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Modelling activated sludge processes

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14.1 WHAT IS A MODEL?

A model can be defined as a purposeful representation or description (often simplified) of a system of interest (Wentzel and Ekama, 1997). This consequently means that a model never exactly reflects the reality. So, the question 'Does this model describe a wastewater treatment plant?' is senseless, unless what part(s) of the treatment plant the model should describe has already been defined. One never develops a model that describes every single organism, every molecule of water or every detail of the process. Models are used as a simplification of reality in such a way that they describe that part of reality that is relevant to understand and to deal with. It is also important to note that a mathematical model can only be successful if it fulfils the expectations people have of it.

There are two aspects that are very relevant in modelling: the aspects of time and of scale. In general, processes can be separated into three groups from the perspective of time. Processes can be in a frozen state, dynamic state, and steady state. Models are usually made to describe the dynamic state, the state where variations occur as a function of time. When a process is in a frozen state it means that the process will change over time, but not in the time interval that one is interested in. For example, if the daily dynamics at a wastewater treatment plant are of concern, the concentration of ammonia in the effluent will vary over time; the concentration of nitrate will vary in the reactors etc. However, within one day, the ammonia and nitrate concentrations in the sludge digester, which is sometimes part of the total activated sludge model, will not change. Usually the hydraulic retention time is 30 days, resulting in a characteristic time of change in this digester in the order of two to three weeks. Consequently one can consider the processes taking place in the digester being in a kind of frozen state. There are hardly any daily variations in the processes in comparison with those taking place in the wastewater treatment line. On the other hand, there are processes that are so fast that they are in steady state or in equilibrium condition. These processes occur so rapidly that the speed of change by far exceeds the dynamics that one is interested in. The changes that are of usual concern in wastewater treatment are, for example, changes in the ammonia concentration which have a rate value in the order of magnitude of hours. The changes that are relevant to process control have a rate value in the order of magnitude of minutes. However, if one considers

chemical precipitation processes, they will occur more or less instantaneously (in a few seconds). These rapid processes do not have to be described in a dynamic way because they proceed so fast that one can assume they are in equilibrium condition or fully performed. Therefore, one of the first considerations in making a model is to consider which processes are of interest, followed by a determination of the relevant timeframe, an assessment of the dynamics of the process, and finally an adequate description of those processes that are time-variable. The other processes, which are in a frozen or steady state, are not of primary importance as they can be introduced in a much quicker, simpler way in the model, or even omitted. This is because they can be considered as continuous processes with stable concentrations under certain conditions (as in digesters). So, the aspect of time is the first major issue in trying to simplify the reality. The recommended approach is to consider the time constants and select those processes that have the dynamics in the order of time constants one is interested in. For wastewater treatment this usually means hourly or daily dynamics, and sometimes yearly dynamics. In the latter case, of course, digestion will become important as over the year the performance of a digester will change because the sludge production will vary during the year.

The second relevant issue for modelling is space resolution. One can theoretically make a model that describes every square inch of an activated sludge plant. However, the question is whether one is interested in such a detailed description in the first place. The answer depends again on the purpose of the model. In general, in wastewater treatment practice, the reactor size is in the order of tens of meters. To describe the concentration gradients of relevant components in the reactor, of which oxygen is the most sensitive one, usually a scale size of a few meters is needed. On a different scale, there is a gradient of concentrations inside the activated sludge floc that can theoretically be described by a model. However, in standard activated sludge modelling it is neglected, as being not relevant enough to be taken into account. This consequently means that activated sludge models are usually not designed to describe a system on the scale of an activated sludge floc but on the scale of a reactor.

The next step in modelling is to look at the relevant level of detail of a microbial model (Figure 14.1).

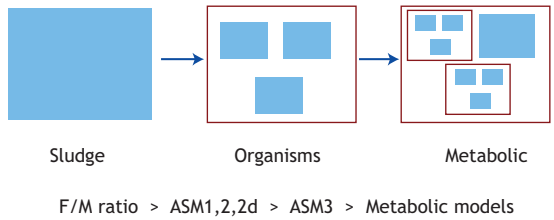

Figure 14.1 Schematic representation of the step-wise refinement of a model (Smolders *et al.*, 1995).

Typical traditional wastewater treatment design methods are based on the 'black-box' approach focusing on plant influent and effluent characteristics, while nothing or very little is known about what is happening inside the wastewater treatment plant. Traditional design parameters, such as the F/M ratio (sludge loading rate), are not based on the understanding of the processes within a wastewater treatment plant. However, one can design a plant reasonably well by applying a proper loading rate, without really knowing what processes are taking place in the plant. So the black-box model can work out well in practice.

The black-box model is not by definition wrong or not scientific, but the application of the black-box approach depends very much on the purpose of the model. If the purpose is to design a wastewater treatment plant, practice has shown that the F/M ratio can be a very good basic approach for the design, despite the fact that it does not give information about the sludge composition. One can refine this approach and move towards grey-box models, as was the case in Activated Sludge Model No.1 (ASM1, Henze *et al.*, 1987a, 1987b), No. 2 (ASM2, Henze *et al.*, 1995), and No. 2d (ASM2d, Henze *et al.*, 1999). Here the sludge was split up into relevant fractions: an inert organic

matter fraction, a fraction of nitrifying bacteria, heterotrophic bacteria, denitrifying bacteria, and a fraction of phosphate-removing bacteria. Different functional aspects of the sludge were specified for a population-based model where selected microbial communities were defined inside the activated sludge and as such incorporated in the model.

Furthermore, the metabolism of the organisms and the metabolic routes inside the organisms can also be described. By such an increase in information, the approach becomes close to glass-box modelling (such as Activated Sludge Model No.3: ASM3, Gujer *et al*., 1999, and the TU Delft EBPR model: TUDP model, Van Veldhuizen *et al.,* 1999). This results in a bigger and more complex model. The challenge here is to figure out for each process what the adequate level of description is. The question is: does the increase in complexity also increase the quality of the model (outputs), in other words, does it provide a better description of the wastewater treatment plant? For example, it has been shown that with an increase in the level of detail in the description of nitrification, a marginal improvement of model performance can be obtained while in the case of phosphate removal, significant improvement can be gained by including a metabolic description. Therefore, the preference for black-, grey-, or glass-box modelling depends very much on the purpose and application of the model. This is the point where modelling often goes wrong as modellers neglect the purpose and make the model itself the purpose of modelling.

Of course, one can even attempt to proceed to the next level of complexity by including fundamentals of microbial genetics and genetic change. Technically and in principle this is possible, but again, must be done depending on the purpose and use of the model. If the model is made too complex and with too many parameters in relation to what one ultimately wants to describe, then such an approach can be generally considered as a waste of time and effort. There is also no absolute need for a model to exactly describe reality. How far reality should be matched depends again on the purpose. For example, if one wants to get an idea about N_2O emission from wastewater treatment plants, maybe three or four theories can be created and incorporated into the model. At this point it is of prime interest to look at the simulation results of different models in terms of trends and to which extent these trends reflect the reality. At this stage one has to focus on trends only and good calibration, exact fitting and accurate knowledge of parameter values are not necessary. On the contrary, as an example, if one needs to predict the performance of a plant to satisfy legislation that requires every sample taken from the effluent to be below 1 mgNH_4/l, then the accuracy of the parameters put in the model must be much higher. In this instance one has to guarantee that the model prediction must be below 1 mgNH_4/l exactly. These two examples show again that the model should always be judged relative to the purpose of its use.

Two extremes in the type of mathematical models can be identified: empirical and mechanistic models. An empirical model is based on recognition of the parameters that seem to be essential to describe the behavioural pattern of interest, and linking these by empirical relationships established by observation. The mechanisms and/or processes operating in the system are not known or are ignored: a classical black-box approach. In contrast, a mechanistic model is based on some conceptualization of the biological/physical mechanisms operating in the system, *i.e.* it is based on a conceptual idea (or model). The complexity of this mechanistic model will depend on the degree of' understanding of the biological and chemical processes occurring in the system. Because mechanistic models have some conceptual basis, they are often more reliable than empirically based models. Because of their black-box approach, empirical models have an application strictly limited by the boundaries (*e.g.* wastewater characteristics, system parameters) within which the model was developed; only interpolation is possible. Being conceptually based, mechanistic models have greater sureness in application outside the boundaries within which the model was developed; both interpolation and extrapolation are possible. However, ultimately all models are only our rationalization of behavioural patterns of processes we conceive to be of interest.

Owing to this rationalization, any model needs to be rigorously calibrated and adequately verified by appropriate tests. Also, the conditions within which the model is expected to operate successfully need to be firmly delineated. For empirical models these are strictly the conditions within which the model was developed, while for mechanistic models these are the conditions under which the conceptualized behaviour is expected to remain valid. It is evident from the discussion above that mechanistically based models have greater potential for application in wastewater treatment plants, and attention will be focused on these models.

Processes operating in a system and the compounds on which these act must be identified in order to set up a conceptual model on which the mechanistic mathematical model is based. The various interactions between the processes, and between the processes and compounds, are delineated descriptively. To develop the mechanistic model from the conceptual model, the process rates and stoichiometric interactions with the compounds are formulated mathematically. The mathematical equivalent of the mechanistic model very probably will not include all the processes and compounds that are present in the system; only those considered to be of significance for fulfilling the objectives set for the model need be included. The art of constructing conceptual and mechanistic models is in eliminating those processes and compounds that contribute little or nothing to fulfilling the objectives set for the model. It is a waste of time and effort to develop a complicated model where a simpler one is adequate. It is most unlikely that a model can be developed that describes a phenomenon completely. Theoretically a complete description should include aspects down to the most fundamental level. The level of organization is usually set by the objectives for the model. For example, in modelling biological behaviour in wastewater treatment systems, we cannot directly implicate biochemical control mechanisms (such as ADP/ATP and NAD/NADH ratios), or even the behaviour of specific microorganism species. The mixed liquor in the activated sludge system contains a wide diversity of different microorganism species for which identification and enumeration techniques have recently become available. These techniques, however, are time and labour-consuming. Instead, microorganisms that fulfil a particular function in the activated sludge system (*e.g.* aerobic degradation of organics or nitrification) are grouped together as a single entity, which is called a 'surrogate' organism. This surrogate organism is assigned a set of unique characteristics that reflect the behaviour of the group but might not reflect the characteristics of any individual organism or species of organisms in the group. To illustrate, this approach is equivalent to modelling the 'macroscopic' behaviour of a forest of trees as opposed to the 'microscopic' behaviour of each individual tree or species of trees that makes up the forest. In considering the behaviour of the forest, a parameter that could be modelled, for example, is carbon dioxide (CO_2) production. The forest as an entity will have defined CO_2 production and consumption rates. Individual tree species within the forest, or even every single tree, might have specific CO_2 production and consumption rates that deviate significantly from those of the forest entity. However, the effect achieved by modelling the forest as an entity will closely equal the net effect of modelling the cumulative contribution of each individual tree or tree species. The great advantage in modelling the forest as an entity over modelling the individuals is that considerably less information is required to develop the model and to calibrate it. In modelling biological wastewater treatment systems, the utilization of substrate by organisms is a typical example: Monod's Equation (Monod, 1949) is used to relate the specific growth rate of the surrogate organism to the surrounding substrate concentration, whereas the organisms making up the surrogate group might have different specific growth rates or might respond differently to the various substrates present in the influent wastewater. Thus, for modelling wastewater treatment systems the organizational level that is modelled is the mass behaviour of a population or group of selected microorganisms. In the models developed for activated sludge systems, the principle organism groups, their functions and the zones in which these functions are performed are summarized in Chapter 2.

The parameters at that level that need to be included in the mathematical model depend greatly on the objectives for the model taking into account the level of organization described above. For mathematical modelling of wastewater treatment systems two different kinds of mathematical models are generally developed: steady state and dynamic models. Steady state models have constant flows and loads, and tend to be relatively simple. This simplicity makes these models useful for design. In these models complete descriptions of system parameters are not required. They are oriented towards determining the more important system design parameters. On the other hand, dynamic models have varying flows and loads and accordingly include time as a parameter. Dynamic models are more complex than steady state ones and are useful in predicting the time-dependent system response of an existing or proposed system. Their complexity means that for application the system parameters have to be completely defined. For this reason, the use of dynamic models for design is restricted. Often steady state design and dynamic kinetic models evolve interactively. Dynamic kinetic models can provide guidance for the development of steady state design models; they help identify the design parameters that have a major influence on the system response and help eliminate those processes that are not of major importance at steady state. For dynamic models, with their greater complexity, only those parameters that seem to be of importance are considered for inclusion in the model.

For activated sludge systems, selecting the level of organization at the surrogate organism or mass behaviour of populations, until recently the dynamic models have been structured to consider only the net effects as present in the bulk liquid. For example, in using Monod's Equation the kinetic rate was determined by the bulk liquid soluble COD and surrogate organism concentrations. However, with the extensions of the models to include enhanced biological phosphorus removal (EBPR), parameters internal to the surrogate biomass have had to be included, *e.g.* poly-β-hydroxyalkanoate (PHA), glycogen and polyphosphate. With this development, although the model might be at a selected level of the organization, information on processes and behaviour from lower levels of the organization is often essential, particularly to identify the key processes that control the response of the system. Usually information from lower levels of the organization is of a microbiological and/or biochemical nature, and the more complete this information is the more reliable the model. To make use of this information, 'model' organisms that are part of the 'surrogate' are identified and the known microbiological and biochemical characteristics of the organism are used to obtain a greater understanding of the surrogate. More recently the surrogate organism approach to modelling has been found to be inadequate to describe completely some behavioural patterns observed in activated sludge systems; for example, the selector effect (Gabb *et al*., 1991), substrate utilization inhibition on transfer from anoxic to aerobic zones (Casey *et al*., 1994), and generation of nitrogen intermediates in denitrification (Casey *et al*., 1994). To describe these and similar observations, it has been found that a lower level of organization needs to be selected: the synthesis and activity of certain key enzymes and the processes they mediate need to be modelled (Wild *et al*., 1994). Modelling at this level of the organization has been termed modelling with structured biomass. Detailed microbiological and biochemical information is required for this modelling approach (Wentzel and Ekama, 1997).

