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Review

A critical comparison of systematic calibration protocols for activated sludge models: A SWOT analysis

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Abstract

Modelling activated sludge systems has gained an increasing momentum after the introduction of activated sludge models (ASMs) in 1987. Application of dynamic models for full-scale systems requires essentially a calibration of the chosen ASM to the case under study. Numerous full-scale model applications have been performed so far which were mostly based on ad hoc approaches and expert knowledge. Further, each modelling study has followed a different calibration approach: e.g. different influent wastewater characterization methods, different kinetic parameter estimation methods, different selection of parameters to be calibrated, different priorities within the calibration steps, etc. In short, there was no standard approach in performing the calibration study, which makes it difficult, if not impossible, to (1) compare different calibrations of ASMs with each other and (2) perform internal quality checks for each calibration study. To address these concerns, systematic calibration protocols have recently been proposed to bring guidance to the modeling of activated sludge systems and in particular to the calibration of full-scale models. In this contribution four existing calibration approaches (BIOMATH, HSG, STOWA and WERF) will be critically discussed using a SWOT (Strengths, Weaknesses, Opportunities, Threats) analysis. It will also be assessed in what way these approaches can be further developed in view of further improving the quality of ASM calibration. In this respect, the potential of automating some steps of the calibration procedure by use of mathematical algorithms is highlighted.

Keywords: Activated sludge models (ASMs); Calibration; Systematic protocols; SWOT analysis

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Nomenclature

ASM	activated sludge model
b_H	endogenous decay coefficient of heterotrophs, d^{-1}
BOD	biological oxygen demand
CFD	computational fluid dynamics
COD	chemical oxygen demand
COD_{tot}	total COD concentration, mgCOD/l
DO	dissolved oxygen, mgO_2/l
EBPR	enhanced biological phosphorous removal
GLUE	generalised likelihood uncertainty estimation
f_p	inert fraction of biomass (ASM1)
f_{SI}	inert fraction of the influent soluble COD
f_{XI}	inert fraction of biomass (ASM3)
FIM	fisher information matrix
MLSS	mixed liquor suspended solids, mgSS/l
NH_4	ammonium, mgN/l
NO_3^-	nitrate, mgN/l
NUR	nitrate uptake rate
OED	optimal experimental design
Q	measurement error matrix
S_I	soluble inert COD, mgCOD/l
S_{ND}	soluble readily biodegradable organic nitrogen, mgN/l
S_S	soluble readily biodegradable COD, mgCOD/l
SA	sensitivity analysis
SBR	sequencing batch reactor
SRT	sludge residence time
SWAT	soil and water assessment tool
SWOT	strength, weaknesses, opportunities, threats
TKN	total Kjeldahl nitrogen, mgN/l
WWTP	wastewater treatment plant
X_{ND}	slowly biodegradable particulate organic nitrogen, mgN/l
X_I	inert particulate COD, mgCOD/l
X_S	slowly degradable particulate COD, mgCOD/l
X_{STO}	storage products of heterotrophs, mgCOD/l
Y_H	heterotrophic yield
y	measured variables vector

Greek symbols

μ_A	maximum growth rate of autotrophic biomass
μ_H	maximum growth rate of heterotrophic biomass
θ	parameter vector

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1. Introduction

Activated sludge models (ASMs) are a compact and elegant summary of the state-of-the-art understanding of activated sludge processes (Henze et al., 2000). Calibration of ASMs is strictly required prior to the application of dynamic models for a wastewater treatment plant (WWTP). It consists of several steps, including lab-scale experiments for the characterisation of the influent wastewater and the determination of the kinetics/stoichiometry of the biological processes ongoing in the WWTP. To this end, numerous experimental methodologies have been developed and applied to full-scale systems (Ekama et al., 1986; Henze et al.,

1987; Sollfrank and Gujer, 1991; Kappeler and Gujer, 1992; Vanrolleghem et al., 1999; Petersen et al., 2003). These experimental designs are often based on respirometric techniques and were developed particularly for calibration of the aerobic processes in ASM1. For a thorough review on this issue the reader is referred to Petersen et al. (2003). In addition to these lab-scale experiments, dedicated measurement campaigns consisting of intensive sampling and measurements of influent and effluent variables every few hours over a period of a few days to a week, are typically used to catch the dynamics in a WWTP (see e.g. Petersen et al., 2002).

The next step in the calibration is to transfer the results collected from the lab experiments into the ASM model parameters. In this step, the influent chemical oxygen demand (COD) fractions, i.e. the ratios of S_S/COD_{tot}, S_I/COD_{tot}, X_S/COD_{tot}, X_I/COD_{tot} and influent nitrogen fractions S_{ND}/TKN, X_{ND}/TKN determined from influent wastewater characterisation experiments are used to construct dynamic influent loading data for the treatment plant model. This is typically performed as follows:

1. The influent COD and nitrogen fractionation results are assumed constant for the particular wastewater under study
2. These influent COD fractions are then multiplied with the dynamic COD and TKN measurements obtained e.g. every 2–4 h from the intensive measurement campaign data. In this way, the dynamic influent S_S, S_I, X_S, X_I, X_{ND} and S_{ND} profiles are estimated.

After the dynamic influent data are constructed, they are used as input to calibrate the kinetic/stoichiometric parameters of the model so as to obtain a good fit to the measured dynamics in the WWTP, e.g. to measure MLSS, measure NO_3–N in the aeration tank, in the effluent, in the return cycle, etc. Currently, the calibration is mostly performed manually. This means the modeller tries to manually change one parameter at a time until a good model fit to the measurements is obtained (visual observation). The information obtained about the kinetic/stoichiometric parameters of the biological processes from the lab-scale experiments is also used in this step. This way of calibration is simply based on expert-knowledge and driven by ad hoc approaches. In fact, calibration of a model without expert-knowledge was reported to be a very dangerous task, bound to lead to nonsense results (Andrews, 1991).

It is striking to observe that each calibration study published in literature has followed its own procedure in choosing the type of lab experiments for the influent characterisation and the kinetic/stoichiometric parameter estimation, parameter subsets to be calibrated, hydraulic characterisation and settling characterisation. This makes it difficult or even impossible to compare and quality check calibration studies since there is no common basis. To address these concerns, recently systematic calibration protocols have been proposed after recognizing this wide range of degrees of freedom used during calibration studies (Hulsbeek et al., 2002; Vanrolleghem et al., 2003; Langergraber et al., 2004; Melcer et al., 2003). Although the objective of these calibration protocols is to aid modellers in calibration studies, the main message is that perhaps a standard procedure for calibration of ASMs (particularly ASM1) would be welcomed and could be used for quality check and comparison reasons.

The objective of this paper is to critically and thoroughly compare the abovementioned systematic calibration protocols. To this end, a SWOT (strengths, weaknesses, opportunities and threats) analysis of these protocols will be performed in view of identifying advantages and disadvantages of each protocol. Following the SWOT analysis, a general discussion of the state-of-the-art of ASM calibration will be provided. Finally, critical issues to be considered in the future development of ASM calibration will be highlighted in view of improving the existing calibration approaches and developing a (partially) automated calibration protocol.

