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Review

Activated sludge wastewater treatment plant modelling and simulation: state of the art

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Abstract

This review paper focuses on modelling of wastewater treatment plants (WWTP). White-box modelling is widely applied in this field, with learning, design and process optimisation as the main applications. The introduction of the ASM model family by the IWA task group was of great importance, providing researchers and practitioners with a standardised set of basis models. This paper introduces the nowadays most frequently used white-box models for description of biological nitrogen and phosphorus removal activated sludge processes. These models are mainly applicable to municipal wastewater systems, but can be adapted easily to specific situations such as the presence of industrial wastewater. Some of the main model assumptions are highlighted, and their implications for practical model application are discussed. A step-wise procedure leads from the model purpose definition to a calibrated WWTP model. Important steps in the procedure are: model purpose definition, model selection, data collection, data reconciliation, calibration of the model parameters and model unfalsification. The model purpose, defined at the beginning of the procedure, influences the model selection, the data collection and the model calibration. In the model calibration a process engineering approach, i.e. based on understanding of the process and the model structure, is needed. A calibrated WWTP model, the result of an iterative procedure, can usually be obtained by only modifying few model parameters, using the default parameter sets as a starting point. Black-box, stochastic grey-box and hybrid models are useful in WWTP applications for prediction of the influent load, for estimation of biomass activities and effluent quality parameters. These modelling methodologies thus complement the process knowledge included in white-box models with predictions based on data in areas where the white-box model assumptions are not valid or where white-box models do not provide accurate predictions. Artificial intelligence (AI) covers a large spectrum of methods, and many of them have been applied in applications related to WWTPs. AI methodologies and white-box models can interact in many ways; supervisory control systems for WWTPs are one evident application. Modular agent-based systems combining several AI and modelling methods provide a great potential. In these systems, AI methods on one hand can maximise the knowledge extracted from data and operator experience, and subsequently apply this knowledge to improve WWTP control. White-box models on the other hand allow evaluating scenarios based on the available process knowledge about the WWTP. A white-box model calibration tool, an AI based WWTP design tool and a knowledge representation tool in the WWTP domain are other potential applications where fruitful interactions between AI methods and white-box models could be developed.

Keywords: Activated sludge; Artificial intelligence; Modelling; Wastewater treatment plant

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Contents

1. Introduction

The activated sludge process is the most generally applied biological wastewater treatment method. In the activated sludge process, a bacterial biomass suspension (the activated sludge) is responsible for the removal of pollutants. Depending on the design and the specific application, an activated sludge wastewater treatment plant (WWTP) can achieve biological nitrogen (N) removal and biological phosphorus (P) removal, besides removal of organic carbon substances. Evidently, many different activated sludge process configurations have evolved during the years. A review on the historical evolution of the activated sludge process can be found in, e.g. Jeppsson (1996).

The first part of this paper will focus exclusively on white-box models for description of activated sludge processes. White-box models, also called deterministic models, are based on first engineering principles, meaning that the model equations were developed from general balance equations applied to mass and other conserved quantities, resulting in a set of differential equations. An overview of the most frequently applied models will be provided, with specific attention for the assumptions or simplifications behind the models. These model assumptions are often not considered carefully by the modeller, although they provide an indication of situations where the white-box models are not valid or provide only a poor description of the process. Specifically in these cases, one could consider other modelling methodologies besides the white-box models. Another modelling approach is to combine the white-box model with knowledge-based information extraction tools. The second part of this paper will therefore focus on such alternative modelling methodologies that make use of data, and on the integration of white-box models with artificial intelligence (AI) methodologies.

2. White-box WWTP modelling

The purpose of the first part of this paper is to demonstrate how the model selection, the data collection and the WWTP model calibration all relate to the modelling purpose. Note that there is an essential difference between an activated sludge model and a WWTP model. A WWTP usually consists of a set of activated sludge tanks, combined with a sedimentation tank, with a range of electron acceptor conditions occurring in the tanks. Depending on the concentrations of dissolved oxygen (DO) and nitrate present in the tanks, aerobic (oxygen present), anoxic (nitrate present, no oxygen) or anaerobic (no oxygen, no nitrate) tanks can be distinguished. Fig. 1 shows a typical activated sludge WWTP lay-out, not

Nomenclature

Symbols and abbreviations

ANN	artificial neural network
AR	autoregressive model
ARX	AR with external input
ARMA	autoregressive moving average model
ARMAX	ARMA with external input
ASM1	Activated Sludge Model No. 1
ASM2	Activated Sludge Model No. 2
ASM2d	Activated Sludge Model No. 2d
ASM3	Activated Sludge Model No. 3
Bio-P	biological phosphorus removal
COD	chemical oxygen demand
DO	dissolved oxygen
GA	genetic algorithm
MIMO	multiple input–multiple output
MPC	model predictive control
MVS	multivariate statistics
NH_4-N	ammonium nitrogen
NO_3-N	nitrate nitrogen
PAO	phosphorus accumulating organism
PCA	principal component analysis
PLS	partial least squares
PO_4-P	orthophosphate phosphorus
S_A	volatile fatty acids (acetate)
SBR	sequencing batch reactor
S_F	readily fermentable substrate
SISO	single input–single output
SRT	sludge retention time
S_S	readily biodegradable substrate
SS	suspended solids
TKN	total Kjeldahl nitrogen
TUDP	metabolic bio-P model of the Delft University of Technology
UCT	University of Cape town process lay-out (bio-P)
VSS	volatile suspended solids
WWTP	wastewater treatment plant
X_I	inert particulate organic material
X_{PHA}	poly-hydroxy alkanoates, an organic storage polymer in bio-P models
X_{STO}	cell internal storage product of heterotrophic organisms (ASM3)

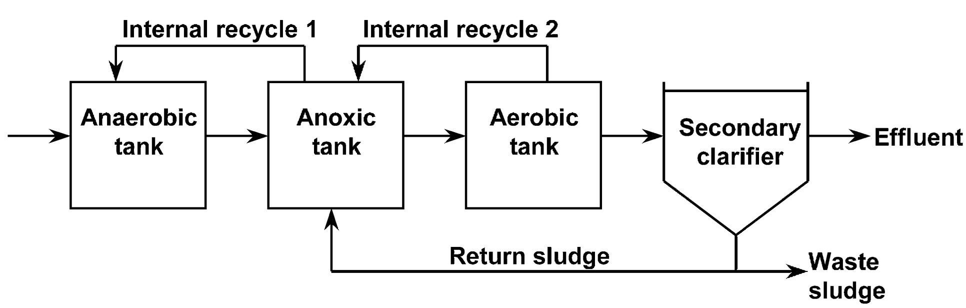

Fig. 1. Scheme of a University of Cape Town (UCT) WWTP lay-out.

considering the different pretreatment steps that normally precede the activated sludge tanks. The term WWTP model is used to indicate the ensemble of activated sludge model, hydraulic model, oxygen transfer model and sedimentation tank model needed to describe an actual WWTP. The term activated sludge model is used in this paper to indicate a set of differential equations that represent the biological (and chemical) reactions taking place in one activated sludge tank. Activated sludge model will thus refer exclusively to white-box models, i.e. models based on first engineering principles. The hydraulic model describes tank volumes, hydraulic tank behaviour (e.g. perfectly mixed versus plug flow behaviour, constant versus variable volume, etc.) and the liquid flow rates in between tanks, such as return sludge flow rate and internal recycle flow rate. The sedimentation tank models are available in varying degrees of complexity. The most popular models are simple ideal point settlers with no retention time, or the one-dimensional layered settler model of Takacs et al. (1991). Dedicated WWTP simulators allow construction of WWTP models based on libraries of activated sludge models, sedimentation tank models, etc.

A number of factors are to be considered with regard to activated sludge modelling and model applications, and a step-wise approach is needed to evolve from the model purpose definition to the point where a WWTP 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 WWTP model purpose or the objectives of the model application (control, design, simulation)
- Model selection: choice of the models needed to describe the different WWTP 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 WWTP or WWTP tanks
- Wastewater and biomass characterisation, including biomass sedimentation characteristics
- Data reconciliation to a steady-state model
- Calibration of the activated sludge model parameters
- Model unfalsification. In this task it is determined whether or not the model is sufficiently accurate for its intended purpose. If this is the case, the model is said to be unfalsified with respect to the available data. If this is not the case, a number of the preceding steps need to be repeated until the model is unfalsified.
- Scenario evaluations

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

This paper will provide the reader with a number of key references as guidance through some of the above-mentioned steps. Hereby we concentrate on the activated sludge models. The paper will summarise the activated sludge models that are most frequently used today, emphasising a number of assumptions behind these models, and, where possible, referring to situations where deviations from the standard models are necessary. Available WWTP simulators will be described briefly. Wastewater and activated sludge biomass characterisation has evolved to a research area on its own. Here a number of recent essential reference papers that can be helpful in this area will be mentioned. The paper will furthermore provide information on how to approach a WWTP model calibration, mainly referring to useful procedures and practical results available in the literature. Finally, an overview of some applications of WWTP models will be included to highlight the potential of WWTP models for different purposes such as WWTP scenario evaluations.

2.1. Activated sludge models

The most frequently used activated sludge models will be considered in an attempt to support the modeller in the model selection phase.

