017).
- Kinetic equations incorporate activation/inhibition terms so that reactions will be activated and deactivated according to the environmental conditions (for example acceptor of electrons, pH, saturation index, gas solubility).

The *second module* will be a set of fast processes (assumed at equilibrium) described using implicit, nonlinear algebraic equations (AEs) that will include chemical reactions required for describing the buffer capacity of the aqueous solution and consequently, the correct description of the weak acid-base chemistry. Two main approaches have been proposed in literature for modelling such reactions:

- Construction of tailor-made solutions suited to the wastewater composition (Lizarralde *et al.*, 2015; Ikumi *et al.*, 2014; Flores-Alsina *et al.*, 2015).
- Connection between WRRF model and external software packages for chemical reactions solution (Barat *et al.*, 2013). One must be careful though because using a full external geochemical library (e.g. PHREEQC) can be quite demanding computationally. Vaneekhaute *et al.* (2017) therefore developed a systematic strategy for selection of relevant species to reduce simulation effort, but still incorporate all species that affect

the model outputs (all potential precipitates, acid-base reactions, complexation reactions, etc.). In this way the advantage of having a full state-of-the-art and up-to-date library with the most efficient numerical solution method is combined with making it tailor-made for the system under study.

This modelling framework should be flexible and expandable, being able to include any new reactions, provided that premises abovementioned are properly guaranteed.

Construction of tailor-made solutions for WRRFs modelling

From the general framework presented above, specific models can be constructed and tailored to the case of study. Thus, the components and transformations considered in the models will be the ones required for describing the processes to be reproduced.

As an example of a procedure to select models, a systematic procedure for constructing WRRF models depending on the processes needed and the scope of the simulation study was presented in Grau *et al.* (2007) and Lizarralde *et al.* (2015). In this procedure, first, the relevant biochemical and precipitation-redissolution reactions for the study are selected. Second, and based on the reactions previously selected, the liquid-gas transfer reactions are added. Finally, depending on the previous transformations, the chemical module will be assigned. Although this methodology could be used as a first approach, one of the goals of the Working Group to be established will be to provide users with systematic procedures, tested guidelines and tools to construct models from the general library of transformations.

Case study

As an example of the potential of WRRF models constructed with the above methodology, a real case study that describes a WRRF for COD and phosphorus removal is presented below. The primary treatment contains 12 rectangular primary settlers. The biological treatment treats domestic wastewater with an annual average flow of 271,000 m³/d (3 million population equivalent) and is divided into six identical lines. Each line contains an anaerobic zone, a facultative zone and an aerobic zone. Alternating anaerobic/aerobic phases enable the activity of phosphorus accumulating organisms (PAOs). In order to guarantee a high solids retention time, the mixed liquor suspended solids are settled within twelve secondary settlers. The waste activated sludge is thickened, then fed to 9 anaerobic digesters. The schematic process diagram of this case study is presented in Figure 1. Two scenario analyses (Scenarios A and B) were used to investigate the optimum phosphorus management in the whole plant in order to maximize the recovery of phosphorus by means of struvite precipitation. The baseline scenario (Scenario A) is based on the current plant configuration. In the second scenario (Scenario B), a precipitation unit is incorporated after the dehydration unit to recover struvite from the supernatant of the digester. Incorporating the reactor unit struvite is recovered and lower phosphate concentrations are taken to the head of the plant.

The biochemical, physico-chemical and chemical reactions required for this case study are those that describe COD removal under aerobic, anoxic and anaerobic conditions, activity of phosphorus accumulating bacteria, struvite precipitation as well as acid-base and ion pairing reactions. As the model is constructed based on the library of transformations described in the previous section, the model will allow for: (1) detailed tracking of COD, N and P (and other elements of interest) and (2) studying different management strategies in order to provide optimum solutions in terms of stability, effluent quality, energy and chemical dosages costs and resource recovery.

Figures 1 and 2 show the complete mapping and characterization of P through the WRRF. Figure 1 shows that a high percentage (70%) of the phosphorus entering the plant is retained in the sludge produced. The 30% of the phosphorus is discharged in the effluent. There are several recycle points in the WWTP that contain phosphorus. The clarified recycle flow of the primary sludge thickener contains 5% of the phosphorus in the influent. The clarified flow of

the secondary sludge thickener is recycled into the activated sludge process, at this point there is 15 % of phosphorus entering the plant. Finally, the last recycle point is the supernatant of the anaerobic digester to the head of the plant. This flow contains 37% of the total phosphorus entering the WWTP.

