

# Modelling wastewater treatment plants – science fiction or approaching reality?

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## Activated sludge models

Over the past twenty years, the knowledge and understanding of wastewater treatment has advanced extensively and moved away from empirically-based approaches to a fundamentally-based ‘first principles’ approach embracing chemistry, microbiology, physical and bioprocess engineering, and mathematics. Many of these advances have matured to the degree that they have been codified into mathematical models for simulation by computers.

Before the 80’s, several research groups worked independently from each other on developing models of activated sludge. Each group developed and applied their own approach and notation, first in steady-state models, and later on, in dynamic models. Table 1 summarizes the essential features of these and several other activated sludge models.

In the early 80’s, Poul Harremoës, President of IAWPRC (The International Association of Water Pollution, Research and Control, later IAWQ, International Association of Water Quality; nowadays, IWA, International Water Association) initiated the idea to combine the most relevant and applied models and to work together at an international level to accelerate development of a common, unified model. As a consequence, in 1982, the "Task Group on mathematical modelling for design and operation of biological wastewater treatment" was established with Gerrit Marais (University of Cape Town), Leslie Grady (Clemson University), Willy Gujer (EAWAG), Tomonori Matsuo (Tokyo University) and Mogens Henze (Technical University of Denmark) as chairman. This joint activity resulted in the development of the first dynamic Activated Sludge Model, called in short ASM1 (Henze *et al.*, 1987b). The ASM1 can be considered as the reference model, since this model triggered the general acceptance of wastewater treatment modelling, first in the research community and later on also in practice. This evolution was undoubtedly supported by the availability of more powerful computers. ASM1 is in essence a consensus model-compromising result of discussions at the time between different modelling groups. Many of the basic concepts of ASM1 were adapted from the activated sludge model defined by Dold *et al.* (1980). A summary of the research developments that resulted in ASM1 was given by Jeppsson (1996) and in a recent chapter of Ekama and Takács (2014) (in Jenkins and Wanner, 2014). Even today, the ASM1 model is still in many cases the state of the art for modelling activated sludge systems (Roeleveld and van Loosdrecht, 2001). ASM1 has become a reference for many scientific and practical projects, and has been implemented (in some cases with modifications) in most of the commercial software available for modelling and simulation of plants for N removal. Copp (2002) reports on experiences with ASM1 implementations on different software platforms. In general, activated sludge models from the ASM ‘family’ are developed to describe the oxygen uptake rate and sludge production (coupled with COD balance), and N and P conversions at domestic wastewater treatment plants. However, despite the fact that they are designed for practical (and therefore not academic) purposes, they are not sanitation models as they do not describe the removal of pathogens. Probably the best way to describe the stepwise activated sludge model development is the original

approach of Marais and Ekama (1976) and Ekama and Marais (1978), later depicted by Dold *et al.* (1980), and further elaborated on in Gujer and Henze (1991). The outcome of this approach is the model which comes close to ASM1.

The ASM1 model is a structured model based on Monod kinetics that predicts the processes of biological (bacteriological) reactions. The ASM1 models COD and N removal, oxygen consumption and sludge production. Wastewater is characterized in terms of 7 dissolved and 6 particulate components that are used to describe 2 biomass groups, 7 fractions of COD (organic material) and 4 fractions of nitrogen (Henze *et al.*, 1987b; Gujer and Henze, 1991). Dissolved oxygen concentration and alkalinity are also included as part of the wastewater characteristics. From the 8 processes of the model, 3 are related to the growth of heterotrophic and autotrophic organisms, 2 describe the biomass decay (death-regeneration theory, Dold *et al.*, 1980), and 3 are related to hydrolysis. The model is presented in a matrix format, also known as the Petersen matrix or Gujer matrix (Petersen, 1965; Takács *et al.*, 2007). This matrix contains stoichiometric coefficients and a kinetic vector. All state variables involved in a process are displayed in columns, and all processes where a state variable is involved are presented in the rows of the matrix. Already in use in chemical modelling (Petersen, 1965), this representation helped to present the model in a condensed form. It facilitated its publication, interpretation and comparison not only between models, but also between processes and compounds. Certain major limitations of ASM1 are, for example, that it only describes heterotrophic and autotrophic reactions under aerobic and anoxic conditions (in which, for instance, ordinary heterotrophs consume carbonaceous substrates and autotrophic nitrifying organisms oxidize ammonia to nitrate), but it does not include enhanced biological phosphorus removal (EBPR) processes (Gujer and Henze, 1991). Despite the fact that to a great extent knowledge of EBPR processes was already available when ASM1 was developed (van Loosdrecht *et al.*, 1997), EBPR was not included in ASM1 since most of the wastewater treatment plants at that time did not incorporate biologically enhanced (or chemical) phosphorus removal (Fenu *et al.*, 2010).

Throughout the years, several research groups started to work on the description of EBPR for its incorporation in the dynamic activated sludge models, mostly based on directly measurable soluble compounds. From the mid 80's to the mid 90's, the EBPR process grew in popularity and the understanding of the underlying bio-chemical mechanisms increased (Henze, 2000). In the meantime, in 1990, the composition of the Task Group changed, when Leslie Grady left and Takashi Mino (Tokyo University) and Mark Wentzel (University of Cape Town) joined the Task Group. The knowledge acquired on EBPR led to the publication of the Activated Sludge Model No. 2 (ASM2) (Henze *et al.*, 1995), which included the EBPR processes. In particular, ASM2 includes Phosphate Accumulating Organisms (PAO), growing only under aerobic conditions, with the correspondingly associated anaerobic, anoxic, and aerobic reactions. ASM2 was a compromise between complexity and simplicity, and between different points of view on how the correct model should look like to be used as a conceptual platform for further model development (Henze *et al.*, 2000). In 1996, Mark van Loosdrecht (Delft University of Technology) became member of the Task Group, following the departure of Tomonori Matsuo, Mark Wentzel and Gerrit Marais. Because the occurrence of denitrifying EBPR was well-established (e.g. Kuba *et al.*, 1997; Murnleitner *et al.*, 1997) the ASM2 model was expanded in 1999 by the inclusion of denitrifying PAO (DPAO). This version of the model was denoted as ASM2d (Henze *et al.*, 1999). Both ASM2 and ASM2d are similar to ASM1 by assuming the cell to be a black box, as opposed to using the metabolic approach to modelling the processes that take place inside the cell. ASM2d appeared to be overparameterized with respect to available data, requiring a more systematic approach for calibration (Brun *et al.*, 2002). Despite that this allowed the model to adapt and describe the dynamic changes in the activated sludge community, it still lacked the ability to entirely describe the observed dynamics particularly with regard to hydrolysis and EBPR processes (Sin and Vanrolleghem, 2006). Parallel to these developments, in 1994, an increasing knowledge of the cell-internal biochemistry of PAO resulted in the development of a metabolic model (TUDP model;

Smolders *et al.*, 1994a, b; Murnleitner *et al.*, 1997) describing the anaerobic and aerobic phases of EBPR based on intracellular storage compounds. This model was later fully integrated with ASM by Meijer (2004).

Table 1. Overview of selected activated sludge models (adopted from Gernaey *et al.*, 2004).

Model	Nitrification	Denitrification	Heterotrophic / autotrophic decay	Hydrolysis	EBPR	Denitrifying PAO	Lysis of PAO / PHA	Fermentation	Chemical P removal	Reactions	State variables	Reference
UCTOLD	●	●	DR, Cst	EA						8	13	Dold <i>et al.</i> , 1980, 1991
ASM1	●	●	DR, Cst	EA						8	13	Henze <i>et al.</i> , 1987b
ASM3	●	●	ER, EA	Cst						12	13	Gujer <i>et al.</i> , 1999
UCTPHO	●	●	DR, Cst	EA	●		Cst	●		19	19	Wentzel, 1988, 1989a,b
ASM2	●	●	DR, Cst	EA	●		Cst	●	●	19	19	Henze <i>et al.</i> , 1995
ASM2d	●	●	DR, Cst	EA	●	●	Cst	●	●	21	19	Henze <i>et al.</i> , 1999
B&D	●	●	DR, Cst	EA	●	●	EA	●		36	19	Barker and Dold, 1997
TUDP	●	●	DR, Cst	EA	●	●	EA	●		21	17	Meijer, 2004
ASM3-bioP	●	●	ER, EA	Cst	●	●	EA			23	17	Rieger <i>et al.</i> , 2001

Den. PAO: Denitrifying Phosphorus Removing Organisms (PAO) activity included in the model; DR: death regeneration concept; EA: electron acceptor depending; ER: endogenous respiration concept; Cst: not electron acceptor depending.

At the same time as the ASM2d model was presented, the Task Group also developed the ASM3 model to correct some of the shortcomings of ASM1. ASM3 was proposed to become the new standard for ASM-based modelling. ASM3 replaced the death-regeneration process for heterotrophic organisms by an endogenous respiration process and also introduced the role of storage of organic substrates (Gujer *et al.*, 1999). In 2000, the Task Group presented the overview of the ASM models 1 to 3 (Henze *et al.*, 2000).

In essence, ASM3 describes the same processes as ASM1, although ASM3 was introduced to correct the deficiencies of ASM1. This is partly based on the observations from oxygen utilization rate (OUR) tests with activated sludge which revealed the fact that bacteria rapidly take-up readily biodegradable COD and store it as internal substrate which will then be converted slowly (conversion of readily biodegradable COD into slowly biodegradable COD). When acetate (defined substrate) is added to the activated sludge the observed OUR suggests the presence of two substrates; a rapid and slow degradation of substrate associated with OUR can be observed (Henze *et al.*, 1992, 2008). In ASM1 it appears as if two substrates are present ( $S_S$  and  $X_S$ ) while in original experiments only acetate ( $S_S$ ) was dosed. In order to describe the observed OUR by ASM1 in this case, it was necessary to define that the acetate is partly soluble and partly particulate, which is not recommended. This deficiency is solved by the introduction of a storage compound,  $X_{STO,S}$ , in ASM3. This means that substrate is taken up rapidly and stored, while growth occurs within the stored substrate. Both models will describe the observed OUR, but only ASM3 will accurately describe the uptake. However, there is no problem in using ASM1 for simulation of nitrogen removal systems because nitrification is a slow process, and thus enough time is available for biodegradation of slowly biodegradable COD.

The second reason to introduce ASM3 was that ASM1 proved to be rather successful for simulation of wastewater treatment plants and consequently too many started to believe that what was in ASM1 was 100% true and the reality. However, the storage mechanisms exhibited by the biomass show that what is in ASM1 is not all true, but close enough to reality to serve its purpose. Therefore, ASM3 has an

added educational value because it demonstrates that there are different (but not necessarily better) ways to model the same treatment plant.

However, the most important reason to introduce ASM3 was the recognition of the importance of three rates of oxygen consumption in the process, namely: the rapid rate of oxygen consumption for degradation of readily biodegradable COD (RBCOD), the slow rate associated with degradation of slowly biodegradable COD (SBCOD), and the even slower endogenous OUR. In contrast, in ASM1 there is only one oxygen-consuming process, so it is very difficult to perform calibration as one needs to calibrate other processes that indirectly influence the processes that consume oxygen.

The other problem is the cycling of the COD in the process, as in the decay process particulate COD is produced, hydrolyzed, and used for growth again. It means that if in the process one parameter is changed, it influences all the other processes due to the cycling, and it is difficult to use automated calibration as every parameter has influences on every process. In ASM3 this issue has been solved as the decay process has been replaced by endogenous respiration which eliminates the COD cycle (Figure 1).

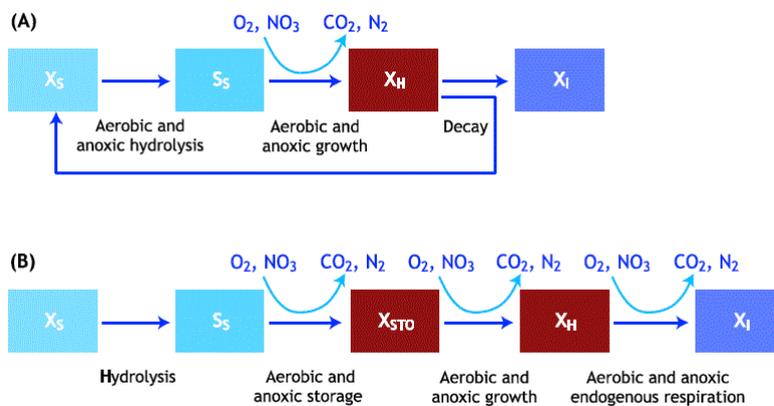


Figure 1. Degradation of COD in (A) ASM1 and (B) ASM3.