It should be noted that there is an essential difference between an activated sludge model and a wastewater treatment (plant) model. The latter term is used to indicate the ensemble of an activated sludge model, hydraulic model, oxygen transfer model and sedimentation tank model, all needed to describe an actual wastewater treatment at a full-scale installation (Gernaey *et al.,* 2004). The wastewater treatment plant model should be furthermore distinguished from a plant-wide model, which combines wastewater treatment models with sludge treatment models.

14.2 WHY MODELLING?

The most important advantages of the use of models in wastewater treatment are: getting insight into plant

performance, evaluating possible scenarios for upgrading, evaluating new plant design, supporting management decisions, developing new control schemes, and providing operator training.

Modelling forces the modeller to make their work explicit. Qualitative comparisons are often found in the literature such as 'better', 'larger', 'smaller', 'higher', etc. Such comparisons are not very useful and are of a subjective nature, as, for instance, the perception of 'large' or 'small' by a researcher in the laboratory or by a person operating a wastewater treatment plant is not necessarily the same. When it comes to modelling it is not possible to use descriptive elements, but it is necessary to use quantitative inputs for sizes, rates, and conversions as the model requires numbers as input. This also forces modellers to become quantitative and objective in their approach and thus the process knowledge is better defined. Of course, one can do without modelling, but very often by making a model one makes a framework that takes into account everything which is considered relevant. It furthermore forces structured and more extensive data collection, and encourages the modeller to be organized. It often exposes knowledge and data limitations and/or incorrect data (such as SRT or flows), supports efforts to improve the quality of data, and enhances good plant monitoring practices. Therefore it is not surprising that getting insight into plant performance (quantification of information, mass balances and data reconciliation) and learning about the wastewater treatment plant in question can be even more important than the modelling itself.

The second main reason for using models is the possibility of saving time and money in the process of the technology/process selection. Comparison of the system performances in a quantitative instead of a qualitative approach allows in many cases for easier decision-making and rapid comparison of options. In comparison with a qualitative description such as 'one system is more efficient than the other', model results showing that 'one system is 2% (or 20%) more efficient than the other' is much more informative and useful. If important information or selection criteria are quantified (such as purification efficiency, effluent quality, sludge production, oxygen requirements, etc), application of modelling for evaluating possible scenarios for upgrading will make the comparison more effective and faster than discussion on such issues that are usually empirical, intuitive, long and often cumbersome. For the purpose of evaluating upgrade scenarios, it is not necessary to make a very accurate model by performing an extensive calibration procedure, as the real uncertainty is associated with the model inputs and not with the model parameters. It is considered much more useful to use trends for comparison as small differences are not relevant in the context of the usual design horizon used in wastewater treatment engineering. In the case of evaluating new plant design, again it is not necessary to have a fine-tuned model due to uncertainty in process conditions in the coming 10 or 20 years. For primary plant design usually static (steady state) models are used while dynamic modelling is applied for sensitivity analysis and optimizing the design. An additional challenge is the fact that wastewater has an extremely complex and uncertain composition. Wastewater flow rate and concentrations are of a highly dynamic nature and are very difficult to control, despite certain limited possibilities to influence the wastewater composition (Chapter 3). Many processes take place within the wastewater treatment plant; some of them are relevant to the treatment and many of them are not. However, many of them occur simultaneously, even in a single process unit. In order to handle such a complex situation, there is a need for a model to support the understanding of those relevant processes. Therefore, despite the fact that from the design perspective, modelling as such is usually not strictly necessary, it is becoming increasingly used as a part of the design process. By applying statistical methods to the occurrence of worst-case scenarios, significant savings can be made and the plant can still achieve its effluent quality standards for approximately 95% of the time. In traditional design all the worst-case scenarios are often assumed to occur simultaneously, leading to a highly unlikely scenario.

Another important reason for using models is the possibility of decreasing or minimizing risks. By using models, 'what-if' scenarios can be examined in

a quantitative way in respect of what the effects of potential risks are. Such a glass-box type (as opposite to the black-box type) quantification is invaluable in the evaluation and selection of acceptable risk, rejecting risks that cannot be taken, and in the identification of upfront measures that can be taken to mitigate or control such risks. For example, questions like 'What will happen if the flow rate doubles?' and 'What is the effect of such an increase on effluent quality?' can be properly addressed by using models. Furthermore, models allow for minimization of risks that are related to the scaling-up of the systems (lab-scale vs. pilot-scale vs. large-scale). Related risks originate from the fact that, for example, mixing conditions, load variations etc., are different for full-scale and lab-scale installations. From the perspective of process control, pilot-scale gives a much faster response in comparison with full-scale plants with greater inertia.

Furthermore, the application of models improves knowledge transfer and decision-making. Wastewater treatment engineering and environmental engineering in general are multidisciplinary fields requiring knowledge of different disciplines, such as microbiology and biochemistry, as well as physical, biological and mechanical engineering. In addition, each expert group involved, be they operators, engineers or scientists, usually has its own perspective of the same subject. By phrasing the subject into a mathematical context the same communication tool (language) is used. Such a multidisciplinary approach allows for a better description of the reality, each discipline delivering its own input for a better understanding of the reality that can be incorporated in a structured, organized and quantitative way into the model. Model-related communication was greatly improved after the introduction of ASM1 in 1987. Prior to the introduction of ASM1, at least five or six different ways of modelling wastewater treatment plants were described; each model had its different approaches in writing up, in notation, and in the implementation of equations, which made it extremely difficult to understand the models and their results. The uniform context and standardization introduced by ASM1, in terms of notations, symbols and structure, made comparison of results and knowledge transfer much easier and further encouraged modelling applications.

Nowadays models are invaluable tools for training. For example, the plant operator can safely investigate by means of modelling what can happen if one takes certain action at a treatment plant without risking upsetting the operation of the plant. Moreover, models can be used to transfer knowledge from design engineers to operators and, of course, in academia worldwide, where modelling is increasingly becoming a part of the curricula for engineers and scientists. From the perspective of process control, in practice there are no direct model-based controllers functional yet, as their application still remains of scientific interest. In practice simple controllers are tuned based on the model, which allows for much quicker optimization of control strategy at full-scale installations (Chapter 15).

In the framework of integrated urban water system modelling, wastewater treatment modelling is an important component and it is necessary to link up wastewater treatment with the sewer system (to take into account the effects of, for example, combined sewer overflows or processes taking place in the sewerage system) on the one hand, or the receiving water's quality and quantity, on the other hand. Integrated modelling is becoming an increasingly popular tool to support decision-making at the level of urban water system management as it brings objectivity and gives quantitative insight into the relevant differences between options.

14.3 MODELLING BASICS

14.3.1 Model building

Many different types of models exist; these can be broadly categorized into (*i*) physical, (*ii*) verbal or conceptual and (*iii*) mathematical models. The physical model is a spatially scaled representation of the system. For example, the laboratory- and pilot-scale experiments used by scientists and engineers to investigate system response and behaviour are

physical models. The verbal or conceptual model provides a qualitative description of the system and is usually developed from detailed observations; these models can be presented as schematic diagrams (*e.g.* flow diagrams) or as a series of narrative statements. Preparation of a verbal model is the most important but also the most complex part of model building. The mathematical model provides a quantitative description of the system. With mathematical models the rates of the processes acting in the system and their stoichiometric interaction with the compounds are formulated mathematically. The mathematical formulations need to be incorporated in a solving procedure that takes account the physical constraints and characteristics imposed by the system in which the processes take place, *e.g.* temperature and mixing conditions. Mathematical models are seldom developed in isolation, but usually evolve interactively from a conceptual model that might be based to some degree on observations made on a physical model, *e.g.* laboratory- or pilot-scale experiments (Wentzel and Ekama, 1997).

Research methodology which combines verbal, mathematical and physical models (Figure 14.2) is very helpful to make rapid progress and to evaluate new systems.

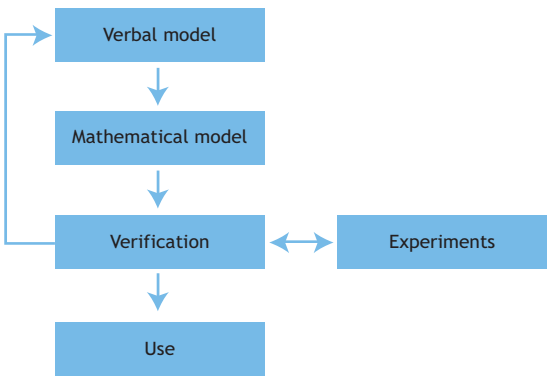

Figure 14.2 The model-building process.

A number of factors are to be considered regarding activated sludge modelling and simulation, and a step-wise approach is needed to progress from the model purpose definition to the point where a wastewater treatment plant model is available for simulations. The following main steps can be distinguished in this process (Coen *et al.,* 1996; Petersen *et al.,* 2002; Hulsbeek *et al.,* 2002):

- definition of the model purpose or the objectives of the simulation study;
- model selection: choice of the models needed to describe the different plant units to be considered in the simulation, *i.e.* selection of the activated sludge model, the sedimentation model, etc.;
- hydraulics, *i.e.* determination of the hydraulic models for the plant or plant tanks;
- wastewater and biomass characterization, including biomass sedimentation characteristics;
- calibration of the activated sludge model parameters;
- model falsification, and
- scenario evaluations.

The methodology is illustrated in detail by Petersen *et al.,* (2002).

14.3.2 General model set-up

Balance equations form the basis of any model description. These equations describe the change in concentration in a reactor over time as the result of chemical and biological conversions and of transport processes. In steady state the change of the concentration as a function of time becomes zero. Transport and conversion processes are two different parts of the model (of a physical and chemical-biological nature, respectively).

The biological processes are only dependent on the concentration in a reactor at the place where the conversion takes place. In essence the conversion processes are therefore independent of the type of reactor or the size of the reactor (microorganisms do not know in which type of rector they are in, concrete or steel, plug-flow or fully-mixed, activated sludge or biofilm reactor, etc.). Therefore the biological and chemical conversions are called micro-kinetics and

can be easily studied in the laboratory and will not change at a full-scale installation. This part of a process model is therefore universal and can be formulated as a general activated sludge model, such as the ASM model family. The local concentrations in a reactor depend on the transport of the reacting compounds in the reactor system or treatment plant. When comparing full-scale systems, the essential differences lie in these transport processes.

The advantage of transport processes (such as convective flow, mixing, aeration) is that they are very well studied and described by general rules. They can therefore be relatively well predicted for different types and scales of processes. One can study biology and chemistry in the laboratory (for instance, the effect of temperature, concentration and pressure on microorganisms) and then use physical transport models to predict what is going to happen at full-scale. Acknowledging the fact that microbes will not undergo change between laboratory and full-scale conditions, as opposed to transport processes, helps to understand the processes and their integration in mathematical models. Such integration allows these models to be used in the process design (selection of bio-reactors, types, stability, optimization, automation and control, scale-up, etc.).

The components of a full wastewater treatment model are schematically given in Figure 14.3. First, measurable wastewater parameters have to be transformed into an influent vector with the concentrations of the different model compounds (Chapter 3). The wastewater treatment plant is modelled hydraulically by describing the different zones/reactor compartments of the plant, including the settler. Each reactor compartment is modelled individually for its mixing and mass transfer (*e.g.* aeration) characteristics. Usually a completely mixed tank reactor is used. A mass balance equation is applied for each reactor. Such a mass balance equation includes a bioconversion model. In the overall model all the compartments are coupled by the state vector including the concentrations and flow rates of the links between the compartments. This overall model is usually numerically solved to give the concentrations of all the compounds as a function of time for each compound included in the model. Therefore, effectively we can speak about four models: the process model, the hydraulic model, the

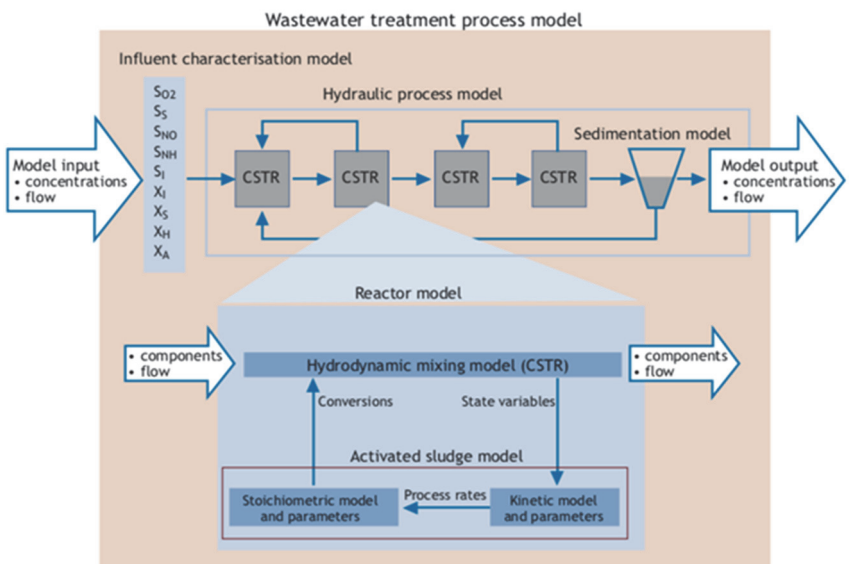

Figure 14.3 Schematic representation of a complete wastewater treatment plant model (Meijer, 2004).

reactor/compartment model and finally the activated sludge model.

The mass balance equation in steady state in mathematical terms reads:

$$\frac{\delta(S_{in} \cdot Q_{in})}{\delta t} = \frac{\delta(S_{out} \cdot Q_{out})}{\delta t} + (\alpha \cdot q \cdot X \cdot V) + (k_l A \cdot (S_{max} - S)) \quad (14.1)$$

where:

α	stoichiometry
A	surface area (m^2)
k_l	external mass transfer coefficient (m/h)
q	specific conversion rate (l/h)
Q_{in}	influent flow (m^3/h)
Q_{out}	effluent flow (m^3/h
S_{max}	saturation concentration (gCOD/m^3)
S	concentration in liquid (gCOD/m^3)
S_{in}	concentration in influent (gCOD/m^3)
S_{out}	concentration in effluent (gCOD/m^3)
t	time (h)
V	volume (m^3)
X	biomass concentration (gCOD/m^3)

Effectively it states that a compound entering a reactor either leaves with the effluent, is converted in the reactor, or is exchanged with the gas phase in the compartment. Each term in the mass balance equation is expressed as mass over time. It is helpful to realize that in order to analyse a complex system it is better to work in these dimensions than with concentration terms.

