Twenty-five years of ASM1: past, present and future of wastewater treatment modelling

M. C. M. Van Loosdrecht, C. M. Lopez-Vazquez, S. C. F. Meijer, C. M. Hooijmans and D. Brdjanovic

ABSTRACT

Activated sludge systems have been applied for 100 years now. Over the course of the years, researchers have developed various models to describe activated sludge processes. The main aim has been to gain a better understanding of the conditions that favour the conversions of carbon, nitrogen and phosphorus present in wastewater, and associated oxygen consumption and sludge production. The current paper presents a reflection on the historical developments, state-of-the-art of activated sludge modelling and future trends. Over the years, many wastewater research groups have benefitted greatly from the development of activated sludge models (ASMs). 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 projects. Although, scientists are still searching for the ideal model, one can say that ASMs are developed to the extent that they can be applied in practice with confidence. New developments are expected to be seen regarding plant-wide modelling, integration with other models at the (urban) system level, organizational and computational infrastructure, and interface and communication with various stakeholders and users.

Key words | activated sludge, application, kinetic, modelling, stoichiometry, wastewater treatment

ACTIVATED SLUDGE MODELS

Over the past 20 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 1980s, 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 (ASMs).

In the early 1980s, 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,
Table 1 | Overview of selected ASMs (adopted from Gernaey et al. 2004)

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

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.
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 result of discussions at the time between different modelling groups. Many of the basic concepts of ASM1 were adapted from the ASM 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 & Takács (2014) (in Jenkins & Wanner 2014). Even today, the ASM1 model is still in many cases the state-of-the-art for modelling activated sludge systems (Roelveld & van Loosdrecht 2002). 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 nitrogen (N) removal. Copp (2002) reports on experiences with ASM1 implementations on different software platforms. In general, ASMs from the ASM ‘family’ are developed to describe the oxygen uptake rate and sludge production (coupled with chemical oxygen demand (COD) balance), and N and phosphorus (P) conversions at domestic wastewater treatment plants (WWTPs). 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 ASM development is the original approach of Marais & Ekama (1976) and Ekama & Marais (1978), later depicted by Dold et al. (1980), and further elaborated on in Gujer & 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 seven dissolved and six particulate components that are used to describe two biomass groups, seven fractions of COD (organic material) and four fractions of N (Henze et al. 1987b; Gujer & Henze 1991). Dissolved oxygen concentration and alkalinity are also included as part of the wastewater characteristics. From the eight processes of the model, three are related to the growth of heterotrophic and autotrophic organisms, two describe the biomass decay (death-regeneration theory, Dold et al. 1980), and three 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 & 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 WWTPs 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 ASM, mostly based on directly measurable soluble compounds. From the mid-1980s to the mid-1990s, the EBPR process grew in popularity and the understanding of the underlying bio-chemical mechanisms increased (Henze et al. 2000). In the meantime, in 1990, the composition of the Task Group changed, when Leslie Grady left and Taka-ishi 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 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 a 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 the fact 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 & 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).

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 1–3 (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 (RBCOD) and store it as internal substrate which will then be converted slowly (suggesting the conversion of RBCOD into slowly biodegradable COD (SBCOD)). When acetate (defined substrate) is added to the activated sludge the observed OUR suggests the presence of two substrates due to a rapid and a slow degradation of substrate associated with OUR (Henze 1992, Henze et al. 2008). In ASM1 it appears as if two substrates are present (S_S and X_S) while in original experiments only acetate (S_A) was dosed. To describe the observed OUR by ASM1 in this case, it was necessary to define 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 SBCOD.

The second reason to introduce ASM3 was that ASM1 proved to be rather successful for simulation of WWTPs 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 RBCOD, the slow rate associated with degradation of 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).

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 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 solids retention time (SRT) (Yuan et al. 2002; Sahlstedt et al. 2004). Here, it makes a substantial difference whether or not readily or SBCOD 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 SBCOD 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 SBCOD 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.

Figure 1 | Degradation of COD in (a) ASM1 and (b) ASM3.
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.

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 CO₂ or nitrate and biomass. They have a rather simple physiology resulting in simple processes. PAOs 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 many 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, 1994b; 1995a, 1995b, 1995c). The model was developed and validated using enriched PAO cultures cultivated on laboratory-scale anaerobic/aerobic 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 OUR, 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 formation (storage polymers) 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 micro-organisms.

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 (rX), poly-P formation (rPP), glycogen formation (rGLY) and maintenance (mO and mPHA). 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. Murnleitner et al. (1997) 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, 1994b; 1995a, 1995b) 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 (rX, rPP, rGLY, rPHA and mPHA) are found but the system can be solved if four out of five rates are determined. van Veldhui-zen et al. (1999) 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 optimized 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 it being 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 & 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.

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 realized when the model is used for educational purposes. However, in modeling 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

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. 1999), 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).
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. (2003) 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 & Daigger (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 GAO, such as Competibacter and Defluvicoccus, has been linked to the suboptimal operation and even failure of the EBPR process performance (Cech & Hartman 1993; Satoh et al. 1994; Saunders et al. 2003). Thus, GAO are seen as undesirable micro-organisms 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).