In other words, once the cells are produced, they start to oxidize themselves and by this means the biomass is reduced by the aerobic mineralization process (the classical endogenous respiration). While this has some conceptual controversy, e.g. why would an organism oxidize itself (i.e. go on a diet) when there is food around, it is useful to eliminate the bioprocess interaction from the substrate recycling of the death–regeneration model.

In addition, in ASM3 the oxygen consumption is divided into three processes (storage, growth and endogenous respiration) instead of having only one as in ASM1. ASM3 allows one of these three rates to be fitted if one knows which process to target, which directly links the measurements and calibration parameter. The fact that the RBCOD<sub>i</sub> is taken up and stored is irrelevant for most plants (and therefore also the choice between ASM1 and ASM3).

One of the most important applications of ASM3 is in plug flow reactors, such as selectors (Makinia *et al.*, 2006). If, for example, acetate must be removed in the aerobic selector to prevent sludge bulking, the design of the selector is governed by the time needed to take up the acetate and by the amount of

oxygen needed for it. If ASM1 is used instead the oxygen requirements in the selector will be significantly overestimated. In reality a large proportion of acetate is stored inside the biomass, and once it is stored, there is no longer a problem with bulking sludge. If one wants to design the aerobic selector and include it in the model, then ASM3 is the best model to use.

Another relevant application of ASM3 is for the description of a pre-denitrifying nitrogen removal plant operating at a short SRT (Yuan *et al.*, 2002; Sahlstedt *et al.*, 2004). Here, it makes a substantial difference whether or not readily or slowly biodegradable COD is present or whether COD is stored or not. In systems with a long SRT (10-20 days depending on temperature, which are more common in practice), a large part of the nitrate removal is effectively associated with the slowly biodegradable COD from the influent and death-regeneration in the pre-denitrification reactor and from death-regeneration only in the post denitrification reactor, so the sensitivity to the exact ratio between readily and slowly biodegradable COD is much less. The same applies for the differentiation between ASM1 and ASM3. In highly loaded systems endogenous respiration is less important and accumulation of COD in the form of storage polymers and the carry over in the aerated phase of a treatment plant might be significant.

In conclusion, ASM3 is recommended to be used for (i) simulation of highly loaded nitrification-denitrification systems with short anoxic retention times (volumes), (ii) supporting selector modelling, (iii) improving aeration demands for tapered systems, during step-feed operations or when high amounts of soluble industrial components are present in the influent, and (iv) easing automatic calibration. Otherwise ASM1 should be equally successful in describing the activated sludge plant.

The consequence of introducing EBPR and Phosphorus Accumulating Organisms (PAO) into ASM is that the model becomes quite complex, as illustrated in Figure 2.

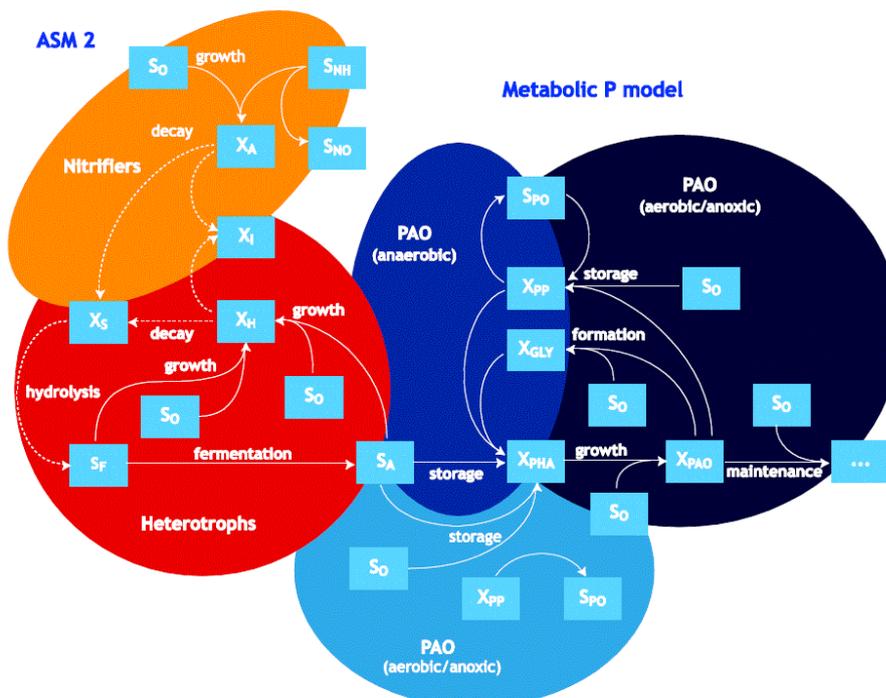


Figure 2. Interactions in the integrated ASM2-TUDP model (Meijer, 2004).

The left side of the figure depicts the part of conversions carried out by nitrifiers and ordinary heterotrophs, while the right side shows the extension needed for the description of the complex physiology of PAO. The nitrifiers and ordinary heterotrophs use oxygen to oxidize their substrate to form CO<sub>2</sub> or nitrate and biomass. They have a rather simple physiology resulting in simple processes. PAO's physiology includes internal storage polymers (poly-hydroxy-alkanoate: PHA, glycogen and poly-P) and their behaviour under anaerobic, anoxic and aerobic conditions is different. They also behave differently under aerobic conditions depending on whether the substrate is present or not. Obviously, there are lots of possible variations and inclusion of EBPR in the model substantially increases its complexity (the number of processes in ASM increases from 11 to 22). The situation becomes even more complex when Glycogen Accumulating Organisms (GAO) are also included. ASM2 and ASM2d are similar to ASM1 in assuming the cell to be a black box as opposed to using the metabolic approach to modelling which takes into account what is happening inside the cell.

In 1994, increasing knowledge of the cell-internal biochemistry of PAO resulted in the development of a metabolic model describing the anaerobic and aerobic phases of EBPR (Smolders *et al.*, 1994a,b; 1995a,b,c). The model was developed and validated using enriched PAO cultures cultivated on lab-scale anaerobic/aerobic (A/O) sequencing batch reactor (SBR) experiments. Why is it useful to use a metabolic model? In the standard model for heterotrophic growth there are seven relevant compounds (substrate, oxygen, charge, carbon dioxide, water, ammonia and biomass), five independent balances (carbon, hydrogen, oxygen, nitrogen and charge), and two degrees of freedom. If one knows one yield and one rate coefficient, it is possible to describe the whole system with one model. If one was to describe COD removal and nitrification at a metabolic level, it would not bring any advantage as the yield and rate coefficients would still be needed. Although the metabolic stoichiometry allows tracking, the C, H, O, N, P and charge flows through a system give more information from a modelling point of view, which makes the model more complex but not more accurate. All the rates are linked through conservation relations (stoichiometry) and, therefore, the choices between the process rate or growth rate, and substrate uptake rate or oxygen utilization rate, is not important.

Thus the black box approach can be used as has been the case with ASM1. So for the activated sludge system itself, C, H, O and charge tracking is not required - COD and N is enough, but when the ASMs are integrated with anaerobic digestion (AD) models to form plant-wide models, it becomes important because AD modelling requires C, H, O and charge tracking to predict gas production and composition and alkalinity generation (Brink *et al.*, 2007).

However, if one needs to describe the situation with heterotrophic growth and product (storage polymers) formation as for PAO in EBPR processes, the number of relevant compounds increases; each additional storage polymer brings an extra compound, but the number of balances does not increase, which means that the degrees of freedom (unknown values) increase as a consequence of the increased number of unknown compounds. In this case, one needs to know at least one yield and rate coefficient, and the choice of the process rate becomes important. For example, during aerobic conditions PAO use internally-stored PHA to produce the intermediate compound Acetyl-CoA, that is used further for biomass growth, glycogen formation and creation of energy required for these processes, and poly-P formation.

Obviously, the introduction of storage compounds creates a more complicated network of processes. In the processes with extra storage polymers, extra yield coefficients will also be introduced. The efficiency of the conversion processes would however be the same for all yields. Within a metabolic model one can link the macroscopic yields to the metabolic yield, which is the efficiency of energy (ATP) generation per unit of substrate oxidized. The substrate oxidation is related to electron transfer to oxygen or nitrate consumption. The yield coefficients are therefore all a function of this basic parameter (ATP

produced per pair of electrons transferred) and the number of independent yield parameters is less in a metabolic description for these complex microorganisms.

Initially, the metabolic model kinetics was chosen as simple as possible. Smolders *et al.* (1994b) proposed a kinetic structure in which the oxygen (or nitrate) consumption and PHA degradation are the net result of biomass growth ( $r_X$ ), poly-P formation ( $r_{PP}$ ), glycogen formation ( $r_{GLY}$ ) and maintenance ( $m_O$  and  $m_{PHA}$ ). Their kinetic structure is expressed by linear equations and led to a set of overall reactions (Meijer, 2004). Soon after, Kuba *et al.* (1996) proposed a metabolic model for denitrifying EBPR. In 1997, Murnleitner *et al.* combined the anaerobic, aerobic and anoxic models, proposing a kinetic structure in which growth was the net result of PHA consumption and poly-P and glycogen formation without changing its original stoichiometry. From an ecological point of view, storage is preferred over growth, suggesting that, in their competition with other micro-organisms, PAO rely on their storage ability. A rapid resupply of storage compounds is a primary condition for long term survival. Thus, the maximum growth rate is no longer an intrinsic property of PAO, but becomes dependent on environmental conditions and the maximum PHA storage capacity (Brdjanovic *et al.*, 1998). With the reformulated kinetic structure, Murnleitner *et al.* (1997) described all experiments performed by Smolders *et al.* (1994a,b; 1995a,b) and Kuba *et al.* (1996) with one set of model parameters. Nevertheless, one must underline that these reactions cannot be read separately, as they are merely the result of the mathematical reformulation.

From the metabolic reactions, an overall anaerobic, aerobic and anoxic stoichiometry was determined. A full description of the TUDP model is given by Meijer (2004) and de Kreuk *et al.* (2007). Overall, the formulation of an overall anaerobic reaction is unambiguous, as there is only one metabolic reaction. As such, by measuring the acetate uptake rate, all other rates are fixed. Concerning the aerobic and anoxic stoichiometry, five overall reactions ( $r_X$ ,  $r_{PP}$ ,  $r_{GLY}$ ,  $r_{PHA}$  and  $m_{PHA}$ ) are found but the system can be solved if four out of five rates are determined. In 1999, van Veldhuizen *et al.* integrated the metabolic EBPR model with the heterotrophic, hydrolytic and autotrophic processes from ASM2d (Henze *et al.*, 1999). With this model a full-scale Modified University of Cape Town (MUCT) process for COD, N and P removal was simulated (Veldhuizen *et al.* 1999). That study showed that the TUDP model was capable of describing full-scale conditions, without significant adjustments. To strengthen the full-scale application of the model, a calibration protocol was developed and tested. Using the same model, Brdjanovic *et al.* (2000) simulated a full-scale side-stream P-removing process. After calibrating glycogen formation, the model described the process without the need to further adjust other parameters. Since temperature plays a major role on microbial conversions, Brdjanovic *et al.* (1998) studied the effect of temperature on EBPR. Their results were incorporated in the TUDP model that was used to simulate a full-scale MUCT process optimised for denitrifying EBPR (WWTP Hardenberg see Meijer *et al.*, 2001). On the basis of all these practical experiments, the updated and validated metabolic TUDP model showed that its stoichiometry is fully reliable and can be used and extrapolated without calibration. To simulate full-scale EBPR, the metabolic model was combined with the heterotrophic, hydrolytic and autotrophic reactions from ASM2d (Henze *et al.*, 1999). Figure 3 shows how the different model structures interact.