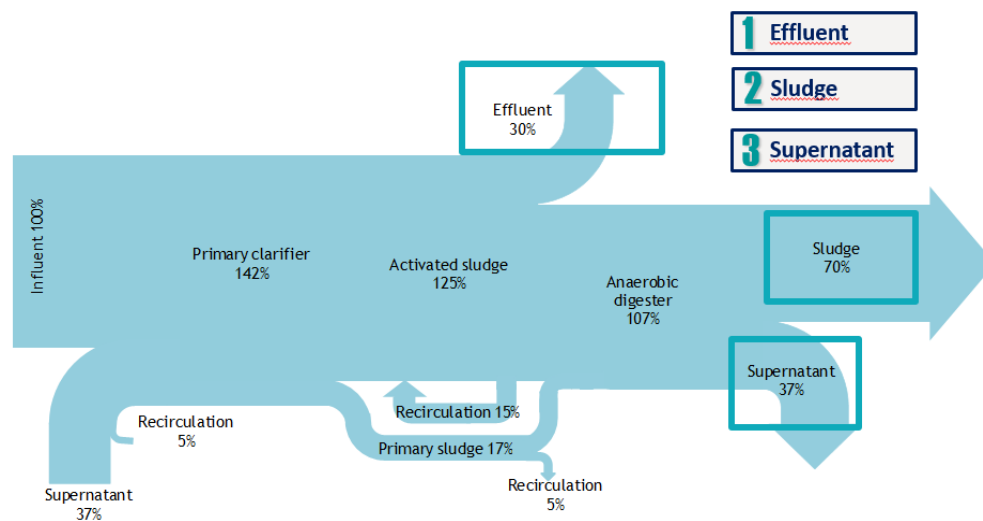


Figure 1. Phosphorus mapping through the plant.

Apart from the total phosphorus fluxes, these models characterise completely the phosphorus throughout the plant, permitting to know the form of phosphorus in each point of the plant, i.e. phosphate, ferric phosphate or biological phosphorus (Figure 2).

This chart enables the visualization of the phosphorus form along the plant. In the influent 72% of the total phosphorus entering the plant is in form of phosphates. This percentage is reduced through the treatment in the water line up to: 19% in the primary sludge, 22% in the effluent and 0.14% in the secondary sludge.

It can be seen in Figure 2 that 73% of the phosphorus is removed biologically in the activated sludge unit. 25% of the phosphorus is removed chemically and contained in the FePO_4 .

Once the primary sludge and secondary sludge are thickened and mixed, only the 0.4% of the total phosphorus in the flux is phosphate. At this point, that corresponds with the entrance to the digester, 83.5 % of the phosphorus is contained in microorganisms and organic matter.

It is remarkable an increase of phosphate concentration in the outflow of the anaerobic digestion. This is caused due to the poly-phosphate release under anaerobic digestion. Moreover, ammonium and other metal cations, such as magnesium and potassium, are also released during anaerobic digestion. However, at this point there is still a high concentration of organic phosphate and consequently high concentration of sludge.

In the clarified outflow of the dewatering unit the dissolved components remain the same as in the outflow of the digester. It must be highlighted that the 99.9% of the total phosphorus is in form of phosphates.