14.3.3 Stoichiometry

From the system definition one takes only those compounds of the system which are considered important and/or make a significant part of the total system mass (being at least a small percentage of it). For example, in the case of nitrification, in most plants the nitrite concentration will remain very low or close to the detection limit, so from the mass balance perspective there is no need to take nitrite into account. In anaerobic digestion, similarly, there is no need to take hydrogen into account, as the hydrogen content of the gas is very low, as almost everything ends up as methane. Such intermediates will only be specified if considered important, for example, when there is nitrite or hydrogen accumulation. Nitrite is not included in the nitrification process in ASM1, while in the Anaerobic Digestion Model (ADM1, Batstone *et al*., 2002) hydrogen is included as it plays an important role in the stability of the anaerobic system. ASM models are specifically designed for applications at lower temperatures (5 to 20ºC), in which no significant accumulation of nitrite is expected to take place. Nitrite will only accumulate at higher temperatures or in the case of unusual toxic events. Thus nitrite is left out of the model. Similarly, in denitrification, only a small amount of nitrate turnover is in the form of N_2O, so from the perspective of describing the N removal it is not relevant to include the contribution of N_2O. However, if the plant has to fulfil N_2O gas limits, then it becomes important to take it into account. Again, this depends on the purpose of the application of the model.

Beside the determination of relevant compounds and processes, defining relevant balances is essential. For each conserved balance the number of atoms of a compound entering the plant is equal to those leaving. Examples of conserved balances are nitrogen, phosphorus, COD or alkalinity conversion. Using balance equations, unknown stoichiometry coefficients can be calculated. This substantially reduces the required information for modelling because the approach allows a number of unknowns to be calculated. The use of BOD measurement to characteristic wastewater is declining and, instead, modern approaches rely on COD. BOD-based design is associated with a black-box approach, it cannot be used for balancing as it is not conserved, and it depends on many factors (*e.g.* reaction time, temperature). In practice it is still mostly used to link the output of ASM regarding effluent impact on receiving waters (where BOD is still a relevant indicator of water quality). In contrast, the COD balance is maintained because COD is by definition the amount of electrons which are transferred to oxygen in order to oxidize all the organic matter in the

system to CO_2 and water. This is why modelling nowadays is based on COD rather than on BOD.

Stoichiometry can be determined based on relevant compounds involved in the reaction and use of balances to calculate the relevant coefficients. For example, in the reaction for heterotrophic growth the relevant compounds are organic matter, oxygen, ammonia, alkalinity, biomass, carbon dioxide and water. At this stage of equation development it is not necessary to determine which compound is utilized and which is produced as it will simply receive a negative or positive sign; in other words, it is not important on which side of the equation the parameter is. The next step is to choose one coefficient as 1 and to use balances to calculate all the other relevant coefficients. In the example here, five balance equations can be made (for carbon, oxygen, hydrogen, nitrogen and charge) and there are seven unknown coefficients. One of these coefficients can be made equal to 1 and there is only one coefficient that we need to know, for example the amount of oxygen consumed per COD converted or the amount of biomass produced per substrate COD mass utilized (yield coefficients).

This is a general approach for setting up the stoichiometry of the reaction for any biological process *e.g.* if organics (or COD) are utilized aerobically (with O_2).

$$?COD + ?O_2 + ?NH_4^+ + ?HCO_3^- \rightarrow ?Biomass\text{-}COD + ?CO_2 + ?H_2O \quad (14.2)$$

In wastewater treatment systems we are usually not interested in the CO_2 and H_2O conversion, and the COD balance is used to replace one of the elemental balances. If one sets the coefficient for substrate COD as 1, and if the yield coefficient for the biomass is known, Eq.14.2 becomes:

$$1COD + (1-Y_H)O_2 + f_N Y_H NH_4^+ + f_N Y_H HCO_3^- \rightarrow Y_H \text{ Biomass COD} \quad (14.3)$$

where:

Y_H heterotrophic yield (gBiomass COD /gSubstrate COD), and

f_N fraction of nitrogen in biomass (gN/gBiomass COD)

To derive this equation we effectively used the COD, nitrogen and charge balance. The COD balance states that oxygen consumption and biomass production are always coupled; it is impossible to save oxygen and produce less sludge as the substrate (COD) is either oxidized by oxygen or becomes sludge. From the N balance the amount of ammonia needed can be calculated, and from the charge balance the amount of bicarbonate (alkalinity) can be determined, etc. The stoichiometric reaction can be written down as a function of the yield coefficient and, in this particular example, the amount of nitrogen inside the biomass. The stoichiometric coefficients for each compound are included in the model matrix (Table 14.1).

14.3.4 Kinetics

Each reaction has its own rate equation. The rate equation specifies the rate of conversion of the compound with the stoichiometric yield coefficient of 1. The conversion rate of the other compounds follows from multiplying each yield coefficient with the rate equation. The model can be based either on substrate-based kinetics (a substrate stoichiometric coefficient is equal to 1) or growth-based kinetics (a biomass stoichiometric coefficient equal to 1). It is not advisable to use both at the same time in one model. In ASM1 the rates are described based on the growth rate; the biomass coefficient is therefore set as 1. In ASM, a saturation equation is used as the standard rate equation. Saturation (Monod) kinetics includes two main parameters, the maximum rate parameter and affinity or saturation constant (the K value, defined as the concentration at half the maximum rate). The saturation term $S/(K+S)$ can have a value between 0 and 1, and can have a different function in the model. Several affinity terms reflect a real value, *e.g.* the oxygen affinity term is an observed parameter. However, in some cases the saturation term is only a switching term. For example, a switching function is

used in the model to stop the growth process when there is no ammonia present (Eq. 14.4). The affinity constant for ammonia is effectively very low and scarcely measurable, so the coefficient placed in the equation has the sole purpose of guaranteeing that there is no further growth when the ammonia is fully consumed. This consequently means that one does not need to calibrate this value. How to distinguish between real measurable parameters and switching functions is a bit vague and inexplicit in activated sludge modelling. Therefore it is important to realize whether the K values are there as real model parameters or as a switching function to stop the process when the relevant compound is no longer present.

$$\mu = \mu^{max} \frac{S}{K_S + S} \cdot \frac{S_O}{K_O + S_O} \cdot \frac{S_N}{K_N + S_N} \cdots \quad (14.4)$$

To describe inhibition kinetics, a similar approach is applied, but now the affinity constant is called the inhibition constant, and consequently it is possible to define an inhibition term (Eq. 14.5), which again has a value between 0 and 1. The inhibition constant is equal to the substrate concentration at which a 50% decrease in the rate is observed. There are also much more complex inhibition terms, but in ASM this is the term that is usually applied, especially for the substrate inhibition.

$$1 - \frac{S}{K_S + S} = \frac{K_S}{K_S + S} \quad (14.5)$$

It is important to note that multiplying so many factors causes deviation because these factors are never exactly 1. If one multiplies two factors with a value of 0.9 with the value of a third factor that is 0.5, the result will be 0.4, while the real value should be 0.5 because this is the limiting factor. This consequently means a 20% lower rate value. Therefore it is better to use a logical operator in the model and choose the minimum factor among the terms (Eq. 14.7) instead of multiplying these factors (Eq. 14.6) as it seems that this better approximates the reality.

$$\mu = \mu^{max} \cdot \frac{S}{K_S + S} \cdot \frac{S_O}{K_O + S_O} \cdot \frac{S_{NH}}{K_{NH} + S_{NH}} \cdot \frac{S_{KI}}{K_I + S_{KI}} \quad (14.6)$$

$$\mu = \mu^{max} \cdot MIN\left(\frac{S}{K_S + S}; \frac{S_O}{K_O + S_O}; \frac{S_{NH}}{K_{NH} + S_{NH}}; \frac{S_{KI}}{K_I + S_{KI}} \right) \quad (14.7)$$

The reason that Eq.14.6 is used is partly an inherited habit (at the time of early model development in the 1970s, computing logical operators by integral differential equations was difficult and extremely time-consuming and thus was not applied). It does not matter so much which equation is used for activated sludge modelling; the point is to understand the reasons for the choices that were made at different stages of the model development.

14.3.5 Transport

A typical wastewater treatment model has several transport terms, which are often time-dependent (Figure 14.3). The model input is the time-variable flow and composition of the wastewater. The process is described in a hydraulic model, representing the hydraulics of a full-scale plant. An example is given in Figure 14.4.

The main problem is associated with making a hydraulic model of a wastewater treatment plant. A rigorous solution would be to make a full computational fluid dynamics model of the plant, which can exactly describe the flow in the reactors. However in general the details obtained for the flow in this way exceed by far the requirements of most conversion models. Since we are mainly interested in the bioconversion we need to adequately describe changes in concentrations in the treatment plant. Measuring several relevant compounds can help to define the hydraulic model. For activated sludge models these compounds are in general oxygen, ammonium and nitrate and, for phosphate removing systems, phosphate. As a first step a clear division can be made between aerobic and anoxic or anaerobic zones in a treatment plant.

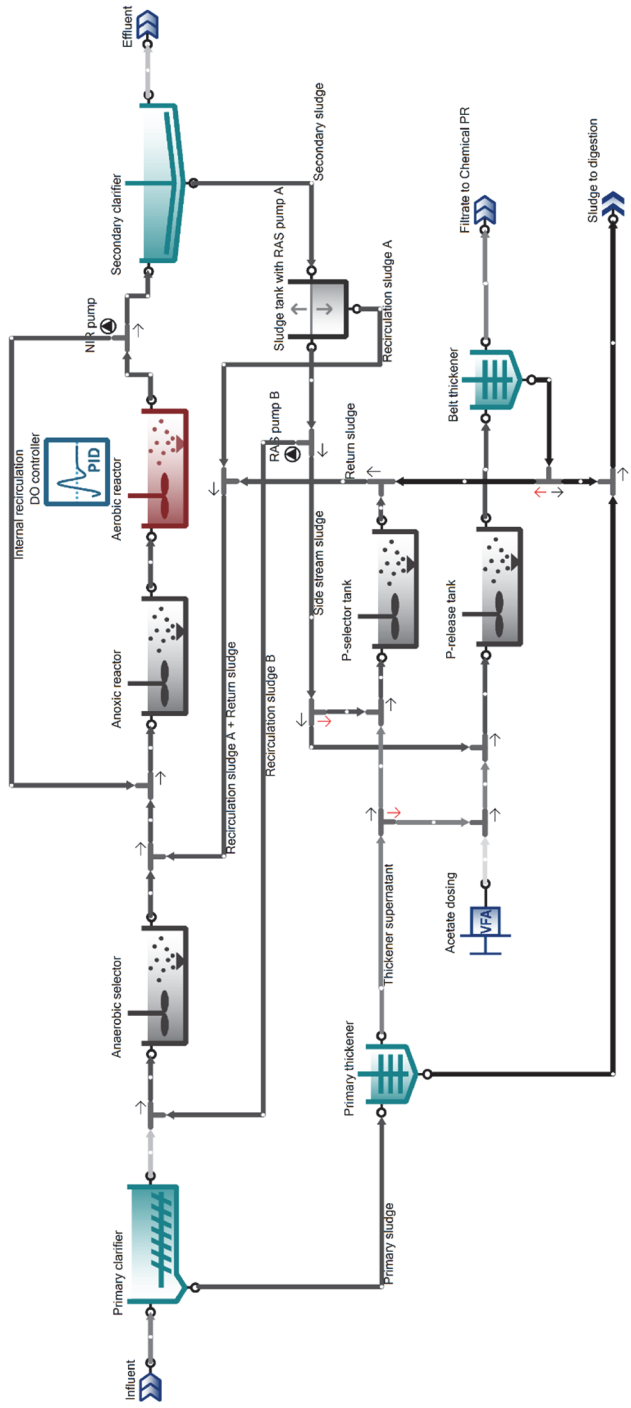

Figure 14.4 Hydraulic process scheme of the PhoStrip® process at WWTP Haarlem Waarderpolder in the Netherlands and its representation in the modelling simulator SUMO (adapted from Brdjanovic *et al.*, 2000 by Dynamita).

Within each zone one then has to observe whether *e.g.* in an aerated tank there exists a gradient in the oxygen concentration. As long as the oxygen concentration is always well above the saturation coefficient for oxygen used in the kinetic equations, there is no direct need to describe the changes in concentration in the aerobic zone, and the tank can be considered fully mixed. If the concentration of the reacting compounds becomes close to or lower than the saturation constants, the hydraulic model should be such that the change in concentrations is clearly described. In general, this means using a plug flow model or describing the system as a series of tanks. If the observed concentration of *e.g.* ammonia in the aeration tank is approximately 4 mg/l across the tank, it can be considered as a fully mixed tank and be represented in the hydraulic scheme of the plant as a single reactor. However, if the observed ammonia concentration changes from 4 mg/l at the inlet to the aeration tank to 0 mg/l at the outlet, this indicates a strong concentration gradient within the tank, and consequently it is much better to model it as a multi-compartmental tank with a number of fully mixed smaller reactors in series. A second aspect taken into consideration is the transfer of compounds between gas and liquid (*e.g.* oxygen) in aerated reactors or between biofilm and liquid. This is described in detail in Chapter 9 and Chapter 17.

14.3.6 Matrix notation

The balance equation (Eq.14.1) can be described for each individual compound. The large number of relevant compounds and conversions make activated sludge modelling complex. A large number of balance equations need to be formulated resulting in a loss of overview. Therefore the IAWQ Task Group (Henze *et al.*, 1987) on 'Mathematical Modelling of Wastewater Treatment' recommends the matrix method for model presentation.

This format facilitates clear and unambiguous presentation of the compounds and processes and their interaction on a single page. In addition, the matrix format allows easy comparison of different models, and facilitates transforming the model into a computer program. The matrix is represented by a number of columns and rows; one column for each compound and one row for each process. A simplified example is given in Table 14.1.

The first step in setting up the matrix is to identify the compounds of relevance in the model. The compounds are presented as symbols listed at the head of the appropriate column including a row with the dimensions.