2. Systematic protocols for activated sludge model calibration

2.1. Summary of the four systematic calibration protocols

2.1.1. The BIOMATH calibration protocol (Vanrolleghem et al., 2003)

The BIOMATH protocol was developed by Vanrolleghem and co-workers (Petersen et al., 2002; Petersen et al., 2003; Vanrolleghem et al., 2003) to meet the need for a standard model calibration procedure. Fig. 1 illustrates the different general steps in this procedure. Depending on the first step of the protocol, which is defining the goal of the model calibration, not all steps may need to be followed. The BIOMATH protocol is further composed of four main stages. These are the plant survey and characterization, steady state calibration, dynamic calibration and evaluation of the calibration result.

The first stage of the protocol consists of a comprehensive plant survey to identify the general plant layout, configuration, operational parameters, average (e.g. yearly) input and output characteristics and plant performance. The quality of data collected at this stage is analysed and verified, using e.g. mass balances, prior to use in the different levels of calibration. The information gathered at this stage is used to select the

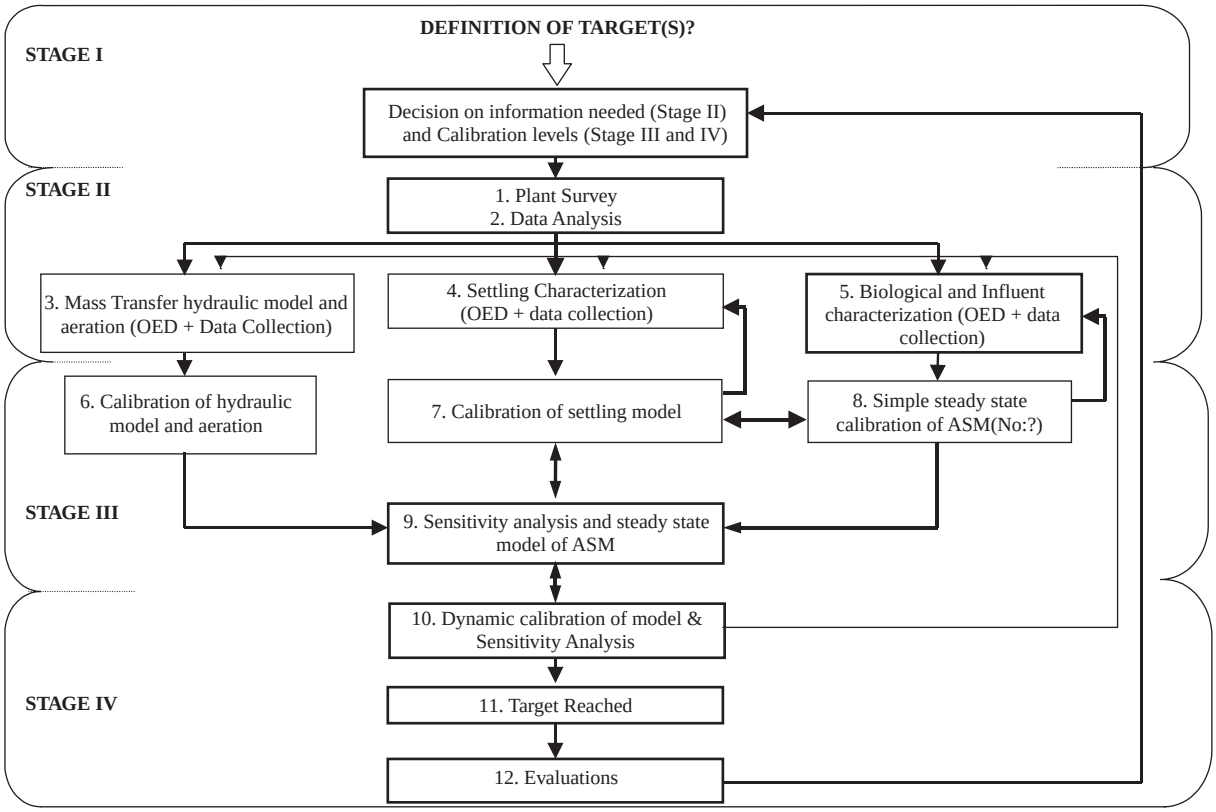

Fig. 1. Schematic/general overview of the BIOMATH calibration protocol (Vanrolleghem et al., 2003).

different sub-models for hydraulic, settling and biological processes of the WWTP.

The full-scale model—which is defined here as the complete model of the full-scale WWTP under study, is partitioned into three compartments: the mass transfer model (hydraulic and oxygen transfer), the settling model and the biological model. Each sub-model is first calibrated separately using the average (flux-based) influent data collected in stage I. After separate calibration, the three models are incorporated into the full-scale model and a steady-state calibration of the model is performed. The ultimate goal of this steady-state calibration is to obtain a good fit to the average sludge production and oxygen consumption of the plant. The parameter subset to be calibrated during steady-state calibration is determined by performing a sensitivity analysis, but usually those parameters which have effect on sludge production on long-term e.g. X_I, b_H, Y_H, f_{XI}, are used.

In case a high calibration accuracy is required, additional data collection can be performed for each sub-model and it is suggested to use optimal experimental design (OED) methodology (Dochain and Vanrolleghem, 2001). The ultimate purpose of using OED is to design data collection campaigns on a quantitative and objective basis to maximise the information content of the data and reduce the associated cost.

After steady-state calibration, dynamic calibration of the full-scale model is performed. In the dynamic calibration step, the influent data obtained from a dynamic measurement campaign (intensive sampling) are used as input to the model. The most sensitive parameter(s) are again determined by analysing the sensitivity functions of the measured variables to the model parameters. The variables to be considered in the sensitivity analysis are usually defined by the goal of the study. For example, if the aim is to minimize the effluent nitrate, then the output variable for the sensitivity analysis is chosen as the nitrate concentration in the effluent.

Lab-scale experiments may be planned to collect more information on the most sensitive parameters. Similar to the preceding step, OED can be used to design information rich (and cost effective) experiments for accurate determination of important parameters determined from the sensitivity analysis. The value of the parameter(s) estimated from lab-scale experiments can then be used in the dynamic calibration. Alternatively, these parameters can be estimated by using the full-scale

data. The same procedure can also be applied for the settling characterization and mass transfer calibration.

After the dynamic calibration is completed, the calibrated model is validated, e.g. using dynamic measurement campaign data collected under different operating conditions of the WWTP. If the predictions of the calibrated model for one or several components (e.g., effluent or in-tank NH_4-N, NO_3-N, MLSS, DO, etc.) are not sufficiently good, then the model has to be re-calibrated.

