A COMPREHENSIVE MODEL CALIBRATION PROCEDURE FOR ACTIVATED SLUDGE MODELS

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ABSTRACT

A methodology for calibration of the activated sludge plant models is proposed on the basis of consolidated engineering experience and a scientific approach. According to the method, the definition of the target(s) plays a crucial role in the selection of the steps incorporated in this so-called 'Biomath-Calibration' protocol. For the activated sludge modelers this protocol tries to combine and link the state of the art methodologies for calibration of different processes in a wastewater treatment plant (hydraulics, biological reactions, sedimentation processes, etc.), and it can thus be used as a complete guideline for extensive model calibration tasks. Finally, an application of the methodology is presented in a case study for a nutrient removing oxidation ditch system.

INTRODUCTION

Robust model-based optimization of wastewater treatment plants necessitates successful calibration of the complex wastewater treatment plant models. The word 'successful' relates to the prediction capability of activated sludge models under variable process conditions, where the model should describe the plant behavior within realistic margins taking into account the uncertainties on the inputs and reactions taking place in the system.

In recent years, the complexity of the models has increased considerably with the discovery of new processes (Henze *et al.*, 2000; Barker and Dold, 1997), and as a result the modelling task became more time consuming with *ad hoc* calibration of the model parameters. In this context, a compromise should be found between the difficulties in parameter estimation with large models and the characterization of important processes taking place in the reactors. The model selection task is based on the target of the model use. Cost reduction and the search for process operating conditions that allow achievement of appropriate effluent quality criteria (N, P) are the most common targets to be achieved with the model studies. After the model selection task, the most important issue is using this model to characterize the overall activated sludge plant behavior including the biological and physico-chemical phenomena (e.g. settling), the so-called model 'calibration'. After a successful validation of the model, it can serve for its purpose.

In this study, a comprehensive model calibration procedure for the activated sludge model is proposed which accounts for the physical and biological processes. The methodology works for different activated sludge models, depending on the targets and the available engineering knowledge.

THE BIOMATH CALIBRATION PROTOCOL

The BIOMATH protocol for the calibration of activated sludge models is composed of four main stages and 12 modules (see Figure 1). The first stage is the definition of the target(s) of the modelling exercise followed by decision making on the necessary information to be obtained from the activated sludge (AS) plant such that the target of the modelling study can be reached. Some of the modules (1-11) can be skipped depending on the general evaluation whether the targets are reached. The second stage is the collection of detailed information on the activated sludge plant. The mass transfer (hydraulic and oxygen transfer), biological, settling and the influent characterizations are included in this step. In addition, the experimental or lab-scale work is incorporated with usage of the Optimal Experimental Design (OED) methodology. By averaging the influent and operational characteristics, steady state modelling is performed for the mass transfer, settler and the biological model (e.g. ASMs). The third step includes the complete calibration of the activated sludge model using the dynamic influent data, and incorporating the parameter values obtained from lab scale experiments or full-scale data. At the last stage, decisions will be made upon eventual re-iteration of a number of the modules.

The proposed protocol for the modelling of the treatment plant is refined on the basis of a previous protocol developed by Petersen (2000). As illustrated in Petersen *et al.*, (2002) the details of the modules underlying each step are shown in Figure 1, and they are summarized below.

I. Stage-1. Definition of a target for modelling

In the first step, the main objectives have to be defined for the modelling of continuous systems, sequencing batch reactors (SBR), alternating activated sludge plants etc. The decision is usually based on the time and/or budget necessary/available for the modelling task. Some of the stages can be omitted depending upon the objectives (see Figure 1). The main objectives for a modelling case can be:

- Optimization and upgrading of an existing activated sludge plant
- Meeting the effluent criteria
- Cost reduction in the operation
- Reuse of effluent wastewater
- Development of control strategies
- Design of the treatment plant or the combination of those.

II. Stage 2. Plant survey/data analysis and process characterization

A general description of the treatment plant to be used in the model calibration can be compiled from the operation database/log files of the activated sludge treatment plant itself, the design documents and/or personal communication with the plant operators. The design data consist of the physical characteristics such as volumes, a number of compartments, pumping capacities, a number of aerators and connections installed. The operational data is mainly the actual working volumes, the flow rates, energy consumption, the distributions of sludge/wastewater over the compartments and specific design parameters for certain treatment plant alternatives.