The second step in setting up a matrix is to identify the biological processes occurring in the system. These are conversions or transformations that affect the compounds considered in the model and are itemized one below the other down the left-hand side of the matrix. The process rates are formulated mathematically and are listed on the right-hand side of the stoichiometry matrix in line with the respective process. Along each process row the stoichiometric coefficient for conversion from one compound to another is inserted so that each compound column lists the stoichiometric coefficients for the processes that influence that compound. If the stoichiometric coefficient equals zero it is for clarity generally not given in the printed matrix. The sign convention used in the matrix for each compound is 'negative for consumption' and 'positive for production'. In this convention the process rates always have a positive sign. Note that oxygen is negative COD because oxygen accepts electrons: electrons are passed from the substrate to oxygen to form water. Care must be taken with the units used in the rate equations for the processes. The stoichiometric coefficients are greatly simplified by working in consistent units.

In the example presented in Table 14.1 the compounds are expressed as COD equivalents. Provided that consistent units are used, continuity can be checked against the stoichiometric parameters by moving across any row of the matrix; the sum of the stoichiometric coefficients must be zero.

This matrix forms a succinct summary of the complex interactions between compounds and processes. It allows alterations in processes,

Table 14.1 Example of a simple stoichiometric matrix for activated sludge modelling (Henze *et al.*, 1987b).

Components i	1: S_O	2: S_S	3: X_H	Process rate equation ρ_j
List of processes j				
Aerobic growth	$-\frac{1}{Y_H}+1$	$-\frac{1}{Y_H}$	+1	$\mu_H^{max} \cdot \frac{S_S}{K_S+S_S} \cdot X_H$
Lysis		+1	–1	$b_H \cdot X_H$
Observed transformation rate r_i	$r_i=\sum_j v_{j,i} \cdot \rho_j$ $[M_i L^{-3} T^{-1}]$			
Definition of stoichiometric parameters: Y_H Heterotrophic yield coefficient $[M_H M_S^{-1}]$	Dissolved oxygen (O_2)	Dissolved organic substrate (COD)	Heterotrophic biomass (COD)	Definition of kinetic parameters: μ_H^{max} Maximum specific growth rate $[T^{-1}]$ K_S Saturation coefficient for substrate $[M_{COD} L^{-3}]$ b_H Rate constant for decay $[T^{-1}]$

compounds, stoichiometry and kinetics to be readily incorporated.

The matrix shows two important process aspects: the reaction equation for each process is represented on the different rows, and in the columns for each compound one can directly observe in which conversions the compound is involved. By multiplying the stoichiometric factors with their respective rate equations one gets the total conversion equation for each compound.

For convenience two extra aspects can be added to the matrix description (Table 14.2). The first aspect is a matrix with the composition in terms of conserved balances, in this case the COD, N and charge balance. Biomass is expressed in the stoichiometric matrix in terms of COD, but it also contains nitrogen. In the composition matrix this is included. Since the composition matrix and the stoichiometry matrix effectively contain all the conserved balances, multiplication of the two matrices therefore leads to zero.

Secondly, we are generally interested not only in the compounds expressed in the dimensions as used in the model, but also in their measured or observed units. For instance, the sludge amount is usually measured as gTSS and not gCOD. The observed matrix contains these conversion numbers between *e.g.* gCOD and gTSS. Other potentially interesting observed quantities are Kjeldahl nitrogen, VSS or BOD.

14.4 STEPWISE DEVELOPMENT OF THE BIOKINETIC MODEL: ASM1

Model development is a step-wise, bottom-up process where only strictly necessary processes for the pre-defined purpose of modelling are included. Starting simple and increasing complexity when needed is the general governing principle in model development. In general, activated sludge models from the ASM family are developed to describe oxygen uptake rate and sludge production (coupled on the COD balance), and N and P conversions at domestic wastewater treatment plants.

Table 14.2 Example of a stoichiometric matrix for activated sludge modelling (adapted from Gujer and Larsen, 1995).

Component	Oxygen	Inert	Substrate	Ammonia	Alkalinity	Biomass	Inert	Substrate	TSS	Rate
Symbol	S_O	S_I	S_S	S_{NH}	S_{HCO}	X_H	X_I	X_S	X_{TSS}	
Unit	gO_2	gCOD	gCOD	gN	mole	gCOD	gCOD	gCOD	gTSS	
Process	STOICHIOMETRY MATRIX									
Hydrolysis			1					–1	–0.75	r_1
Aerobic growth	–0.5		–1.5	-0.08	–0.005714	1			0.9	r_2
Lysis				0.07	0.005	–1	0.2	0.8	–0.12	r_3
Conservatives	COMPOSITION MATRIX									
ThOD-COD	–1	1	1	0		1	1	1		
N		0.02		1		0.08	0.05	0		
Charge				0.071429	–1					
Observables										
TSS						0.9	0.9	0.75		

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 stepwise activated sludge model development is the original approach of Ekama and Marais (1978), later depicted by Dold *et al*., (1980), and further elaborated in Gujer and Henze (1991). The outcome of this approach is a model which comes close to ASM1 and as such is briefly described here. The experimental system used in this approach comprised a completely mixed activated sludge system using settled domestic wastewater, and the basic influent and sludge characterization and operational conditions are listed in Table 14.3.

The objective of the study was to use the model to correctly describe the biomass content in the system, oxygen uptake by the biomass, and nitrogen conversion. To begin, one can use a very simple model consisting of only three relevant components (dissolved oxygen S_O, dissolved organic substrate S_S, and heterotrophic biomass X_H) and two relevant conversion processes (aerobic biomass growth and

Table 14.3 Experimental system summary data, Ekama and Marais (1978).

Parameter	Value
Feeding regime	12 h/d turned on between 02 and 14 hrs
Flow	18 l/d
Reactor volume	6.73 l
Processes	COD removal and nitrification (fully aerobic)
Biomass content in the reactor	1,375 mgVSS/l or 2,090 mgCOD/l
Sludge retention time (SRT)	2.5 d
Operating temperature	20.4°C
Influent COD concentration	570 mgCOD/l
Influent TKN concentration	46.8 mgN/l

lysis). With an increase in SRT, the biomass (live organisms) as a fraction of the sludge mass (VSS) in the system decreases. To describe this, the lysis process or death regeneration was used *i.e.* disintegration of death cells resulting in the generation of soluble biodegradable substrate available for the generation of new biomass (Chapter 4). Lysis of heterotrophic biomass here summarizes all the processes which lead to a loss of biomass (decay, lysis, endogenous respiration, predation etc). Maintenance or endogenous decay could have also been used here to describe the reduction in biomass. For the aerobic growth process all three components are relevant; dissolved oxygen and organic substrate are utilized by the biomass under aerobic conditions (thus negative coefficient) to produce biomass (positive coefficient). In general, a matrix can be simplified if one can choose to freely assign for each process one stoichiometric coefficient with a value of +1 or –1. The choice of the yield coefficient Y_H (0.67 gCOD/gCOD) together with the COD conservation equation is sufficient to determine all the stoichiometric coefficients for aerobic growth (Figure 14.5). For both processes one can define the rate; for aerobic growth it is a product of the maximum specific growth rate, the affinity for substrate and the biomass concentration (assuming that the oxygen is not limiting the growth).

For lysis, it is a sort of 1st order process where the biomass falls apart in proportion to the biomass concentration present and the constant of proportionality is called the rate constant for decay. Substituting the coefficients in the biokinetic model gives the matrix for Model A (Table 14.4).

If this model is used to compare the experimentally observed oxygen uptake rate (OUR), it can be seen that the experimental observations deviate considerably from the model predictions, except for the period between 0 and 2 hrs and at the very end of the experiment (endogenous respiration). In general, if the model predictions are deviating in terms of the levels of parameter of interest, this can be relatively straightforwardly adjusted by changing the value of the selected model parameter(s). However, if the model predictions in terms of trends and shapes are wrong, very likely the relevant process or processes have been overlooked. In this particular experiment, the difference between the total oxygen consumption observed over 24 hrs and the one predicted by the model seems to be quite close. However, it was the deviation between the model prediction and experimental results that led Dold *et al*. (1980) to suggest splitting the degradation of organic matter in wastewater into two processes (fractions): the relatively rapid process of biodegradation of part of the COD comprising of organics such as VFAs and glucose, and the relatively slow process of COD degradation (cellulose, starch, proteins etc). This fractionation of biodegradable COD into readily and slowly biodegradable COD (RBCOD and SBCOD, respectively) was triggered by the experimental observation of the OUR profile which showed a very sharp drop almost immediately after feeding stopped (14 hrs), followed by a slow decrease observed until the end of the experiment where it reached the steady value observed during the first two hours of the test. Therefore, the lysis process was reasonably well described by the model. It was furthermore concluded that the SBCOD is converted into RBCOD by the relatively slow process of hydrolysis (Figure 14.5).

Table 14.4 Matrix presentation of Model A.

Component	S_O	S_S	X_H	Rate
Growth	–0.5	–1.5	1.0	$\mu_H^{max} \cdot \frac{S_S}{K_S+S_S} \cdot \frac{S_O}{K_{O,H}+S_O} \cdot X_H$
Lysis		+1.0	–1.0	$b_H \cdot X_H$

This implies that there is a need to extend Model A by introducing two types of substrate (RBCOD and SBCOD) and one additional process (hydrolysis). In ASM1 it was also assumed that slowly biodegradable substrate consists entirely of particulate substrate (X_S), which is not necessarily true, but in ASM1 accepted as such. A distinction between soluble (S) and particulate (X) material is necessary in order to determine which compound will settle in the clarifier and which will leave the system with the effluent.

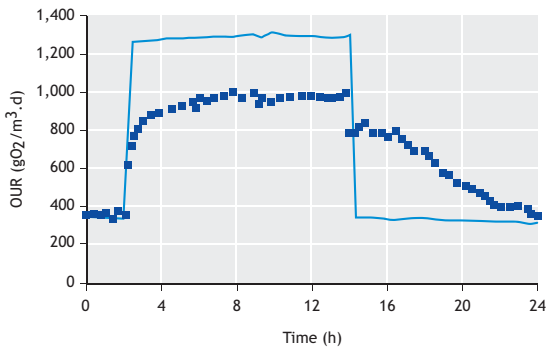

Figure 14.5 Model A: a comparison of experimentally observed values (data points) with a theoretically predicted oxygen uptake rate (continuous line) (adapted from Ekama and Marais, 1978; Gujer and Henze, 1991).

The introduction of a SBCOD fraction (X_S) did not affect the heterotrophic growth process as it is assumed that growth is not directly based on SBCOD. Also, the lysis processes were adjusted by the assumption that the lysis products are slowly biodegradable and, as such, are added to the pool of X_S. These products are made available for aerobic heterotrophic growth by hydrolysis. This means that there are two types of particulate substrate: one derived from the influent wastewater, and the second generated by the biomass decay. In some cases these are lumped together (as in this case), while in some models they are taken into account separately. However, both options result in virtually zero net difference. Furthermore, hydrolysable material X_S is assumed to adsorb onto heterotrophic biomass X_H resulting in a kind of Lagrangian kinetic expression as the rate equation for hydrolysis. Therefore it is the amount of substrate per biomass which is important here (rate limiting) and not the substrate concentration with respect to the bulk liquid as in the case for the RBCOD. By implementing this, Model B was formed (Table 14.5).

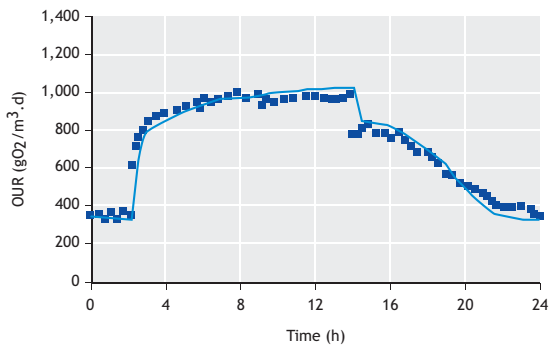

Figure 14.6 Model B: comparison of experimentally observed values (data points) with theoretically predicted oxygen uptake rate (continuous line) (adapted from Ekama and Marais 1978; Gujer and Henze 1991).

Model B describes the OUR very accurately (Figure 14.6). However, the predicted activated sludge concentration was 22% less than the measured concentration. This indicated the need to increase the sludge production by introduction of an influent non-

Table 14.5 Matrix presentation of Model B.

Component	S_O	S_S	X_H	X_S	Rate
Growth	–0.5	–1.5	1.0		$\mu_H^{max} \cdot \frac{S_S}{K_S+S_S} \cdot \frac{S_O}{K_{O,H}+S_O} \cdot X_H$
Lysis			–1.0	+1.0	$b_H \cdot X_H$
Hydrolysis		+1.0		–1.0	$k_H \cdot \frac{(X_S/X_H)}{K_x+(X_S/X_H)} \cdot X_H$

biodegradable fraction of COD (being inert and also particulate organic matter which accumulates in the reactor: X_I). The term 'non-biodegradable' is used in the context of wastewater treatment for a compound which is not degraded by microorganisms during its retention in the treatment system. Materials such as plastics, wood-based and fibrous materials, nails, and hairs are all organic and strictly speaking considered biodegradable, but not in wastewater treatment systems. Even a compound such as cellulose is considered non-biodegradable in high-loaded wastewater treatment plants but biodegradable in low-loaded systems. Besides inert particulate material derived from the influent wastewater, there is also the second component generated by the biomass decay. The latter arises from the fact that cell walls are made of COD which biodegrades very slowly and is considered non-biodegradable, resulting in the experimentally-determined division of lysis process products of 92% being X_s (biodegradable) and 8% X_I (unbiodegradable). Consequently the rates in Model B are not changed given the fact that the OUR profile was described correctly.

Inclusion of X_I resulted in the new Model C shown in Table 14.6. The observed biomass concentration in the reactor was very well predicted by Model C; however, due to higher sludge (COD) production/removal from the system, the oxygen consumption was significantly underestimated by the model (despite the fact that the general OUR profile was well matched, Figure 14.7).

This is to be expected as oxygen consumption and sludge production are coupled via the COD balance, and consequently, an increase in sludge production will cause a decrease in oxygen demand. It was not possible to predict correctly both oxygen consumption and sludge production by Model C.

From the experimental observations (results not shown) it was clear that the effluent from the treatment plant contained nitrate which implied that nitrification should be included.