Despite that it would be possible to reformulate the auto- and heterotrophic processes of ASM2d in a metabolic form, such a model would have the same number of yields as the original model. Therefore, it would not be smaller and, moreover, it would not improve the model performance. Therefore, in the TUDP model, the ASM2d processes were maintained in their original form and the integration of the two models was relatively simple. This could increase the reliability of the EBPR process description that ASM2d previously appeared to lack (Sin and Vanrolleghem, 2006). Nevertheless, where the two models are merged a new form of substrate competition develops (e.g. between Ordinary Heterotrophic Organisms: OHO and PAO). Moreover, with the EBPR also the fermentation and hydrolysis processes

in the model become more sensitive and two concepts of endogenous respiration/maintenance are used simultaneously.

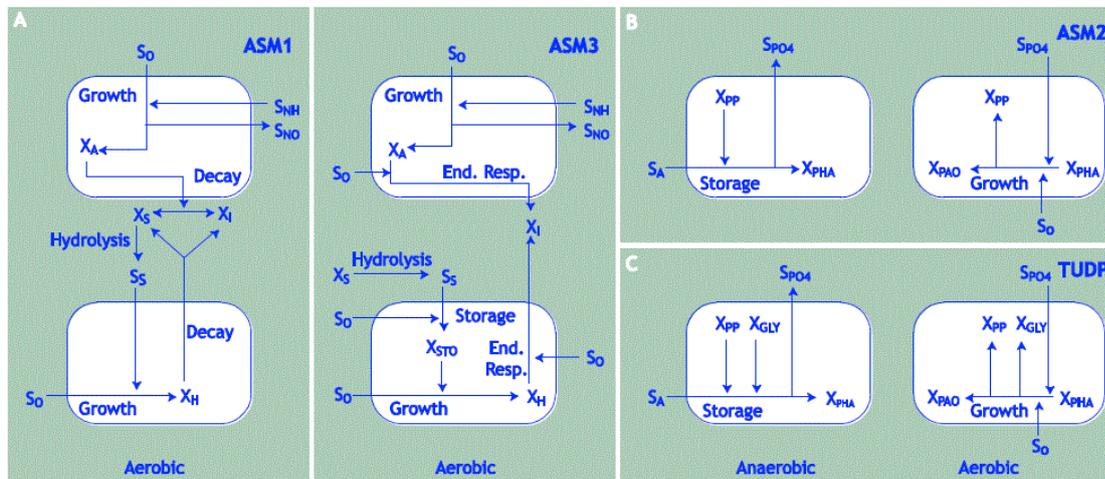


Figure 3. Simplified schemes of substrate flows for (A) autotrophic and heterotrophic biomass in the ASM1 and ASM3 models (modified from Gujer *et al.*, 1999), (B) storage and growth of PAO in the ASM2 model (Henze *et al.* 1995), and (C) storage and aerobic growth of PAO in the TUDP model (van Veldhuizen *et al.*, 1999; Brdjanovic *et al.*, 2000). Adapted from Gernaey *et al.* (2004).

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In the TUDP metabolic model, the kinetic structure results in a set of atypical model reactions. These reactions are the mathematical result of the kinetic formulation, and cannot be seen independently. For those not aware, this could easily lead to misinterpretations of the model matrix, as the individual stoichiometric reactions do not exemplify the actual EBPR process. This should be realised when the model is used for educational purposes. However, in modelling practice, working with the metabolic concept has important advantages over other model approaches. The main advantage is the solid stoichiometric base of the metabolic model. This solid stoichiometric base is largely owed to the inclusion of glycogen and the simultaneous modelling of the counteracting dynamics of glycogen and PHA.

It is clear that when using metabolic information the degrees of freedom in the model can be reduced. Better understanding of the metabolic processes of the organism will close the gap to a fully white box situation. The increased complexity of processes is consequently reflected in the models. However, improved understanding of the complex interactions within the cell and the introduction of the metabolic approach gives more confidence and consistency in the application of models to describe activated sludge processes. It is in effect gathering information from a lower level of organization to help

understand and model the processes at a higher level of organization. For further details on ASM2, ASM2d, ASM3 and metabolic models the reader is referred to Henze *et al.* (2000), Gernaey *et al.* (2004) and Meijer (2004).

Following the work on the metabolic modelling of the Delft group, Filipe *et al.* (2001) improved the model for anaerobic acetate uptake. A kinetic poly-P dependency was included, which improved the description of acetate uptake under varying initial poly-P concentrations. Also a different pH dependency for anaerobic acetate uptake was suggested that becomes critical when anaerobic substrate uptake is limiting. In the TUDP model, anaerobic acetate uptake was modelled according to Smolders *et al.* (1994a). Also, Filipe *et al.* (1999) proposed improvements for the anoxic acetate uptake model according to Smolders *et al.* (1994a). These improvements were however not incorporated in the TUDP model. Despite that the EBPR process can reach relatively high phosphorus removal efficiency (effluent phosphorus concentrations lower than 1 mg/L), it may experience process upsets and deterioration due to factors that are not completely understood yet (Oehmen *et al.*, 2007). In this regard, the appearance of Glycogen Accumulating Organisms (GAO), such as *Competibacter* and *Defluviicoccus*, has been linked to the suboptimal operation and even failure of the EBPR process performance (Cech *et al.*, 1993; Satoh *et al.*, 1994; Saunders *et al.*, 2003). Thus, GAO are seen as undesirable microorganisms in wastewater treatment since they do not contribute to the EBPR process but compete with PAO in the anaerobic stage for the same carbon source (RBCOD, e.g. volatile fatty acids: VFA).

In 2009, Lopez-Vazquez *et al.* incorporated the influence of carbon source (such as acetate and propionate), temperature (from 10 to 30°C) and pH dependency of PAO and GAO (from pH 6.0 to 7.5) in the metabolic model amended by Murnleitner *et al.* (1997). Thus, using a mechanistic model, Lopez-Vazquez *et al.* (2009) were able to evaluate the carbon source, pH and temperature influence on the PAO and GAO interaction and their effects on EBPR stability aiming at facilitating improved process efficiency and robustness. They concluded that PAO are favoured by temperatures lower than 20°C and pH levels higher than 7.0. Building on the research carried out by Lopez-Vazquez *et al.* (2009), Oehmen *et al.* (2010) expanded the competition between PAO and GAO to sequential anaerobic-anoxic-aerobic conditions which are typically found in most of the biological nutrient removal (BNR) systems. This implied to incorporate up to six different biomass groups consisting on *Accumulibacter Types I and II* and denitrifying and non-denitrifying *Competibacter* and *Defluvicoccus* in accordance to their observed denitrifying capabilities. Their model also included a multistep denitrifying process (from nitrate to dinitrogen gas). Overall, the model of Oehmen *et al.* (2010) with minimum adjustments was able to successfully describe the EBPR biomass activities observed in lab-scale anaerobic-anoxic-aerobic SBR data. Since the application to full-scale conditions of the metabolic model developed by Oehmen *et al.* (2010) is not straight-forward (e.g. due to the absence of organic matter and nitrogen oxidation processes as well as practical limitations concerning the elemental balances), recent attempts have been made towards the development of a more friendly-user ASM type model (Ramirez-Higareda *et al.*, 2012). Such an integrated model may prove useful to describe the relevant EBPR microbial populations of interest with the objective of exploring the environmental and operational conditions beneficial for the EBPR process.

In some cases, such as high pH (>7.5) and high Ca<sup>++</sup> concentrations, it may be necessary to add biologically induced P precipitation to the EBPR model (Maurer *et al.*, 1999; Maurer and Boller, 1999). Indeed, under certain conditions the EBPR reactions coincide with a natural precipitation that can account for an important P removal effect that is not related to the EBPR reactions included in the models described thus far. The formation of these precipitates, mostly consisting of calcium phosphates, is promoted by the high P concentration and increased ionic strength during the anaerobic P release by the PAO. Model equations and components necessary to describe this precipitation process were given by Maurer and Boller (1999).

## Current developments

Currently, activated sludge models are considered reliable and capable of describing complex wastewater treatment plants. From the practical perspective, for most engineering applications, models are considered sufficiently developed. Within the context of model development it is also important to mention the role of hardware. The development of the models and computer capacity (CPU) grew hand-in-hand (Gujer, 2006). From a technical perspective, it became feasible to work with models that contained a large number of process descriptions and variables. In the 90's, models were increasingly used by researchers, but also mathematical modelling became also popular among practitioners. Today, mathematical models are commonly used in the North America, Australia and many countries in Europe (Hauduc *et al.*, 2009). To facilitate its application, software has been developed to assist in design, optimisation, operation and training. Modelling simulators provide a better understanding of wastewater treatment plants since they allow users to view the response of the treatment systems to changes in a number of different variables, and are also used to optimize wastewater treatment plants and to train plant operators. Examples of commercial packages are GPS-X, SIMBA, STOAT, WEST, BioWin etc. For research and training SSSP, ASIM, AQUASIM and even Microsoft Excel are regularly used (references to packages are provided at the end of the paper). Significant benefits are associated with the use of simulators in the analysis, design, and operation of wastewater treatment systems (Meijer and Brdjanovic, 2012).

To make modelling closer to practitioners and facilitate its use in a structured and organized manner, several practical guidelines on how to model a wastewater treatment plant, and protocols on how to characterize the wastewater/sewage and sludge, have been developed during the last years around the world. In 2004, at the 4<sup>th</sup> IWA World Water Congress in Marrakech, groups that developed various protocols (Hochschulgruppe, STOWA, BIOMATH and WERF) came together to develop plans to synthesize the best modelling practices available. A new IWA Good Modelling Practice Task Group (GMP-TG) was formed on the use of Activated Sludge Models, parallel to and with the full support from the Task Group on mathematical modelling for design and operation of biological wastewater treatment. The website of this and other relevant IWA Task Groups in the field of mathematical modelling are presented in the Annexes. The GMP-TG consists of an international team of modellers collecting experience and knowledge on activated sludge modelling to provide guidance to practitioners (Rieger *et al.*, 2012). One of the aims of GMP-TG was to prepare a scientific and technical report to propose simple and effective procedures for the use of ASM-type models (Rieger *et al.*, 2012). In preparation of this report, the GMP-TG developed and sent out a questionnaire in 2007 to benchmark and collect relevant information on the practical use of modelling. The objectives were to better define the profile of ASM users, to identify the tools/procedures that are used (models, guidelines, protocols) and to highlight the main limitations encountered while building and using ASM-type models (Hauduc *et al.*, 2009). The outcome of the questionnaire, filled in by 96 respondents, showed that models are used by researchers for optimisation purposes, as well as by modellers employed by private companies to carry out design studies. Modelling is seen as an engineering tool, needing relevant training that is often lacking. The most used biokinetic models were ASM1 (57%) and ASM2d (32%), followed by ASM3, other (non-specified), ASDM (BioWin), Mantis (GPS-X) and TUDP model. The study also revealed that models are sometimes not properly applied, which might be due to a lack of knowledge and standardised procedures. The development of standardised modelling procedures and better knowledge transfer by making available some practical case studies were mentioned as key instruments to address certain obstacles like the complexity of the model theories and procedures, the time consuming steps and finally the reliability of the models.

Besides sending out the questionnaire several workshops, meetings and courses on activated sludge modelling were organised, such as the wastewater treatment modelling seminars. The GMP-TG was

involved in the development of a new IWA Model Notation System (Corominas *et al.*, 2010), and interviewed several distinguished modellers (Peter Dold, George Ekama, Willi Gujer, Mogens Henze, Mark van Loosdrecht, among others). One of the suggestions was to suggest typical values for regularly used ratios, variables and parameters in wastewater modelling. The feedback was compiled in the IWA book "Guidelines for Using Activated Sludge Models", Scientific and Technical Report No. 22 (Rieger *et al.*, 2012). Obviously, IWA played an important role in the evolution of wastewater modelling by facilitating its development, providing a platform for various communities of practice and promoting modelling research and practice through various publications.