The ***design data*** consist of the general plant layout and configuration, compartments/process units, volumes/areas/depths, water and sludge lines, installed capacities, pumps, aerators, P&I diagrams, hydraulic layout. On the other hand, the ***operational data*** concern the flow rates for influent, sludge recycles, sludge wastage and internal recirculation; sludge/wastewater distributions over parallel lines, step feed *etc.*; location, type and implementation of control strategies. The most important issue is the (available) ***measured data*** comprising the conventional characterization of influent & effluent (e.g. COD, TKN, PO_4, TP, NO_3, NH_4, TSS, pH, T (°C)); on-line measurements from the treatment plant (dissolved oxygen, NO_3, SVI, ML(V)SS, PO_4, NH_4 , pH, T (°C)); sludge blanket height in the clarifier, TSS concentration in the return sludge and effluent, P and N content of sludge, sludge age and daily sludge production, VSS/SS ratio of the sludge.

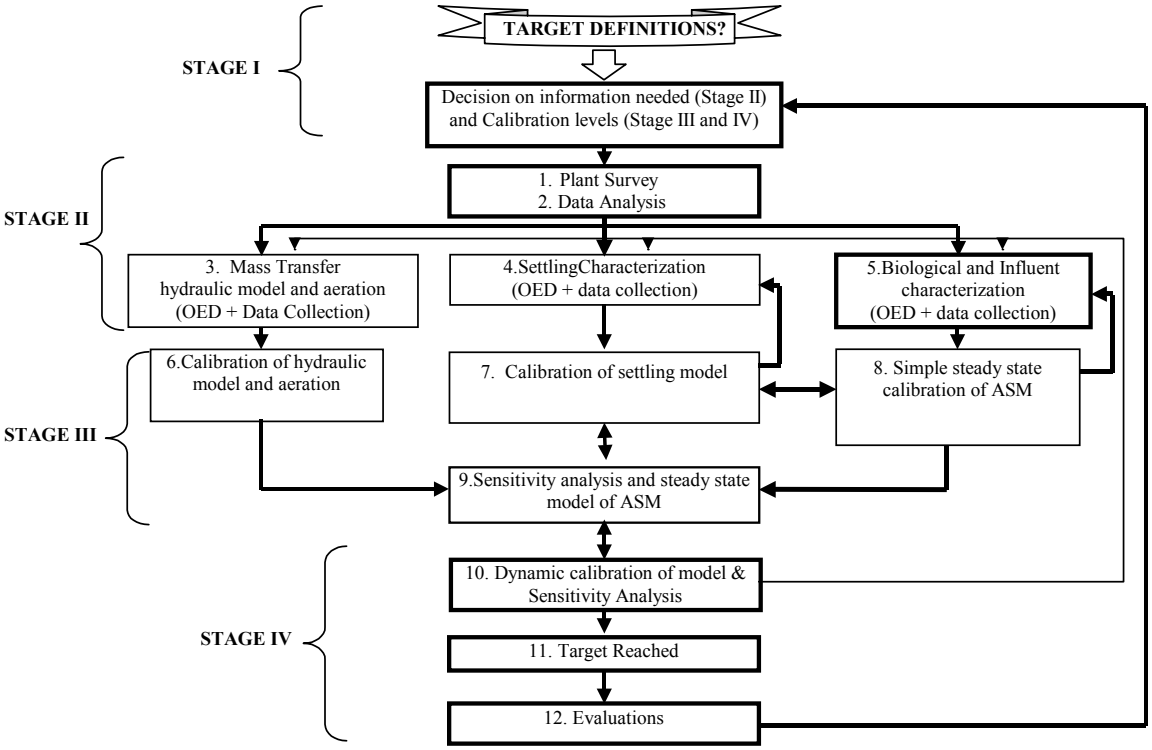

Figure 1. The BIOMATH model calibration protocol

The information collected in this step is of great importance for the understanding of the capacity and the behaviour of the system. So, the design, the operational data and the measured data should be evaluated and processed for understanding of the entire process. For data quality assessment, outlier detection is applied here and interpolation of data can be done whenever it is appropriate and possible. Mass balances regarding the flow rate and the sludge (considering the N and P content) are crucial for the model calibration; particularly for the accurate estimation of the system sludge age (Barker and Dold, 1995; Nowak *et al.*, 1999). From the modelling point of view, it should be noted that the sludge age is the most sensitive parameter with respect to all model outputs.
In addition, some other factors that exert a critical influence on the system performance such as pH, temperature changes, industrial discharges, addition of auxiliary chemicals, energy consumption and generation of daily and monthly operational and maintenance costs etc., should be evaluated in this step.