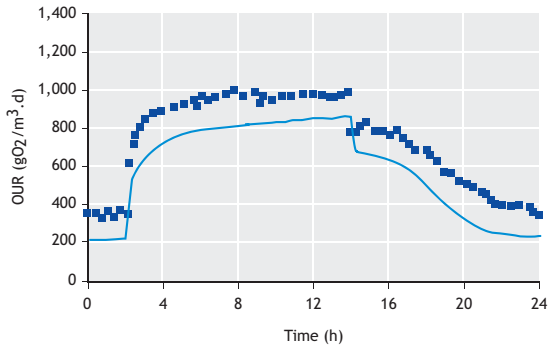

Figure 14.7 Model C: comparison of experimentally observed values (data points) with theoretically predicted oxygen uptake rate (continuous line) (adapted from Ekama and Marais, 1978; Gujer and Henze, 1991).

By inclusion of nitrification the model had to be extended by the addition of three materials and two processes, namely ammonium (NH_4^+, S_{NH}), nitrate (NO_3^-, S_{NO}) and nitrifying autotrophic biomass (X_A), and aerobic (nitrifier) growth and nitrifier lysis. Again, it was necessary to evaluate the influence of each of the additional materials on the existing reactions. Ammonia is not only used in nitrification, but also for cell growth, so therefore it was necessary to add a stoichiometric factor for ammonia in the growth relation. If the biomass contains 8% nitrogen (0.08 mgN/mgCOD), then the factor becomes 0.08.

Table 14.6 Matrix presentation of Model C.

Component	S_O	S_S	X_H	X_S	X_I	Rate
Growth	-0.5	–1.5	1.0			$\mu_H^{max} \cdot \frac{S_S}{K_S+S_S} \cdot \frac{S_O}{K_{O,H}+S_O} \cdot X_H$
Lysis			-1.0	+0.92	+0.08	$b_H \cdot X_H$
Hydrolysis		+1.0		-1.0		$k_H \cdot \frac{(X_S/X_H)}{K_x+(X_S/X_H)} \cdot X_H$

Furthermore, it was assumed that in the lysis process nitrogen remains within the biomass. However, in the hydrolysis process the biomass SBCOD is degraded (*e.g.* proteins into amino acids) resulting in a release of ammonia. As a consequence, besides one unit of substrate, 0.08 units of ammonia is also produced. This also happens with the influent SBCOD: as the protein part of it is hydrolysed, ammonia is released, and the proteins are measured in the influent as organic N, *i.e.* the difference between the TKN and FSA. So for nitrification, a certain amount of oxygen and ammonia are consumed, and nitrate and biomass are produced. The amount of ammonia consumed is not exactly the same as the amount of nitrate produced, due to dual use of the ammonia, namely (*i*) for energy generation in the nitrification process, and (*ii*) as a nitrogen source for the heterotrophic biomass growth. The difference between the ammonia consumed and nitrate formed is 0.08, representing the nitrogen content of the heterotrophic biomass. The overall N balance in this case will fit (4.25 = 4.17 + 0.08 · 1.0). Furthermore, the lysis process for the autotrophs was assumed to be the same for the heterotrophs, by which particular substrate and a small amount of inert substrate are produced. The process rate for growth for autotrophs is generated analogously to heterotrophs with saturation terms for ammonia and oxygen. By the inclusion of an additional three materials and two processes, Model D was created which satisfied both the COD and N balance. By having such a model it was possible to split the total oxygen consumption into oxygen consumption for ammonium oxidation and oxygen consumption for COD degradation. This shows the added value of using the model by providing insight into where the oxygen is used and for which processes (known as process analysis).

The results of the simulation of the OUR by Model D are presented in Figure 14.8.

There were a few dilemmas at this stage of the model development such as 'Is the match sufficiently accurate?' or 'Is deviation, for example, in OUR of 5 to 10% at 14.00 h acceptable?'. The answers to these questions depends entirely on the quality of the experimental data. If the COD and N balances of the data are exactly 100%, then it may be worth pursuing refinements in the model to get a better prediction because the data are reliable and accurate. However, if the COD and N balances are not 100% but in the 95-105% range, then there is not much sense in making the model very much more accurate. Making models is relatively easy but getting reliable and accurate experimental data is the most difficult part of developing models for wastewater treatment systems. If the equipment results in an inaccuracy of 5-10% there is no sense in making the model more accurate.

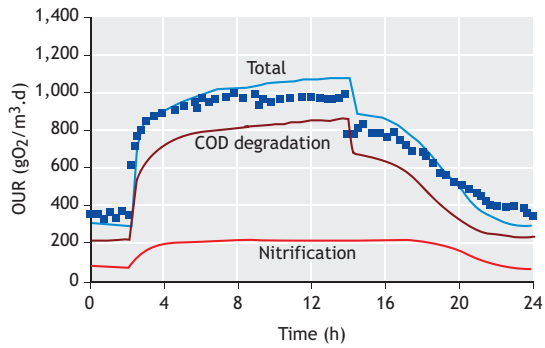

Figure 14.8 Model D: comparison of experimentally observed values (data points) with theoretically predicted total oxygen uptake rate (continuous line). Oxygen uptake for COD degradation and nitrification are separated out (adapted from Ekama and Marais, 1978; Gujer and Henze, 1991).

One should not forget that a model can only be successful if it fulfils the expectations the modeller has of it. If the purpose of the model is to correctly describe general trends, there is no need for further refinements. Of course, fine-tuning and calibration for a more accurate fit are possible, but this increases the model complexity. Here, it was decided not to add extra compounds or processes, as the last part of calibration can be done by straightforward shifting some model parameters. In general, the model simulations showed that the measured line and model line fit rather well: OUR, sludge production and nitrification (data not shown, see Dold *et al.*, 1980; Gujer and Henze, 1991) are predicted correctly. For the pre-defined goal, the model is considered correct,

Table 14.7 Matrix presentation of Model D.

Component	So	S_S	S_{NH}	S_{NO}	X_H	X_S	X_I	X_A	Rate
Growth	-0.5	–1.5	–0.08		+1.0				$\mu_H^{max} \cdot \frac{S_S}{K_S+S_S} \cdot \frac{S_O}{K_{O,H}+S_O} \cdot \frac{S_{NH}}{K_{N,H}+S_{NH}} \cdot X_H$
Lysis					–1.0	+0.92	+0.08		$b_H \cdot X_H$
Hydrolysis		+1.0	+0.08			–1.0			$k_H \cdot \frac{(X_S/X_H)}{K_x+(X_S/X_H)} \cdot X_H$
Autotrophic growth	–18.0		–4.25	+4.17				+1.0	$\mu_A^{max} \cdot \frac{S_O}{K_{O,A}+S_O} \cdot \frac{S_{NH}}{K_{N,A}+S_{NH}} \cdot X_A$
Autotrophic lysis						+0.92	+0.08	–1.0	$b_A \cdot X_A$

but this does not necessarily mean that the assumptions used are correct. Indeed, by using those assumptions, a mathematical description sufficiently appropriate for the purpose of its use is obtained. However, Model D omitted some processes which in reality play an important role, such as protozoa activity (Table 14.7). In this case, it was evaluated that inclusion of protozoa in the model would not increase its descriptive power and consequently this process was not included.

The next step in model development was the inclusion of the denitrification process. There are in general two approaches possible that ultimately lead to the same end results. It can be assumed that there is either a special group of bacteria which perform denitrification or that all heterotrophic microorganisms can denitrify, but at a fraction of their rate under aerobic conditions. In other words, there is either a specialized population which can utilize both oxygen and nitrate, and another part of the population which can only use oxygen, or all heterotrophs can denitrify but at a reduced rate, corrected by the η factor (reduction factor for growth rate under anoxic conditions). These are different assumptions conceptually but mathematically they come down to the same equation. Since the last assumption simplifies the model, it has been chosen to use stoichiometry for denitrification and the bacteria that are ordinary heterotrophic organisms. Although the reality is probably much more complex, it was demonstrated that this simplified approach works satisfactorily in practice.

Another important aspect concerned the differentiation between fractions of inert material and nitrogen which is one of the items that differs from one commercial model to another. As mentioned earlier, inert material can originate from influent or from the degradation of biomass, and the end content of the degraded biomass, inert material, might be different in composition to that of inert material in the influent. This can also be taken into account in the model; the inert material can be either separated or lumped together. In principle, it is not strictly necessary to define these fractions separately, but sometimes this is done based on aesthetic reasons or for the specific purpose of the model application. Similar reasoning applies for nitrogen fractionation. The model development as described by Ekama and Marais (1978) is still considered valid and Model D extended with denitrification becomes close to ASM1 (Henze *et al*., 1987b). For further details on ASM1 the reader is referred to Dold *et al.,* 1980; Van Haandel *et al.,* 1981; Alexander *et al.,* 1983; Warner *et al.,* 1986; Henze *et al.,* 1987a, 1987b, 2000.

One of the most important limitations of ASM is that it does not describe the sludge bulking phenomenon. Therefore, if ASM is used, for example to improve the nitrification process, it is necessary to

check if the proposed changes create bulking sludge. Limited aeration, which is beneficial for nitrogen removal, will almost inevitably induce bulking sludge. Sludge bulking itself cannot be modelled in a way that is sufficiently reliable for implementation in commercial software packages despite some attempts described in the literature (Krebs, 1995). This consequently means that the model cannot be accurately applied to predict very low effluent concentrations when highly efficient processes are implemented. Furthermore, this analogous consideration is valid for the denitrification process as well. On the other hand, even if the model is able to predict the concentration of ammonia at 0.5 mg/l, there are always some inaccuracies and imperfections in the analytical procedures for determining ammonia concentration, as well as in the sampling procedure and sample handling.

Another ASM limitation is that it does not take into account the removal of micropollutants such as metals, xenobiotics or oestrogenic endocrine-disrupting compounds. This is partially due to the required increase in the complexity of the model and partially due to lack of knowledge about the microorganisms and biochemical reactions involved in the conversion of these compounds. In some cases, such as in modelling of the wastewater treatment at oil refineries, it is necessary to predict the phenol reduction. To support denitrification, methanol is often added under anoxic conditions and its conversion needs to be included. There are also cases when, for example, one is interested in sulphite reduction. In all these cases a new specialized organism must be included in the model, as the biomass included in ASM1 does not convert these micropollutants. Examples of such extensions can be found in the literature, and nowadays some commercial software packages include for example methanol utilization. In the case of other COD compounds such as volatile fatty acids (VFAs), the ordinary organisms which remove COD from the wastewater will convert them and therefore the model does not have to be extended for this purpose. Beyond the ASM1 level, the model can be extended to take into account oxygen transfer, pH and alkalinity, anaerobic digestion, chemical phosphorus removal and precipitation, additional units (such as settlers etc), side-stream processes, the gas phase etc. Again, whether the model needs to be extended depends on the purpose of the model.

14.5 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 1980s, several research groups worked independently of each other on developing models for activated sludge. Each group developed and applied their own approach and notation, first in steady-state models, and later on, in dynamic models. Table 14.8 summarizes the essential features of these and several other activated sludge models.

In the early 1980s, Poul Harremoës, President of IAWPRC (the International Association of Water Pollution, Research and Control, which later became IAWQ, the International Association of Water Quality, and which is nowadays the IWA, the International Water Association) initiated the idea of combining the most relevant and applied models and working 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),

Table 14.8 Overview of selected activated sludge models (based on 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 *et al*., 1980, 1991
ASM1	●	●	DR, Cst	EA						8	13	Henze *et al*., 1987b
ASM3	●	●	ER, EA	Cst						12	13	Gujer *et al*., 1999
UCTPHO	●	●	DR, Cst	EA	●		Cst	●		19	19	Wentzel *et al.*, 1988, 1989a,b
ASM2	●	●	DR, Cst	EA	●		Cst	●	●	19	19	Henze *et al*., 1995
ASM2d	●	●	DR, Cst	EA	●	●	Cst	●	●	21	19	Henze *et al*., 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 *et al*., 2001

DR, death regeneration concept; EA, electron acceptor dependent ER, endogenous respiration concept; Cst, not electron acceptor dependent

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). 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, 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 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 a 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. 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 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 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 the state variables involved in a process are displayed in columns, and all the 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. This facilitated its publication, interpretation and comparison not only between models, but also between processes and compounds. However, 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), and 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 (Comeau *et al.*, 1986; 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).

In recent years several research groups have started to work on the description of EBPR for its incorporation in dynamic activated sludge models, 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 Takashi Mino (Tokyo University) and Mark Wentzel (University of Cape Town) joined. The knowledge acquired on EBPR led to the publication of 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 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 in that they assume the cell to be a black box, as opposed to using the metabolic approach to modelling the processes that take place inside the cell. However, ASM2d appeared to be overparameterized with respect to the available data, requiring a more systematic approach for calibration (Brun *et al*., 2002). Although this allowed the model to adapt and describe 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 internal cell 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 with 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 the 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; both a rapid and a slow degradation of substrate associated with OUR can be observed (Henze*,* 1992; Henze *et al.,* 2008).

In ASM1 it appears as if two substrates are present (S_S and X_S) while in the 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 so successful for simulation of wastewater treatment plants that 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. This 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 14.9). 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.

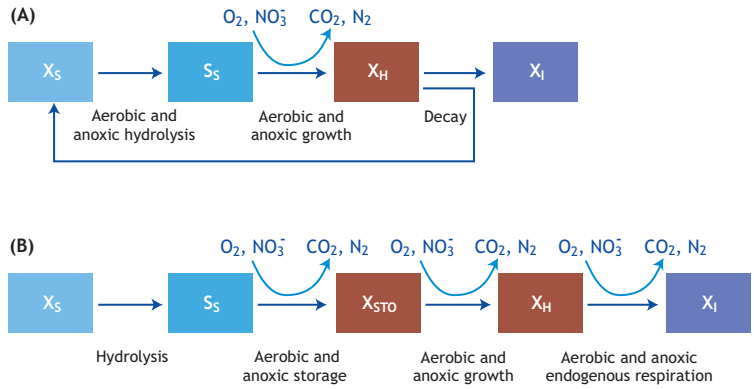

Figure 14.9 Degradation of COD in (A) ASM1 and (B) ASM3.

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 then 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 therefore the 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*) simulating 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 an 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 14.10.