On the same website of the GMP-TG (<https://iwa-gmp-tg.irstea.fr/>) adjusted 'Gujer matrices' for 7 published models can be downloaded as an MS Excel spreadsheet: (1) ASM1 (Henze *et al.*, 1987a,b, 2000); (2) ASM2d (Henze *et al.*, 1999); (3) ASM3 (Gujer *et al.*, 1999); (4) ASM3+BioP (Rieger *et al.*, 2001); (5) ASM2d+TUD (Meijer, 2004); (6) Barker & Dold model (Barker and Dold, 1997); and (7) UCTPHO+ (Hu *et al.*, 2007). In the same website, a comparison of different parameter-naming rules including the new IWA Model Notation System (Corominas *et al.*, 2010) can also be found.

Recently, among other initiatives to improve the knowledge transfer by facilitating and making available some practical case-studies (Hauduc *et al.*, 2009), UNESCO-IHE published the book "A Practical Guide to Activated Sludge Modelling" (Meijer and Brdjanovic, 2012) which is used in the modelling course delivered every year at UNESCO-IHE in cooperation with Delft University of Technology (<http://www.unesco-ihe.org/modelling-wastewater-treatment-processes-and-plants>). With a very practical focus, it presents all the steps performed as a part of a modelling project where five WWTPs were subject to upgrade to EU effluent discharge standards in a new EU member state. Besides the general modelling protocols and guidelines for wastewater characterization and fractionation, methods for quantitative influent assessment, addressing different components of the urban wastewater chain and introducing a methodology for quantification of sewage components are presented. Guidelines for plant flows and measurement points necessary for the preparation of an additional sampling program are also shown, as well as an inventory of all the regular day-to-day sampling to be used in a modelling project, a methodology for activated sludge plant assessment and methods to evaluate raw plant data and to filter out possible errors which affect the model reliability and results. Practical methods for wastewater data evaluation were developed by Meijer *et al.* (2002). New developments on data evaluation are also presented in this book in relation to a well-documented recent case study performed on a plant in the Netherlands. A methodology for secondary settlers' design and assessment is also described, including the five most commonly used settler design and operation procedures such as the empirical, flux-theory, WRC, ATV (recently DWA) and the STOWA design guidelines (Henze *et al.*, 2008). The last part of the book elaborates on the methodology applied in model calibration and the main steps thereof.

The authors of this paper also recently published a book which describes their selection of fifteen municipal and industrial activated sludge model applications carried out over last two decades by the Delft modelling group (Brdjanovic *et al.*, 2015). Besides a number of examples from the Netherlands, this book includes some pioneering studies on activated sludge modelling in India (Brdjanovic *et al.*, 2007; Lopez-Vazquez *et al.*, 2013), Bosnia and Herzegovina (Hodzic *et al.*, 2011, Price and Vojinovic, 2010), Mexico (Fall *et al.*, 2012), Croatia (Meijer and Brdjanovic, 2012) and Uruguay (Betancur, 2014). This demonstrates that efforts are undertaken also in developing countries to apply the models to existing activated sludge systems (mostly for optimization or upgrade).

It is too soon to assess whether the efforts of the IWA GMP-TG, in the form of the standardized procedures, available 'Gujer matrices' for all models, and the publication of the Guidelines on Good Modelling Practice in 2012 will lead to an increased work on modelling and increased number of publications. As a mean to assess the development and historical impact of mathematical modelling on

the wastewater treatment field, a statistical analysis of the scientific literature was recently carried out (Brdjanovic *et al.*, 2015). Most of the top 50 most cited papers deal with protocols for characterization and modelling closely followed by papers on modelling development and metabolic modelling, but by far by the applied modelling papers. Nevertheless, when looking at the cumulative number of citations of the top 50 most cited papers the papers on model development and presentation have the highest number of citations. Such a distribution can suggest that there has been an increasing need to use well-established protocols to understand and implement the mathematical models but, logically, they cannot outnumber the basic modelling papers since they are indeed the subject of study and application. Remarkably, the papers on metabolic modelling rank third close to the first two groups. This is a clear indication that metabolic modelling has been widely accepted particularly for its contribution to modelling the EBPR process (e.g. Comeau *et al.*, 1986; Smolders *et al.*, 1994a). It should be underlined that applied modelling papers received the lowest number of citations. This can be a reflection of the findings of the GMP-TG regarding the need to make available more practical case-studies (Hauduc *et al.*, 2009). In practice, possibly the modelling studies are so case-specific that they offer a limited interest to a broad scientific audience, which limits the potential number of citations that an applied modelling paper could get. But also, it cannot be discarded that the present degree of maturity and reliability of the models reduces the chances to find a novelty in the field. Thereby in any case, the historical links between academia and industry have been a key catalyser and should continue to work hand-in-hand for the future development and establishment of mathematical modelling in the wastewater treatment field.

In parallel, a search was done on the citations of the five publications on the different ASM models. This included the technical reports on ASM1, ASM2, ASM1-ASM3, and papers on ASM2d and ASM3 (which are only published in papers and not as a technical report). Between 1998 and 2000, more than 10 years after the publication of ASM1, there was a boost in the number of citations to the ASM models. Simulation tools were already available from the early 90's (like GPS-X and SIMBA), indicating that the software capabilities were not a factor that delayed their implementation (and possibly the hardware was not either). Interestingly, the ASM started to have more citations after the publications of the most cited papers on characterization and modelling protocols (like the papers of Sollfrank and Gujer, 1990; Kappeler and Gujer, 1992; Mamais *et al.*, 1993; Orhon *et al.*, 1997; Spanjers and Vanrolleghem, 1999; Vanrolleghem *et al.*, 1995,1999; Hulsbeek *et al.*, 2002; and Roeleveld and van Loosdrecht, 2002). Possibly, the lack of understanding and confidence to apply the ASM models delayed their implementation, which was overcome by the availability of reliable characterization, modelling protocols as well as enough satisfactory and promising full-scale demonstrations and applications. Furthermore, the publication of the ASM1-ASM3 technical report (Henze *et al.*, 2000), which consolidated in a single publication the contents and features of all ASM models, could be another important driver that helped to promote the ASM models, increasing the number of citations after 2000. Due to the popularity of the ASM1-ASM3 technical report practically all the latest publications refer to it. This makes it difficult to clearly distinguish which model was used for a particular study, possibly overestimating the popularity or application of some ASM models and underestimating the others. Importantly, the yearly number of citations to ASM reports is stabilizing or even decreasing. Apparently, the number of citations per year has passed its exponential growth and started to level off since 2009.

In an effort to get an estimation of the individual potential application of the ASM models, an additional search was carried out, looking at the yearly number of publications that refer to each model. Compared to the previous search, the difference is that the focus is not on the technical reports, but on the number of yearly citations to the models themselves. The results show that ASM1 is still the model of reference, followed by ASM3, ASM2 and ASM2d. Its simplicity and flexibility to apply it, not only to municipal activated sludge systems, but also to industrial conditions (Petersen *et al.*, 2002) and even to other wastewater treatment technologies (e.g. biofilm systems and wetlands) (Wanner *et al.*, 2006; Langergraber *et al.*, 2009) may have contributed to its popularity. The maximum number of citations

was reached around the years 2009-2010. Thereafter, a decrease in the number of citations is observed. A similar trend was observed by Gujer (2006) when searching the Web of Science. The fact that the number of citations to the ASM models decreases does not automatically mean that the number of studies performed has progressively reduced. As previously discussed (Gujer, 2006), it could likely be a consequence of the fact that mathematical modelling is mature, standardized and well-established and that publications on modelling are not easy to publish in peer-reviewed journals due to a lack or insufficiency of scientific novelty.

The number of citations to the ASM models has currently decreased, likely because mathematical modelling is becoming a standardized and mature practice in developed countries. On the opposite, case-studies and publications from developing countries are limited, which might be partly caused by the fact that activated sludge treatment systems are mainly found in developed countries. Likewise, the questionnaire prepared by the GMP-TG (Hauduc *et al.*, 2009) also showed that among the 96 responses, 65% came from European countries and 20% from North America. Other continents (South America, Africa, Asia and Australia) were under-represented.

#### Challenges for ASM and future trends

Concerning the future development of activated sludge modelling, it is important to take into consideration the current and future needs and developments. The trends regarding existing wastewater process technologies will likely need to further focus on providing a better description of the nutrient removal processes, not only for the sake of the nutrient removal itself, but also to reduce the associated energy costs and environmental impact. Modelling of nitrous oxides emissions in nutrient removal plants (Ni *et al.*, 2013; Nopens *et al.*, 2014) as well as achieving a satisfactory description of the actual (anaerobic, aerobic and anoxic) metabolic activities of the relevant EBPR populations (e.g. *Accumulibacter* type I and type II) and their interactions with 'new' bacterial populations (such as GAO) (Lopez-Vazquez *et al.*, 2009; Oehmen *et al.*, 2010) can be some examples of the required developments. In this regard, the IWA Task Group on Greenhouse Gas plays a major role towards the design and operation of environmentally-friendly wastewater treatment systems. Regarding innovative wastewater treatment technologies, a stronger focus can be expected on modelling the bioprocesses and hydrodynamics involved in the aerobic granular sludge (de Kreuk *et al.*, 2007), on the implementation of the Anammox process and related N-removal processes in the mainstream treatment line (Kartal *et al.*, 2010; Wett *et al.*, 2013; Lackner *et al.*, 2014), and even on the intracellular storage processes of organics for bioplastic production (Bengtsson *et al.*, 2008; Jiang *et al.*, 2012; Nopens *et al.*, 2014). While the aerobic granular technology offers significant benefits for WWTP optimization on both resources and footprint, the last two open new doors towards the conversion of existing WWTP from 'removal-type systems' towards 'resource-recovery systems' and 'energy-factories' (Kartal *et al.*, 2010; van Loosdrecht and Brdjanovic, 2014). Also, the application of the sulphur-cycle processes to wastewater treatment will likely continue to attract attention for the treatment of sulphate rich waters resulting from saline water intrusion, use of seawater for sanitation to alleviate water scarcity, cooling purposes, and industrial activities (Wang *et al.*, 2009; Hao *et al.*, 2014). Undoubtedly, mathematical modelling will be a strong tool to get a better understanding of the factors affecting these processes and facilitate their implementation. Such efforts may imply the need to incorporate and take into account more complex biokinetic models (Nielsen *et al.*, 2010; Oehmen *et al.*, 2010), elemental balance approaches (Takács *et al.*, 2007; Lu *et al.*, 2009), and likely also to establish stronger links with genomics, molecular techniques and metabolome analyses (Fiehn, 2001) as well as to develop the required experimental methods to determine and understand the microbial activities involved. The incorporation of the new processes (e.g. Anammox, and sulphur conversions) will likely follow the IWA GMP-TG concepts (Rieger *et al.*, 2012) and certainly most of the developments could be expected on the implementation of Anammox processes. The increased complexity of these combined biological processes require development of

effective process controls in which application of dynamic ASMs could become crucial for successful full-scale application.

One should not overlook that despite the significant advances and the development of even more (complex and) complete mathematical models, a common issue can be the lack of (quality and reliable) input data to feed the models or the potential influence of regularly dynamic and even extreme scenarios affecting the quality and characteristics of the influent wastewater quality and consequently the reliability of models. Furthermore, as underlined by Nopens *et al.* (2014) more methods are needed to assess the probability of compliance, quantify uncertainty and its sources and evaluate how risks, benefits and costs are or can be distributed among stakeholders (consultants, contractors, operators and owners). One of the objectives of the recently conceived IWA Task Group on Design and Operations Uncertainty (DOU) is to overcome such limitations with actions like the development of influent generator models to provide relevant input data and incorporate explicit uncertainty evaluations in model-aid design and operation of wastewater treatment systems (Gernaey *et al.*, 2011; Flores-Alsina *et al.*, 2014; Nopens *et al.*, 2014).