II.1. Mass transfer characterization

In the mass transfer characterization; two main aspects have to be considered. The first one is the determination of the oxygen transfer efficiency (K_La) in all reactors (e.g. surface aerators, compressed air). The second aspect is the hydraulic characterization of the treatment plant.

Oxygen transfer characterization

Regarding the determination of the K_La for aeration, first, the influences of operational and biological factors on the oxygen transfer have to be considered (i.e. temperature, salt content). The volumetric mass transfer coefficient, (K_La) should be estimated under process conditions. A variety of methods have been developed over the last 2 decades (Boyle and Campbell, 1984; Capela *et al.*, 1999; Gillot, *et al.* 1997; Mueller and Boyle, 1988). Daily power consumptions of the aerators and/or the information provided from the manufacturers may give hints about the oxygen transfer coefficient of the aeration system.

Hydraulic characterization

The second aspect concerns the question whether hydraulic characterization is needed or not. The reactor configuration and the modelling objectives will have an influence on the selection of the degree of accuracy required from the hydraulic characterization. Importantly, complex hydraulics may affect sampling location for representative measurements for the calibration. In case it is difficult to understand the hydraulics of the plant from experience, the plant layout and the survey of the plant (e.g. higher volumes and dispersions), a detailed hydraulic characterization is essential.

For this, a "tracer test" can be performed in order to obtain information about the mixing characteristics allowing for determination of the number of tanks in series (see Figure 2-right). It should be noted here that the transient hydraulic behavior of the treatment system due to flow changes, on/off controls of the pumps-aeration etc. can also be important factors (De Clercq *et al.*, 1999). Alternatively, dispersion models (or terms) can be incorporated in the models for the hydraulic characterization (Stamou, 1997). The tracer experiment may also provide more information about the dead volumes and/or recycles in the reactors. If a detailed hydraulic characterization is not required, possible assumptions can be made on the number of tanks-in-series based on the configuration/dimensions of the compartments or by using empirical equations (Chambers, 1992).

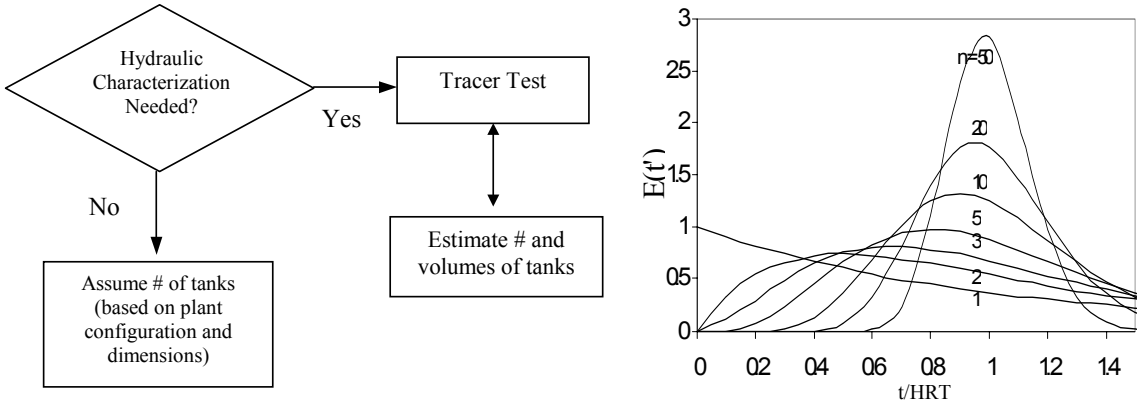

Figure 2. Decision chart for hydraulic characterization (right) and hydraulic residence time distribution function, E(t') for different numbers of tanks in series (left)

II.2. Settling Characterization

A detailed settling characterization is necessary if the settling performance and the reactions during settling influence the overall system behaviour (e.g. effluent COD, N and P). In addition, the target(s) might be the optimization of settling or may be the amendment of effluent suspended solid removal. From a modelling point of view, the investigation could be focused on either settling in the primary and/or final clarifier. If a detailed settling characterization is necessary, settling experiments (Daigger and Roper, 1985; Ekama and Marais, 1986b) and/or other relevant measurements such as SVI have to be carried out before selecting the settling model.