2.1.1. Activated sludge model development

The focus will be on the recent developments of activated sludge models, mainly the family of activated sludge models developed by the International Water Association (IWA) and the metabolic model developed at the Delft University of Technology (TUDP model). Table 1 summarises essential features of these and several other activated sludge models.

The Activated Sludge Model No. 1 (ASM1; Henze et al., 1987) can be considered as the reference model, since this model triggered the general acceptance of WWTP modelling, first in the research community and later on also in industry. This evolution was undoubtedly supported by the availability of more powerful computers. 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).

Even today, the ASM1 model is in many cases still 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 WWTPs for N removal. Copp (2002) reports on experiences with ASM1 implementations on different software platforms. For a full description of the ASM1 model, as well as a detailed explanation on the matrix format used to represent activated sludge models, the original publication Henze et al. (1987) should be consulted.

Table 1
Overview of activated sludge models included in this review. Den. PAO, denitrifying PAO activity included in the model; DR, death regeneration concept; EA, electron acceptor depending; ER, endogenous respiration concept; Cst, not electron acceptor depending

Model	Nitrification	Denitrification	Heterotrophic/ autotrophic decay	Hydrolysis	Bio-P	Den. PAOs	Lysis of PAO/PHA	Fermentation	Chemical P removal	Reactions	State variables	Reference
ASM1	X	X	DR, Cst	EA						8	13	Henze et al. (1987)
ASM3	X	X	ER, EA	Cst						12	13	Gujer et al. (1999)
ASM2	X	X	DR, Cst	EA	X		Cst.	X	X	19	19	Henze et al. (1995)
ASM2d	X	X	DR, Cst	EA	X	X	Cst.	X	X	21	19	Henze et al. (1999)
B&D	X	X	DR, Cst	EA	X	X	EA	X		36	19	Barker and Dold (1997)
TUDP	X	X	DR, Cst	EA	X	X	EA	X		21	17	Brdjanovic et al. (2000)
ASM3-bio-P	X	X	ER, EA	Cst	X	X	EA			23	17	Rieger et al. (2001)

ASM1 was primarily developed for municipal activated sludge WWTPs to describe the removal of organic carbon compounds and N, with simultaneous consumption of oxygen and nitrate as electron acceptors. The model furthermore aims at yielding a good description of the sludge production. Chemical oxygen demand (COD) was adopted as the measure of the concentration of organic matter. In the model, the wide variety of organic carbon compounds and nitrogenous compounds are subdivided into a limited number of fractions based on biodegradability and solubility considerations.

The ASM3 model (Gujer et al., 1999) was also developed for biological N removal WWTPs, with basically the same goals as ASM1. The ASM3 model is intended to become the new standard model, correcting for a number of defects that have appeared during the usage of the ASM1 model (Gujer et al., 1999). The major difference between the ASM1 and ASM3 models is that the latter recognises the importance of storage polymers in the heterotrophic activated sludge conversions. In the ASM3 model, it is assumed that all readily biodegradable substrate (S_S) is first taken up and stored into an internal cell component (X_{STO}) prior to growth (see Fig. 2). The heterotrophic biomass is thus modelled with an internal cell structure, similar to the phosphorus accumulating organisms (PAOs) in the biological phosphorus removal (bio-P) models. The internal component X_{STO} is subsequently used for biomass growth in the ASM3 model. Biomass growth directly on external substrate as described in ASM1 is not considered in ASM3. A second difference between ASM1 and ASM3 is that the ASM3 model should be easier to calibrate than the ASM1 model. This is mainly achieved by converting the circular growth–decay–growth model, often called death–regeneration concept, into a growth-endogenous respiration model (Fig. 2). Whereas in ASM1 effectively all state variables are directly influenced by a change in a parameter value, in ASM3 the direct influence is considerably lower thus ensuring a better parameter identifiability. Koch et al. (2000) concluded that ASM1 and ASM3 are both capable of describing the dynamic behaviour in common municipal WWTPs, whereas ASM3 performs better in situations where the storage of readily biodegradable substrate is significant (industrial wastewater) or for WWTPs with substantial non-aerated zones. The ASM3 model can be extended with a bio-P removal module (Ky et al., 2001; Rieger et al., 2001).

The overview of models including bio-P will start with the ASM2 model (Henze et al., 1995), which extends the capabilities of ASM1 to the description of bio-P. Chemical P removal via precipitation was also included. The ASM2 publication mentions explicitly that this model allows description of bio-P processes, but does not yet include all observed phenomena. For example, the ASM2d model (Henze et al., 1999) builds on the ASM2 model, adding the denitrifying activity of

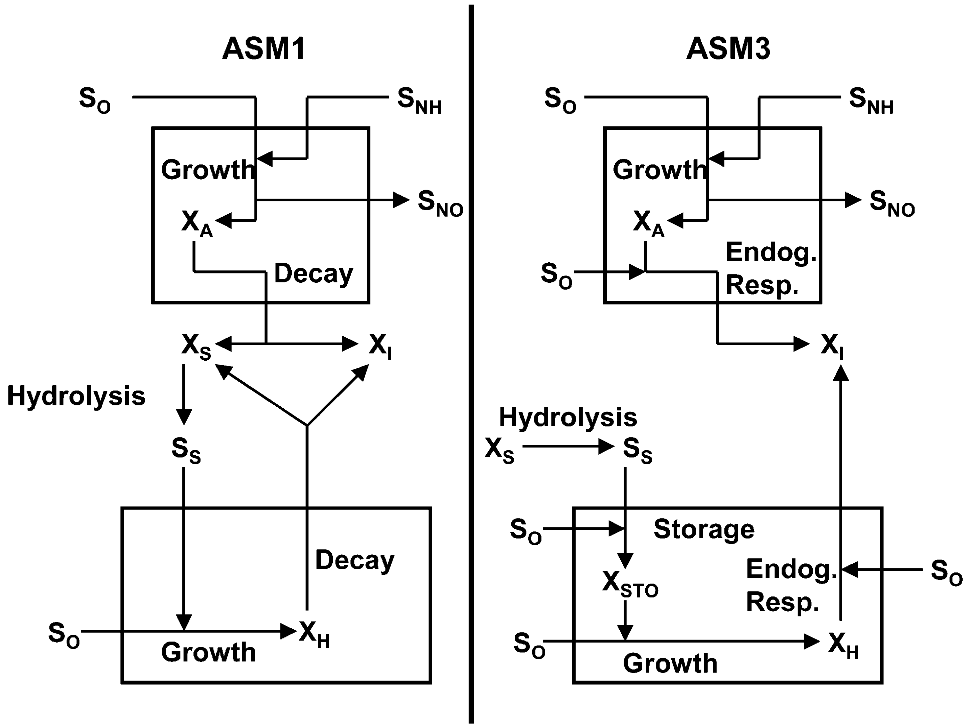

Fig. 2. Substrate flows for autotrophic and heterotrophic biomass in the ASM1 and ASM3 models (modified from Gujer et al., 1999).

PAOs which should allow a better description of the dynamics of phosphate and nitrate. Bio-P modelling in ASM2 is illustrated in Fig. 3: the PAOs are modelled with cell internal structure, where all organic storage products are lumped into one model component (X_{PHA}). PAOs can only grow on cell internal organic storage material; storage is not depending on the electron acceptor conditions, but is only possible when fermentation products such as acetate are available. In practice, it means that storage will usually only be observed in the anaerobic activated sludge tanks.

The TUDP model (van Veldhuizen et al., 1999; Brdjanovic et al., 2000) combines the metabolic model for denitrifying and non-denitrifying bio-P of Murnleitner et al. (1997) with the ASM1 model (autotrophic and heterotrophic reactions). Contrary to ASM2/ASM2d, the TUDP model fully considers the metabolism of PAOs, modelling all organic storage components explicitly (X_{PHA} and X_{GLY}), as shown in Fig. 4. The TUDP model was validated in enriched bio-P sequencing batch reactor (SBR) laboratory systems over a range of sludge retention time (SRT) values (Smolders et al., 1995), for different anaerobic and aerobic phase lengths (Kuba et al., 1997), and for oxygen and nitrate as electron acceptor (Murnleitner et al., 1997). A full description of the TUDP model is currently in preparation.

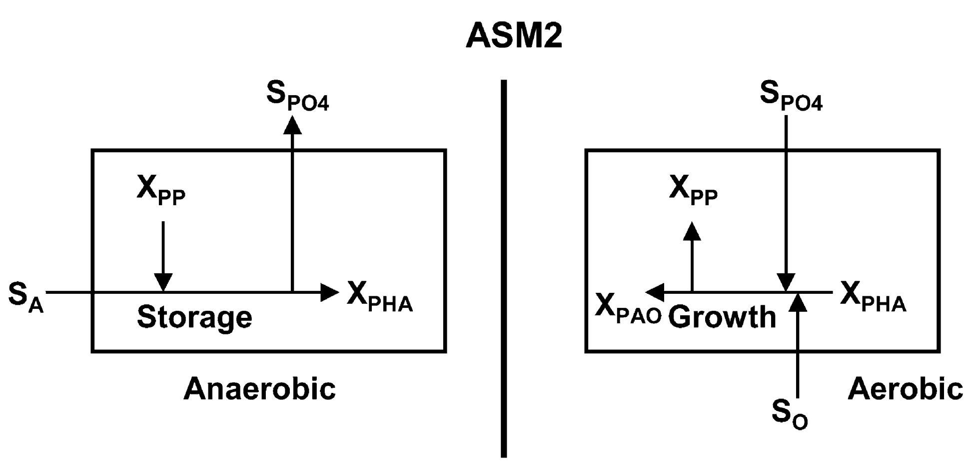

Fig. 3. Substrate flows for storage and growth of PAOs in the ASM2 model (Henze et al., 1995).