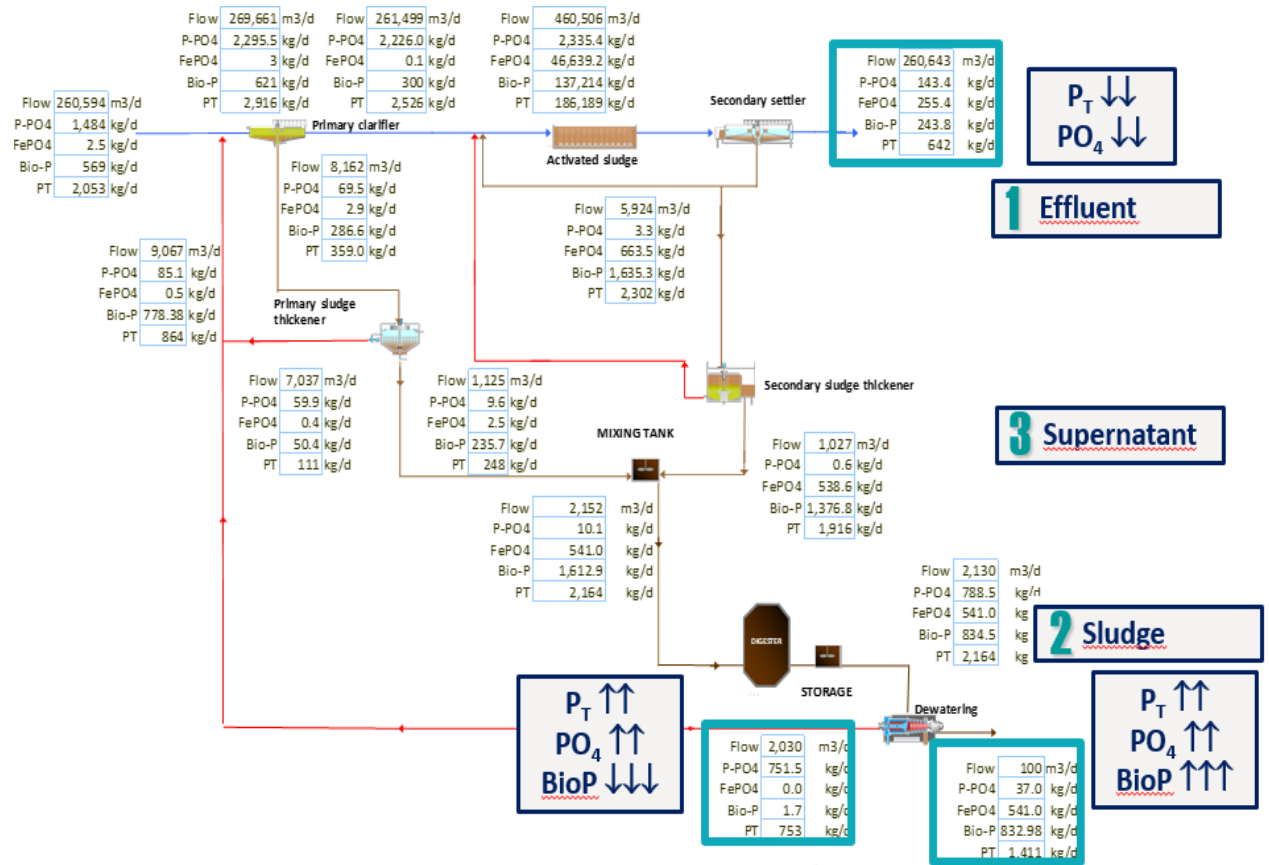


Figure 2. Phosphorus characterization through the plant.

From this analysis, an optimum alternative for recovering P is shown in Figure 3 and Table 1.

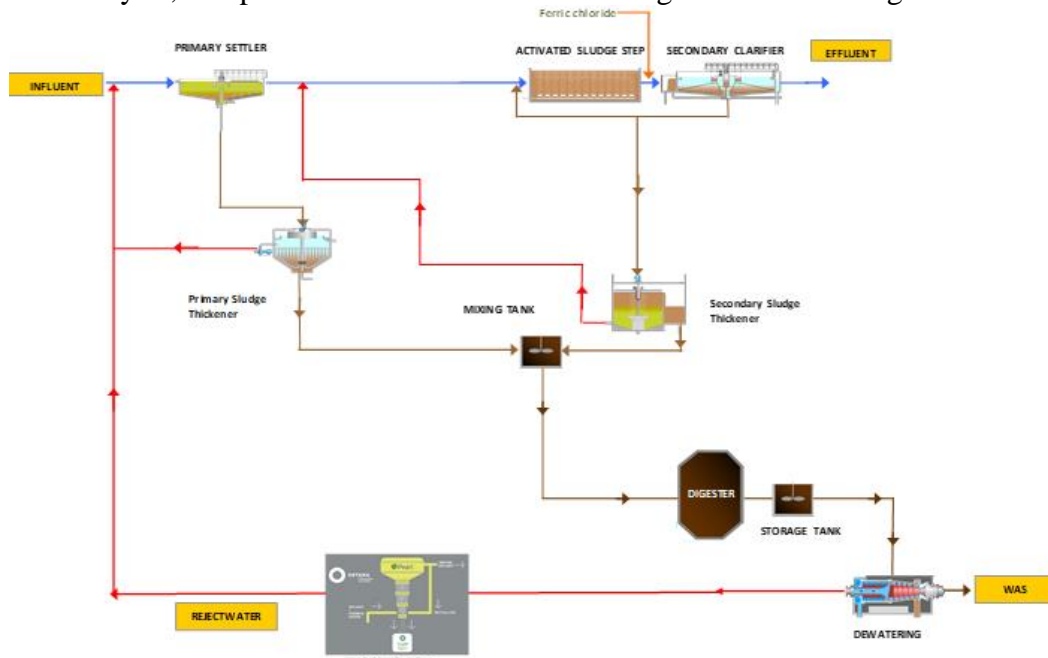


Figure 3. Scenario B alternative for struvite recovery.