As a consequence of the interaction between the existing but also for the implementation of new technologies, plant-wide modelling will acquire and deserve special attention to: (i) develop an optimal WWTP control strategy, (ii) increase the efficiency of the WWTP removal processes, (iii) reduce the operating costs, (iv) maximize energy recovery through biogas production, and (v) maximize the removal and recovery of nutrients in the side-stream processes. In this regard, the IWA Task Group on Benchmarking of control strategies for wastewater treatment plants (BSM) has played and continues to play a prominent role towards achieving these goals (Copp, 2002; Jeppsson *et al.*, 2013; Gernaey *et al.*, 2014). As a plant-wide modelling starting point, the mathematical description of the separation processes in the primary settling tanks (PST) affecting the COD fractions needs to improve (Nopens *et al.*, 2014; Vanrolleghem *et al.*, 2014). This will contribute to maximize the recovery of energy via the anaerobic digestion of organics and favour the role of WWTP as energy factories (Kartal *et al.*, 2010, Energiefabriek, 2015). Currently, most of PST separation processes are still modelled as black boxes with lumped and gross removal coefficients assigned to all particulate organics, whereas unbiodegradable particulate organics have shown to be subject to higher removal efficiencies than the biodegradable organics (Ikumi *et al.*, 2014a,b).

Another important aspect in plant-wide modelling is the coupling of the state variables (Volcke *et al.*, 2006) from the activated sludge process tanks and those from secondary settling tanks (SST) (Bürger *et al.*, 2011; Torfs *et al.*, 2013). Models for clarifiers use total suspended solids as a state variable, which is not explicitly used in ASM models and need to be calculated as a composite variable of the activated sludge processes. In addition, due to the different redox conditions created, the bottom of a clarifier needs to be dynamically modelled in a similar way like a bioreactor to take into account the potential redox effects on the active biological processes. Among them, rising sludge due to denitrification under anoxic conditions in nitrogen removal plants, secondary P-release under anaerobic conditions in EBPR systems and the description of the sludge settleability are some examples of the need to secure a satisfactory modelling description of the operation of SST. So far, some of the mentioned processes could be mimicked by the addition of an anoxic (denitrifying) tank in addition to the secondary settling tank (Brdjanovic *et al.*, 2000). However, this 'trick' is more an intermediate than the final solution to the problem. Computational fluid dynamics (CFD) can help to improve the description and operation of SST (Plósz *et al.*, 2012; Laurent *et al.*, 2014; Nopens *et al.*, 2014). Furthermore, by studying the influence of diffusion limitations and gradients through CFD, the interactions between bacterial morphology and bacterial competition could be better understood and lead to a better prediction of the sludge bulking phenomenon (Martins *et al.*, 2004a,b). The latter affecting not only the SST performance but also the whole WWTP efficiency and capacity by reducing the sludge settleability. However, besides

the added complexity, reliable experimental methods and set-ups are still needed to support model development and cope with the lack of (quality) data that has limited the use of advanced settling models (Piósz *et al.*, 2012; Bürger *et al.*, 2011, 2012). Such an approach requires tightening the collaboration links between practice and research to assess and provide feedback on newly developed models under real case scenarios.

Nevertheless, to apply plant-wide modelling the biggest challenges can be found when coupling ASM models with anaerobic digestion models (like the ADM1) (Batstone *et al.*, 2002). Those challenges are related not only to the description of the sludge digestion processes that take place in sludge thickeners and anaerobic sludge digesters, but also to the physicochemical processes occurring within these systems. One of the first challenges is the different sets of state variables used by ASM models and ADM1. Overall, there are two different ways to deal with this issue: (1) the ‘super model’ approach where a complete set of variables valid for both aerobic and anaerobic environments is defined (Grau *et al.*, 2009), which is also available in e.g. the BioWim simulator, and (2) the use of established interlinked models by applying a set of algebraic transformation equations (‘transformers’) based on a ‘Gujer matrix’ description of the two models (Vanrolleghem *et al.*, 2005; Volcke *et al.*, 2006; Nopens *et al.*, 2009). A pioneering and successful attempt of plant-wide modelling and coupling ASM and ADM models using a designed interface/transformer was demonstrated on the WWTP Anjana in India (Brdjanovic *et al.*, 2007), arguably the first published application of activated sludge modelling in a developing country. Overall, the previous approaches can satisfactorily help out to apply a plant-wide model, the supermodel having the biggest potential. However, they cannot be directly applied to the plant-wide model description of a system performing EBPR. The latter because the anaerobic digestion fate of EBPR sludge (highly rich in phosphorus and intracellular compounds) is not included in ADM1 (Ikumi *et al.*, 2014a,b). Thus, the anaerobic endogenous processes at which an enriched EBPR sludge is exposed in anaerobic digesters cannot be currently described by ADM1. This is also directly linked with the strong need to achieve a satisfactory description of the metabolism of the dominant EBPR populations since it will define the fractions of the different intracellular compounds (from poly-P to glycogen and PHA) contained in the sludge.

Concerning the physical-chemical processes occurring within the anaerobic systems, ASM models contain only the alkalinity state, which acts mostly as an indicator of the potential inhibition of a biological process if alkalinity decreases, and a single gas transfer model. Whereas the pH description in ADM1 is only valid for dilute systems and do not include a mechanistic (pH-based) precipitation (Batstone *et al.*, 2012). However, if EBPR sludge is anaerobically digested the related physical-chemical processes that take place in the anaerobic sludge digestion systems are required to be modelled. Of particular importance are the physical-chemical processes affecting the multi-mineral precipitation (with cations such as iron and aluminium and anions like ortho-phosphate, carbonate and even sulphur) and the prevailing pH in anaerobic sludge digesters. In this regard, in recent years, an IWA Task Group was initiated for the development of a Generalized Physical-chemical Framework (Batstone *et al.*, 2012). Although the fundamentals of the physical-chemical reactions are well understood, available from other disciplines, and do not need calibration (since thermodynamics define the end points of the kinetic processes), the organic compounds driving the bioprocesses and the thermodynamics of the precipitation rates are not yet defined/known, implying that the end points of these reactions need to be known, involving considerable calibration efforts (Ekama, *personal communication*, 2014). These plant-wide modelling aspects require further research involving both experimental and modelling development activities to clarify and achieve a satisfactory modelling of the physical-chemical processes. Together with those concerning the implementation of recently developed technologies (such as the implementation of Anammox for the treatment of nitrogen-rich reject waters) it can contribute to reach the objectives of the plant-wide modelling philosophy. Ikumi *et al.* (2011, 2014a) have made one of the

first steps towards upgrading ADM1 and account for the potential effects of the anaerobic digestion of EBPR sludge.

Besides the potential energy savings that hydroinformatics tools (such as CFD) could bring (Rieger *et al.*, 2012), with an increasing need and interest in water reuse and integrated modelling the biological and physical-chemical removal processes of micro-pollutants will be another modelling area of major expansion and development (Gujer *et al.*, 2006; Clouzot *et al.*, 2013) where CFD could also be applied (Radu *et al.*, 2010; Laurent *et al.*, 2014). Moreover, a growing interest in integrated (urban) water modelling will continue to motivate integration of wastewater treatment process models with receiving water quality (RWQM) and sewer models (Gujer, 2006; Vanrolleghem *et al.*, 2014). Until a few years ago, only hydraulics and pollutant transport phenomena in the sewers were taken into account (Hvitved-Jacobsen, 2013). However, recent models start to consider the chemical and biological processes that take place in the sewer system, looking at the sewers as physical, chemical and biological reactors (Rauch *et al.*, 2002). One of the first examples of holistic modelling (combined sewage network, WWTP and the recipient/river) using different models (combining Mike Urban, BioWin and HEC-RAS), although carried out in a sequential mode (as opposite to a better and more realistic but much more complex real-time approach), showed great advantages of such modelling application (Hodzic *et al.*, 2011, Price and Vojinovic, 2010). This is of major importance for the design, operation and maintenance of sewer networks, not only from a holistic water management perspective but also from a potential future asset management focus (which needs a satisfactory modelling description of the removal of micro-pollutants). In collaboration with the University of Cape Town, WEST, a hydraulic modelling software developed by Gent University (Vanhooren *et al.*, 2003) and nowadays held by the Danish Hydraulic Institute (DHI), has been upgraded to make one of the prime efforts to link wastewater treatment models with RWQM and sewer models (Ikumi *et al.*, 2014b) in addition to other recent developments (Benedetti *et al.*, 2013a; Langeveld *et al.*, 2013). Together with the plant-wide modelling advances, this can open promising lines towards the development of an integrated urban water model suitable and capable to describe and optimize the entire urban water system (Benedetti *et al.*, 2013b). Likely, such a holistic approach will be also of importance and useful when dealing with secondary quality water sources for sanitation to contribute to alleviate water scarcity issues (like the use of saline water for sanitation and the implementation of the SANI process) (Lu *et al.*, 2009; Wang *et al.*, 2009).

Bearing in mind that 2.6 billion people still do not have access to sanitation, that most of the population in developing countries is not connected by sewer systems, and that only a small fraction of sewage in developing countries is treated, brings the issue of holistic modelling where the urban drainage and sewerage models and wastewater treatment models (not only ASM and ADM) will be complemented by and integrated with (de)centralized sanitation models in cities which are not fully covered by sewerage. There are several similar examples worldwide, especially in developing countries. Recent advances in this direction include a decentralized sanitation model created by the software developers of the SIMBA simulator (funded by the Bill & Melinda Gates Foundation and therefore expected to be freely accessible) and a decision support tool called WAMEX by UNESCO-IHE and funded by the Asian Development Bank (and also freely available) which include sanitation (Brdjanovic *et al.*, 2014), sewerage (Abbot and Vojinovic, 2009; Sanchez *et al.*, 2013; Vojinovic *et al.*, 2014), and sewage treatment components (von Sperling and Chernicharo, 2005).

Cloud computing has gained in interest lately (Armbrust *et al.*, 2010), by joining efforts and contributing to standardize approaches and notation (Corominas *et al.*, 2010), sharing wastewater treatment models between researchers, software developers, and practitioners, while being in different longitudes and latitudes, may not be far from reality. This can be a strong tool to facilitate the application of plant-wide and integrated urban water modelling to contribute to optimize the water quality and quantity transported through the aquatic veins and arteries of an urban settlement.

From a commercial and practical perspective, the incorporation of the processes and approaches described previously will considerably increase the model complexity. However, understandably, practitioners feel uncomfortable working with increasingly complex models. So, possibly, vendors with specific modelling skills will appear on the market, since conventional wastewater treatment 'generalists' will not be able to cope with the fast release and development of more complex models for particular applications. Thus, like in other fields, in the near future consultants will outsource their modelling activities to specific vendors (Ekama, *personal communication*, 2014).

It is not impossible to imagine that sooner or later new interfaces and way of interactions between (probably or even likely less specialized) users and models will be created. Maybe, in the form of multi-layer serious gaming and using 3D urban water system simulators with simplified 'surface' user interfaces and more complex expert models running 'invisibly' in the background (Ekama, *personal communication*, 2014). An expected future development is the use of models built in data acquisition systems (SCADA) of larger wastewater treatment facilities. Thereby the complex knowledge contained in ASMs is made available for process operators making more efficient and safe plant operation possible on a daily basis. It is also expected that the modelling boundaries will be further extended reaching trans-disciplinary character as other issues will be included, e.g. emergencies, risks, and social aspects (Abbott and Vojinovic, 2010a,b; Vojinovic and Abbott, 2011; Abbott and Vojinovic, 2013; Brdjanovic *et al.*, 2014; Zakaria *et al.*, 2015). By doing so, modelling will come closer to decision makers and increase and facilitate the use of models by different and currently not involved stakeholders.

Last but not least and despite all the expected developments (van Loosdrecht and Brdjanovic, 2014) and release of more complex models for several wastewater treatment applications and further, one must keep in mind that a model is still a mere representation of reality, generally, applied as a tool for improvement and optimization purposes. A model must by no means be used as a substitute of an educational programme or design criterion, but rather as a complement.