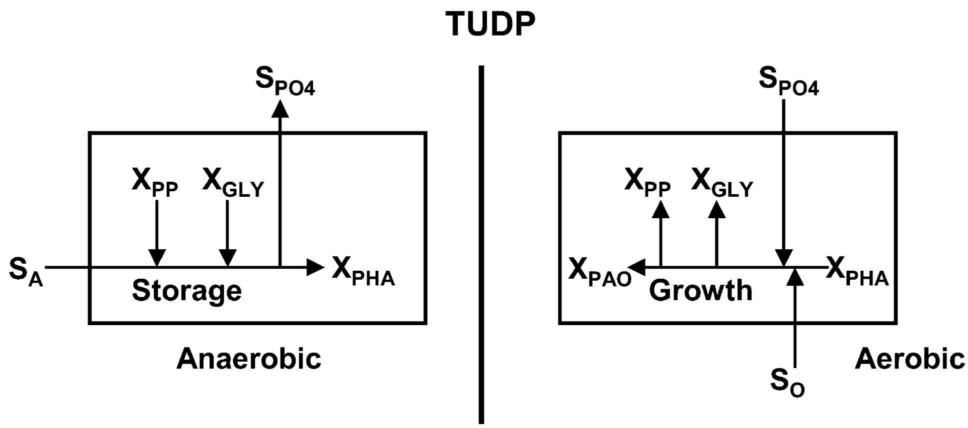

Fig. 4. Substrate flows for storage and aerobic growth of PAOs in the TUDP model (van Veldhuizen et al., 1999; Brdjanovic et al., 2000).

In some cases, such as high pH (>7.5) and high Ca^{2+} concentrations, it can be necessary to add biologically induced P precipitation to the bio-P model (Maurer et al., 1999; Maurer and Boller, 1999). Indeed, under certain conditions the bio-P reactions coincide with a natural precipitation that can account for an important P removal effect that is not related to the bio-P reactions included in the models described thus far. The formation of these precipitates, mostly consisting of calcium phosphates, is promoted by the high P concentration and increased ionic strength during the anaerobic P release of the PAOs. Model equations and components necessary to describe this precipitation process were given by Maurer and Boller (1999).

2.1.2. Activated sludge model assumptions and limitations

Some of the main assumptions of the ASM1 model, the reference model in this paper, will be highlighted and the implications of some of these assumptions for practical model application will be discussed. Where possible it will be indicated how the model assumptions were modified in later models.

2.1.2.1. Influence of environmental effects

- *Temperature*: Kinetic model parameters are temperature dependent, and consequently one has either to estimate the model parameters when calibrating the model for a specific temperature, or to develop appropriate temperature correction factors to include the temperature dependency of the reaction kinetics in the simulations. Henze et al. (1987) provide two sets of typical parameters for 10 and 20 °C, respectively. Later models, such as ASM2 (Henze et al., 1995) and the TUDP model (van Veldhuizen et al., 1999), use an Arrhenius type temperature dependence. Different reactions have different temperature dependencies, where nitrification is generally most sensitive. Hellinga et al. (1999) provide a detailed explanation of the influence of temperature on nitrification kinetics. Finally, Henze et al. (1995) warn that the ASM2 temperature coefficients are only valid between 10 and 25 °C.
- *pH*: In ASM1, it is assumed that the pH is constant and near neutrality. Including alkalinity as one of the state variables in the model allows detection of possible pH problems. For some reactions, specific functions can be added to the model to describe inhibitory pH effects, as illustrated by Hellinga et al. (1999) for the nitrification reaction.
- *Toxic components*: Nitrification is especially sensitive to inhibition by toxic components. In ASM1, the nitrification parameters are assumed to be constant. This means that any inhibitory effect of the wastewater on the nitrification kinetics is assumed to be included in the calibrated nitrification parameters. It is thus only possible to represent an “average inhibitory effect” of the wastewater. Alternatively, the nitrification rate equation can be extended to represent sudden acute inhibition by specific chemicals (Nowak et al., 1995). It is then up to the modeller to select the best inhibition kinetics model for the actual inhibition problem.
- *Wastewater composition*: The models in Table 1 were developed for simulation of municipal WWTPs. Model modifications are typically needed for WWTP systems where industrial contributions dominate the wastewater characteristics. Acute nitrification inhibition by toxic components related to industrial activity is one of the model modifications that are often necessary. Ky et al. (2001) combined the ASM3 model with the bio-P reactions of the TUDP model. In their modelling study, the simulation of a SBR treating the wastewater of a cheese industry, Mg^{2+} Monod switching functions were added to specific bio-P model reactions to account for Mg^{2+} limited kinetics. Coen et al. (1998) proposed a modified ASM1 model extended to three different soluble biodegradable organic substrates to describe a WWTP in the pharmaceutical industry.

2.1.2.2. Biodegradation kinetics

- Cell growth limitations due to low nutrient concentrations (e.g. N and P) are not considered in ASM1. Later models have included these limitations, e.g. the ASM3 model includes N and alkalinity limitations (Gujer et al., 1999). The bio-P models usually include P limitations too.
- Biomass decay in ASM1 is modelled according to the death–regeneration concept (Dold et al., 1980). In the ASM3 model this was replaced by the endogenous respiration or maintenance concept (see Table 1). As a result, the conversion reactions of both autotrophs and heterotrophs are clearly separated in ASM3, whereas the decay product regeneration cycles of the autotrophs and heterotrophs are strongly interrelated in ASM1 (see Fig. 2). Moreover, the use of the endogenous respiration concept in the ASM3 model should allow easier comparisons between the results of kinetic parameters derived from respirometric batch experiments with activated sludge of the plant to be modelled (Vanrolleghem et al., 1999), and the activated sludge model used to describe the phenomena in the full-scale plant. Note that the TUDP model uses the death regeneration concept for the autotrophic and heterotrophic (non-PAO) reactions, whereas the maintenance concept is used for the PAOs. Effectively you want to describe maintenance, viruses, decay, protozoa, rotifers, nematodes, etc., in the model, since all these processes lead to a decreased sludge production or oxygen consumption in the absence of external substrate in the full-scale WWTP (van Loosdrecht and Henze, 1999). It has been shown that all these processes can conveniently be lumped in one activated sludge model reaction. The names of the reactions should therefore not be taken too literally.
- The hydrolysis of organic matter and organic nitrogen are coupled and occur simultaneously with equal rates. In the bio-P models this was extended to include also organic phosphate.
- ASM1 can not deal with elevated nitrite concentrations, i.e. nitrification is modelled as a one-step process thereby ignoring the possible appearance of nitrite, a nitrification intermediate, in full-scale WWTPs. Typically, the assumption of one-step nitrification is acceptable. However, when modelling a WWTP where considerable nitrite concentrations occur, or where the temperature is above 20 °C, a two-step nitrification model with nitrite as intermediate might be useful. Examples of two-step nitrification models were proposed by Nowak et al. (1995) and Hellinga et al. (1999). The influence of nitrite on the bio-P reactions was investigated by Meinhold et al. (1999).
- Nitrogen gas, a denitrification product, is not included in the ASM1 model. As a consequence, the model does not allow checking the N balances. Most of the later models included nitrogen gas as a model component (Henze et al., 1995, 1999; Gujer et al., 1999; Brdjanovic et al., 2000). Clearly, the modeller can easily add nitrogen gas to the model as an extra component. The P-balances in the bio-P models are always closed.
- In ASM1, the type of electron acceptor present does not affect the biomass decay rate. In contrast, ASM3 allows differentiation between aerobic and anoxic heterotrophic biomass, storage product (X_{STO}) and autotrophic biomass decay rates. According to the experimental results reported in Siegrist et al. (1999), this differentiation between aerobic, anoxic, and if necessary anaerobic autotrophic biomass decay rates seems to be justified.
- In ASM1, the type of electron acceptor does not affect the heterotrophic biomass yield coefficient, whereas the ASM3 model (Gujer et al., 1999) and the model of Barker and Dold (1997) allow inclusion of different aerobic and anoxic heterotrophic biomass yield coefficients in the model. It has been theoretically proven, based on metabolic process energetics, that anoxic yields are consistently lower than aerobic ones (Orhon et al., 1996). Indeed similar differences between aerobic and anoxic yield were obtained experimentally with activated sludge (McClintock et al., 1988; Spérandio et al., 1999). A metabolic model takes this explicitly into account because a different energetic efficiency for the different electron acceptors is included.
- In the ASM1 model, hydrolysis reaction rates depend on the electron acceptor present (aerobic or anoxic conditions). In the ASM3 model, hydrolysis is independent of the available electron acceptor (Gujer et al., 1999). ASM2 acknowledges that hydrolysis reaction rates may depend on the available electron acceptor, also under anaerobic conditions (Henze et al., 1995).
- The bio-P models cannot handle two extreme situations (van Veldhuizen et al., 1999): (1) full depletion of the organic storage product pool X_{PHA} in the PAOs; (2) simultaneous presence of volatile fatty acids (=substrate for storage reactions) and electron acceptors. Model extensions are needed to handle these two situations.
- Storage of substrate by non-PAOs is not accounted for in ASM2/ASM2d and TUDP.
- The models are not able to describe filamentous biomass growth and sludge bulking.