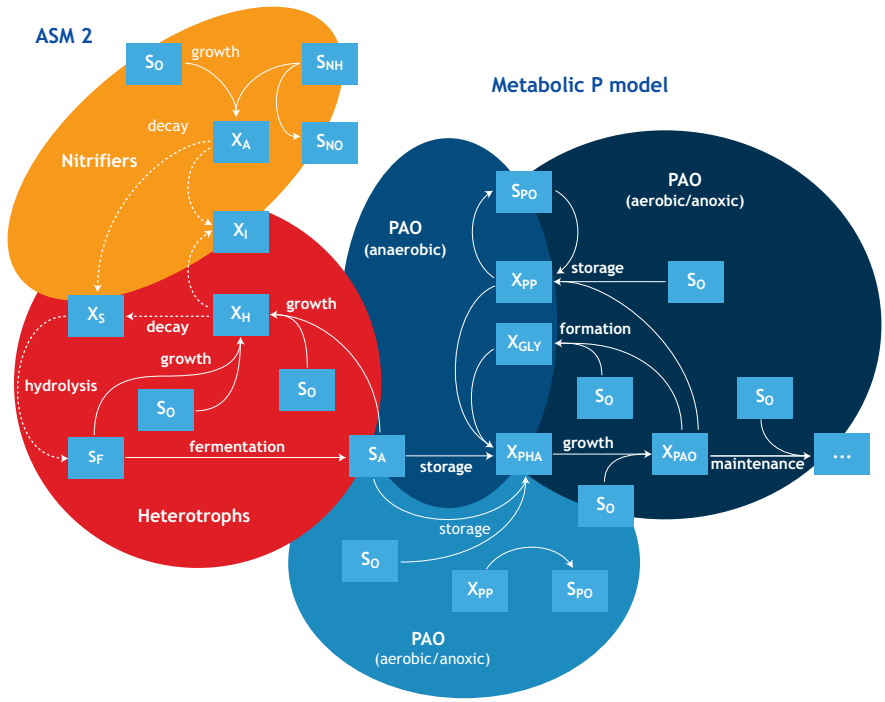

Figure 14.10 Interactions in the integrated ASM2-TUDP model (Meijer, 2004).

The left side of Figure 14.10 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_2 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 internal cell 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 in 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 the substrate uptake rate or oxygen utilization rate, are not important.

Thus the black box approach can be used, as is also 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 which is used further for biomass growth, glycogen formation and creation of the energy required for these processes, and for 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 the 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 simplest metabolic model kinetics were chosen. 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 which lead 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 the 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 the 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*)*. This study showed that the TUDP model was capable of describing full-scale conditions without any 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 in 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 14.11 shows how the different model structures interact.

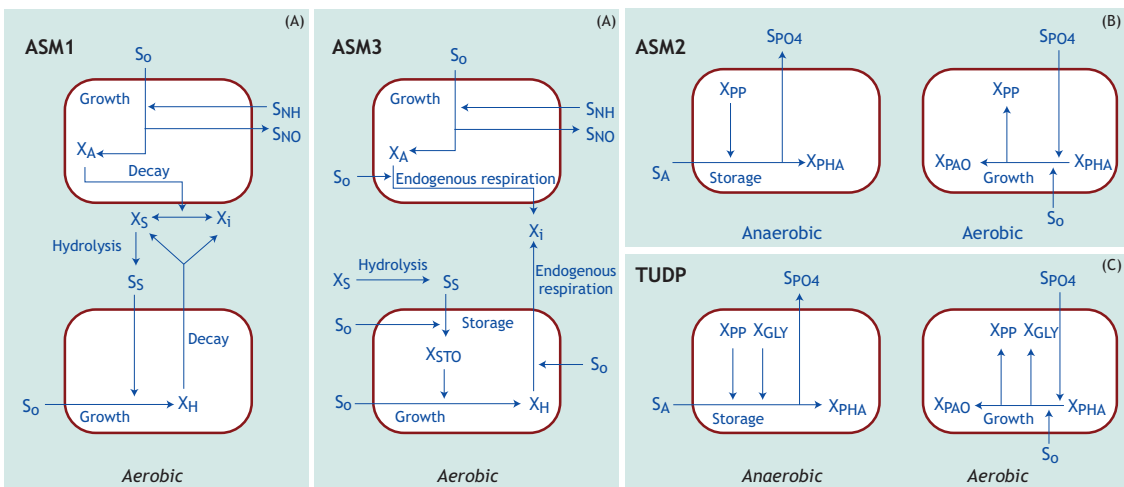

Figure 14.11 Simplified schemes of substrate flows for (A) autotrophic and heterotrophic biomass in the ASM1 and ASM3 models (modified from Gujer *et al.*, 1999), (B) storage and growth of PAO in the ASM2 model (Henze *et al.*, 1995), and (C) storage and aerobic growth of PAO in the TUDP model (Van Veldhuizen *et al.*, 1999; Brdjanovic *et al.*, 2000). Adapted from Gernaey *et al.* (2004).

Although 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.

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 of this, 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 being 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 metabolic modelling by 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). However, these improvements were not incorporated in the TUDP model.

14.6 THE ASM TOOLBOX

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 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 the application of mathematical models, 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, SUMO, 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 chapter). 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 it easier for practitioners to use 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 around the world over the last few years. 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 Activated Sludge Models, parallel to and with the full support of the original 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. 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, 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 the TUDP model. The study also revealed that models are sometimes not properly applied, which might be due to a lack of knowledge and to standardised procedures. The development and improvement of standardised modelling procedures and better knowledge transfer by making available some practical case studies were mentioned as key instruments to addressing certain obstacles such as 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 also organised, such as wastewater treatment modelling seminars. 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 recommend 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 GMP-TG website, adjusted 'Gujer matrices' for seven published models can be downloaded as an MS Excel spreadsheet: (*i*) ASM1 (Henze *et al*., 1987a,b, 2000); (*ii*) ASM2d (Henze *et*

al., 1999); (*iii*) ASM3 (Gujer *et al.,* 1999); (*iv*) ASM3+BioP (Rieger *et al.,* 2001); (*v*) ASM2d+TUD (Meijer, 2004); (*vi*) the Barker & Dold model (Barker and Dold, 1997); and (*vii*) UCTPHO+ (Hu *et al.,* 2007). On 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.

More recently, among other initiatives to improve knowledge transfer by facilitating and making available some practical case studies (Hauduc *et al.,* 2009), IHE Delft 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 IHE Delft [1] in cooperation with Delft University of Technology. 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. Furthermore it includes 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 the design and assessment of secondary settlers 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. In addition, another recent publication describes the selection of fifteen municipal and industrial activated sludge model applications carried out over the 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 (Bentancur, 2014). This demonstrates that efforts are also being undertaken in developing countries to apply the models to existing activated sludge systems (mostly for optimization or upgrade).

Overall, mathematical modelling is becoming a standardized and mature practice, mostly in developed countries, and the efforts made by the IWA GMP-TG and the publication of diverse modelling guidelines (*e.g.* Rieger *et al.*, 2012; Meijer and Brdjanovic, 2012; Brdjanovic *et al.,* 2015) will ultimately contribute to increasing their reliability and application.

14.7 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 current and novel nutrient removal processes, not only for the sake of the removal of nutrients but also to reduce the associated energy costs and the environmental impact of wastewater treatment plants.

[1] www.un-ihe.org/modelling-wastewater-treatment-processes-and-plants

Such efforts, in combination with the recovery of resources (not only of the nutrients themselves but also of other valuable products) will contribute to moving forward from conventional treatment concepts towards achieving the goals outlined for Water and Resource Recovery Facilities (WRRF), wastewater treatment plants as energy factories, and biorefineries (Kartal *et al.*, 2010; Van Loosdrecht and Brdjanovic, 2014; Energiefabriek, 2015).

With regard to new developments, although the EBPR process can reach relatively high phosphorus removal efficiency rates (with effluent phosphorus concentrations lower than 1 mg/l), it tends to experience process upsets and deterioration due to factors not yet completely understood (Oehmen *et al*., 2007). In this regard, the appearance of Glycogen Accumulating Organisms (GAO), such as *Competibacter* and *Defluviicoccus*, has been tentatively 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 biological nutrient removal (BNR) systems. This suggested 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 to 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 lab-scale anaerobic-anoxic-aerobic sequencing batch reactor (SBR) data. However, the application to full-scale conditions of the metabolic model developed by Oehmen *et al.* (2010) is not that straightforward (*e.g.* due to the absence of organic matter and nitrogen oxidation processes as well as practical limitations concerning the elemental balances). Recently, SUMO, a model developed by Dynamita [2] has not only incorporated an extended PAO-GAO module to take into account the interactions between these organisms but also a relatively new type of PAO with fermentative capabilities (arguably *Tetrasphera*, Liu *et al.*, 2019). This 'new type of PAO' appears to be active in side-stream EBPR systems (S2EBPR) and therefore proliferates in these systems, as suggested by practical observations (Dunlap *et al.*, 2016; Barnard *et al.,* 2017; Varga *et al.,* 2018). Following this conceptual model, in addition to the 'conventional PAO' (active in the main-stream line) a second group of PAO, a 'side-stream PAO', has been incorporated into the EBPR models. As such, in the newly added EBPR SUMO module, the 'side-stream PAO' becomes active and is able to take up VFA when the oxido-reduction potential in the side-stream line (calculated in terms of the concentrations of oxygen, nitrate, and sulphate in the liquid phase) decreases to below -200 mV. Despite this, although such a modelling approach would likely require further improvements, mostly because the actual biological mechanisms and the dominant microorganisms involved are not completely known (Onnis-Hayden *et al*., 2019; Liu *et al.,* 2019), it has so far satisfactorily described the biological P-removal activity observed in S2EBPR systems. Overall, such integrated models

[2] www.dynamita.com

seem to be useful to describe the relevant EBPR microbial activities and the 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^{++} concentrations, it may be necessary to add biologically induced P precipitation to ASM models (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 phosphate, 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). Furthermore, Flores-Alsina *et al.* (2015) developed a plant-wide aqueous phase chemistry module able to describe the pH variations in activated sludge systems. Mbamba *et al.* (2016) further studied and applied the model developed by Flores-Alsina *et al.* (2015) to describe the precipitation of minerals with specific emphasis on P precipitates. Furthermore, with an increasing interest in improving the P-removal process in existing activated sludge plants through the implementation of chemical P removal, Mbamba *et al.* (2019) modelled the iron (Fe) addition. The authors successfully described the chemical P-removal process in a pilot plant. Most commercial simulators have already incorporated similar functionalities (like BioWin, SUMO and GPS-X) but future research and developments will likely focus on the implementation of such models in full-scale plant-wide systems with particular interest in P recovery.

Regarding the implementation of innovative wastewater treatment technologies, a stronger focus can be expected on modelling the bioprocesses involved and related to the implementation of the anammox process in the mainstream treatment line and on aerobic granular sludge technology (De Kreuk *et al.,* 2007; Kartal *et al.,* 2010; Wett *et al.,* 2013; Lackner *et al.,* 2014). In the case of the anammox process and aerobic granular sludge technologies, one of the first challenges to overcome is to satisfactorily describe the 2-step nitrification process (the ammonium and nitrite oxidation activities, respectively) as well as their strong interaction with the anammox and EBPR-related organisms (Dapena-Mora *et al.,* 2004; Wyffels *et al.,* 2004). As such, for both mainstream anammox and aerobic granular sludge modelling applications, it becomes rather important to describe the substrate, product reactions and conversions considering the redox gradients within the corresponding flocs or granules and the populations involved, taking into account their symbiosis and/or competition. In this regard, factors such as diffusion (which depends on floc properties and these ones on shear conditions, cohesion, expolymeric substances and turbulence intensity, Arnaldos *et al.,* 2015; Regmi *et al.,* 2019) play an important role in particular in describing the simultaneous nitrification-deamonification process observed in anammox-driven and simultaneous nitrification-denitrification P removal in aerobic granular sludge systems (Kagawa *et al.,* 2015; Baeten *et al.,* 2018a, 2018b). Apparent half-saturation coefficients (that lump the reaction-diffusion processes inside dense flocs or granules) when applying ASM models instead of biofilm models have proven successful in describing the macro-scale activity (*e.g.* predicting effluent concentrations) but mostly under rather stable population dynamics (Baeten *et al.,* 2018a). Therefore, it will be useful when defining the operational ranges to use either a lumped approach (Arnaldos *et al*., 2015; Baeten *et al.*, 2018a) or a biofilm-based model (Picioreanu *et al.*, 2004; Kagawa *et al.,* 2015). This choice depends considerably on the modelling goal ranging from understanding the micro- and macro-scale phenomena and reactor operation to process optimization and design of microbial activities (Baeten *et al.,* 2018b). However, the choice made will determine whether to use a less or more complex model. So far, existing modelling simulators, such as BioWin and SUMO, have specific modules and extensions to describe the applications of anammox-based and aerobic granular sludge technologies, but still further research needs to

focus on the goal definition and consequently on the definition of the level of model complexity.

The application of the sulphur conversion in wastewater treatment will likely continue to be a viable option for the treatment of sulphate-rich waters generated by industry, saline water intrusion, and even the use of seawater for sanitation to alleviate water scarcity (Hvitved-Jacobsen *et al.,* 1998; Huisman and Gujer, 2002; Wang *et al.,* 2009; Hao *et al.*, 2014; Cui *et al.*, 2019).

Undoubtedly, mathematical modelling can be a useful tool to get a better understanding of the factors affecting these processes and facilitate their implementation. However, the application of sulphate or sulphur conversion models in municipal wastewater treatment systems is limited to only a few studies despite the fact that several wastewater treatment plants may be exposed to relatively high influent sulphate concentrations due to saline water intrusion or the use of alternative water sources (Lu *et al.*, 2009), particularly in regions with a warm climate (Sharma *et al.,* 2008; Choubert *et al.,* 2012). Moreover, the potential positive or negative influence of sulphur-driven processes on municipal wastewater treatment systems (Rubio-Rincon *et al.,* 2017; Cui *et al.,* 2019) increases the need to further develop sulphate and/or sulphur models. On the other hand, most of the commercial software simulators (*e.g.* BioWin, GPS-X or SUMO) have suitable additional simulation modules to describe sulphur conversions but only for industrial applications (*e.g.* usually sulphate-rich effluents from petrochemical industries) and are therefore limited to specific applications beyond the industrial sector. The need to describe and assess the corrosion of concrete structures, process upsets or process improvements as well as changes in dominant microbial populations caused by the presence of relatively high influent sulphate concentrations will likely expand the application of sulphur and sulphate-related models to the municipal sector.