Table 1. Comparison of performance of the two scenarios

Variable	Scenario A	Scenario B
Struvite production (Ton/year)	---	1499
MgCl ₂ dosage (Ton/year)	---	763
NaOH dosage (Ton/year)	---	450
Natural struvite precipitation (Ton/year)	139	105
Sludge production (Ton/year)	16490	15400
FeCl ₃ dosage (Ton/year)	4742	2371
Biogas production (m ³ /d)	30422	31001

The recovery of phosphorus as struvite has a positive effect on the overall performance of the plant. Primarily, since less phosphorus is recycled into the head of the plant, less struvite precipitates naturally, leading to less pipe clogging problems (Drechsel *et al.*, 2015). It can be seen that incorporating a precipitation unit into the plant reduces sludge production by 6.6%, reducing economical costs. Recovering struvite in the sludge line implies that a lower orthophosphate quantity is recycled into the water line. Consequently, the ferric chloride dosage required to achieve the effluent quality in terms of phosphorus concentration is lowered by up to 50%.

Finally, the effect of the new technologies on biogas production is evaluated. It can be seen that biogas production is not altered by addition of the precipitation units. These technical benefits can be translated into economical savings. First, the economic costs and benefits of producing struvite are estimated and, second, the cost savings associated with phosphorus recovery are estimated.

This study illustrated the benefits of having a plant-wide model that describes the behaviour of the complete plant. Having the complete plant described enables the study of optimum management strategies of resources.

Discussion and future needs around new WWRF models

It is clear that new scenarios require new models for describing new processes. It is not only a question of considering more components or transformations but also a question of model structure. As the previous and other examples demand, IWA's biological models should evolve to models where elemental mass and energy fluxes can be mapped and tracked allowing users to select the best mass and energy management solution in order to operate the facility considering new and conventional technologies. Thus, elemental mass characterization, mass, charge and energy continuity in all transformations, gas and aqueous phases consideration in reactors, dynamic/algebraic equations, etc. are aspects that need to be considered in the new modelling framework.

The consideration of all these aspects considerably increases the complexity of the internal structure of the models. The model constructed to describe the case study considers 24 soluble compounds, 25 particulate compounds and 7 gaseous compounds; and 31 intracellular reactions, 16 hydrolysis reactions, 36 biomass decay reactions and 56 equilibrium reactions. However, at this point it is important to highlight what is understood when referring to more complex models and analyse in each case how this complexity is increased and if that is the case, how can it be dealt with given current measurement tools, computational capacity, numerical knowledge, etc. Some questions that could be raised for further discussion would be: Which is more complex? A model that considers a high number of processes/components or one that is simplified based on assumptions and simplifications? Is a model that includes more parameters always more complex? Do parameters which can be fundamentally

determined (e.g., equilibrium constants) contribute to the parameter count? Should we consider the difficulty to include new processes or state variables in the existing models a complexity aspect? Should a more complex internal model structure always imply a complexity in the use of the model or longer simulations times? From the authors' view, the challenge for model developers nowadays would be to build guidelines, procedures and tools that make the new models easy to use, even if they consider a large number of processes and variables or more complex numerical methods. An analysis of different tools to simplify the use of models is proposed and adapted to the new model structure:

- New influent characterization methods and tools based on mass and charge elemental description of components.
- New measurement techniques. For example, the recovery of volatile fatty acids is becoming prominent, thus techniques for their measurement may become very important.
- Computational requirements, numerical solution techniques.
- User-friendly interfaces.
- Tools for the selection of the most relevant parameters for the description of the processes.
- Tools for parameter calibration. Parameters that are specific and affect only one process may be calibrated using traditional analytical methods, by calculation of Jacobian matrix. Where the parameter shape function is highly non-linear incremental search techniques that are computationally expensive, such as MC-Monte Carlo Bayesian estimation may be required.

ACKNOWLEDGEMENT

The authors would like to thank the Spanish Education and Culture ministry for the Research Project MODYREC (CTM2015-70794-R) and the COST Action ES1202: Conceiving Wastewater Treatment in 2020 – “Water2020”. Peter Vanrolleghem holds the Canada Research Chair on Water Quality Modelling.