2.1.3. Activated sludge model selection for specific model application purpose

The definition of the WWTP model purpose or the objectives of the model application will influence the activated sludge model selection. This will be illustrated with an example. Assume a modelling study where the influence of process modifications such as tank volume extensions or implementation of improved process control on an existing biological N removal plant combined with chemical P precipitation should be investigated, aiming at improved process operation. It is thus not necessary to consider the bio-P models, for reasons of model parsimony. Chemical P precipitation reactions contribute substantially to the waste sludge production. In that case, combining the model for the biological N removal reactions with a chemical P precipitation model, such as for example the one included in the ASM2 model description (Henze et al., 1995), offers an advantage. Indeed, it will lead to more realistic biomass yield coefficients in the calibrated model because the chemical sludge production will no longer be lumped with the biological sludge production.

2.2. Simulator environments

A WWTP simulator environment can be described as software that allows the modeller to simulate a WWTP configuration. A rather detailed overview of simulator environments for WWTP models can be found in Olsson and Newell (1999) and Copp (2002). General-purpose simulator environments can be distinguished from specific WWTP simulator environments. General-purpose simulator environments normally have a high flexibility, but the modeller has to supply the models that are to be used to model a specific WWTP configuration. The latter task can be very time consuming. However, it is better to spend sufficient time on the model implementation and debugging, to avoid running lots of simulations with a model that afterwards turn out to be erroneous for the specific application task. As a consequence, general-purpose simulator environments require a skilled user that fully understands the implications of each line of code in the models. A popular example of a general-purpose simulator environment is MATLAB/Simulink (http://www.mathworks.com). Specific WWTP simulator environments usually contain an extended library of predefined process unit models, for example a perfectly mixed ASM1 or ASM2d bioreactor, and a one-dimensional 10-layer settler model. The process configuration to be simulated can easily be constructed by connecting process unit blocks. Pop-up windows allow modifying the model parameters. Examples of specific commercial WWTP simulator environments are (in alphabetic order): AQUASIM (http://www.aquasim.eawag.ch), BioWin (http://www.envirosim.com), EFOR (http://www.dhisoftware.com/efor), GPS-X (http://www.hydromantis.com), SIMBA (http://www.ifak-system.com), STOAT (http://www.wrcplc.co.uk/software), and WEST (http://www.hemmis.com). More information about a specific simulator environment can be found in Olsson and Newell (1999) or on the respective websites. On the websites it is often possible to download a demo version of the simulator environments for evaluation purposes. Specific WWTP simulator environments allow the modeller to easily produce the desired WWTP configuration by connecting predefined model blocks. As such, this involves a danger that the user is simulating process configurations without fully understanding the model structure, implicating that model assumptions and limitations can also easily be overlooked.

2.3. Model applications

A model may be applied in the following roles (Russel et al., 2002): (1) a service role, where the model, when solved, provides the needed numerical values for further analysis; (2) an advice role, where the model provides insights that help to understand and solve related subproblems contributing to the solution of an overall problem; (3) an analysis role, where simulations with the model indicate how to use models to solve a specific task.

Table 2 summarises a selected number of papers that give rather detailed information on WWTP model applications. The purpose for WWTP model studies can be (Hulsbeek et al., 2002; Petersen et al., 2002): (1) learning, i.e. use of simulations to increase process understanding, and to develop people's conception of the system; (2) design, i.e. evaluate several design alternatives for new WWTP installations via simulation; (3) process optimisation and control, i.e. evaluate several scenarios that might lead to improved operation of existing WWTPs. The two latter are applications of the model in a service role. An application of the model in an analysis role can for example be a study where the suitability to describe a particular process is evaluated for several modelling concepts enclosed in different activated sludge models.

2.3.1. WWTP model simulations for learning

Simulations with WWTP models can be applied in different ways to increase the process understanding of the user. For the WWTP operator, simulations might for example be useful to indicate the consequences of process operation modifications on the activated sludge composition and the WWTP effluent quality. Similarly, simulations with e.g. the ASM1 benchmark plant (Copp, 2002) for different weather disturbance scenarios are very informative to get an idea of the behaviour of a WWTP under variable weather conditions.

From a research perspective, Brdjanovic et al. (2000) used the TUDP model to increase their understanding of a full-scale bio-P process. Siegrist et al. (1999) noticed in their experimental work that the decay rate of autotrophic bacteria is lower under anaerobic and anoxic conditions, compared to aerobic conditions. Simulations

Table 2
Overview of recently published WWTP model applications. AT, aeration tank; DT, denitrification tank; NBR, nitrifying biofilm reactor; RWT, reject water treatment; SC, secondary clarifier; ST, storm water tank; StT, storage tank; PC, primary clarifier

Reference	Model	Purpose	WWTP	Scenarios								
				Extra tanks added	Tanks removed	Load modified	Step feed	Aeration	Internal recirculation flow rates	Sludge recycle	SRT	Carbon addition
Coen et al. (1996)	ASM1	WWTP upgrade; N removal	Continuous, plug flow	ST	PC		X	X	X	X		
Çinar et al. (1998)	ASM2	WWTP upgrade; P removal	Continuous, plug flow+oxidation ditch/carrousel					X				X
Yuan et al. (1998)	ASM1	Design: Evaluate process alternative	Continuous	StT							X	
Ladiges et al. (1999)	ASM1	WWTP upgrade; N removal	Continuous	StT		X			X		X	X
Hao et al. (2001)	TUDP	Evaluate process alternatives	Continuous	SC, NBR					X	X		
Salem et al. (2002)	TUDP	Design: Evaluate process alternatives	Continuous	AT, DT, RWT				X	X	X	X	X

with a WWTP model incorporating this hypothesis showed that avoiding excess aeration in the activated sludge tanks, for example via intermittent aeration, not only saves aeration energy but also improves the nitrification capacity of the plant.

2.3.2. *WWTP model simulations for design*

During the design phase, process alternatives can be evaluated via simulation. Such a model study was presented e.g. by Salem et al. (2002), where different alternatives for the upgrade of a biological N removal plant were evaluated with focus on appropriate treatment of sludge reject water. The WWTP model simulations provided the knowledge basis that was needed to decide on full-scale implementation of one of the proposed alternatives. In this context, modelling can substantially reduce the scale-up time, because different options can be evaluated before a pilot plant is built. The model thus contributes significantly in bridging the gap between lab and full-scale application (Hellinga et al., 1999). A WWTP model thus transforms data obtained from lab-scale experiments into quantitative knowledge, which helps in decision-making processes.

Based on the presence of denitrifying PAOs in the TUDP model, Hao et al. (2001) used WWTP model simulations to compare the traditional UCT bio-P plant lay-out with an innovative alternative two-stage WWTP configuration (A_2N process) that fully exploits the capabilities of the denitrifying PAOs by introducing a separate nitrifying biofilm reactor in the process. The total aerobic tank volume is thus no longer dominated by the slow growth of the autotrophic organisms, leading to a more compact WWTP process.

Yuan et al. (1998) evaluated a sludge storage concept via ASM1 simulations, based on the reduced decay of autotrophic bacteria under anaerobic conditions. The concept provides spare nitrification capacity for nitrogen shock load situations by storing the waste activated sludge temporarily in an anaerobic tank with a retention time of a few days, whereas the SRT in the activated sludge plant is reduced considerably. The concept thus results in a WWTP with less sludge but a similar nitrification capacity compared to traditional reactor design, and was successfully evaluated in pilot plant studies (Yuan et al., 2000). Savings on reactor volume were evaluated to be around 20%, but increased sludge production could be a problem with respect to operational costs.

2.3.3. *WWTP model simulations for process optimisation*

Process optimisation can be used in different contexts. Off-line process optimisation refers to applications where off-line simulations with the calibrated model are used to determine how to optimally run the process, whereas the result is later on implemented and tested on the full-scale plant. In on-line process optimisation simulations with the calibrated model are applied in an on-line optimisation scheme, for example in the frame of a plant-wide supervisory control system (Rodriguez-Roda et al., 2002) or a model predictive control (MPC) optimisation algorithm. On-line process optimisation will be considered in more detail in Section 4 of this paper.

Off-line process optimisation is often needed because new stricter demands are imposed to existing WWTPs, or considerable changes in the plant load have occurred, or deficiencies have appeared during WWTP operation such that the initially required effluent quality cannot any longer be obtained. In this context, simulations are often used to evaluate whether the pollutant removal efficiencies can be improved within the existing plant lay-out, e.g. via improved process control. The ASM1-based benchmark WWTP (Copp, 2002) was specifically developed for simulation-based objective evaluation of different control strategies on a N removal WWTP, and includes several criteria to evaluate the WWTP performance.

Scenario evaluations with ASM1/ASM3 usually aim at upgrading a WWTP for biological N removal (Coen et al., 1996), evaluating the possibilities for improved biological N removal within an existing WWTP configuration (Ladiges et al., 1999), or predicting the effect of a change in load on the WWTP performance. During scenario evaluations with bio-P models, evaluation of different process alternatives often results in a trade-off between bio-P capacity and nitrification, where increased DO concentrations will promote nitrification but negatively influence the bio-P process due to increased aerobic decay of PAO storage products (Çinar et al., 1998). Gernaey et al. (2002) illustrate the implementation of chemical P precipitation on an existing N removal WWTP. Fig. 5 illustrates the difference in effluent orthophosphate concentrations obtained before and after the introduction of a constant $Fe(OH)_3$ dosage.