2.1.2. *The STOWA calibration protocol (Hulsbeek et al., 2002)*

This protocol has been developed in the Netherlands, and was the result of extensive experiences obtained from calibration of over 100 WWTPs (Hulsbeek et al., 2002). Fig. 2 illustrates the main flowchart of this protocol. Similar to the BIOMATH protocol it starts with the formulation of the objectives. After this, a definition of the relevant processes can be made. In the data collection and verification stage the composition and rates of the flows to the different process components, as well as the volume of the process components are defined. Mass balances are strongly advised in order to check data consistency, e.g. to check the SRT of the system, erroneous flow rates etc. In case the data is not consistent or the mass balances are not closed, then the operational parameters (e.g. the SRT or the recycle flowrate) should be corrected before proceeding further into calibration of the model (see details in Meijer et al., 2001, 2002).

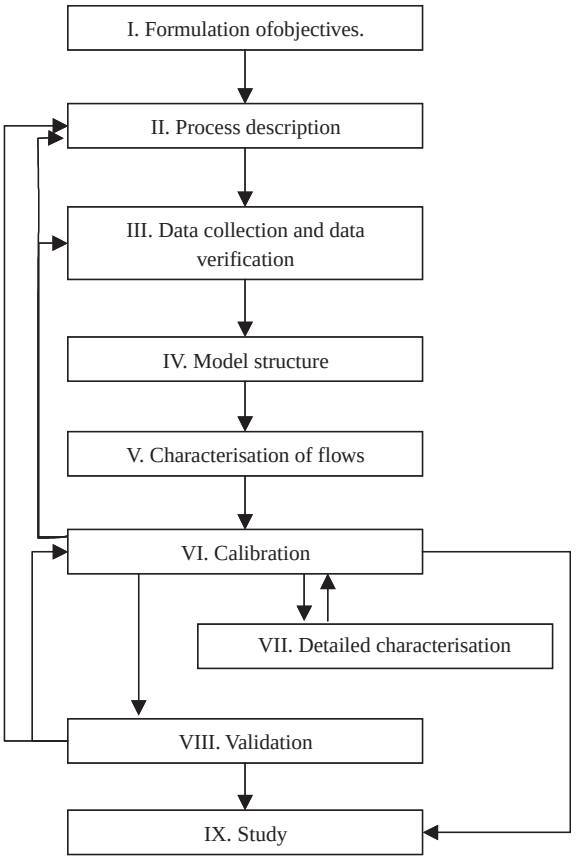

Fig. 2. General overview of the STOWA protocol (Hulsbeek et al., 2002).

In the fourth step of the protocol, the model structure of the WWTP is defined. This comprises the selection of sub-models for the description of hydraulics, aeration, settlers and the controllers of the WWTP. In the following step, information concerning the different flows in the WWTP is collected, i.e. influent, effluent, recycle, waste and internal recirculation flows are all quantified.

Finally, the ASM can be calibrated. At this stage, the protocol advises to perform an initial calibration and to compare the simulation results with the plant data. If there is a considerable discrepancy between model and measurements, the protocol advises to check the data quality again by performing additional measurements/checking again the mass balances. After verifying (or correcting if appropriate) the mass balances, the detailed calibration can be performed. To this end, the STOWA protocol provides a manual calibration procedure in which parameters of different biological processes are calibrated one at a time until a good fit is obtained to the plant data.

In the STOWA protocol, influent wastewater characterization is based on physical-chemical methods combined with biological oxygen demand (BOD) tests. A detailed discussion on the use of BOD tests and their shortcomings are also provided.

A step-wise procedure is proposed to manually calibrate the full-scale model considering the available measurements obtained from a detailed dynamic measurement campaign data. Different parameter subsets of the ASM model to be calibrated with respect to different variables are presented in an order of importance resulting from the experiences of STOWA.

After the calibration is completed, the model should be validated using plant data from a period different than the period used in the calibration. After the model has successfully passed the validation stage, it can finally be used for its ultimate purpose.

2.1.3. *The Hochschulgruppe (HSG) guidelines (Langergraber et al., 2004)*

This calibration protocol was introduced by several academic institutes (Hochschulgruppe) working on simulations of ASMs from Germany, Austria and Switzerland (Langergraber et al., 2004). The general structure of this protocol is shown in Fig. 3. Similar to the other protocols, the first step is the definition of the objectives of the calibration study. Then, complete

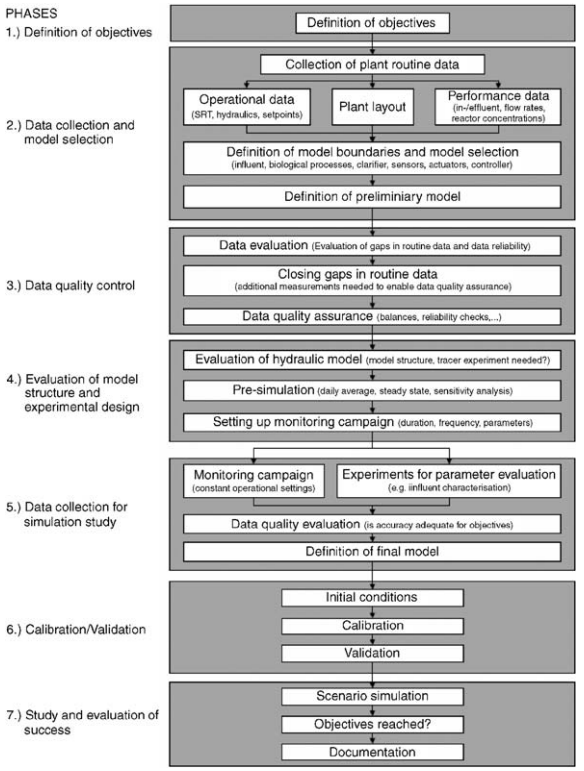

Fig. 3. Flowchart of a simulation study according to the HSG guideline (Langergraber et al., 2004).

information on plant layout, operation and plant performance is collected. Using this general plant information the preliminary model for the WWTP under study is selected. It consists of sub-models for hydraulics, settler, controllers and biological compartments. In the third step of the protocol, the quality of the plant data is checked and verified using mass balances, similar to the other protocols.

Prior to dynamic calibration of the model, i.e. at the fourth phase, the hydraulic sub-model is calibrated. A tracer experiment or, alternatively, computational fluid dynamics (CFD) is proposed to determine the required number of tanks in series for adequate modelling of the aeration tank mixing behaviour. After the hydraulic sub-model is calibrated, a pre-simulation is performed. In this step, a steady-state simulation of the model is performed and the results are compared with average plant data. Also, a sensitivity analysis is performed to determine the most influential parameters.

In the fifth phase, a measurement campaign is set-up and performed to collect data about the plant dynamics for use in the dynamic calibration of the full-scale model. The frequency and location and type of measurements should be determined based on the evaluation of the model in the preceding steps. The duration of the dynamic measurement campaign is advised to be 10 days long to include the plant performance of at least one weekend. At this step, also a data quality and consistency check is applied.