In addition to the aforementioned developments, the application of new technologies, such as anammox, sulphur-related processes and aerobic granular sludge, may imply the need to incorporate more complex biokinetic models (Nielsen *et al.,* 2010; Oehmen *et al.*, 2010), elemental balance approaches (Takács *et al.*, 2007; Lu *et al.*, 2009), and is likely also to establish stronger links with genomics, molecular techniques and metabolome analyses (Fiehn, 2001) as well as to develop the required experimental methods in order to determine and understand the microbial activities involved (Van Loosdrecht *et al.,* 2015).

The incorporation of new processes (*e.g.* anammox, aerobic granular sludge and sulphur conversions) will likely follow the IWA GMP-TG concepts (Rieger *et al.*, 2012). The increased complexity of these combined biological processes requires the development of effective process controls in which application of dynamic ASMs could become crucial for successful full-scale application (Regmi *et al.,* 2019).

Modelling of nitrous oxide emissions in nutrient removal plants (Ni *et al.,* 2013; Nopens *et al.*, 2014) is another emerging topic. In this regard, the IWA Task Group on Greenhouse Gas (GHG) is playing a major role in the design and operation of environmentally-friendly wastewater treatment systems. Robust and relevant developments in mathematical modelling have been made to describe N_2O and CH_4 emmissions (Flores-Alsina *et al.,* 2011; Corominas *et al.*, 2012; Mampaey *et al.,* 2019). Such advances have led to the assessment of specific parameters to reduce GHG emissions and also to evaluate the performance of wastewater treatment plants (Flores-Alsina *et al.,* 2014a). Undoubtedly, further modelling efforts will continue to focus on the assessment of the biological mechanisms and operational conditions that lead to GHG emissions and the development of minimization strategies linked to process control and automation (Regmi *et al.,* 2019).

As a consequence of the interaction between the existing but also for the implementation of new technologies, plant-wide modelling will pay special attention to: (*i*) developing an optimal plant control strategy, (*ii*) increasing the efficiency of the removal

processes, (*iii*) reducing the operating costs, (*iv*) maximizing energy recovery through biogas production, and (*v*) maximizing 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 particular attention (Nopens *et al*., 2014; Vanrolleghem *et al.,* 2014). This is mostly because a PST can contribute to maximizing the recovery of energy via the anaerobic digestion of organics and favouring the conversion of existing plants from 'removal-type systems' towards 'resource-recovery systems' and 'energy factories' (Kartal *et al.,* 2010; Van Loosdrecht and Brdjanovic, 2014; Energiefabriek, 2015). Until a few years ago, most PST separation processes were still modelled as black boxes with lumped and gross removal coefficients assigned to all the particulate organics, whereas unbiodegradable particulate organics have been shown to be subject to higher removal efficiencies than the biodegradable organics (Ikumi *et al*., 2014a,b). Bachis *et al.* (2015) developed a model for a PST based on the settling velocity distributions determined by Maruejouls *et al.* (2012) observing that the removal process that takes place in PST affects the (settled) wastewater characteristics as well as the generation and quality of the settled sludge (which is usually anaerobically digested for biogas generation). In addition to PST modelling, Torfs *et al.* (2016) proposed a unified model framework described with a set of partial differential equations (PDEs) to model the settling processes that occur in PST and secondary settling tanks (SST). This set of equations is able to describe the discrete settling process that takes place in PST as well as the compression settling observed in SST. This proposal was further amended by Bürger *et al.* (2017) who suggested a numerical solution to increase the versatility of the unified settling theory. These advances are contributing to tackling the long-standing limitations of PST and SST which have been neglected up to now but are relatively important in achieving the ultimate goals of the WRRF.

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 the SST (Bürger *et al.,* 2011, 2012; Torfs *et al.,* 2013). Models for clarifiers use total suspended solids as a state variable, which is not explicitly used in ASM models and needs 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. Some examples of the need to have a satisfactory modelling description of the operation of SST are 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. Some of these processes can 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. Nevertheless, to apply plant-wide modelling the biggest challenges can be found when coupling ASM models with anaerobic digestion models (such as ADM1) (Batstone *et al*., 2002). These 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: (*i*) 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.* BioWin, SUMO or GPS-X simulators, and (*ii*) 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; Solon *et al.,* 2017). Overall, these previous approaches can satisfactorily help to apply a plant-wide model. Recently, plant-wide models have also been developed to describe the P transformations throughout the whole plant including the anaerobic digestion fate of EBPR sludge (highly rich in phosphorus and intracellular compounds) by including the required processes in ADM1 (Ikumi *et al.*, 2014a,b; Ikumi and Ekama, 2019) and the development of a new set of biological (activated sludge, anaerobic digestion), physical-chemical (aqueous phase, precipitation, mass transfer) process models and model interfaces (between water and sludge line) to describe the required tri-phasic (gas, liquid, solid) compound transformations and the close interlinks between the P and the sulphur (S) and iron (Fe) cycles (Flores-Alsina *et al.,* 2016; Mbamba *et al.*, 2016; Solon *et al.,* 2017). These models have contributed not only to expanding the ASM models but also ADM1 (Batstone *et al.,* 2012), including relevant processes to assess the anaerobic digestion of EBPR sludge, chemical precipitation of P compounds, gas composition (involving S-related compounds) and mineral precipitation. In this regard, the IWA Task group on the development of a generalized physical-chemical framework (Batstone *et al.,* 2012) contributed to this achievement. Although the fundamentals of the physical-chemical reactions are well understood, are available from other disciplines, and do not need calibration (since thermodynamics define the end points of the kinetic processes), further research is needed to validate the fate of the organic compounds driving the bioprocesses and the thermodynamics of the precipitation rates in full-scale systems. These plant-wide modelling aspects require additional 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), this can contribute to reaching the objectives of the WRRF.

Computational fluid dynamics (CFD) can potentially help to improve the description and operation of practically all the process units of wastewater treatment plants (from primary to secondary settling tanks including the aeration and biological processes, Plósz *et al.*, 2012; Laurent *et al.*, 2014; Nopens *et al.*, 2014; Wicklein *et al.,* 2015; Karpinska and Bridgeman, 2016; Samstag *et al.,* 2016). By studying the influence of diffusion limitations and gradients through CFD, the interactions between bacterial morphology, bacterial competition and their physical and hydrodynamic interactions can be better understood and therefore lead to better operation and control practices. However, despite the added complexity, reliable experimental methods and set-ups are being developed to support model development and increase their reliability and application. So far, by coupling CFD with bio-kinetic and chemical models, this has led to a better description of the residence time distribution and cross-flow gas-liquid interactions (Le Moullec *et al.*, 2008), improved mixing and aeration as well as better assessments of the biological reactions in process reactors (Le Moullec *et al.*, 2010; Meister and Rauch, 2016; Rehman *et al.,* 2017) and even to the study of N_2O emissions (Bellandi *et al.,* 2019) and to the improved description of nutrient recovery via struvite formation (Rahaman and Mavinic, 2009). Besides the potential energy savings that hydroinformatics tools (such as CFD) can bring (Rieger *et al.*, 2012), with the increasing need and interest in water reuse and integrated modelling, the biological and physical-chemical removal processes of micropollutants will be another modelling area of future 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). It is likely that, due to its rather practical approach, further efforts will continue hand-to-hand with stronger collaborative links between practice and research to assess and provide feedback on newly developed models under real-case scenarios. A clear and promising example of such development is the establishment of the AM Team (Advanced Modelling

for Process Optimization [3]), a spin-off of Gent University for CFD-based wastewater treatment modelling. This close collaboration between academia and practice has contributed to the application of CFD to improve effluent quality, reduce energy consumption, and increase the capacity and reliability of wastewater treatment and resource recovery. Probably other specialist CFD companies will emerge in the coming years. To support the application of CFD models in a structured and reliable manner, IWA has helped to establish the Working Group on CFD for Unit Processes[4] with the main aim of developing and establishing modelling guidelines for the application of CFD models in wastewater treatment. Towards this goal, Nopens *et al.* (2012), Laurent *et al.* (2014) and Wicklein *et al.* (2015) have proposed structured guidelines and protocols towards the development of good modelling practices when applying CFD in wastewater treatment plants. There is no doubt that CFD modelling will be further developed and expanded, yet its use and application needs to be well-defined by first answering what the goal of modelling is and consequently selecting an appropriate modelling approach, *e.g.* a CFD-based model or a (simpler) ASM model.

A growing interest in integrated (urban) water modelling will continue to motivate the 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 and simulators (*e.g.* SUMO) are starting 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 (a combined sewage network, plants and the recipient/river) using different models (combining Mike Urban, BioWin and HEC-RAS), although carried out in a sequential mode (as opposed to a better and more realistic but much more complex real-time approach), showed great advantages with this type of modelling application (Hodzic *et al.,* 2011, Price and Vojinovic, 2010). At the moment a large holistic modelling study is being carried out in Croatia (Brdjanovic, personal communication) which combines a large sewer system, four wastewater treatment plants and seawater quality modelling along a shoreline of 23 km[5].

Such an integrated approach 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 micropollutants). In collaboration with the University of Cape Town, WEST, 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 could lead to promising opportunities for the development of an integrated urban water model suitable for and capable of describing and optimizing the entire urban water system, including receiving waters (Benedetti *et al.*, 2013b).

However, one should not overlook the fact that despite these significant advances and the development of more (complex and) complete mathematical models, a common issue is still 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,

[3] www.am-team.com

[4] www.iwa-connect.org/group/working-group-on-computational-fluid-dynamics-cfd-for-unit-processes/about

[5] http://odvodnjaporec.hr/projekti/projekt-porec/

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 such as 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*., 2014b; Nopens *et al.*, 2014).

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 to sewer systems, and that only a small fraction of sewage in developing countries is treated, this raises 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 entirely covered by sewerage. There are several examples of this worldwide, especially in developing countries. Recent advances in this direction include the development of an excreta flow diagram (also often described as a shit flow diagram, SFD[6]) which is a tool to help understanding and communicate the management of excreta in a city or town. Another novelty is a decentralized sanitation concept and its model which considers all the major components of the sanitation service chain (Brdjanovic *et al.,* 2015). This non-sewered sanitation decision support tool has been incorporated in a decision support tool called WaMEX by IHE Delft which also includes sewerage (Abbot and Vojinovic, 2009; Sanchez *et al*., 2013; Vojinovic *et al*., 2014), and sewage treatment components (Von Sperling and Chernicharo, 2005).

Another interesting modelling aspect is modelling of the influence of faecal and septic sludge discharge (load) to sewage treatment plants, a practice regularly applied in many (especially low and middle income) countries (Strande *et al.,* 2014). More interesting faecal sludge management modelling tools are to be found in the Faecal Sludge Management (FSM) Toolbox[7]; however, FSM modelling falls outside the scope of this book and for more information the reader is referred to Strande *et al.,* 2014 and Velkushanova *et al.,* 2020.

Further, cloud computing has gained in interest lately (Armbrust *et al.,* 2010) by joining efforts and contributing to standardized approaches and notation (Corominas *et al.*, 2010), and therefore sharing wastewater treatment models between researchers, software developers, and practitioners, despite them being in different longitudes and latitudes, may not be far from reality. This could be a powerful tool to facilitate the application of plant-wide and integrated urban water modelling to contribute to optimizing 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. Therefore, vendors with specific modelling skills might 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 modelling specialists.

It is not impossible to imagine that sooner or later new interfaces and methods of interaction between (very probably less specialized) users and models will be created. These could be in the form of multi-layer serious gaming and use 3D urban water system simulators with simplified 'surface' user interfaces and more complex expert models running 'invisibly'

[6] www.sfd.susana.org

[7] www.fsmtoolbox.com/

in the background. Another expected future development is the use of models built in the data acquisition systems (SCADA) of larger wastewater treatment facilities; thereby the complex knowledge contained in ASMs would be made available to process operators, making more efficient and safe plant operation possible on a daily basis. It is also expected that modelling boundaries will be further extended reaching a 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 the decision makers and increase and facilitate the use of models by different and currently not involved stakeholders. Last but not least, despite all these expected developments (Van Loosdrecht and Brdjanovic, 2014) and the release of more complex models for several wastewater treatment applications, 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 for an educational programme or design criterion, but rather as a complement.

14.8 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 30 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 the 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 that this chapter will be useful to inspire future engineers to use models as central tools in their work on improving wastewater treatment technology through innovation and optimization.

Table 14.9 A stoichiometric matrix and a component composition matrix (Meijer, 2004).