In addition, reactions such as denitrification and phosphorus release in the settler may have to be considered (Henze *et al.*, 1993; Koch *et al.*, 1999; Wouters-Wasiak *et al.*, 1996). This can be checked by calculating the mass balance over nitrate-phosphate or by site observations such as the occurrence of nitrogen gas bubbles entrapped in the flocs (Henze *et al.*, 1993).

If the solid separation in the settler is working well, no detailed settling characterization is necessary (Figure 3). So, a point settler model can be used to describe the separation of the suspended solid flux from the main stream. If a considerable amount of sludge is maintained in the settler, a virtual reactor can be defined next to the point settler. The residence time in the settler can then be modeled by placing a CSTR with a volume equal to the sludge-blanket volume of the settler in series with the settler. The smoothing effect of the secondary clarifier on the effluent quality with respect to COD, total nitrogen and phosphorus etc. should be accounted for.

As mentioned above, if a specific analysis of the plant is required and if the settler affects the performance of the plant critically, then a more detailed model for the settler should be used. This can be done via one-, two- or three-dimensional settling models. Of course, the complexity of the model should meet the requirements. For operation and control of a WWTP a one-dimensional model is advised. The most commonly used one-dimensional model is the settling model presented in Takács *et al.* (1991), but alternatives (both simpler and more complex) exist (Krebs *et al.*, 2000).

Selection of the appropriate model is based on the measurement of concentration profiles or sludge-blanket-height time profiles (De Clercq *et al.,* 2003). The model, which fits the measured concentration profiles or the sludge blanket heights best, should be selected. The reactions should be included in the settler model if they significantly affect the performance. The flow diagram for the settling characterization is given in Figure3.