During the sixth phase, the dynamic calibration of the model is performed. First, the model variables should be initialized by simulating the model several weeks depending on the SRT of the plant. Then the model parameters should be calibrated following an iterative procedure similar to the STOWA protocol. The success of the model calibration is judged through visual checks considering peak and median values of the simulation results. Similar to the above protocols, the HSG guidelines also advise to perform model validation. The calibrated model is confronted with plant data under conditions different than those of the calibration period (e.g. different temperatures, sludge ages, etc.).

In the seventh and final step, the calibrated and validated model is used to simulate different scenarios defined according to the objectives of the study. A performance index criterion is proposed to compare these scenarios. Finally, the calibration study is completed by thoroughly documenting all details and steps followed until the target was reached i.e. a successfully calibrated and validated model.

2.1.4. *The WERF protocol for model calibration (Melcer et al., 2003)*

This protocol reflects the North American (United States and Canada) practice of ASM calibration and is based on a large number of experiences of consultants and researchers with modelling of full-scale activated sludge treatment plants for a wide range of purposes. Unfortunately, a general structure/scheme summarizing each step of the proposed WERF protocol is not available (yet) (see Melcer et al., 2003).

The general methodology of the WERF protocol can be summarized as follows: in the first step, the plant configuration is set-up in the simulator (collection of physical plant data, influent loading data and plant performance data). In the second step, additional data is gathered about the WWTP under study. This step includes collection of historical data, new measurements (full-scale and lab-scale) and clearly stating underlying assumptions. The third step is the calibration step, which is performed differently at different calibration levels (a *tiered approach,* see below). The fourth step is the model validation. Finally, upon successful validation, the model is ready for full-scale application.

Similar to the other protocols, the WERF protocol depends very much on the objective of calibration and it proposes a tiered approach with four different calibration levels. In this approach, the model calibration starts from a simple level and advances to a more sophisticated/complicated levels. With each increasing level, the accuracy of the calibration increases too. Calibration

level 1 uses default values and assumptions for the full-scale model. This level of calibration is used for designing a new WWTP where no information about the process and the influent wastewater is available.

The calibration level 2 only uses historical data for calibration of the WWTP. An important point of attention is the so-called data conditioning, which includes processing, cleaning and correction of the raw historical data. In this step, time series analysis of data and statistical methods can be used to detect sensor-fouling, outliers etc. The filtered data set is then subjected to the *data reconciliation* step. In this step, the quality of the plant data is checked using mass balances and expert engineering knowledge. For this calibration level 2, several parameters that can be determined from the historical data are also indicated (e.g. f_{SI}, f_{XI}, SRT, affinity constants, etc.)

Calibration level 3 aims to further improve the results of the calibration by setting up a dynamic monitoring/measurement campaign to collect high frequency data about plant dynamics and influent characteristics. *Stress tests* are also performed to determine the maximum capacity of the plant under extreme conditions, e.g. when the plant is under extreme influent loading, or when failure of clarifiers occurs, etc. Moreover, hydraulic (mixing behavior) characteristics of the aeration tanks can also be determined, e.g. by performing tracer tests or using empirical formulae.

In calibration level 4, direct parameter measurements are included. In other words, detailed influent wastewater characterization and detailed kinetic/stoichiometric parameter estimation is performed. This calibration level is advised in case calibration level 3 fails to deliver a successful calibration result due to the poor information content of the dynamic measurement campaign data or the complexity of model. The main focus in lab-scale experiments is given to the determination of the nitrification parameters (particularly the growth and decay rate of autotrophs) and influent characterization. Usually an SBR-based experimental procedure is used/proposed.

2.2. SWOT analysis of the systematic calibration protocols

The systematic calibration protocols have a lot in common. First of all, all of them start with a clear definition of the objective of the model calibration and emphasise the importance of data quality checking and verification (and ultimately correcting). Further, they all demand a similar validation step after the calibration. However, there are also significant points where each protocol has a different approach. For example, the experimental methods for determining influent wastewater characterisations, kinetic/stoichiometric parameter estimation are all different in the BIOMATH, STOWA and WERF protocols. The same holds for the design of a dynamic measurement campaign, or how to perform the calibration of model parameters etc.

In order to make the picture clearer and thoroughly compare these protocols, a SWOT analysis was performed and it is summarised in Table 1.

2.2.1. The BIOMATH calibration protocol

The BIOMATH protocol has a detailed procedure for the characterisation of settling, hydraulic and biological sub-models of the WWTP. For characterization of each sub-model, several (at least two) methods are proposed, each associated with different underlying assumptions and calibration accuracies.

As the characterisation of settling and hydraulic models are usually more straightforward, the BIOMATH protocol focuses more on the identification of the biological sub-model, i.e. the influent wastewater characterisation and parameter estimation of the biological processes. The latter heavily rely on respirometric measurements. These respirometry-based methods have both positive and negative aspects. First of all, it is a more ASM-related approach because it analyses the biomass response to different fractions of wastewater in contrast to the physical–chemical methods, which only evaluate physical properties of the wastewater. However, it is not always straightforward to interpret respirograms and quantitatively determine readily biodegradable COD, (S_S), and slowly biodegradable COD, (X_s), without the use of a model. Moreover, storage phenomena are increasingly shown to occur in activated sludge treatment plants which make it difficult to separate the degradation of the X_S wastewater fraction from the utilisation of internal storage polymers, X_{STO}. This will add some uncertainty to the correct determination of the S_S and the X_S fractions in the influent wastewater.

The estimation of kinetic and stoichiometric parameters of the biological model from OUR measurements has been shown to be possible with a high accuracy. Moreover, the parameter estimation can be performed simultaneously with the wastewater characterisation. The respirometric methods require model-based interpretation and demand dedicated software and trained users. As the interpretation of the respirometric methods depends on the initial conditions used in the test, i.e. the biomass composition, care should be exercised. The biomass composition is typically estimated from steady-state simulations taking into account the history of the plant at least 3 times SRT days before the biomass sample was taken. For this, the actual data that have to be collected anyway for the steady-state calibration of the full-scale model can be used (see the existing protocols).