				1	2	3	4	5	6
			Component →	S_O	S_F	S_A	S_{NH}	S_{NO}	S_{N2}
↓ Process				gO_2/m^3	$gCOD/m^3$	$gCOD/m^3$	gN/m^3	gN/m^3	gN/m^3
1	r_h^O	Aerobic hydrolysis	$gCOD_{XS}/d$		$1-f_{SI}$		$c_{N,1}$		
2	r_h^{NO}	Anoxic hydrolysis	$gCOD_{XS}/d$		$1-f_{SI}$		$c_{N,1}$		
3	r_h^{AO}	Anaerobic hydrolysis	$gCOD_{XS}/d$		$1-f_{SI}$		$c_{N,1}$		
Regular heterotrophic organisms X_H									
4	r_{SF}^O	Aerobic growth on S_F	$gCOD_{XH}/d$	$-(1/Y_H-1)$	$-1/Y_H$		$c_{N,4}$		
5	r_{SA}^O	Aerobic growth on S_A	$gCOD_{XH}/d$	$-(1/Y_H-1)$		$-1/Y_H$	$c_{N,5}$		
6	r_{SF}^{NO}	Anoxic growth on S_F	$gCOD_{XH}/d$		$-1/Y_H$		$c_{N,6}$	$-\frac{(1/Y_H-1)}{2.86}$	$\frac{(1/Y_H-1)}{2.86}$
7	r_{SA}^{NO}	Anoxic growth on S_A	$gCOD_{XH}/d$			$-1/Y_H$	$c_{N,7}$	$-\frac{(1/Y_H-1)}{2.86}$	$\frac{(1/Y_H-1)}{2.86}$
8	r_{fe}^{AN}	Fermentation	$gCOD_{SF}/d$		-1	1	$c_{N,8}$		
9	r_{HL}	Heterotrophic lysis	$gCOD_{XH}/d$				$c_{N,9}$		
Phosphorus-accumulating organisms X_{PAO}									
10	r_{SA}^{AN}	Anaerobic storage of S_A	$gCOD_{SA}/d$			-1			
11	r_M^{AN}	Anaerobic maintenance	gP/d						
12	r_{SA}^{NO}	Anoxic storage of S_A	$gCOD_{SA}/d$			-1		$-\frac{(1-Y_{SA}^{NO})}{2.86}$	$\frac{(1-Y_{SA}^{NO})}{2.86}$
13	r_{PHA}^{NO}	Anoxic PHA consumption	$gCOD_{PHA}/d$				$c_{N,13}$	$-\frac{(1-1/Y_{PHA}^{NO})}{2.86}$	$\frac{(1-1/Y_{PHA}^{NO})}{2.86}$
14	r_{PP}^{NO}	Anoxic storage of polyP	gP/d				$c_{N,14}$	$-\frac{(1/Y_{PP}^{NO})}{2.86}$	$\frac{(1/Y_{PP}^{NO})}{2.86}$
15	r_{GLY}^{NO}	Anoxic glycogen formation	$gCOD_{GLY}/d$				$c_{N,15}$	$-\frac{(1/Y_{GLY}^{NO}-1)}{2.86}$	$\frac{(1/Y_{GLY}^{NO}-1)}{2.86}$
16	r_M^{NO}	Anoxic maintenance	$gCOD_{PAO}/d$				$c_{N,16}$	$-1/2.86$	$1/2.86$
17	r_{PHA}^O	Aerobic PHA consumption	$gCOD_{PHA}/d$	$1/Y_{PHA}^O-1$			$c_{N,17}$		
18	r_{PP}^O	Aerobic storage of polyP	gP/d	$-1/Y_{PP}^O$			$c_{N,18}$		
19	r_{GLY}^O	Aerobic glycogen formation	$gCOD_{GLY}/d$	$1-1/Y_{GLY}^O$			$c_{N,19}$		
20	r_M^O	Aerobic maintenance	$gCOD_{PAO}/d$	-1			$c_{N,20}$		
Autotrophic nitrifying organisms X_A									
21	r_A^O	Autotrophic growth	$gCOD_{XA}/d$	$1-4.57/Y_A$			$c_{N,21}$	$1/Y_A$	
22	r_{AL}	Autotrophic lysis	$gCOD_{XA}/d$				$c_{N,22}$		

			1	2	3	4	5	6
		Component →	S_O	S_F	S_A	S_{NH}	S_{NO}	S_{N2}
↓ Composition			gO_2	gCOD	gCOD	gN	gN	gN
1	COD	gCOD	-1	1	1		-2.86	…
2	TOC/COD	gC/gCOD		…	0.4			
3	Nitrogen	gN		$i_{N,SF}$	$i_{N,SA}$	1	1	1
4	Phosphorus	gP		$i_{P,SF}$	$i_{P,SA}$			
5	Ionic charge	mole			-1/64	+1/14	-1/14	
6	TSS	g						

Table 14.9 ... continued (for definition of the symbols see Meijer (2004)).

7	8	9	10	11	12	13	14	15	16	17	18
S_{PO}	S_I	S_{HCO}	X_I	X_S	X_H	X_{PAO}	X_{PP}	X_{PHA}	X_{GLY}	X_A	X_{TSS}
gP/m^3	$gCOD/m^3$	$mole/m^3$	$gCOD/m^3$	$gCOD/m^3$	$gCOD/m^3$	$gCOD/m^3$	gP/m^3	$gCOD/m^3$	$gCOD/m^3$	$gCOD/m^3$	g/m^3
$c_{P,1}$	f_{SI}	$c_{e,1}$		-1							$c_{TSS,1}$
$c_{P,1}$	f_{SI}	$c_{e,1}$		-1							$c_{TSS,1}$
$c_{P,1}$	f_{SI}	$c_{e,1}$		-1							$c_{TSS,1}$
$c_{P,4}$		$c_{e,4}$			1						$c_{TSS,4}$
$c_{P,5}$		$c_{e,5}$			1						$c_{TSS,5}$
$c_{P,6}$		$c_{e,6}$			1						$c_{TSS,6}$
$c_{P,7}$		$c_{e,7}$			1						$c_{TSS,7}$
$c_{P,8}$		$c_{e,8}$									$c_{TSS,8}$
$c_{P,9}$		$c_{e,9}$	$f_{XI,H}$	$1- f_{XI,H}$	-1						$c_{TSS,9}$
Y_{PO}^{AN}		$c_{e,10}$					$-Y_{PO}^{AN}$	Y_{SA}^{AN}	$1-Y_{SA}^{AN}$		$c_{TSS,10}$
1		$c_{e,11}$					-1				$c_{TSS,11}$
Y_{PO}^{NO}		$c_{e,12}$					$-Y_{PO}^{NO}$	Y_{SA}^{NO}			$c_{TSS,12}$
$c_{P,13}$		$c_{e,13}$				$1/Y_{PHA}^{NO}$		-1			$c_{TSS,13}$
$c_{P,14}$		$c_{e,14}$				$-1/Y_{PP}^{NO}$	1				$c_{TSS,14}$
$c_{P,15}$		$c_{e,15}$				$-1/Y_{GLY}^{NO}$			1		$c_{TSS,15}$
$c_{P,16}$		$c_{e,16}$				-1					$c_{TSS,16}$
$c_{P,17}$		$c_{e,17}$				$1/Y_{PHA}^{O}$		-1			$c_{TSS,17}$
$c_{P,18}$		$c_{e,18}$				$-1/Y_{PP}^{O}$	1				$c_{TSS,18}$
$c_{P,19}$		$c_{e,19}$				$-1/Y_{GLY}^{O}$			1		$c_{TSS,19}$
$c_{P,20}$		$c_{e,20}$				-1					$c_{TSS,20}$
$c_{P,21}$		$c_{e,21}$								1	$c_{TSS,21}$
$c_{P,22}$		$c_{e,22}$	$f_{XI,A}$	$1- f_{XI,A}$						-1	$c_{TSS,22}$
7	8	9	10	11	12	13	14	15	16	17	18
S_{PO}	S_I	S_{HCO}	X_I	X_S	X_H	X_{PAO}	X_{PP}	X_{PHA}	X_{GLY}	X_A	X_{TSS}
gP	gCOD	mole	gCOD	gCOD	gCOD	gCOD	gP	gCOD	gCOD	gCOD	g
	1		1	1	1	1		1	1	1	
	…		…	…	…	0.334 (α)		0.334	0.375	…	
	$i_{N,SI}$		$i_{N,XI}$	$i_{N,XS}$	$i_{N,XH}$	$i_{N,BM}$				$i_{N,BM}$	
1	$i_{P,SI}$		$i_{P,XI}$	$i_{P,XS}$	$i_{P,XH}$	$i_{P,BM}$	1			$i_{P,BM}$	
-1.5/31		-1					-1/31				
			$i_{TSS,XI}$	$i_{TSS,XS}$	$i_{TSS,BM}$	$i_{TSS,BM}$	$i_{TSS,PP}$	$i_{TSS,PHA}$	$i_{TSS,GLY}$	$i_{TSS,BM}$	1

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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
- Task Group on Good Modelling Practices (GMP) - Guidelines for use of activated sludge models: http://www.iwa-network.org/task/good-modelling-practice-gmp-guidelines-for-use-of-activated-sludge-models
- 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 Physicochemical Framework (GPCF): http://www.iwa-network.org/task/generalized-physicochemical-framework

References for software simulators (websites)

- AQUASIM: http://www.eawag.ch/en/department/siam/software
- ASIM: http://www.asim.eawag.ch/
- BioWin: https://envirosim.com/getbw
- GPS-X: http://www.hydromantis.com/GPS-X.html
- HEC-CRAS: http://www.hec.usace.army.mil/software/hec-ras/
- Mike Urban: http://www.mikebydhi.com/products/mike-urban
- STOAT: http://www.wrcplc.co.uk/software-development
- SUMO: http://www.dynamita.com/
- WEST: http://www.mikebydhi.com/products/

NOMENCLATURE

Symbol[1)]	Symbol[2)]	Description	Unit
A	A	Surface area	m^2
b_A	b_{ANO}	Specific rate of endogenous mass loss of nitrifying organisms	1/d
b_H	b_{OHO}	Specific rate of endogenous mass loss of ordinary heterotrophic organisms (OHOs)	1/d
F/M	F/M	Food to microorganism ratio or load factor (LF)	gCOD/gVSS.d
f_H	$f_{XE,OHO}$	Unbiodegradable fraction of OHOs	mgCOD/mgCOD
f_N	f_n	Nitrogen content of VSS	mgN/mgVSS
FSA	FSA	Free and saline ammonia	mgN/l
K	K	Half saturation constant	-
k_H	K_h	Maximum specific hydrolysis rate of SBCOD by OHOs under aerobic conditions	mgCOD/mgCOD.d
K_I		Half saturation constant for inhibition compound	mg/l
K_l		External transfer coefficient	m/h
K_N	K_{NHx}	Half saturation constant for growth of organisms with nitrogen (FSA)	mgN/l
$K_{N,A}$	K_{ANO}	Half saturation constant for growth of nitrifiers with nitrogen (FSA)	mgN/l
$K_{N,H}$	$K_{OHO,NHx}$	Half saturation constant for growth of OHOs with nitrogen (FSA)	mgN/l
K_O	KO	Half saturation constant for dissolved oxygen	mgO_2/l
$K_{O,A}$	$K_{ANO,O2}$	Half saturation constant for nitrifiers for dissolved oxygen	mgO_2/l
$K_{O,H}$	$K_{OHO,O2}$	Half saturation constant for OHOs for dissolved oxygen	mgO_2/l
K_S	KS	Half saturation concentration for soluble organics utilization	mgCOD/l
K_x	Kx	Half saturation concentration for utilization of SBCOD by OHOs	mgCOD/mgCOD.d
q		Specific conversion rate	l/h
Q_{in}	Q_i	Influent flow rate	m^3/h
Q_{out}	Q_e	Effluent flow rate	m^3/h
r_i		Observed transformation rate for process i	$ML^{-3}T^{-1}$
S	S	Soluble concentration in bulk liquid	mgCOD/l
S_{HCO}		Bicarbonate concentration	mg/l
S_I	S_U	Soluble unbiodegradable COD concentration	mgCOD/l
S_{in}	S_i	Influent substrate concentration	mgCOD/l
S_{KI}		Inhibition compound concentration	mg/l
S_{max}		Saturation concentration	$gCOD/m^3$
S_N		Nitrogen concentration (ammonia or nitrate)	mgN/l
S_{NH}	S_{NHx}	Free and saline ammonia concentration	mgFSA-N/l
S_{NO}	S_{NO3}	Nitrate concentration	$mgNO_3$-N/l
S_O	S_{O2}	Dissolved oxygen concentration	mgO_2/l
S_{out}	S_e	Effluent substrate concentration	mgCOD/l
S_S	S_S	Soluble readily biodegradable (RB)COD concentration	mgCOD/l
t	t	Time	h
V	V_R	Reactor volume	m^3
$v_{j,i}$		General stoichiometry term in model matrix for component i in process j	
X	X	Biomass concentration	$gCOD/m^3$

X_A	X_{ANO}	Nitrifier biomass concentration	mgCOD/l
X_H	X_{OHO}	Ordinary heterotrophic (OHO) biomass concentration	mgCOD/l
X_I	XI	Unbiodegradable particulate organics from influent wastewater	mgCOD/l
X_S/X_H	XS/X_{OHO}	SBCOD/OHO concentration ratio	mgCOD/mgCOD
X_S	XS	Slowly biodegradable (SB)COD concentration	mgCOD/l
$X_{STO,S}$		Intra-cellularly stored organic concentration	mgCOD/l
X_{TSS}	X_{TSS}	TSS concentration in reactor	mgTSS/l
Y_H	Y_{OHO}	Yield of OHOs	mg COD/mgCOD

[1)] Symbols used in this chapter are the original symbols reported as such in the source literature. Consequently, no attempt has been made by the authors of this chapter to align the symbols with the symbols used in chapters 3, 4, 5, 6, 7 and 17. [2)] Instead, an additional column with relevant symbols from these chapters was added to this table, for comparison.

Abbreviation	Description
ADM	Anaerobic digestion model
ASM	Activated sludge model
BOD	Biological oxygen demand
COD	Chemical oxygen demand
CSTR	Complete stirred tank reactor
DO	Dissolved oxygen
DR	Death regeneration
EA	Electron acceptor
EBPR	Enhanced biological phosphorus removal
ER	Endogenous respiration
GAO	Glycogen accumulating organism
IWA	International Water Association
OUR	Oxygen utilization rate
OHO	Ordinary heterotrophic organism
PAO	Phosphorus accumulating organism
PHA	Polyhydroxyalkanoate
RBCOD	Readily biodegradable COD
SBCOD	Slowly biodegradable COD
SRT	Sludge retention time
TKN	Total Kjeldahl nitrogen
TSS	Total suspended solids
TUDP	Delft University of Technology EBPR model
VFA	Volatile fatty acid

Greek symbol[1)]	Greek symbol[2)]	Description	
α		Represents a stoichiometric formula	-
η		Reduction factor for utilization of SBCOD under anoxic conditions	-
μ	μ	Specific growth rate of organisms	1/d
μ_A^{max}	$\mu_{ANO,max}$	Maximum specific growth rate of nitrifiers	1/d
μ_H	μ_{OHO}	Specific growth rate of OHOs	1/d
μ_H^{max}	$\mu_{OHO,max}$	Maximum specific growth rate of OHOs	1/d
μ^{max}	μ_{max}	Maximum specific growth rate of organisms	1/d
ρ_j		Kinetic rate of process j	$ML^{-3}T^{-1}$

[1)] Greek symbols used in this chapter are the original symbols reported as such in the source literature. No attempt has been made by the authors of this chapter to align the symbols with the symbols used in chapters 3, 4, 5, 6, 7 and 17. [2)] Instead, an additional column with relevant symbols from these chapters was added to this table, for comparison.