### Practical examples

First examples of application of ASM date from late 80's and today there is about 4,000 publications on activated sludge modelling, some of them including the modelling full-scale WWTPs. A collection of 15 applications of models on full-scale carried out by the modelling research group from Delft, The Netherlands is presented in the book *Applications of Activated Sludge Models* (Brdjanovic *et al.*, 2015). For the purpose of this conference probably the most illustrative examples are: a) WWTP Haarlem Waarderpolder (The Netherlands) which describes the first complex application of the new TUD Bio-P model in practice where for the first time simulation of a plant was combined and supported by simulations of batch activity tests (Brdjanovic *et al.*, 2000), b) WWTP Shell Godorf (Germany) which is the first reported application of ASM for optimization of an oil refinery plant (Pinzon *et al.*, 2007), c) WWTP Anjana (India) which is the first application of ASM on a plant in developing country and the first reported successful application of integrated wastewater and sludge line modelling (combination of ASM and ADM) for upgrade of the plant (Brdjanovic *et al.*, 2007; Lopez-Vazquez *et al.*, 2013), d) WWTP Sarajevo (Bosnia and Herzegovina) which is the first ASM modelling study reported in the region and one of the first studies in general which integrated modeling of the sewage network, WWTP and recipients River Miljacka and River Bosnia (Meijer and Brdjanovic, 2010; Hodzic *et al.*, 2011), and finally e) WWTP Varaždin (Croatia) in which the ASM model was used for the first time in the region for the expansion of the existing plant. The WWTP Varaždin was one of the 5 WWTPs in Croatia (Varaždin, Zagreb, Čakovec, Vinkovci and Belišće) which were modelled as part of the project completed in 2014. Due to the extensive length of this paper author opted to provide more space for the practical examples in his platform presentation at the

conference, while for additional information the reader is referred to the reference book mentioned earlier. In addition, detailed modeling guidance are also available (Meijer and Brdjanovic, 2012) also in Croatian language (not readily available, so please request it directly from the author).

## Conclusions

Modelling is an important activity in the development of science. Modelling not only requires the explicit and quantitative formulation of theoretical concepts, it also allows transfer of complicated knowledge between scientific disciplines as well as between theoretical and practical applications. For 25 years, activated sludge models have played a crucial role in the development of the activated sludge process. These models are not typically academic; they do not aim to include every potential sub-process involved in the activated sludge process. Instead, they are formulated with the minimum complexity needed to describe the relevant features of the process in practice. They also provide a systemized platform for the description of environmental biotechnological models in general, through the use of standardized notation and a matrix presentation. Over the years, many wastewater research projects have benefitted greatly from the development of activated sludge models. On one hand, modelling has been expanded through the development of novel theoretical concepts and their application in new fields. On the other hand, models have been used for practical applications. While models have been considered as a standard tool in professional practice in developed world, its applications in south-eastern Europe and the Balkans are limited. However, even few in numbers, they demonstrate that the modelling is not a science fiction but approaching and unavoidable reality in the region, so get ready for it!

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## References

- Abbott M.B., Vojinovic Z. (2009) Applications of numerical modelling in hydroinformatics. *J Hydroinformatics*, 11(3-4): 308-319.
- Abbott M.B., Vojinovic Z. (2010a) Realising Social Justice in Water Sector: Part 1, *J Hydroinformatics*, 12(1):110–130.
- Abbott M.B., Vojinovic Z. (2010b) Realising Social Justice in Water Sector: Part 2, *J Hydroinformatics*, 12(2):225–239.
- Abbott M.B., Vojinovic Z. (2013) Towards a hydroinformatics praxis in the service of social justice, *J Hydroinformatics*, 16(2):516–530.
- Armburst M., Fox A., Griffith R., Joseph AD., Katz R., Konwinski A., Lee G., Patterson D., Rabkin A., Stoica I., Zaharia M. (2010) A view of cloud computing. *Communications ACM*, 53(4):50-58.
- Barker P.S., Dold P.L. (1997) General model for biological nutrient removal activated-sludge systems: model presentation. *Water Environ Res*, 69(5): 969-984.
- Batstone D.J., Keller J., Angelidaki I., Kalyuzhnyi S.V., Pavlostathis S.G., Rozzi A., Sanders W.T.M., Siegrist H., Vavillin V.A. (2002) The IWA Anaerobic digestion model No. 1 (ADM1). *Wat Sci Tech*, 45(10):65-73.
- 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., Volcke E. (2012) Towards a generalized physicochemical framework. *Wat Sci Tech*, 66(6):1147-1161.
- Benedetti L., Langeveld J., van Nieuwenhuijzen A.F., de Jonge J., de Klein J., Flameling T., Nopens I., van Zanten O., Weijers S. (2013a) Cost-effective solutions for water quality improvement in the Dommel River supported by sewer–WWTP–river integrated modelling. *Water Sci Technol*, 68(5): 965-973.

- Benedetti L., Langeveld J., Comeau A., Corominas L., Daigger G., Martin C., Mikkelsen P.S., Vezzaro L., Weijers S., Vanrolleghem P. A. (2013b) Modelling and monitoring of integrated urban wastewater systems: review on status and perspectives. *Water Sci Technol*, 68(6):1203-1215.
- Bengtsson S., Werker A., Christensson M., Welander T. (2008) Production of polyhydroxyalkanoates by activated sludge treating a paper mill wastewater. *Biores Technol*, 99(3):509-516.
- Bentancur S. (2014) Evaluation and modelling of UPM pulp mill wastewater treatment plant in Fray Bentos, Uruguay. MSc. Thesis. UNESCO-IHE Institute for Water Education. Delft, the Netherlands.
- Brdjanovic D., Logemann S., van Loosdrecht M. C. M., Hooijmans C. M., Alaerts G. J. and Heijnen J. J. (1998) Influence of temperature on biological phosphorus removal: process and ecological studies. *Wat Res*, 32(4): 1035-1048.
- Brdjanovic D., Meijer S.C.F., Lopez-Vazquez C.M., Hooijmans C.M., van Loosdrecht M.C.M. (2015) Applications of Activated Sludge Models. IWA Publishing. London, UK. ISBN: 9781780404639.
- Brdjanovic D., Moussa M.S., Mithaiwala M., Amy G., van Loosdrecht M.C.M. (2007) Use of plant-wide modelling for optimization and upgrade of a tropical wastewater treatment plant in a developing Country. *Water Sci Tech*, 56(7):21-31.
- Brdjanovic D., van Loosdrecht M.C.M., Versteeg P., Hooijmans C.M., Alaerts G.J., Heijnen J.J. (2000) Modelling COD, N and P removal in a full-scale wwtp Haarlem Waarderpolder. *Water Res*, 34(3):846–858.
- Brdjanovic D., Zakaria F, Mawioo P.M., Garcia H.A., Hooijmans C.M., Curko J., Pean Y.P., Setiadi T. (2014) eSOS – Emergency Sanitation Operation System. *J Water Sanitation Hygiene Develop*, 5(1):156-164.
- Brdjanovic D., Meijer S.C.F., Lopez-Vazquez C.M., Hooijmans C.M., van Loosdrecht M.C.M. Ed. (2015). Applications of Activated Sludge Models. *IWA Publishing*, pg. 500. ISBN 9781780404639.
- Brink I.C., Wentzel M.C. and Ekama G.A. (2007) New developments in modeling wastewater treatment plants – Using stoichiometry to build a plant-wide mass balance based steady state WWTP model. In: Proceedings 10th IWA Conference on Design, Operation and Economics of WWTP. September 9th-13th, 2007. Vienna, Austria.
- Brun R., Kühni M., Siegrist H., Gujer W., Reichert P. (2002) Practical identifiability of ASM2d parameters—systematic selection and tuning of parameter subsets. *Water Res*, 36(16):4113-4127.
- Bürger R., Diehl S., Nopens I. (2011) A consistent modelling methodology for secondary settling tanks in wastewater treatment. *Water Res*, 45:2247-2260.
- Bürger R., Diehl S., Farås S., Nopens I. (2012) On reliable and unreliable numerical methods for the simulation of secondary settling tanks in wastewater treatment. *Computers Chem Eng*, 41:93-105.
- Cech, J.S., Hartman, P. (1993) Competition between phosphate and polysaccharide accumulating bacteria in enhanced biological phosphorus removal systems. *Water Res*, 27:1219-1225.
- Clouzot L., Choubert J.M., Cloutier F., Goel R., Love N.G., Melcer H., Ort C., Patureau D., Plósz B.G., Pomiès M., Vanrolleghem P.A. (2013) Perspectives on modelling micropollutants in wastewater treatment plants. *Water Sci Tech*, 68(2):448-461.
- Comeau Y., Hall K.J., Hancock R.E.W., Oldham W.K. (1986) Biochemical model for enhanced biological phosphorus removal. *Wat Res*, 20(12):1511–1521.
- Copp J.B. (2002) The COST Simulation Benchmark: Description and Simulator Manual. Office for Official Publications of the European Community. Luxemburg, Luxembourg. ISBN: 92-894-1658-0.
- Corominas L., Rieger L., Takács I., Ekama G., Hauduc H., Vanrolleghem P.A., Oehmen A., Gernaey K.V., Comeau Y. (2010) New framework for standardized notation in wastewater treatment modelling. *Water Sci Tech*, 61(4):841–857.
- de Kreuk, M. K., Picioreanu, C., Hosseini, M., Xavier, J. B., van Loosdrecht, M. C. M. (2007) Kinetic model of a granular sludge SBR: influences on nutrient removal. *Biotechno Bioeng*, 97(4):801-815.
- Dold P.L., Ekama G.A., Marais G.v.R. (1980) A General Model for the Activated Sludge Process. *Progress Water Tech* 12(6):47-77.
- Dold P.L., Wentzel M.C., Billing A.E., Ekama G.A., Marais G.v.R. (1991) Activated sludge simulation programs: Nitrification and nitrification/denitrification systems (version 1.0). Report TT 52/91. Water Research Commission, Pretoria, South Africa. ISBN: 0 947.
- Ekama G.A., Marais G.v.R. (1978) The dynamic behaviour of the activated sludge process. Research Report W27. Dept. of Civil Eng., University of Cape Town. Rondebosch, South Africa.
- Ekama G.A., Takács I. (2014) Modelling. In: Activated sludge: 100 years and counting. Eds. Wanner J. and Jenkins D. IWA Publishing. London, U.K. ISBN: 9781780404936.