Sensitivity analysis is proposed as a tool to point out the parameters that influence the process behaviour

Table 1
Strengths, weaknesses, opportunities and threats (SWOT) of the different calibration protocols

	Strengths	Weaknesses	Opportunities	Threats
BIOMATH	Detailed settling, hydraulic & biological characterization Detailed influent characterization Biomass characterization Sensitivity analysis/parameter selection OED for measurement campaign design Structured overview of protocol Feedback loops	Respirometric influent characterisation requires model-based interpretation OED has not been applied yet in practice but research is ongoing OED software and specialist required No detailed methodology for data quality check No practical procedure for parameter calibration	Generally applicable Works efficiently once implemented in a simulator Dynamic measurement campaigns can be designed and compared based on OED	Not all modelling and simulation software have OED/Sensitivity analysis (SA) High degree of specialisation is required for the application
STOWA	Detailed settling and biological characterization Process control Time estimate for different calibration steps Detailed data quality check Step-wise calibration of biological process parameters Structured overview of protocol Feedback loops	No detailed hydraulic characterization BOD test gives problems (f_p) No biomass characterization No guidance for measurement campaign design No detailed info on sensitivity analysis Fixed parameter subsets for calibration of biological processes	Easy to use Practical experimental methods No specialist required Good for consultants and new modelers	No mathematical/statistical approach for parameter selection for calibration May not be applicable for different systems since parameter subset for calibration may change for different WWTPs
HSG	CFD for hydraulic characterization Biological characterization Design of measurement campaign A standard format for documentation Data quality check Structured overview of protocol	No feedback loops in overview diagram Provides only general guidelines No detailed settling characterisation No particular methods for influent characterisation or parameter estimation No detailed sensitivity analysis/ parameter selection	Generally applicable A standard format for thorough documentation/reporting of calibration studies	Not detailed/practical enough for new practitioners The free choice of experimental methodologies for influent/kinetic characterisation may jeopardise standardization of calibration studies
WERF	Detailed influent characterization Detailed μ_A and b_A determination Biomass characterization Sensitivity analysis/parameter selection Detailed data quality check A *tiered approach* for calibration Several examples of case studies	No feedback loops Settling process less emphasized Almost no emphasise on other kinetic parameters than nitrification No structured overview of protocol	Based on practical experience A tiered approach for calibration provides different calibration levels for different goals and accuracy of calibration Good for consultants and new modelers	Focus on μ_A determination and influent characterization Ignoring the significance of the other compartments of the full-scale model Laborious methods

most. Based on this sensitivity analysis the selection of parameters to be calibrated can be made. Moreover, OED is proposed for design and comparison of (dynamic) measurement campaigns and dedicated batch experiments. As such it contributes to increasing the parameter accuracy from both full-scale and lab-scale data collection steps. The downside of the use of the sensitivity analysis and OED is that not all modelling and simulation software have such modules and so far a high degree of specialisation is required for the use of such a tool. However, the increased automation and efforts in improving user support should alleviate this.

The BIOMATH protocol does not emphasise in sufficient detail the methods for data reconciliation as the STOWA and WERF protocols do. From the structure of the BIOMATH protocol, it is also not clear to determine how the objective of the calibration study determines the specific calibration procedure to follow for a particular case study. This could be improved and clarified by mentioning the different calibration levels and associated procedures from the start, similar to the *tiered approach* used in the WERF protocol.

Overall, the BIOMATH protocol is oriented at employing scientifically more exact methods rather than using more empirical methods. This makes the BIOMATH protocol the most sophisticated of all four protocols but it may not be the most user friendly for new modellers entering the field. Still, once the OED methodology and sensitivity analysis can be incorporated into the calibration procedure by automating these activities, it may provide a good opportunity to improve the efficiency of model calibration (see below).

2.2.2. The STOWA calibration protocol

In the STOWA calibration protocol, the influent wastewater characterisation is based on combined BOD and physical–chemical measurements. Although physical–chemical methods give reproducible/consistent results, the BOD method leads to a major uncertainty with the determination of the inert particulate fraction, f_P (Roeleveld and van Loosdrecht, 2002). The results of the BOD method are very important since they determine the inert fraction of the wastewater, which is a key factor in determining the remaining fractions of the influent COD. To extend the STOWA protocol, Weijers (1999) has investigated the use of model-based interpretation of the BOD profiles using a simplified ASM1 model. Further investigation to improve the reproducibility of the BOD method could significantly improve this part of the STOWA protocol.

The steady-state calibration of the protocol is not acknowledged in the main structure of the model calibration. However, steady-state calibration results could be used to double-check the results of the mass balances similar to the three other protocols.

Biomass characterisation, i.e. the determination of the initial autotrophic and heterotrophic biomass concentrations in the WWTP, is not specified in the protocol. Moreover, guidelines or remarks concerning the design of dynamic measurement campaigns are not discussed in detail, even though this is the most expensive aspect of a model calibration study.

The STOWA protocol is the only protocol where a time estimate for the different steps involved in calibration is mentioned. However, it may not generally be applicable for different systems as the protocol is based on a range of studied WWTPs. Settling and biological characterization are addressed in detail, but relatively few details are provided on hydraulic characterization of the aeration tanks.

Further, the protocol puts little emphasis on mathematical and/or statistical methods such as OED that can be used for better design of measurement campaigns and lab-scale batch tests. Moreover, although the proposed manual calibration procedure is a great help for beginners, it may be dangerous to generalize it for full-scale applications. By definition, it is too difficult if not impossible to expect that the fixed parameter subsets proposed by the STOWA protocol (and the order of calibration of these parameter subsets) remain valid for different WWTPs. The possibility to calibrate these parameter subsets given in the STOWA protocol depends on the available information content of the plant data (quality, quantity, etc.) and plant operation/configuration. It would therefore be useful to check whether these proposed parameter subsets remain indeed the most sensitive in each calibration study.

Overall, the STOWA protocol appears to be the most straightforward, practical, easy to follow and implement protocol. In that context, this protocol (in addition to the WERF protocol, see below) is most suited for practical applications and as such it is expected to become popular among consultants. A very important function of the STOWA protocol could also be to guide the inexperienced modeller to understand the significant steps underlying a calibration study and perform a good quality calibration study.

2.2.3. The HSG guidelines

This protocol presents general guidelines to be followed and documented during a calibration study and is therefore generally applicable. It is aimed to provide a reference standard for the highest requirements regarding model calibration and validation studies. The ultimate goal is to systematize the documentation of the overall calibration study. However, no feedback loops are incorporated in the scheme implying that all calibration steps are straightforward and no internal check of each step is necessary.

On the other hand, the HSG guidelines do not emphasise the standardization of the calibration process

itself. The goal is that the whole simulation study is systematized, i.e. that all important factors to guarantee a good quality simulation study are considered. However, getting a good quality simulation study can be achieved in different ways. This certainly gives extra freedom for the modellers to decide which experimental methodologies to employ. However, in this way it may be questionable to what extent the calibration procedure is systematized. In other words, not imposing certain experimental methods may conflict with the ultimate aim of the protocol, which is to bring a standard for the overall calibration study. Also, new practitioners are not guided by the protocol to find adequate experimental methods for parameter determination and influent characterization.

Similarly, the choice of the parameters to be calibrated is also left to the practitioners. However, sensitivity analysis is proposed to identify the most sensitive parameters, which may help improving the choice of parameters subsets for calibration. Still, quantitative criteria are needed to rank the parameters, e.g. as suggested in Weijers et al. (1997) and Brun et al. (2002).

As an alternative to the traditional tracer test, the HSG guidelines proposes to use CFD to characterize the hydraulic (mixing behaviour) of the aeration tanks. This indeed could provide a better description of the hydrodynamics of WWTPs which may contribute to improving the quality of modelling of WWTPs. However, the use of CFD would further complicate the model calibration study, as it is currently a computationally demanding and time-consuming task.