Lopez-Vazquez et al. (2009) 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 systems. This implied the incorporation of up to six different biomass groups consisting of Accumulibacter Types I and II and denitrifying and non-denitrifying Competibacter and Defluvicoccus in accordance with their observed denitrifying capabilities. Their model also included a multistep denitrifying process (from nitrate to di-nitrogen gas). Overall, the model of Oehmen et al. (2010) with minimum adjustments was able to successfully describe the EBPR biomass activities observed in laboratory-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 straightforward (e.g. due to the absence of organic matter 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 GAO, such as Competibacter and Defluvicoccus, has been linked to the suboptimal operation and even failure of the EBPR process performance (Cech & Hartman 1993; Satoh et al. 1994; Saunders et al. 2003). Thus, GAO are seen as undesirable micro-organisms 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).

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CURRENT DEVELOPMENTS

Currently, ASMs are considered reliable and capable of describing complex WWTPs. 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 1990s, models were increasingly used by researchers, but also mathematical modelling became popular among practitioners. Today, mathematical models are commonly used in 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 WWTPs 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 WWTPs 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 & 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 WWTP and protocols on how to characterize the wastewater/sewage and sludge, have been developed during recent years around the world. In 2004, at the 4th 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 ASMs, 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 at the end of this paper. The GMP-TG consists of an international team of modellers collecting experience and knowledge on activated sludge modelling to provide guidance to practitioners (Rieber 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 (Rieber 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 standardized procedures. The development of standardized 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 organized, 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 (Rieber 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 seven 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 & 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 & Brdjanovic 2012) which is used in the modelling course delivered every year at UNESCO-IHE in cooperation with Delft University of Technology (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 a model-based upgrade scenario analysis to meet 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 programme 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 15 municipal and industrial ASM applications carried out over the last two decades by the Delft modelling group (Brdjanovic et al. 2013). 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 & Vojinovic 2010), Mexico (Fall et al. 2011), Croatia (Meijer & Brdjanovic 2012) and Uruguay (Betancur 2014). This demonstrates that efforts are also undertaken 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 increased work on modelling and an increased number of publications. As a means 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. 2013). 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).
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 catalyst 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 1990s (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 & Gujer 1990; Kappeler & Gujer 1992; Mamais et al. 1995; Vanrolleghem et al. 1995, 1999; Orhon et al. 1997; Spanjers & Vanrolleghem 1999; Hulsbeek et al. 2002; Roeleveld & 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. Owing 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 obtain 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. However, 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 Green-house Gas towards the Anammox process and related N-removal and footprint, the last two open new doors towards the con-
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Trends 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 & Brdj&n&v&c 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 (Riger 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 (DOUT) 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 existing and 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 AD of organics and favour the role of WWTP as energy factories (Kartal et al. 2010; Energiefabriek 2015). Currently, most 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 to 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 SST (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 (Plösz 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 (Plösz 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 physico-chemical 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 for example the BioWin 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 AD 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). 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 AD of EBPR sludge.

Besides the potential energy savings that hydronformatics 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 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 et al. 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 (Price & Vojinovic 2010; Hodzic et al. 2011). 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. 2005) and nowadays held by the Danish Hydraulic Institute, 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 decentralized sanitation models 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 & Vojinovic 2009; Sanchez et al. 2013; Vojinovic et al. 2014), and sewage treatment components (von Sperling & Chernicharo 2009).

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).

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 and Brdjano-ovic, personal communication). 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 & Vojinovic 2010a, b, 2013; Vojinovic & Abbott 2011; Brdjano-ovic 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 & Brdjano-ovic 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.

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, ASMs 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 ASMs. 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. We trust this paper will inspire future engineers to use models as central tools in their work on improving the wastewater treatment technology through innovation and optimization.

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WEBSITES OF MODEL-RELEVANT TASK GROUPS FROM THE INTERNATIONAL WATER ASSOCIATION

Task Group on Green-House Gas (GHG):
http://www.iwa-network.org/task/task-group-on-green-house-gas
https://www.linkedin.com/groups?home=&gid=4365414&trk=anet_ug_hm&goback=%2Egna_4365414

Task Group on Good Modelling Practices (GMP)-Guidelines for use of ASMs:
www.modelEAU.org/GMP_TG
https://iwa-gmp-tg.irstea.fr/

Task Group on Benchmarking of control strategies for wastewater treatment plants (BSM):
http://www.iwa-network.org/task/benchmarking-of-control-strategies-for-wastewater-treatment-plants
http://www.benchmarkwwtp.org/

Task Group on Generalized Physico-chemical Framework (GPCF):
http://www.iwa-network.org/task/generalized-physico-chemical-framework
http://www.iwawaterwiki.org/xwiki/bin/view/WorkGroup_IWA+Task+Group+for+Physico-Chemical+Modelling/WebHome

IWA Task Group on Design and Operations Uncertainty (DOUT):
http://www.iwawaterwiki.org/xwiki/bin/view/WorkGroup_DOUT/WebHome

REFERENCES FOR SOFTWARE SIMULATORS (WEBSITES)

WEST: http://www.mikebydhi.com/products/west
STOAT: http://www.wrcplc.co.uk/software-development
SSSP: http://www.clemson.edu/ces/eees/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
SUMO: http://www.dynamita.com/
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