- Energiefabriek (2015) *Energiefabriek: een initiatief van de Nederlandse Waterschappen (In Dutch: Energy factories: An initiative of the Dutch Waterboards)*. Website: <http://energiefabriek.com>.
- Fall C., Flores-Alamo N., Esparza-Soto M., Hooijmans C.M. (2012) Tracer test and hydraulics modelling of a large WWTP. *Water Practice Technol*, 7(1).
- Fenu A., Guglielmi G, Jimenez J., Spèrandio M., Saroj D., Lesjean B., Brepols C., Thoeye C., Nopens I. (2010) Activated sludge model (ASM) based modelling of membrane bioreactor (MBR) processes: a critical review with special regard to MBR specificities. *Water Res*, 44(15): 4272-4294.
- Fiehn O. (2001) Combining genomics, metabolome analysis, and biochemical modelling to understand metabolic networks. *Comparative Functional Genomics*, 2(3):155-168.
- Filipe C. D. M., Daigger G. T. (1999) Evaluation of the capacity of phosphorus-accumulating organisms to use nitrate and oxygen as final electron acceptors: A theoretical study on population dynamics. *Wat Environ Res*, 71(6): 1140-1150.
- Filipe C. D. M., Daigger G. T. and Grady C. P. L. (2001) Stoichiometry and kinetics of acetate uptake under anaerobic conditions by an enriched culture of phosphorus-accumulating organisms at different pHs. *Biotechnol Bioeng*, 76(1):32-43.
- Flores-Alsina X., Saagi R., Lindblom E., Thirsing C., Thornberg D., Gernaey K.V., Jeppsson U. (2014) Calibration and validation of a phenomenological influent pollutant disturbance scenario generator using full-scale data. *Water Res*, 51:172-185.
- Gernaey K.V., Flores-Alsina X., Rosen C., Benedetti L., Jeppsson U. (2011) Dynamic influent pollutant disturbance scenario generation using a phenomenological modelling approach. *Environ Model Software*, 26(11):1255-1267.
- Gernaey K.V., Jeppsson U., Vanrolleghem P.A., Copp J.B. (2014) Benchmarking of Control Strategies for Wastewater Treatment Plants. IWA Scientific and Technical Report No. 23. IWA Publishing. London, UK. ISBN: 9781843391463.
- Gernaey K.V., van Loosdrecht M.C.M., Henze M., Lindd M., Jørgensen S.B. (2004) Activated sludge wastewater treatment plant modelling and simulation: state of the art. *Environ Modelling Software*, 19(9):763-783.
- Grau P., Copp J., Vanrolleghem P.A., Takács I., Ayesa E. (2009) A comparative analysis of different approaches for integrated WWTP modelling. *Wat Sci Tech*, 59(1):141-147.
- Gujer W. (2006) Activated sludge modelling: past, present and future. *Water Sci Tech*, 53(3):111-119.
- Gujer W., Henze M. (1991) Activated sludge modelling and simulation. *Wat Sci Tech*, 23:1011-1023.
- Gujer W., Henze M., Mino T., van Loosdrecht M.C.M. (1999) Activated Sludge Model No. 3. *Water Sci Tech*, 3:183-193.
- Hao T.W., Xiang P.Y., Mackey H.R., Chi K., Lu H., Chui H.K., van Loosdrecht M.C.M., Chen G.H. (2014) A review of biological sulfate conversions in wastewater treatment. *Wat Res*, 65:1-21.
- Hauduc H., Gillot S., Rieger L., Ohtsuki T., Shaw A., Takács I., Winkler S. (2009) Activated sludge modelling in practice-An international survey. *Water Sci Tech*, 60(8):1943-1951.
- Henze M. (1992) Characterization of wastewater for modelling of activated sludge processes. *Water Sci Tech*, 25:1-15.
- Henze, M., Gujer, W., Mino, T., van Loosedrecht M. (2000) Activated sludge models ASM1, ASM2, ASM2d and ASM3. IWA Scientific and Technical Report No. 9. IWA Publishing, London, U.K. ISBN: : 1900222248.
- Henze M., Grady J.R.C.P.L, Gujer W., Marais G.v.R. and Matsuo T. (1987b) Activated sludge model No 1. IAWPRC Scientific and Technical Report No. 1. IAWQ. London, U.K.
- Henze M., Grady J.R.C.P.L., Gujer W. (1987a) A general model for single-sludge wastewater treatment systems. *Water Res*, 21(5):505-515.
- Henze M., Gujer W., Mino T., Matsuo T., Wentzel M.C., and Marais G. V. R. (1995) Activated Sludge Model No. 2. IAWQ Scientific and Technical Report No. 3. IAWQ. London, U.K.
- Henze M., Gujer W., Mino T., Matsuo T., Wentzel M.C., Marais G.VR., van Loosdrecht M.C.M.(1999) Activated sludge model No. 2d, ASM2d. *Water Sci Tech*, 39(1):165-182.
- Henze M., van Loosdrecht M.C.M., Ekama G.A., Brdjanovic D. (2008) Biological wastewater treatment. Principles, modelling and design. IWA Publishing. London, UK. ISBN: 1843391880.
- Hodzic A., Vojinovic Z., Seyoum S.D., Pathirana A., Meijer S.C.F., Brdjanovic D. (2011) Model-based evaluation of the urban wastewater infrastructure reconstruction options in a developing country: Case study Sarajevo in Bosnia and Herzegovina. In: Proceedings 2nd IWA Development Congress. November 21st-24th, 2011. Kuala Lumpur, Malaysia.

- Hu Z.R., Wentzel M.C., Ekama G.A. (2007) A general kinetic model for biological nutrient removal activated sludge systems: Model development. *Biotechnol Bioeng*, 98(6):1242-1258.
- Hulsbeek J.J.W., Kruit J., Roeleveld P.J., van Loosdrecht M.C.M. (2002) A practical protocol for dynamic modelling of activated sludge systems. *Water Sci. Tech.*, 45:127-136.
- Hvitved-Jacobsen T., Vollertsen J., Nielsen, A.H. (2013) Sewer processes: microbial and chemical process engineering of sewer networks. CRC press. ISBN: 9781439881774.
- Ikumi D.S., Brouckaert C.J. and Ekama G.A. (2011) A 3-phase anaerobic digestion model. In: Proceedings of the 8th IWA International Symposium on Systems Analysis and Integrated Assessment in Water Management (Watermatex2011). June 20th-22nd, 2011.San Sebastian, Spain.
- Ikumi D.S., Harding T.H., Ekama G.A. (2014a) Biodegradability of wastewater and activated sludge organics in anaerobic digestion. *Water Res*, 56:267-279.
- Ikumi D.S., Harding T.H., Vogts M., Lakay M.T., Mafungwa H., Brouckaert C.J., Ekama G.A. (2014b) Mass balances modelling over wastewater treatment plants III. Final Report. Water Research Commission. South Africa.
- Jenkins D., Wanner J. (2014) Activated sludge - 100 years and counting. IWA publishing. London, UK. ISBN: 9781780404936.
- Jeppsson U. (1996) Modelling aspects of wastewater treatment processes. PhD thesis. Lund University of Technology. Lund, Sweden. ISBN: 91-88934-00-4.
- Jeppsson U., Alex J., Batstone D., Benedetti L., Comas J., Copp J.B., Corominas L., Flores-Alsina X., Gernaey K.V., Nopens I., Pons M.-N., Rodriguez-Roda I., Rosen C., Steyer J.-P., Vanrolleghem P.A., Volcke E.I.P., Vrecko D. (2013) Benchmark simulation models, quo vadis?. *Wat Sci Tech*, 68(1):1-15.
- Jiang Y., Marang L., Tamis J., van Loosdrecht M.C.M., Dijkman H., Kleerebezem, R. (2012) Waste to resource: Converting paper mill wastewater to bioplastic. *Water Res*, 46(17):5517-5530.
- Kappeler J., Gujer W. (1992) Estimation of kinetic parameters of heterotrophic biomass under aerobic conditions and characterization of wastewater for activated sludge modelling. *Water Sci Tech*, 25(6):125-139.
- Kartal B., Kuenen J.G., van Loosdrecht MCM (2010) Sewage treatment with anammox. *Science*, 328(5979): 702-703.
- Kuba T., Murnleitner E., van Loosdrecht M.C.M., Heijnen J. J. (1996) A metabolic model for biological phosphorus removal by denitrifying organisms. *Biotechnol Bioeng*, 52(6):685-695.
- Kuba T., van Loosdrecht M.C.M., Brandse F.A., Heijnen J.J. (1997) Occurrence of denitrifying phosphorus removing bacteria in modified UCT-type wastewater treatment plants. *Water Res*, 31:777-786.
- Lackner S., Gilbert E. M., Vlaeminck S. E., Joss A., Horn H., van Loosdrecht M. (2014) Full-scale partial nitrification/anammox experiences—An application survey. *Water Res*, 55:292-303.
- Langeveld J., Nopens I., Schilperoort R., Benedetti L., de Klein J., Amerlinck J., Weijers S. (2013) On data requirements for calibration of integrated models for urban water systems. *Water Sci Technol*, 68(3):728-736.
- Langergraber G., Rousseau D.P.L., Garcia J., Mena J. (2009) CWM1 - A general model to describe biokinetic processes in subsurface flow constructed wetlands. *Wat Sci Tech*, 59(9):1687-1697.
- Laurent J., Samstag R.W., Ducoste J.M., Griborio A., Nopens I., Batstone D.J., Wicks J. D., Saunders S., Potier O. (2014) A protocol for the use of computational fluid dynamics as a supportive tool for wastewater treatment plant modelling. *Water Sci Technol*, 70(10): 1575-1584.
- Lopez-Vazquez C.M., Mithaiwala M., Moussa M.S., van Loosdrecht M.C.M., Brdjanovic D. (2013) Coupling ASM3 and ADM1 for wastewater treatment process optimisation and biogas production in a developing country: case-study Surat, India. *J Water Sanitation Hygiene Develop*, 3(1):12-25.
- Lopez-Vazquez C.M., Oehmen A., Hooijmans C.M., Brdjanovic D., Gijzen H.J., Yuan Z., van Loosdrecht M.C.M. (2009) Modelling the PAO–GAO competition: effects of carbon source, pH and temperature. *Water Res*, 43(2): 450-462.
- Lu H., Wang J., Li S., Chen G.H., van Loosdrecht M.C.M., Ekama GA (2009) Steady-state model based evaluation of sulfate reduction, autotrophic denitrification and nitrification integrated (SANI) process. *Water Res*, 43(14):3613-3621.
- Makinia J., Rosenwinkel K., Phan L. (2006) Modification of ASM3 for the determination of biomass adsorption/storage capacity in bulking sludge control. *Water Sci Technol*, 53(3):91-99.
- Mamais D., Jenkins D., Pitt P. (1993) A rapid physical-chemical method for the determination of readily biodegradable soluble COD in municipal wastewater. *Water Res*, 27(1):195-197.

- Marais G.v.R., Ekama G.A. (1976) The activated sludge process Part 1 - Steady-state behaviour. *Water SA*, 2(4):164-200.
- Martins A.M.P., Pagilla K., Heijnen J.J., van Loosdrecht M.C.M. (2004a) Filamentous bulking sludge—a critical review. *Water Res*, 38(4):793-817.
- Martins A.M.P., Picioreanu C., Heijnen J.J., van Loosdrecht M.C.M. (2004b) Three-dimensional dual-morphotype species modelling of activated sludge flocs. *Environ Sci Tech*, 38(21):5632-5641.
- Maurer M., Boller M. (1999) Modeling of phosphorus precipitation in wastewater treatment plants with enhanced biological phosphorus removal. *Wat Sci Tech*, 39(1):147-163.
- Maurer M., Abramovich D., Siegrist H., Gujer W. (1999) Kinetics of biologically induced phosphorus precipitation in waste-water treatment. *Water Res*, 33:484-493.
- Meijer S.C.F. (2004) Theoretical and practical aspects of modelling activated sludge processes. PhD Thesis. Delft University of Technology. Delft, The Netherlands. ISBN: 9090180273.
- Meijer S.C.F., Brdjanovic D. (2012) A practical guide to activated sludge modelling. Lecture Notes. UNESCO-IHE Institute of Water Education. Delft, The Netherlands. ISBN: 9073445264.
- Meijer S.C.F., van der Spoel H., Susanti S., Heijnen J.J., van Loosdrecht M.C.M. (2002) Error diagnostics and data reconciliation for activated sludge modelling using mass balances. *Water Sci Tech*, 25(6):145-156.
- Meijer S.C.F., van Loosdrecht M.C.M., Heijnen J.J. (2001) Metabolic modeling of full-scale biological nitrogen and phosphorus removing WWTP's. *Water Res*, 35, 2711-2723.
- Meijer S.C.F. and Brdjanovic D. (2010) Upgrading Large Wastewater Treatment Plants: Use of Modeling as a Decision-making Tool. IWA Specialist Conference on Water and Wastewater Treatment Plants in Towns and Communities of the XXI Century: Technologies, Design and Operation, Moscow, Russia, June 2010.
- Murnleitner E., Kuba T., van Loosdrecht M.C.M., Heijnen J.J. (1997) An integrated metabolic model for the aerobic and denitrifying biological phosphorus removal. *Biotech Bioeng*, 54(5):434-450.
- Ni B.-J., Yuan Z., Chandran K., Vanrolleghem P.A., Murthy S. (2013) Evaluating four mathematical models for nitrous oxide production by autotrophic ammonia-oxidizing bacteria. *Biotechnol Bioeng*, 110(1):153-163.
- Nielsen P.H., Mielczarek A.T., Kragelund C., Nielsen J.L., Saunders A.M., Kong Y., Hansen A.A., Vollertsen J. (2010) A conceptual ecosystem model of microbial communities in enhanced biological phosphorus removal plants. *Water Res*, 44(17): 5070-5088.
- Nopens I., Batstone D.J., Copp J.B., Jeppsson U., Volcke E., Alex J., Vanrolleghem P.A. (2009) An ASM/ADM model interface for dynamic plant-wide simulation. *Water Res*, 43(7):1913-1923.
- Nopens I., Arnaldos M., Belia E., Jeppsson U., Kinnear D., Lessard P., Murthy S., O'Shaughnessy M., Rieger L., Vanrolleghem P., Weijers S. (2014) Maximising the benefits of activated sludge modelling. *Water 21 Magazine*. October 2014, 31-33.
- Oehmen A., Carvalho G., Lopez-Vazquez C.M., van Loosdrecht M.C.M., Reis M.A.M. (2010) Incorporating microbial ecology into the metabolic modelling of polyphosphate accumulating organisms and glycogen accumulating organisms. *Water Res*, 44(17): 4992-5004.
- Oehmen A., Lemos P.C., Carvalho G., Yuan Z., Keller J., Blackall L.L., Reis M.A.M. (2007) Advances in enhanced biological phosphorus removal: from micro to macro scale. *Water Res*, 41(11):2271-2300.
- Orhon D., Ateş E., Sözen S., Çokgör E.U. (1997) Characterization and COD fractionation of domestic wastewaters. *Environ Pollution*, 95(2):191-204.
- Petersen B., Vanrolleghem P.A., Gernaey K., Henze M. (2002) Evaluation of an ASM1 model calibration procedure on a municipal-industrial wastewater treatment plant. *J Hydroinformatics*, 4:15-38.
- Petersen E.E. (1965) Chemical reaction analysis. Prentice-Hall, Englewood Cliffs, N.J., USA. ISBN: 0131287281.
- Plózc B.G., Nopens I., Rieger L., Griborio A., De Clercq J., Vanrolleghem P.A., Daigger G.T., Takács I., Wicks J., Ekama G.A. (2012) A critical review on clarifier modelling: state-of-the-art and engineering practices. In: Proceedings 3rd IWA/WEF Wastewater Modelling Seminar. Feb 26-28th, 2012. Mont-Sainte-Anne, Québec, Canada.
- Price R.K., Vojinovic Z. (2010) Urban hydroinformatics: data, models and decision support for integrated urban water management. IWA Publishing. London, U.K. ISBN: 1780401361.
- Radu A. I., Vrouwenvelder J. S., van Loosdrecht M.C.M., Picioreanu C. (2010) Modelling the effect of biofilm formation on reverse osmosis performance: Flux, feed channel pressure drop and solute passage. *J Membrane Sci*, 365(1):1-15.
- Ramirez-Higareda B.L., Lopez-Vazquez C.M., Hooijmans C.M., Brdjanovic D. (2012) Modelling the effects of process configurations on the occurrence of microbial populations and their impact on the performance of