At present, the HSG guidelines do not yet present a case study where the implementation of the protocol is illustrated on a full-scale WWTP. This would have improved the transfer of the protocol among practitioners. Overall, the HSG guidelines are the only protocol which proposes a certain format for reporting the overall calibration study, and this may indeed remarkably improve the ability to read and compare different calibration studies.

2.2.4. *The WERF protocol*

The WERF protocol lacks a clear, explicit structure of the different levels of the calibration procedure, which makes it not user-friendly to read and follow. Further, the WERF protocol presents detailed experimental methods for influent wastewater characterization and fractionation of active biomass, yet it provides relatively few explanations and methods for hydraulic and settling characterisation of the treatment plant. It is particularly important to note that the WERF protocol misses to adequately discuss the significance of biological reactions (particularly denitrification) ongoing in clarifiers and the need to consider them in the model-formulation step.

The experimental methodologies were particularly oriented at determination of nitrification parameters. On the one hand, this is a good point since methods for the determination of, for instance, the decay rate of autotrophs was lacking in the existing literature. However, the significance of the nitrification kinetics should not undermine the significance of adequately describing the kinetics of other biological processes, e.g. denitrification, EBPR, etc. The SBR-based experimental methodologies proposed to determine the growth rate of autotrophs could be powerful in providing information about wastewater and sludge characteristics, particularly for design of new WWTPs where no sludge is available yet. However, when sludge can be sampled from an already existing plant, the proposed methods may be rather laborious and not cost-effective, e.g. compared to batch respirometric experiments (Spanjers and Vanrolleghem, 1995). Further the SBR-based methods may involve the risk of triggering physiological changes in activated sludge thereby causing kinetic and stoichiometric behaviour which may not be representative to the original system (Grady et al., 1996) (see also below for a detailed discussion).

General guidelines to design a dynamic measurement campaign are proposed. However, these guidelines are still plant-specific and cannot readily be extrapolated to other WWTPs. In that sense, the design of a measurement campaign is left to the practitioners. Moreover, the proposed length of the dynamic measurement campaign is rather short i.e. 1–2 days. This short-term is not expected to adequately reflect the long-term dynamics of the plant. In that respect, the WERF protocol may imply that the model calibration results aim to catch daily dynamics of the plant rather than slower dynamics.

Overall the WERF protocol summarises a huge number of full-scale model calibration experiences. It manages also to present a so-called *tiered approach* for model calibration, which makes it possible for new modellers to choose a calibration procedure depending on the goal of the calibration. A very important point in this respect is the calibration level 2, which is based on the historical data of the plant. Such data are available for most of the WWTPs and can be used by the new modellers as a stepping-stone before starting to collect dynamic measurement campaign data, which is the most expensive step of a calibration study. In that respect, this protocol, in addition to the STOWA protocol, is expected to be attractive for inexperienced modellers and consultants.

3. General discussion

The SWOT analysis of the protocols shows that all protocols have comparable advantages and disadvantages and a large degree of similarities as well as

differences. Based on this SWOT analysis one could work towards a unified protocol, which should be evaluated and considered critically on various experiences with full-scale practitioners. Although all protocols highlight the very important point of standardisation of the calibration efforts, it is important to keep in mind that these protocols are the first steps in solving a very complex problem: calibration of ASMs. The state of the art of calibration of ASMs as summarised in these four systematic protocols, still faces several challenges, which are identified as follows:

1. Range of applicability of the protocols.
2. Technical limitation of tools/sensors for data collection.
3. Limitations in transferring lab-scale data to full-scale models.
4. Design of data collection (measurement campaigns): ad hoc versus mathematical approaches.
5. Complexity of model calibration: limited data versus complex model structure.

These challenges are further discussed below.

3.1. Range of applicability of the protocols

In general the calibration protocols have been developed for municipal WWTPs performing COD, nitrogen and to a lesser extent, phosphorous removal. Therefore, inherently, the calibration protocols are specialised to support the calibration of such full-scale WWTPs. However, some deficiencies in some of the existing protocols were observed when applied to guide application of ASMs to non-municipal WWTPs.

Particularly the proposed methods for wastewater characterization and parameter estimation may not be readily applicable to an industrial and non-domestic WWTP. For example, the determination of the maximum specific growth rate of ammonium and nitrite oxidizers in recently developed autotrophic nitrogen removal processes (e.g. the SHARON process (van Dongen et al., 2001)) will not be as straightforward as described in the WERF or the BIOMATH protocol, since ammonium and nitrite are present in such amounts that they will inhibit the ammonium and nitrite oxidation processes. Moreover, pH and salinity play an important role in the affinity and inhibition kinetics of these processes (Van Hulle et al., 2004; Moussa, 2004). When modelling an industrial tannery WWTP with high saline characteristics (Moussa et al., 2004), it was reported that the general experiences of the STOWA protocol with modelling municipal WWTPs, e.g. mass-balancing of plant flow data, the calibration procedure of parameters, etc. were indeed useful. However, at the other stages of model calibration, a great deal of expert knowledge and dedicated laboratory tests were required for successful characterisation of the tannery wastewater as well as to get adequate insight into the activity of nitrifiers under salt stress.

By the same token, it can be expected that the existing protocols may not be of great guidance when calibrating a WWTP with a biofilm reactor, e.g. trickling filter (Vanhooren, 2001). In the biofilm systems, it is believed that physical factors (mass transfer limitations, biofilm detachment (high shear forces), etc.) on top of the biological factors play a significant role. This unique feature of biofilm systems limits the ability to transfer the experiences gathered on suspended activated sludge systems. As such, the existing systematic protocols need to be extended to address these specific characteristics of the biofilm systems, e.g. determination of the active fraction of biomass, biofilm growth and detachment processes, mass transfer limitation, etc. (Vanhooren, 2001; van Loosdrecht et al., 2002).

In short, it is expected that the general structure of the protocol and the mathematical methods (sensitivity analysis, OED) may be useful for the modeller when calibrating a totally different WWTP than municipal plants with suspended cultures. It is proposed that the existing protocols are extended to include separate modules of calibration guidance for different WWTP systems (non-domestic, industrial, biofilm systems, etc.). In that context, it may also be useful for the calibration protocols to establish a field of applicability (which systems are they tailored for?) and validity (what are the limitations of the protocols?).

3.2. Technical limitation of tools/sensors for data collection

An important issue in model calibration concerns the availability of data. Strictly speaking the quantity and quality of input data determine the quality of the output of calibration (garbage in = garbage out). In that respect, the development of sensors and experimental methods for data collection has an important impact on the quality of model calibration, which also implies that the existing limitations in data collection may limit the quality of model calibrations.