REFERENCES

- Barat, R., Serralta, J., Ruano, M.V., Jiménez, E., Ribes, J., Seco, A. and Ferrer, J. (2013). Biological Nutrient Removal Model No 2 (BNRM2): A general model for wastewater treatment plants. *Wat. Sci. Tech.* 67(7), 1481-1489.
- Drechsel, P., Wichelns, D. and Qadir, M. (2015). Wastewater Economic Asset in an Urbanizing World. Springer.
- Ekama, G.A. (2009). Using bioprocess stoichiometry to build a plant-wide mass balance based steady-state WWTP model. *Wat. Res.* 43(8), 2101-2120.
- Feldman, H., Flores-Alsina, X., Ramin, P., Kjellberg, K., Batstone, D.J., Jeppsson, U. and Gernaey, K.V. (2017). Modelling an industrial anaerobic granular reactor using a multi-scale approach. *Wat. Res.* 126, 188-200.
- Fernández-Arevalo, T., Lizarralde, I., Grau, P. and Ayesa, E. (2014). New systematic methodology for incorporating dynamic heat transfer modeling in multi-phase biochemical reactors. *Wat. Res.* 60(1), 141-155.
- Fernández-Arevalo, T., Lizarralde, I., Fdz-Polanco, F., Pérez-Elvira, S.I., Garrido, J.M., Puig, S., Poch, M., Grau, P. and Ayesa, E. (2017). Quantitative assessment of energy and resource recovery in wastewater treatment plants based on plant-wide simulations. *Wat. Res.* 118, 272-288.
- Flores-Alsina, X., Kazadi-Mbama, C., Solon, K., Vrecko, D., Tait, S., Batstone, D.J., Jeppsson, U. and Gernaey, K.V. (2015). A plant-wide aqueous phase chemistry module describing pH variations and ion speciation/pairing in wastewater treatment models. *Wat. Res.* 85, 255-265.
- Flores-Alsina, X., Solon, K., Kazadi-Mbamba, C., Tait, S., Gernaey, K.V., Jeppsson, U. and Batstone, D.J. (2016). Modelling phosphorus (P), sulfur (S) and iron (Fe) interactions for dynamic simulations of anaerobic digestion processes. *Wat. Res.* 95, 370-382.

- Gernaey, K.V., Jeppsson, U., Vanrolleghem, P.A. and Copp, J.B. (2014). Benchmarking of Control Strategies for Wastewater Treatment Plants. IWA Publishing. London, UK. IWA Scientific and Technical Report No. 23.
- Grau, P., de Gracia, M., Vanrolleghem, P.A. and Ayesa, E. (2007). A new plant-wide modelling methodology for WWTPs. *Wat. Res.* 41(19), 4357-4372.
- Ikumi, D.S., Harding, T.H. and Ekama, G.A. (2014). Biodegradability of wastewater and activated sludge organics in anaerobic digestion. *Wat. Res.* 56(1), 267-279.
- Kazadi Mbamba, C., Flores-Alsina, X., Batstone, D.J. and Tait, S. (2015). A systematic study of multiple minerals precipitation modelling in wastewater treatment. *Wat. Res.* 85, 359-370.
- Lizarralde, I., Fernández-Arévalo, T., Brouckaert, C. J., Vanrolleghem, P.A., Ikumi, D.S., Ekama, G.A., Ayesa, E. and Grau, P. (2015). A new general methodology for incorporating physico-chemical transformations into multi-phase wastewater treatment process models. *Wat. Res.* 74, 239-256.
- Solon, K., Flores-Alsina, X., Kazadi-Mbamba, C., Ikumi, D.S., Volcke, E., Vaneeckhaute, C., Ekama, G., Vanrolleghem, P.A., Batstone, D.J., Gernaey, K.V. and Jeppsson, U. (2017). Plant-wide modelling of phosphorus transformations in wastewater treatment systems: Impacts of control and operational strategies. *Wat. Res.* 113, 97-110.
- Vaneeckhaute, C., Claeys, F.H.A., Tack, F.M.G., Meers, E., Belia, E. and Vanrolleghem, P.A. (2018). Development, implementation, and validation of a generic nutrient recovery model (NRM) library. *Environ. Model. Software* 99, 170-209..
- van Rensburg, P., Musvoto, E.V., Wentzel, M.C. and Ekama, G.A. (2003). Modelling multiple mineral precipitation in anaerobic digester liquor. *Wat. Res.* 37(13), 3087-3097.