- enhanced biological phosphorus removal (EBPR) systems. In: Proceedings IWA Nutrient Removal and Recovery 2012: Trends in Nutrient Removal and Recovery. September 23-25th, Harbin, China.
- Rauch W., Bertrand-Krajewski J.L., Krebs P., Mar O., Schilling W., Schutze M., Vanrolleghem P.A. (2002) Deterministic modelling of integrated urban drainage systems. *Wat Sci Tech*, 45(3):81-94.
- Rieger L., Gillot S., Langergraber G., Ohtsuki T., Shaw A., Takács I., Winkler S. (2012) Guidelines for using activated sludge models. IWA Task Group on Good Modelling Practice. Scientific and Technical Report No. 22. IWA publishing. London, UK. ISBN: 9781843391746.
- Rieger L., Koch G., Kühni M., Gujer W., Siegrist H. (2001) The EAWAG Bio-P module for activated sludge model No. 3. *Water Res*, 35(16):3887-3903.
- Roeleveld P.J., van Loosdrecht M.C.M. (2002) Experience with guidelines for wastewater characterisation in the Netherlands. *Water Sci Tech*, 45:77-87.
- Sahlstedt K., Aurola A.M., Fred T. (2004) Practical modelling of a large activated sludge DN-process with ASM3. *Water Intelligence Online*. <http://test.iwaponline.com/wio/2004/08/pdf/wio200408017.pdf>
- Sanchez A., Medina N., Vojinovic Z., Price R. (2013) An integrated cellular automata evolutionary-based approach for evaluating future scenarios and the expansion of urban drainage networks. *J Hydroinformatics*, 16(2):319-340.
- Satoh H., Mino T., Matsuo T. (1994) Deterioration of enhanced biological phosphorus removal by the domination of microorganisms without polyphosphate accumulation. *Water Sci Technol*, 30(6):203-211.
- Saunders, A.M., Oehmen, A., Blackall, L.L., Yuan, Z., Keller, J. (2003) The effect of GAO (glycogen accumulating organisms) on anaerobic carbon requirements in full-scale Australian EBPR (enhanced biological phosphorus removal) plants. *Water Sci Technol*, 47(11):37-43.
- Sin G., Vanrolleghem P.A. (2006) Evolution of an ASM 2 d-like model structure due to operational changes of an SBR process. *Water Sci Technol*, 53(12):237-245.
- Smolders G.L.F., Klop J.M., van Loosdrecht M.C.M., Heijnen J.J. (1995b) A metabolic model for the biological phosphorus removal process: Effect of the sludge retention time. *Biotechnol Bioeng*, 48:222-233.
- Smolders G.L.F., van der Meij J., van Loosdrecht M.C.M., Heijnen J. J. (1994a) Model of the anaerobic metabolism of the biological phosphorus removal process: stoichiometry and pH influence. *Biotechnol Bioeng*, 43(6):461-470.
- Smolders G.L.F., van der Meij J., van Loosdrecht M. C. M., Heijnen J. J. (1995a) Structured metabolic model for anaerobic and aerobic stoichiometry and kinetics of the biological phosphorus removal process. *Biotechnol Bioeng*, 47:277-287.
- Smolders G.L.F., van der Meij J., van Loosdrecht M.C.M., Heijnen J.J. (1994b) Stoichiometric model of the aerobic metabolism of the biological phosphorus removal process. *Biotechnol Bioeng*, 44(7):837-848.
- Smolders G.J.F., Bulstra, D. J., Jacobs, R., van Loosdrecht M.C.M., Heijnen, J.J. (1995c) A metabolic model of the biological phosphorus removal process: II. Validation during start-up conditions. *Biotechnol Bioeng*, 48(3):234-245.
- Sollfrank U., Gujer W. (1990) Characterisation of domestic wastewater for mathematical modelling of the activated sludge process. *Water Sci Tech*, 23(4-6):1057-1066.
- Spanjers H., Vanrolleghem P. (1999) Respirometry as a tool for rapid characterization of wastewater and activated sludge. *Water Sci Tech*, 31(2):105-114.
- Takács I., Vanrolleghem P., Wett B., Murthy S. (2007) Elemental balance based methodology to establish reaction stoichiometry in environmental modelling. *Water Sci Tech*, 56(9):37-41.
- Torfs E., Vlasschaert P., Amerlinck Y., Bürger R., Diehl S., Faràs S., Nopens I. (2013) Towards improved 1-D settler modelling: calibration of the Bürger model and case study. In: Proceedings 86th Annual Water Environment Federation Technical Exhibition and Conference (WEFTEC 2013). Water Environment Federation (WEF). October 5th-9th, 2013. Chicago, Ill. U.S.A.
- van Loosdrecht M.C.M., Brdjanovic D. (2014) Anticipating the next century of wastewater treatment. *Science*, 344(6191):1452-1453.
- van Loosdrecht M.C.M., Hooijmans C.M. Brdjanovic D., Heijnen J.J. (1997) Biological phosphorus removal processes: a mini review. *Applied Microbiol Biotechnol*, 48:289-296.
- Vanhooren H., Meirlaen J., Amerlinck Y., Claeys F., Vangheluwe H., Vanrolleghem P.A. (2003) WEST: modelling biological wastewater treatment. *J Hydroinformatics*, 5(1):27-50.
- Vanrolleghem P., Flores-Alsina X., Guo L., Solon K., Ikumi D., Batstone D., Brouckaert C., Takács I., Grau P., Ekama G.E., Jeppsson U., Gernaey K. (2014) 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. In: Proceedings 4th IWA/WEF Wastewater Treatment Modelling Seminar (WWTmod2014). March 30th-April 2nd, 2014. Spa, Belgium.
- Vanrolleghem P.A., Rosen C., Zaher U., Copp J., Benedetti L., Ayesa E., Jeppsson U. (2005) Continuity-based interfacing of models for wastewater systems described by Petersen matrices. *Wat Sci Tech*, 52(1-2):493-500.
- Vanrolleghem P.A., Spanjers H., Petersen B., Ginestet P., Takács I. (1999) Estimating (combinations of) Activated Sludge Model No. 1 parameters and components by respirometry. *Water Sci Tech*, 39(1):195-214.
- Vanrolleghem P.A., Van Daele M., Dochain D. (1995) Practical identifiability of a biokinetic model of activated sludge respiration. *Water Res*, 29(11):2561–2570.
- Veldhuizen van H.M., van Loosdrecht M.C.M., Heijnen J.J. (1999) Modelling biological phosphorus and nitrogen removal in a full scale activated sludge process. *Water Res*, 33(16):3459–3468.
- Vojinovic Z., Abbott M.B. (2011) Flood risk and social justice: from hydroinformatics of quantities to hydroinformatics of qualities. IWA Publishing. London, U.K. ISBN: 1843393875.
- Vojinovic Z., Sahlou S., Torres A.S., Seyoum S.D., Anvarifar F., Matungulu H., Barreto W., Savic D., Kapelan Z. (2014) Multi-objective rehabilitation of urban drainage systems under uncertainties. *J. Hydroinformatics*, 16(5):1044–1061.
- Volcke E.I., van Loosdrecht M.C.M., Vanrolleghem P.A. (2006) Continuity-based model interfacing for plant-wide simulation: A general approach. *Water Res*, 40(15): 2817-2828.
- Von Sperling M., Chernicharo C.A.L. (2005) Biological wastewater treatment in warm climate regions. IWA Publishing. London, UK. ISBN: 1 84339 002 7
- Wang J., Lu H., Chen G.H., Lau G.N., Tsang W.L., van Loosdrecht M.C.M. (2009) A novel sulfate reduction, autotrophic denitrification, nitrification integrated (SANI) process for saline wastewater treatment. *Water Res*, 43(9):2363-2372.
- Wanner O., Eberl H.J., Morgenroth E., Noguera D.R., Picioreanu C., Rittman B.E., van Loosdrecht M.C.M. (2006) Mathematical modelling of biofilms. IWA Publishing. London, UK. ISBN: 1843390876.
- Wentzel M.C., Loewenthal R.E., Ekama G.A., Marais G.v.R. (1988) Enhanced polyphosphate organism cultures in activated sludge systems. Part I: Enhanced culture development. *Water SA*, 14(2): 81-92.
- Wentzel M.C., Ekama G.A., Loewenthal R.E., Dold P.L., Marais G.v.R. (1989a) Enhanced polyphosphate organism cultures in activated sludge systems. Part II: Experimental behaviour. *Water SA*, 15(2):71-88.
- Wentzel M.C., Dold P.L., Ekama G.A., Marais G.v.R. (1989b) Enhanced polyphosphate organism cultures in activated sludge systems. Part III: Kinetic model. *Water SA*, 15(2):89-102.
- Wett B., Omari A., Podmirseg S.M., Han M., Akintayo O., Gómez Brandón M., Murthy S., Bott C., Hell M., Takács I., Nyhuis, O'Shaughnessy M. (2013) Going for mainstream deammonification from bench-to full-scale for maximized resource efficiency. *Water Sci Tech*, 68(2): 283-289.
- Yuan Z., Oehmen A., Ingildsen P (2002) Control of nitrate recirculation flow in predenitrification systems. *Water Sci Technol*, 45(4): 29-36.
- Zakaria F., Garcia H.A., Hooijmans C.M., Brdjanovic D. (2015) Decision support system for the provision of emergency sanitation. *Sci Tot Environ*, 512-513:645-658.

#### References for software simulators (websites):

- SIMBA: [http://nl.mathworks.com/products/connections/product\\_detail/product\\_35797.html](http://nl.mathworks.com/products/connections/product_detail/product_35797.html).
- BioWin: <http://envirosim.com/products/biowin>.
- WEST: <http://www.mikebydhi.com/products/west>
- GPS-X: <http://www.hydromantis.com/GPS-X.html>
- STOAT: <http://www.wrcplc.co.uk/software-development>
- SSSP: <http://www.clemson.edu/ces/ees/outreach/sssp.html>
- ASIM: <http://www.asim.eawag.ch/>
- AQUASIM: <http://www.eawag.ch/forschung/siam/software/aquasim/index>
- Mike Urban: <http://www.mikebydhi.com/products/mike-urban>
- HEC-CRAS: <http://www.hec.usace.army.mil/software/hec-ras/>