At the full-scale WWTP level, the development of on-line, robust and reliable sensors for determination of influent COD and or COD fractions (S_S, X_S, X_I, acetate, etc.) may lead to a substantial improvement in the model calibration results. Indeed, in this way it will be possible to measure the input dynamics to WWTPs with a high frequency (currently, the influent COD is usually measured off-line every 2 h, similar to other influent components). On the market, UV- and UV/VIS-based sensors are already available to this purpose, however these sensors still require a rather tedious calibration procedure to provide measurements with good accuracy

that can be used for quantitative purposes (see e.g. Langergraber et al., 2003). More research is needed to improve these sensors to a level sufficiently reliable for use in model calibration purposes, especially for the measurement of different COD fractions. The authors still believe in the potential of on-line, automatic wastewater fractionation by using respirometry but further developments are needed to make this fully reliable (Vanrolleghem et al., 1996).

At lab-scale, the development and further fine-tuning of the existing experimental methods to determine kinetic and stoichiometric parameters of activated sludge is also a quite significant aspect by which model calibration accuracy can be improved. A very significant example is the fact that aerobic respirometry has been so far the most dominantly used experimental method to quantify influent COD fractions and kinetic/stoichiometric parameters of activated sludge. Thanks to the recent development of a reliable and accurate nitrate biosensor (Larsen et al., 2000), it was only recently possible to develop an anoxic respirometer –with a measurement accuracy and frequency similar to an aerobic respirometer (Sin and Vanrolleghem, 2004).The nitrate uptake rate (NUR) data obtained from this anoxic respirometer was also shown to be useful for determination of kinetic/stoichiometric parameters of the denitrification process (Sin, 2004).

Additional examples can be provided, e.g. experimental methods able to measure active fraction of biomass etc. However, the aim of this section is to emphasise the significance of data collection (quantity and quality), which may ultimately change the existing calibration protocols. In that context, the protocols should encourage the use and/or development of high quality methods for data collection and use these in the model calibration.

3.3. Limitations in transferring lab-scale data to full-scale models

Lab-scale experiments may offer a significant contribution to obtain additional information about activated sludge systems that can be used in the calibration of full-scale WWTP models. Numerous experimental methods have been developed to this purpose (see for a review, Petersen et al., 2003). However, the transferability and representability of results obtained from lab-scale experiments to full-scale models is still under discussion (Chudoba et al., 1992; Novak et al., 1994; Grady et al., 1996). The initial substrate/biomass (S/X) ratio was identified, among others, to be an important factor that determines the behaviour/response of activated sludge in lab-scale batch tests. However, there is no common agreement on this S/X ratio and, generally, the experimental procedures.

Recently, it was demonstrated that biomass sampled from full-scale WWTP displays various transient responses in typical batch experiments designed for calibration of ASMs (Vanrolleghem et al., 2004; Sin, 2004). For example, a fast-transient phenomenon occurring in the first 5 min of a respirometric experiment was observed to induce bias in parameter estimates (particularly the estimate of yield coefficient) unless the transient phenomenon is properly accounted for (see Vanrolleghem et al., 2004).

Particle size of activated sludge flocs was also shown to considerably influence the estimation of the substrate affinity constants from batch oxygen uptake rate (OUR) data (Gapes et al., 2004; Chu et al., 2004). In Gapes et al. (2004), the estimated oxygen affinity constant for the same nitrifying sludge obtained from a lab-scale SBR were found different for different particle sizes of activated sludge. It is noteworthy that in the same study the oxygen affinity constant for granular activated sludge was found to be 4.9 mgO_2/l. These results clearly show the impact of mass transfer limitations (either external (from bulk to liquid) or internal (from liquid to cell), see Gapes et al. (2004) and Wilén et al. (2004) on the estimation of parameters of suspended activated sludge cultures (Stenstrom and Poduska, 1980). Concerning model calibration, the activated sludge floc properties in combination with the hydrodynamics of the medium, i.e. mixing or aeration intensity, might influence the results obtained from lab-scale reactors too (Chu et al., 2004; Pérez et al., 2005). This in turn may add another challenge to their transferability to the full-scale WWTP model that has different reactor size, configuration and hydrodynamics.

In short, there is a need to further develop and standardize the experimental methodologies for data collection at lab-scale. The transferability problem of the lab-scale results is very significant and further research should be performed to resolve this issue. Solution of this problem is expected to directly contribute to the standardization of the experimental methodologies too.

3.4. Design of data collection (measurement campaigns): ad hoc versus mathematical approaches

So far measurement campaigns are designed mostly on the basis of ad hoc expert knowledge/experience, often resulting in sub-optimal and even poor data quality in view of model calibration. To better design experiments, mathematical techniques can be used. One of the existing techniques for this purpose is optimal experimental design based on the fisher information matrix (Eq. (1)) (Dochain and Vanrolleghem, 2001).

$$\mathrm{FIM} = \sum_{i=0}^{N} \left(\frac{\partial y}{\partial \theta}\right)_i^{\mathrm{T}} Q_i^{-1} \left(\frac{\partial y}{\partial \theta}\right)_i. \quad (1)$$

This matrix represents the information content of a specific experiment. It is calculated based on two components: sensitivity functions $\partial y/\partial\theta$ and measurement error (Q_i). Sensitivity functions express how sensitive certain measured variables are with respect to the model parameters. Measured variables, which are sensitive to certain parameters, contribute to the information content of the experiment in the sense that they, if measured, will provide useful data for calibration. Having sensitive measurement variables is not the only prerequisite for a well designed experiment, correctly quantifying measurement error is equally important. Measurement errors express how much trust one can have in the measurements and to what extent they contribute to the information content of the experiment.

The inverse of the fisher information matrix is the lower bound of the parameter estimation variance-covariance matrix which is expected after calibration on the data gathered from the proposed experiment. The diagonal elements of this variance–covariance matrix represent the variances of the parameter estimates and thus indicate how accurate a certain parameter will be estimated. Together with the diagonal elements, the off-diagonal elements (the covariances between parameters) can be used to calculate parameter correlations. Both information on variances and parameter correlations can be used to select parameters, which are practically identifiable. As such the parameter subset can be determined which can be estimated by model calibration techniques once the experiment is performed (Weijers and Vanrolleghem, 1997; De Pauw, 2005).

OED is based on model simulations and is therefore a very useful technique since it quantifies the information content of the data of a certain experiment before it is performed in practice. Using this technique, different experiments can be proposed based on the experimental degrees of freedom of the system under study: available measurements and experimental manipulations. The proposed experiments can be "virtually" simulated and their information content determined. Once the optimal experiment is found it can be performed in reality to collect the data. Based on this data the model can be (re)calibrated resulting in a model with more accurately estimated parameters.

Besides information content, other properties of experiments like cost of the measurement campaign, process stability under the proposed experimental conditions, … can also be evaluated based on the "virtually" simulated experiments (De Pauw, 2005). Taking all of these objectives into account may result in better designed experiments (e.g. higher information content, cost effective).

3.5. Complexity of model calibration: limited data versus complex model structure

An important step in the overall model calibration is the step where the (sensitive) parameter subset of the model is calibrated until a good/acceptable fit to the measurements is found. This calibration is predominantly performed ad hoc, manually and based on expert knowledge. The reproducibility of this (manual) calibration approach may therefore be questionable and introduces uncertainty into the model calibration. An alternative method to the manual calibration is obviously automatic calibration. However, until now we are not aware of any study where automatic calibration is successfully implemented (e.g. based on optimisation algorithms, see e.g. Wanner et al., 1992).