2.4. Model calibration

Model calibration is understood as the estimation of the model parameters to fit a certain set of data obtained from the full-scale WWTP under study. The need for a model calibration depends on the model purpose. In case the model is to be used for educational purposes (e.g. to increase basic understanding of the processes), for comparison of design alternatives for non-existing municipal WWTPs or in other situations where qualitative comparisons are sufficient, default parameter values can be applied (Petersen, 2000). However, if the model is to be used for process performance evaluation and optimisation, it may be necessary to have a more accurate description of the actual processes under study, and thus data collection and model calibration are needed (Petersen, 2000). Different calibration levels can be distinguished. Henze et al. (1995) distinguish a calibration using static (non-dynamic) data (composite 24 h samples available) and a model calibration using dynamic data (dynamic profiles of influent and effluent composition available). This nomenclature (static versus dynamic) has also been used in Table 3, a table that refers to recent experiences with model calibrations for full-scale WWTPs.

The starting point for the model calibration is usually the default parameter set provided with the activated sludge model descriptions. Two model calibration approaches can be distinguished: the mathematical optimisation approach which relies purely on mathematical optimisation, and the process engineering approach which is based on understanding of the process and the model structure.

2.4.1. Mathematical optimisation model calibration approach

A purely mathematical optimisation of the WWTP model will be problematic due to the complexity and resulting unidentifiable nature of the highly non-linear (and for ASM1 also circular via the death–regeneration concept) activated sludge models. A major problem encountered in calibration of WWTP models is indeed the lack of identifiability of the model parameters: more than one combination of influent characteristics and model parameters can give a description of the available data of a similar quality. It therefore becomes important to obtain informative data that allow constraining the model parameters within realistic boundaries. Obtaining informative data on a full-scale installation is often difficult in practice, because many WWTPs were overdesigned and thus show only little effluent dynamics that could be used during the calibration. In-process measurements, taken at several points in the bioreactors, can then be very helpful. Mathematical optimisation can undoubtedly be useful in WWTP model calibration, but only when supported by sufficient expert process knowledge. An optimisation algorithm cannot differentiate between more defined (e.g. stoichiometric model parameters) or less defined model parameter values, and will often end up giving rather small modifications to a considerable number of parameters (Weijers and Vanrolleghem, 1997).

The mathematical optimisation and process engineering model calibration approach were evaluated by van Veldhuizen et al. (1999). The mathematical optimisation approach was evaluated based on sensitivities of the WWTP model to kinetic and stoichiometric model parameters, to changes in the influent composition and the set point for control handles (flow rates, etc.). The conclusion was that more parameters would have been modified when following the mathematical optimisation approach compared to the process engineering approach.

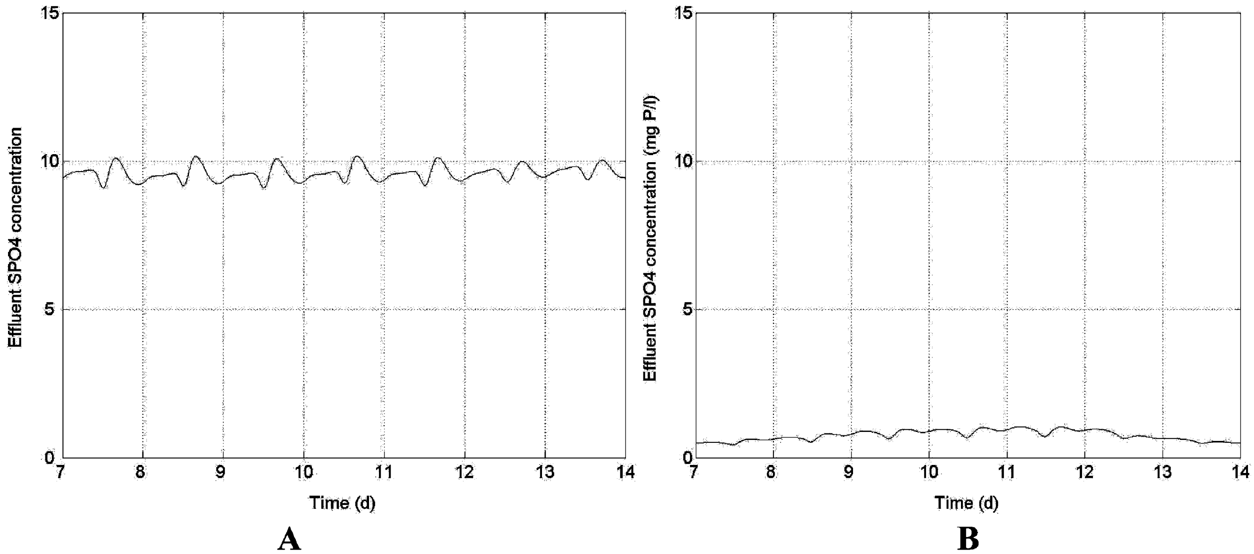

Fig. 5. Simulation results illustrating the effect on effluent orthophosphate concentrations of implementing a continuous metal salt dosage (in this case $Fe(OH)_3$) to induce chemical P precipitation (Gernaey et al., 2002): (A) no metal salt dosage; (B) metal salt dosage.

A model calibration based on process knowledge is more sensible, but requires a considerable level of expert process knowledge. In many WWTP model studies, the process engineering calibration approach is combined with the mathematical approach, by applying sensitivity analysis in verifying whether the model is indeed sensitive to changes in the parameters that were modified during the calibration procedure (van Veldhuizen et al., 1999; Meijer et al., 2001; Petersen et al., 2002).

2.4.2. Process engineering model calibration approach

In the process engineering model calibration approach, the model parameters are adjusted one by one, mainly based on the experience and the process understanding of the modeller, until the model fits the available WWTP data reasonably well. The result is not a unique set of parameters but a parameter set that results in acceptable predictions of the effluent concentration, the sludge production, and also the internal concentration dynamics (if data are available) for the WWTP under study. Often the gains (sensitivities) of the plant model are not properly calibrated in this approach in case no data are available on the internal concentration dynamics.

Detailed procedures for activated sludge model calibration will not be repeated here, only the main steps in the step-wise model calibration procedure were given in the introduction of this paper. Recent key publications on activated sludge model calibration are Hulsbeek et al. (2002) and Petersen et al. (2002). Petersen et al. (2002) describe a general step-wise procedure relying on a sequence of steady state, static and dynamic models that is applied to an ASM1 model calibration, and explain how, depending on the purpose of the model, a number of steps in the proposed procedure can be omitted. Hulsbeek et al. (2002) also present a step-wise model calibration protocol, making a clear distinction between COD, nitrification and denitrification, aiming mostly at practical applicability instead of scientific exactness. Both publications agree that there is an iterative interaction between WWTP model parameter calibration and wastewater characterisation, i.e. a modification of a model parameter can for example lead to a subsequent modification of the wastewater fractionation, which can then again result in a change of an activated sludge model parameter. This is mainly due to the influence of wastewater characterisation on the WWTP model parameters. The models are very sensitive to a modification of the influent composition, especially the inert particulate fractions (X_I) which will affect the sludge production (Brdjanovic et al., 2000; Petersen et al., 2002), and the readily biodegradable substrate fraction (S_S or S_A+S_F) which will affect the denitrification and/or bio-P capability of the WWTP. Koch et al. (2000) for the ASM3 model, and Rieger et al. (2001) for the ASM3-bio-P model, calibrated the full-scale plant model via an iterative procedure that uses a combination of batch experiments, weekly wastewater variations, diurnal variations and long-term simulations. In many cases (see Table 3) batch experiments with the activated sludge of the WWTP are indeed used to determine sludge kinetic parameters and wastewater biodegradability. These experimentally determined parameters can be used during the model calibration to provide values for a number of model parameters (Brdjanovic et al., 2000; Rieger et al., 2001) or during the model unfalsification phase to evaluate whether a model parameter value is within a realistic range (Brdjanovic et al., 2000; Petersen et al., 2002). Koch et al. (2000), Rieger et al. (2001) as well

Table 3
Overview of papers describing detailed practical experiences with full-scale WWTP model calibration (Dyn., dynamic; St., static)

Reference	Model	Data			Model		Remarks
		Static	Dynamic	Batch exp.	Calibration	Unfalsification	
Coen et al. (1996)	ASM1	X	X	X	Dyn.	St.	Dynamic influent profile was designed based on the measurement campaign
Çinar et al. (1998)	ASM2	X			St.	St.	
van Veldhuizen et al. (1999)	TUDP	X	X		St.	Dyn.	
Brdjanovic et al. (2000)	TUDP	X	X	X	St.	St.	Use of batch experiments mainly during model unfalsification phase
Koch et al. (2000)	ASM3	X	X	X	Dyn.	Dyn.	Use of batch experiments before the full-scale model calibration phase
Meijer et al. (2001)	TUDP	X	X		St.		
Rieger et al. (2001)	ASM3-bio-P	X	X	X	St./Dyn.	St./Dyn.	Use of batch experiments during calibration; iterative calibration procedure
Hulsbeek et al. (2002)	ASM1/general	X	X		St./Dyn.	St./Dyn.	Type of data depending on model purpose
Petersen et al. (2002)	ASM1/general	X	X	X	St./Dyn.	St.	Type of data depending on model purpose; Use of batch experiments for calibration (wastewater) and unfalsification

as Petersen et al. (2002) emphasise the importance of batch experiments with activated sludge in the determination of model parameters, whereas Hulsbeek et al. (2002) promote a methodology without specific batch experiments. Brdjanovic et al. (2000) mainly used the batch test results for model unfalsification. Petersen et al. (2002) apply the results of batch experiments both during the model calibration (e.g. for wastewater characterisation) and model unfalsification. Koch et al. (2000) and Rieger et al. (2001) first adjust a number of model parameters based on the batch experiments (with sludge and wastewater), and only afterwards involve the plant data in the WWTP model calibration. In general, care should be taken when transferring model parameters obtained from lab-scale experiments with activated sludge to the full-scale installation. A batch experiment with activated sludge provides much more detailed information about the reaction kinetics compared to the full-scale WWTP data. The model calibration approach of Hulsbeek et al. (2002) implies that the results obtained from batch experiments are not really needed by the practitioner.