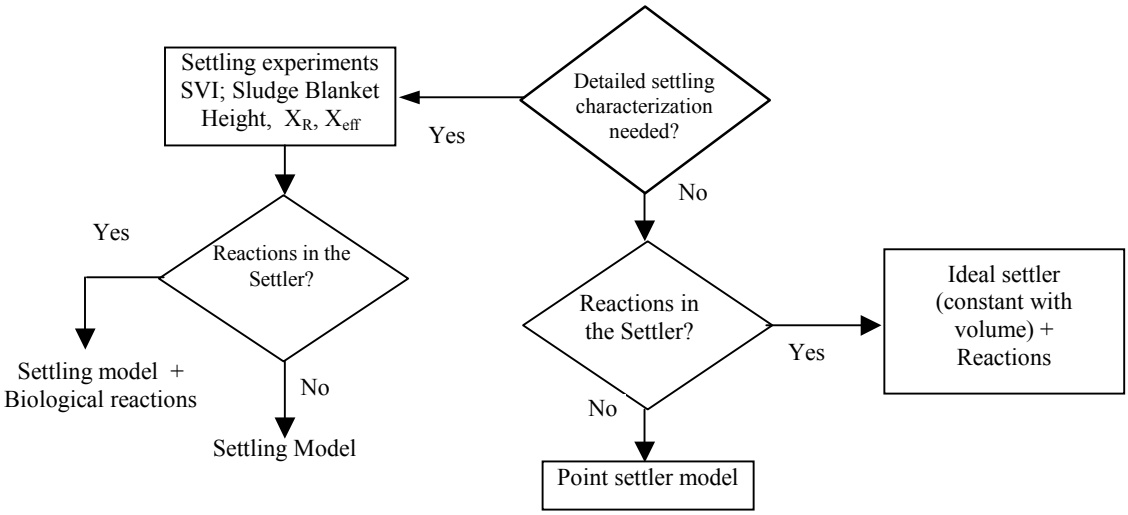

Figure 3. Decision chart on settling characterization

The primary clarifiers ahead of the biological reactors also have a vital importance since there might be activation and/or interactions between physico-chemical and biological reactions. For instance, in addition to biological reactions, the COD removal can be expressed as a physico-chemical reaction such as flocculation and solubilization of the particulate COD fractions into soluble fractions. A large amount of COD up to 50% is removed by gravity settling (Orhon *et al.*, 2002). The biomass in wastewater leads to biological processes such as fermentation, acidification and ammonification due to heterotrophic activity and depending on the environmental conditions in the primary clarifier (Gernaey *et al.*, 2001). The settling and biological reactions should be incorporated in the model if the effect of the primary clarifier on the overall process performance is evident. The effect of the primary clarifier can be evaluated by performing some relevant on-site experimental analyses such as filtered/unfiltered COD, NH_4-N, P, pH and VFA analysis etc. in the influent and the effluent streams of a primary clarifier. Sometimes modelling of the primary settling tank is not carried out by considering the pre-settled influent as a starting point to the aeration tank.

II. 3. Biological Characterization

Activated Sludge Models (ASM1, ASM2-ASM2d, ASM3) proposed by the IWA (formerly IAWPRC, then IAWQ) task group on Mathematical Modeling for Design and Operation of Biological Wastewater Treatment are the most commonly applied mathematical models for the modelling of the biological compartments of wastewater treatment plants. The ASM family models has been successfully applied to full-scale treatment plants and shown to be a good compromise between the complexity of the activated sludge processes and prediction of the plant behavior under dynamic conditions. Therefore, in the proposed BIOMATH protocol, the calibration methodology focuses on the ASM models.

Model selection for the modelling of the biological activity is dependent on: (a) biological processes/activity (e.g. COD removal, N & P removal) occurring in the treatment plant and (b) on the purpose of the model application. Model selection should be based on the targets of the modelling in order to optimize the calibration efforts in accordance with the modelling objectives. Appropriate modifications or extensions of the proposed models can also be considered (i.e. build-up of nitrite during nitrification or denitrification or the fate of specific chemicals).

The determination of all model components is an expensive and time-consuming process. Therefore, whenever possible it is suggested that the default values reported in previous applications should be assigned to the model parameters (Henze *et al.*, 2000). In this context, a sensitivity analysis allows, based on the target of the modelling exercise, to discriminate between the relatively less sensitive and the most sensitive parameters (De Pauw *et al.*, 2003; Weijers and Vanrolleghem, 1997). This information should be used in the calibration protocol and is expected to minimize the calibration efforts and therefore optimize the overall calibration procedure towards the objectives of the modelling. For instance the most important (sensitive) parameters for the prediction of MLSS in the system are mainly the particulate inert materials concentration (or COD) in the influent (X_I), the heterotrophic biomass yield coefficient (Y_H), the heterotrophic biomass decay coefficient, (b_H) and the sludge retention time (Nowak *et al.*, 1999).

Optimal Experimental Design (OED)

Calibration of a mathematical model asks for at least the determination of a couple of parameters that can be selected among all model parameters by analysing the sensitivity functions of the parameters with respect to the model component explicitly specified in the target of the modelling exercise (e.g.

minimum nitrate concentration in the effluent). Another approach for the selection of the parameter subset for the calibration is to apply the collinearity index (Brun *et al.*, 2002; Reichert and Vanrolleghem, 2001) In the context of calibration of the Activated Sludge Models, several lab-scale experiments and full-scale measurement campaigns are usually needed (Henze *et al.,* 1987; Carucci *et al.,* 1999; Coen *et al.*, 1997; Petersen *et al.,* 2002, 2003b) which are expensive and time consuming. The OED concept should be incorporated into the experimental work of the calibration to maximize the information content of each of the experiments (Dochain and Vanrolleghem, 2001). This approach therefore, is expected to minimize time and cost aspects of the laboratory work. Optimal experimental design methodology can be applied for lab-scale experimental set-ups or even for full-scale systems. However, OED applications to full-scale systems need a high level of *a priori* information and expert knowledge.

Estimation of Activated Sludge Model parameters

The ASM1 introduced by Henze *et al.* (1987) essentially describes a single-stage activated sludge system performing simultaneous COD oxidation, nitrification and denitrification processes. A detailed description and explanation of the model processes and components can be found in the technical report of the IWA task group. Application of the ASM1 to a specific treatment plant, i.e. simulation of an activated sludge system based on ASM1, requires the calibration of the ASM1 model to the system under study. That requires the calibration of the stoichiometric and kinetic parameters and characterization of wastewater and biomass of the system in accordance with the ASM1 model. This overall process is called calibration of the ASM1 model.