The main reason behind this failure is most probably due to the complex interaction between parameters of the different modules (e.g. hydraulic, settling and biological processes) of the full-scale WWTP model (Weijers et al., 1996; Weijers and Vanrolleghem, 1997; Brun et al., 2002). Assuming that the model structure is correct, the complexity of the model structure (e.g. the non-linearity of the model) becomes an issue when the available data is not informative enough –in terms of quality (e.g. noise level, accuracy etc.) and quantity- to determine all the model parameters (Beck, 1987; Dochain and Vanrolleghem, 2001). In practice, the full-scale WWTP data often require some consistency check. This is felt essential prior to any model calibration step. However, even abundant consistency checked data may be information poor (Beck and Lin, 2003) to identify all model parameters.

Not surprisingly, similar problems were encountered and reported in modelling other large-scale environmental systems (see e.g. Alewel and Manderscheid, 1998; Omlin et al., 2001). The common problem in this wide range of large-scale ecosystem models is that the model structure is too complex to successfully calibrate under the limited available data. To resolve this issue, usually advanced statistical/mathematical tools are applied. It is also believed that the use of advanced mathematical/statistical approaches (as opposed to expert-based/ad hoc/heuristic calibration approaches) will increase the accuracy of the calibration and contribute to further standardization of the calibration studies in activated sludge systems. In the following, the automatic calibration approach applied in the calibration of river quality models and a proposal for an automatic calibration methodology for activated sludge models are presented.

3.5.1. Automatic parameter uncertainty methodology as applied in hydrological modeling

In the field of hydrology, the problem of non-identifiability of parameters has led to an acceptance of the possible "equifinality" of models, which means that there is not one "optimal" parameter set to represent the system, but that there are many combinations of parameter values for a chosen model structure that may be equally good in fitting the data (Beven and Binley, 1992). These parameter sets may be distributed

across a wide range of values for each parameter, reinforcing the conclusion that it is the combined set of parameters that is important (Freer et al., 2001).

The generalised likelihood uncertainty estimation (GLUE) methodology (Beven and Binley, 1992) is able to define these parameter sets through the scanning of the entire parameter space. Since this requires a very large number of Monte Carlo simulations, it is very computationally demanding.

A much more efficient and statistically based method is ParaSol (van Griensven and Meixner, 2004) that is built on the global optimisation technique of the Shuffled Complex Evolution algorithm (SCE-UA) (Duan et al., 1992). ParaSol is able to perform multi-objective optimisation and parameter uncertainty estimation in an efficient way. It has been applied with success on a river water quality model-using SWAT (van Griensven and Meixner, 2004).

3.5.2. A partially automated calibration methodology for complex activated sludge models

In this section, it will be illustrated how some steps of the ASM calibration process can be facilitated by use of mathematical algorithms. The term partially automated calibration methodology refers to the procedure in which some steps among many others involved in model calibration (see e.g. steps 9 and 10 of the BIOMATH protocol in Fig. 1) are supported by computer programs while other steps will still depend on expert knowledge. It can be implemented as follows: before any calibration can be started the data should be verified. Once this is accomplished a parameter subset should be selected from the model, which can be calibrated based on the available data. One possible technique is the calculation of the Fisher Information Matrix (as discussed in Section 3.4). This combines sensitivity analysis and knowledge about measurement errors to determine the information content of the experiment and an estimate of the parameter estimation accuracy and correlations. From these results, parameters with predicted estimation accuracies higher than for example 30% and correlations higher than 50% should be regarded as unidentifiable. These cut-off values (30% and 50%) can be altered based on expert knowledge or preferences. Once the parameter subset is determined an optimisation algorithm can be employed to fit the model parameters within a realistic range to the data. Because of the selection of an adequate parameter subset, many of the numerical problems often encountered with classical search algorithms are avoided.

4. Future perspectives of Activated sludge model calibration

The SWOT analysis of the four systematic calibration protocols performed in this study revealed that these protocols have many similarities as well as differences. The major common points of the protocols are:

- Definition of goal—determines the overall calibration procedure.
- Data collection, verification and reconciliation is very significant (both design, operational data (SRT, flows, controllers, etc.) and additional measurements (intensive measurement campaigns).
- Validation—calibrated models should be validated using a data set obtained under different operating conditions than those of the calibration period.

The major differences of the protocol are:

- Design of the measurement campaign: frequency, location, duration of measurements.
- Experimental methods for influent characterisation and kinetic/stoichiometric parameter estimation.
- Calibration of the model parameters: selection of parameter subset, how to calibrate.

In view of the future of calibration of ASMs, it is strongly suggested to test these different protocols on a case study and to develop a unified protocol combining all the strengths and opportunities of each protocol.

From a scientific point of view, on the other hand, several problems still remain to be bottlenecks to the application of the existing calibration protocols as summarised below.

1. The range of applicability of the protocols should be extended to include WWTP systems other than municipal plants.
2. Technical limitations of tools/sensors in data collection still exist. The protocols should be regularly updated in parallel to new developments in this field.
3. Lab-scale data can be an important additional source of information to the calibration of full-scale model parameters. However, serious limitations do exist in transferring the lab-scale data to the full-scale model. Also important is the need to standardise lab-scale experiments to ascertain a high accuracy of lab results.
4. The design of data collection (measurement campaigns) should be based on more advanced mathematical tools rather than expert knowledge. By designing clever data collection campaigns (information rich but low cost), a considerable cost reduction can be achieved for the overall calibration study.
5. Full-scale ASMs are rather complex models to identify under limited and information-poor data. This aspect of model calibration may be improved by applying partially automated calibration procedures, e.g. for the selection of an identifiable parameter

subset and the estimation of the identifiable parameters using mathematical/statistical approaches (sensitivity analysis, FIM, collinearity index), as it is currently practised in other large-scale complex ecosystem models (Beck, 1987; Beven and Binley, 1992; van Griensven and Meixner, 2004).

Further the SWOT analysis also reveals that from an application/engineering point of view, calibration studies have to seek a balance between more scientific approaches and pragmatic approaches constrained by the time, budget, qualified personnel and equipment available for the task at hand. This issue should be considered in the development of better calibration protocols.

The recently introduced calibration protocols have attempted to tackle the rather complex calibration issue of ASMs, but still remains to be the weakest link in the overall modelling of activated sludge systems. Results of the SWOT analysis as well as the abovementioned problems may benefit from a multidisciplinary approach to improve the identifiability of ASMs: advanced mathematical/statistical tools, development of robust sensors, improvement of batch experiments, understanding of the transient response of biomass in batch tests, etc. With this critical review and the discussion provided in this study, it is hoped to contribute to the further advancement of the calibration practice of ASMs.

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