Generally speaking, the activated sludge model parameters are calibrated in the following order: sludge production and sludge balance, nitrification, denitrification, and bio-P (Brdjanovic et al., 2000; Meijer et al., 2001; Hulsbeek et al., 2002; Petersen et al., 2002). A basic rule in WWTP model calibration seems to be that only a few model parameters usually need to be changed in order to calibrate the model to experimental data (Henze et al., 1995; Çinar et al., 1998; van Veldhuizen et al., 1999; Brdjanovic et al., 2000; Meijer et al., 2001; Petersen et al., 2002).

Hulsbeek et al. (2002) indicate that calibrated model parameters deviating substantially from default parameter values usually indicate errors in the hydraulic WWTP model, e.g. that the WWTP configuration is not correctly described or due to errors in the available concentration and flow rate data. A critical but too often neglected factor is indeed that the system parameters (SRT, flow rates, DO, etc.) obtained from the WWTP may not be correct. This needs some extra attention in general. In some model calibrations it is even considered that most “calibration” is due to in-correct primary data (e.g. SRT or recycle flow rate), and as a consequence data should be reconciled (Hulsbeek et al., 2002). A proper wastewater characterisation is thus not a guarantee for a successful model calibration. Data reconciliation is needed, as illustrated by Meijer et al. (2002). Meijer et al. (2001) used a sensitivity analysis to show the relatively large influence of operational data, (such as internal flow rates) on the model output, compared to many kinetic activated sludge model parameters. Meijer et al. (2001, 2002) therefore proposed to use the P balance, and in some cases N and flow balances to validate the data quality via consistency checking and data reconciliation before moving on with the calibration. After reconciling the operational data with average static balances, no major calibration effort was needed to fit the model to experimental data. It is also essential for the predictive capacities of the model to verify whether flows are equally distributed between parallel WWTP units (Coen et al., 1998; Hulsbeek et al., 2002).

During the model calibration, especially for bio-P models, in-process measurements can be much more informative than the effluent concentrations for calibration of the model parameters. Indeed, van Veldhuizen et al. (1999) observed large deviations between the measured and simulated nitrate and phosphate concentration profiles for different in-process locations during the model calibration, although the model fit to effluent concentrations seemed reasonable. Thus, in-process measurements contribute substantially to proper calibration of the plant model gains.

Local factors may influence the model calibration procedure. For the Dutch situation a static model calibration using 24-h flow proportional samples is normally considered as sufficient (Hulsbeek et al., 2002), because the influent concentration variations are limited, i.e. only the diurnal flow rate variations need to be considered. This was explained by the long residence time of the wastewater (0.8–1.5 days) in the sewer systems (van Veldhuizen et al., 1999). The long residence time in the sewer, especially when combined with anaerobic conditions in the sewer, also implies that the WWTP is fed with a wastewater that contains considerable amounts of readily biodegradable substrate. As a consequence, hydrolysis and fermentation processes will be less influential on the modelling of the overall performance of the WWTP (van Veldhuizen et al., 1999). This results in a simpler model calibration, since the modeller can exclusively focus on the nutrient removal process instead of the less understood and therefore less well-described hydrolysis and fermentation processes.

Çinar et al. (1998) calibrated a WWTP model for one WWTP, and afterwards attempted to transfer the activated sludge model parameters of the calibrated WWTP model to three other WWTPs, with varying degree of success. Poor characterisation of the reactor hydraulics was believed to be the major reason for the poor predictions obtained on two WWTPs. One can indeed partially compensate for a poor hydraulic WWTP model by selecting a biased set of activated sludge model parameters.

2.4.3. Data collection for model calibration

The purpose of the model application determines how to approach a model calibration, e.g. which data are needed (averages or dynamic profiles) and to which level of detail the model should be calibrated (Hulsbeek et al., 2002; Petersen et al., 2002). Dynamic influent and effluent concentration profiles are needed in case one is interested in describing the fast process dynamics. An example of dynamic influent and effluent profiles is given in Figs. 6 and 7, respectively. Data collection is an essential part in several model calibration steps. Petersen et al. (2002) distinguish the following data sources for a model calibration:

1. Design data: e.g. reactor volumes, maximum pump flow rates and aeration capacities.
2. Operational data:
   - Flow rates, as averages or dynamic trajectories, of influent, effluent, recycle and waste sludge flows.
   - pH, aeration (flow rates, valve openings, etc.) and temperatures.
3. Tracer tests for the characterisation of the hydraulic model.
4. Sedimentation tests for the determination of the settler model parameters.
5. Data for the characterisation of:
   - Concentrations of influent and effluent, in-process measurements (as well as some intermediate streams between the WWTP unit processes), as averages or dynamic trajectories: e.g. SS, COD, TKN, NH_4-N, NO_3-N, PO_4-P, etc.
   - Sludge composition: e.g. SS, volatile suspended solids (VSS), COD, N and/or P content.
   - Reaction kinetics: e.g. growth and decay rates.
   - Reaction stoichiometry: e.g. yields.
6. Process gains, i.e. sensitivities of the process variables to changes in model parameters, influent composition and set points of control handles.

The available data set can vary considerably, depending on the specific WWTP (size, process lay-out, presence of industrial activity) and on the model purpose (Petersen et al., 2002). A typical municipal wastewater composition is usually provided together with the activated sludge model descriptions, and can serve as a first guidance for the wastewater fractionation, a procedure that converts the available influent and effluent measurement data into the model component fractions. The activated sludge model descriptions also contain information on the wastewater fractionation and the methods that could be used to determine the different wastewater fractions (Henze et al., 1987, 1995). An extensive review on advantages and disadvantages of wastewater fractionation methods for the ASM1 model, and on ASM1 model calibrations, can be found in Petersen (2000). Petersen et al. (2002) describe a protocol for ASM1 influent fractionation, including the use of respirometric experiments to evaluate the readily biodegradable fraction of the wastewater. Roeleveld and van Loosdrecht (2002) provide a detailed wastewater characterisation procedure that mainly relies on physico-chemical and chemical analysis methods supplemented with BOD tests. This procedure is applicable for ASM1 and ASM2d.

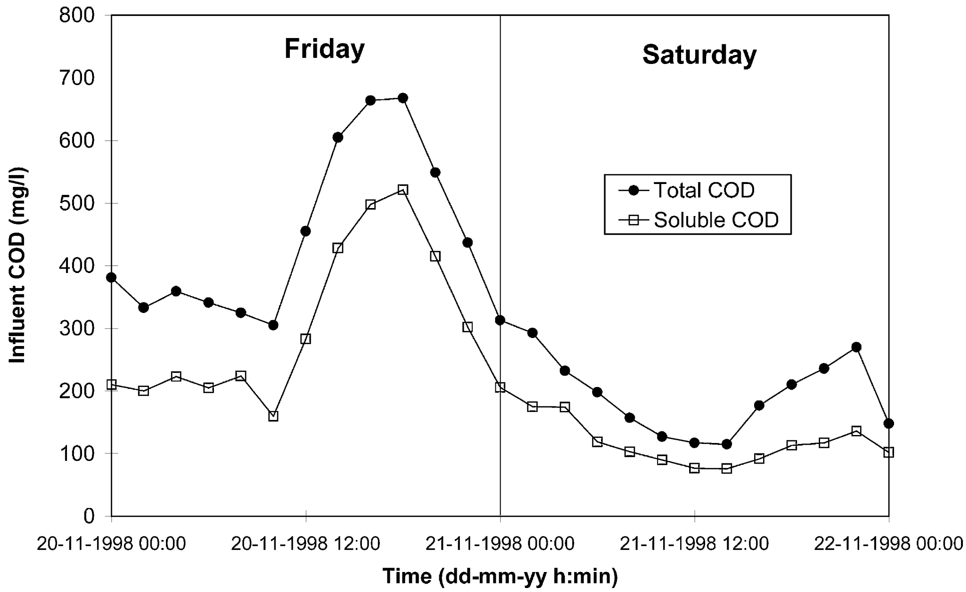

Fig. 6. Influent COD concentrations for a mixed industrial–municipal WWTP, illustrating diurnal load variations and weekend versus working day load variations (Petersen et al., 2002).

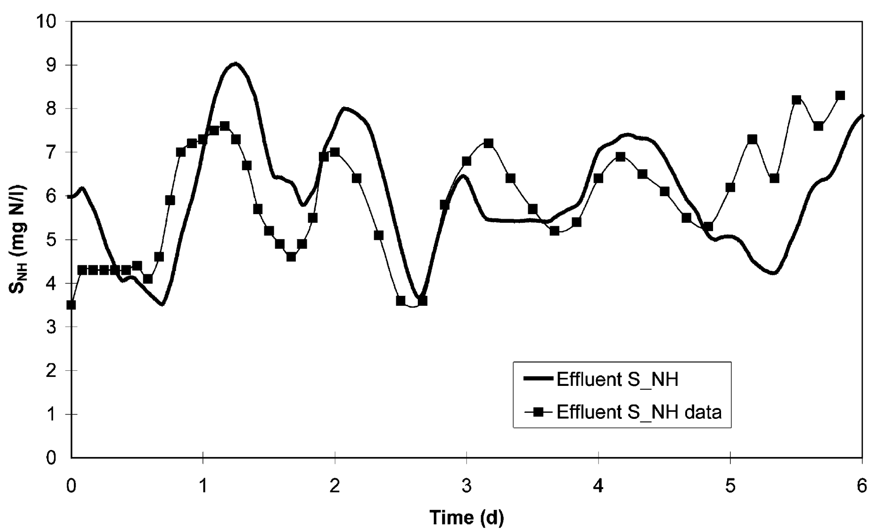

Fig. 7. Results of a model calibration. Model fit of an ASM1 based WWTP model to dynamic effluent ammonium (S_{NH}) concentrations (Petersen et al., 2002).

3. Alternative modelling methodologies

The first part of this paper has exclusively focussed on the selection, calibration and usage of white-box models for description of activated sludge processes. However, it is clear that other modelling methodologies are available and applied to the activated sludge process too. In many ways, alternative modelling methodologies are complementing and supporting the knowledge about the wastewater treatment process and its operation that is summarised in the white-box plant model. This is especially useful in situations where the white-box plant model assumptions are not valid: (1) For many applications insufficient data are available for calibration of a white-box plant model. (2) Furthermore, the white-box models do not accurately describe the layered activated sludge floc structure, which in full-scale results in simultaneous nitrification and denitrification. (3) The white-box models do not sufficiently describe full-scale activated sludge sedimentation processes. (4) The white-box models are usually calibrated for dry weather situations, resulting in model predictions that might be less accurate when rain events occur in the influent data.

Prediction of sludge sedimentation problems such as sludge bulking is a good example to illustrate this. The white-box WWTP models were not developed to provide information on changes in the sludge sedimentation properties, although deterioration of sludge sedimentation properties is one of the major causes of process upsets in full-scale WWTPs. Therefore, black-box models, i.e. models entirely identified based on input–output data without reflecting physical, biological or chemical process knowledge in the model structure can be applied to provide an indication of occurrence of sludge sedimentation problems in the full-scale plant, thus triggering appropriate control actions in good time.

Typical black-box model examples applied for time series modelling are autoregressive (AR) models, autoregressive moving average (ARMA) models, AR with external input models (ARX), ARMA models with external input (ARMAX) and Box–Jenkins (transfer function) models. A recent example of the use of Box–Jenkins models for prediction of the behaviour of a primary sedimentation tank in a WWTP can be found in El-Din and Smith (2002). Another example of input–output models, usually classified as an AI methodology, is the use of artificial neural networks (ANN). ANNs are normally very effective to capture the non-linear relationships that exist between variables in complex systems, and can also be applied in situations where insufficient process knowledge is available to construct a white-box model of the system. A recent example of ANN models applied for the estimation of the influent COD load to a WWTP can be found in Baeza et al. (2002). In this application, the ANN model allowed to differentiate between situations of low, normal and high influent loads mainly based on oxygen uptake rate measurements in the activated sludge tanks.

Multivariate statistical methods (MVS) form another promising black-box modelling approach that is used for wastewater system monitoring and for time series modelling for predictions. Standard MVS methods such as principal component analysis (PCA) and partial least squares (PLS) have been used in many industrial applications for process monitoring, fault detection and isolation (e.g. Gregersen and Jørgensen, 1999). In recent years, a number of attempts have been made to implement MVS modelling methodologies on WWTPs. Several applications are focussing on predictions of quality parameters of the WWTP influent or effluent. However, a considerable amount of the reported results are based on daily average values of the on-line measured variables combined with off-line measured variables (Mujunen et al., 1998; Eriksson et al., 2001). Mujunen et al. (1998) used PLS models to predict deterioration of sludge sedimentation properties, and indicated that the PLS model was usually able to predict deterioration of sludge sedimentation properties 2–4 days in advance. Eriksson et al. (2001) applied MVS methods to predict the influent COD load to a newsprint mill WWTP. Real on-line prediction of deteriorating plant performance and sludge washout could be used to induce suitable control actions on a full-scale plant. Advanced MVS tools, such as adaptive PCA and multi-scale PCA, have been used for WWTP monitoring by Rosen and Lennox (2001). In adaptive PCA, the PCA model is continuously updated, thereby compensating for the fact that the WWTP data usually are not stationary. The latter is a basic assumption in standard PCA. In multi-scale PCA, the data are decomposed using wavelets, thus resulting in different time-scales with decreasing level of detail or resolution. Theoretically this should allow separating faults in the different time scales relevant for the WWTP process. The challenge for these MVS methods, however, is to interpret and link the results of the advanced process monitoring model to the occurrence of significant events of interest in the full-scale process, and to subsequently use that information for process operation improvement.

The advantages of white-box and black-box modelling can be combined in a hybrid modelling scheme. Hybrid model is a term that is used to designate models based on first engineering principles, where specific functionalities, e.g. reaction kinetics, have to be estimated from process data. An example is the combination of a set of differential equations with an ANN, where the differential equations incorporate the a priori process knowledge, whereas the ANN is used to predict a number of key parameters (e.g. Thibault et al., 2000; Ignova et al., 2002). Côté et al. (1995) coupled a white-box activated sludge model with an ANN model. In this application, the ANN model was used to model the errors between the simulation output of the white-box model and the corresponding experimental values. If the prediction of a state variable was significantly improved by the ANN model, this gave an indication that the experimental data contained dynamics that were not yet included in the white-box model, i.e. the white-box model structure could be improved further. Crowley et al. (2001) developed a hybrid model consisting of a combination of a first engineering principles based model part with an MVS model part, where the MVS model was used to correct for modelling errors.

Kristensen et al. (2003) proposed a hybrid modelling methodology by combining stochastic grey-box modelling with non-parametric kernel estimators. The latter estimators provide functional relations for the specific unknown terms in the white-box model structure based upon data. The hybrid modelling methodology of Kristensen et al. (2003) cannot be applied to the complete white-box model but only to parts of it, since the method is rather computationally expensive. Hybrid models can be used for process optimisation (Crowley et al., 2001; Ignova et al., 2002).

Stochastic grey-box models only describe the most important relationships of the deterministic theory, and can also be identified from on-line data. In the WWTP area, stochastic grey-box models have been developed for the description of SS transport and deposition in sewer system (Bechmann et al., 1998, 1999). When these stochastic grey-box models for build-up of pollutants are identified, they can be combined with WWTP influent flow rate predictions. Carstensen et al. (1998) showed that simple regression models and stochastic grey-box models perform better than white-box sewer models for influent flow rate predictions. The predictions of flow rate and pollutant concentrations in the influent to the WWTP can provide valuable information to adjust the WWTP control strategy to the influent load variations.

The alternative modelling methodologies, some of which were mentioned in this overview, are especially useful for predictions of the influent load, for estimation of biomass activities and effluent quality parameters. In other words, these modelling methodologies are available to complement the process knowledge included in white-box models with predictions based on data in areas where the white-box model assumptions are not valid or where white-box WWTP models do not provide accurate predictions. In addition they can generate data, for example as influent flow rate and concentration profile predictions, which can subsequently be applied as input for simulations with the white-box model.

4. Combining artificial intelligence and white-box WWTP models

The last part of this review paper focuses on the combination of AI and (mainly) white-box WWTP models. The ambition of this part of the paper is not to give a complete overview of AI applications in relation to WWTPs, but rather to provide the authors' viewpoints on promising interactions between AI and white-box models in this field.

AI is a research area that involves use of ANN, genetic algorithms (GA), fuzzy logic, rule-based systems, knowledge-based systems, ontologies, case-based systems, agents, etc. An overview of AI methodologies often applied in the environmental field can be found in Rizzoli and Young (1997) and Cortés et al. (2000). Currently, the main AI applications are in data interpretation and data mining techniques, in problem diagnosis and decision support (Cortés et al., 2000).

4.1. Supervisory control systems

WWTPs are complex multivariable systems. Similar to chemical production plants, the developments in sensor equipment and automatic control techniques can also result in a significant improvement of the plant performance. However, such developments also increase system complexity and, consequently, increase demands on the skills of plant operators. To support plant operators in overcoming problems of system complexity supervisory control systems have been developed with the overall purpose of improving plant performance and increasing operational reliability of the plants through automation and efficient man–machine interface functionalities. Both AI methods and white-box models can play an important role in supervisory control systems: AI methods can maximise the knowledge extracted from data and operator experience and subsequently apply this knowledge to improve WWTP control, whereas white-box models allow evaluating scenarios based on the available process knowledge about the WWTP.

A scheme of the control hierarchy in an industrial process plant is given in Fig. 8. Process monitoring, including both fault detection and controller performance monitoring, fault diagnosis, process optimisation, setpoint generation for SISO control loops and decision support are important tasks for a supervisory control system. Ideally, the supervisory control system should consist of modular agents, i.e. systems that independently handle parts of the over-all problem based on small amounts of locally stored information. Expert systems, a simulator environment with the white-box plant model, a case-based reasoning system, etc., are all examples of agents that can be active in the supervisory control system. An integrated multi-level architecture for WWTP supervision was already proposed some time ago (Sànchez et al., 1996).

A number of AI methods applied for fault detection and diagnosis were summarized and illustrated with

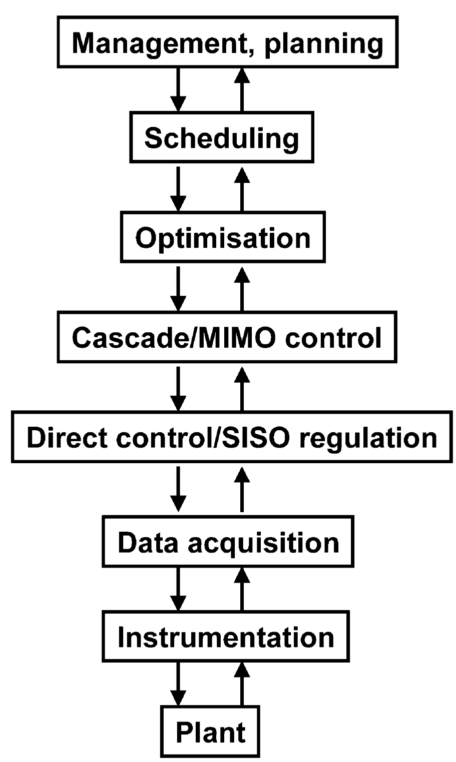

Fig. 8. Scheme of the control hierarchy in a process plant (Yazdi, 1997).

examples by Chiang et al. (2001). Chong and Walley (1996) concluded that probabilistic approaches, in that case Bayesian belief networks, performed considerably better than rule-based approaches (expert systems) for fault diagnosis in WWTP processes. This was attributed to the fact that the probabilistic approaches were better in representing the inherently uncertain behaviour of complex WWTP systems.

Evolutionary techniques are increasingly used in multi-objective optimisations, e.g. related to on-line optimisations in process control applications. Rauch and Harremoës (1999) presented a modelling study where GAs were applied to the control system of an urban wastewater system in the search for an optimal solution in a set of feasible candidate strategies. Chen et al. (2001) applied a three-stage analysis integrating different AI methods in their hybrid fuzzy-neural controller developed for an industrial WWTP. GAs were combined with ANNs in the first layer of this system, where the ANN represented the behaviours of the process states, and the GA was used to optimise the structure of the ANN model. A GA-based global search algorithm was applied in the second layer. Finally, an integrated fuzzy–ANN was proposed to auto-tune the fuzzy control rules.

Fuzzy logic, GAs, ANNs, probabilistic reasoning and rough set theory are AI methods that can be applied for predicting the input–output behaviour of a WWTP (Belanche et al., 1999), similar to black-box models. In the work of Baeza et al. (2002) an intelligent control system, including a number of expert rules, was used to adjust the aerated volume in a pilot plant based on influent load estimates obtained via an ANN model. The advantage of AI based prediction tools is that qualitative information can also be considered (Belanche et al., 2000). The combined use of several methods can result in reasonable prediction models, even in cases where data are missing. This was illustrated by Belanche et al. (2000) for a case study aiming at the prediction of sludge bulking in WWTPs.

Learning from previously successful situations or process failures is a key issue in improving the performance of the supervisory system. Sànchez-Marrè et al. (1999) present an approach to apply case-based reasoning to continuous domains such as WWTP systems. Deciding which elements constitute a case and efficient management of a considerable number of cases in the case library were considered as major problems. Basically, one day of WWTP system data were considered to constitute a case. However, one could easily imagine other ways of classifying cases. Rain events resulting in sludge wash-out or events with reduced sludge sedimentation properties are two examples of cases that could contain relevant information on WWTP operation that could be applied for learning how to better handle or prevent future events. In both cases, the duration and the intensity of the event can vary a lot. Thus, a number of rules or criteria need to be developed to decide on for example the beginning and the ending of relevant rain event cases.

AI methods and simulations with a calibrated white-box model of the treatment plant can be applied to support a supervisory control system as complementary techniques (Rodriguez-Roda et al., 2002). The white-box model incorporates the knowledge about the process, and also can be used in the frame of an on-line process optimisation scheme. Parallel application of different AI methods, of black-box (see Section 3), stochastic grey-box and white-box models should result in increased reliability of the supervisory control system (Cortés et al., 2000; Rodriguez-Roda et al., 2002). Again it should be emphasised that modular agent-based systems provide great potential. An obvious application of AI methods in supervisory control systems would be to distinguish between dry weather and rain weather situations based on on-line WWTP data, and to subsequently introduce a modification of the control objectives of the WWTP related to the change in weather conditions. In dry weather conditions operating cost minimisation while satisfying effluent pollutant concentration limits could be the main objective, whereas in rain weather it could be avoidance of sludge wash-out from the WWTP.

Rodriguez-Roda et al. (2002) successfully evaluated an agent-based supervisory system with three layers. The lowest layer was responsible for data gathering from different sources, for data validation (outlier detection, missing value replacement, filtering) and for a number of calculations with the validated data. Calculations included for example derivatives of some variables, and averages calculated over different time windows. The middle layer consisted of a parallel expert system and a case-based reasoning system. The expert system, consisting of three modules, was used for detection of faults, plant operational problems and transition process states evolving as a result of the problems related to the other two modules. The knowledge base of the expert system, summarised literature data, WWTP expert knowledge and knowledge obtained from the WWTP database. The case-based reasoning system allowed classifying each day with operational WWTP data as a case, and by comparison with a historic case library, to learn from past operating experiences.

4.2. Potential application of AI methodologies to WWTP modelling

This last part of this paper is probably the most speculative part, as it will try to provide an indication on how AI tools could interact with WWTP models to support the modeller in a range of model application tasks. As illustrated in Section 2 of this paper, examples of white-box WWTP model applications are simulation, design and control. It was explained in detail that the development of a calibrated white-box WWTP model is a rather complicated process that involves a considerable level of expert knowledge. Ideally, a modelling tool should be available to guide the modeller through the different steps of the model development process. AI methodologies could be very useful to support the modeller in this process, and to provide guidance through the different modelling steps, from the definition of the model purpose and the model selection to providing support in the data collection, the data reconciliation and the model parameter calibration. Already in the model purpose definition step, AI tools could play an important role, for example via pattern recognition methods to extract knowledge from a historic library of white-box WWTP models resulting from earlier model applications. As soon as the purpose for a new modelling task is defined AI methodologies, for example case-based reasoning, could search in the WWTP model library and, if available, automatically retrieve information on similar cases that have been solved in the past. AI methodologies could thus provide a structured way to learn from past modelling experiences, resulting in a more efficient model development process. Indeed, ideally a model retrieved from the historical model database could be reused with only few modifications to obtain the WWTP model of a similar plant in the modelling application that is currently at hand.

When applying a model for control purposes, AI methods could be applied to provide support in sensor–actuator pairing and control structure selection tasks. Ideally, a plant-wide control system should be developed as a number of agents such as SISO control loops, AI based fault diagnosis and decision support tools that interact with each other.

WWTP design is mainly based on standard design rules and knowledge of human experts. Clearly, there is a great potential to apply AI methods in this area. Finally, AI methods could also be applied to represent the knowledge about a domain, in this case WWTP plants. The knowledge represented in the AI system could subsequently be applied for automatic generation of the differential equations that constitute the white-box model. For example, if the WWTP plant under study includes biological nitrogen removal and often shows inhibition of nitrification by toxic components, then the AI based system could automatically generate a parsimonious set of differential equations that can describe such a process.

5. Conclusions

Activated sludge modelling and simulation are widely applied. Learning, design and process optimisation are the main application areas of white-box WWTP models. The introduction of the ASM model family by the IWA task group was of great importance in this field, providing researchers and practitioners with a standardised set of basis models. These basis models are mainly applicable to municipal wastewater systems, but can be adapted easily to specific situations such as the presence of industrial wastewater. A step-wise procedure leads from the model purpose definition to applications using a calibrated WWTP model. It was illustrated how the model purpose influences the model selection, the data collection and the model calibration.

A second part of the paper focussed on alternative modelling methodologies such as black-box, stochastic grey-box and hybrid modelling. It was illustrated how the different modelling methodologies can complement and support the process knowledge included in the white-box activated sludge models, for example in situations where the white-box models are not valid or provide predictions that are not sufficiently accurate.

AI methodologies and white-box models can interact in many ways. Supervisory control systems for WWTPs are one application. A white-box model calibration tool, an AI based WWTP design tool and a knowledge representation tool in the WWTP domain are potential applications where a fruitful interaction between AI methods and white-box models could be developed.

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