Parameter estimation consists of determining the ‘optimal’ values of the parameters of a selected model with the aid of measured data (Petersen *et al.*, 2003b). Initially, the model structure, of which parameter(s) need to be estimated, initial concentration of the components and experimental data are necessary. According to Figure 4, the initial values of the parameters (or combinations) and initial conditions have to be defined. By application of this routine, the parameter estimation is terminated when the objective function reaches a minimum with a certain accuracy. The numerical techniques for parameter estimation can be found in Dochain and Vanrolleghem (2001).

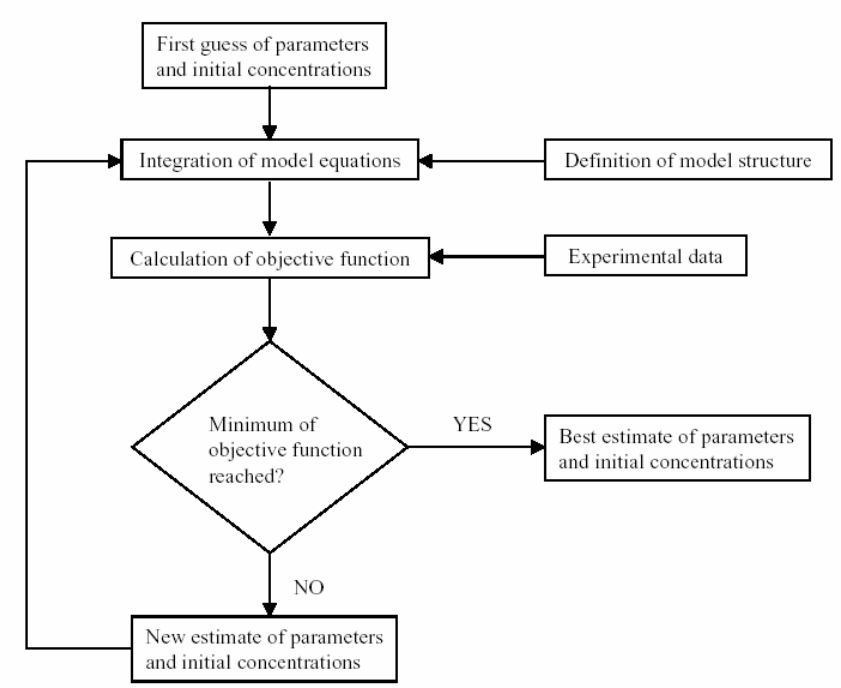

Figure 4. Parameter estimation routine (Wanner *et al.*, 1992)

In this section, a calibration protocol for ASM1 will be presented mainly based on dedicated lab-scale experimental methods for wastewater characterization and estimation of the kinetic and stoichiometric parameters. However, it is important to stress that not all experiments presented in this section should be performed. Only the experiments aiming at providing data to identify the relevant parameters shown to be influential in the sensitivity analysis should be carried out. In other words, the experiments that have to be performed will be dependent on the system under study as well as on the target of the modelling study. In this context, the proposed model calibration procedure is not fixed but it should be considered as dynamic depending on each specific case study. In the following, the methods for the influent wastewater characterization and kinetic/stoichiometric parameters for ASM1 and ASM2d are summarized.

Influent Wastewater Characterization

In most of the cases, the daily monitoring of an ordinary wastewater treatment plants consists of measuring influent and effluent COD, TKN, NH_4 and PO_4-P. On the other hand, the wastewater components included in the ASM1 are different from those being measured in the treatment plant. In the following an experimental methodology for determining the remaining fractions of the influent COD are presented. From the modelling point of view, the biomass fractions in the influent COD are assumed to be negligible (Henze, 1992). Alternatively, the heterotrophic biomass fraction in wastewater can be measured via long-term respirometric experiments applied to raw wastewater without any biomass inoculation (Sperandio and Paul, 2000). Otherwise, it can be incorporated in slowly biodegradable COD, X_S fraction. The methodology is based on the combination of biological (respirometric) and physical-chemical methods. The influent COD is subdivided into several components as illustrated in Figure 5.

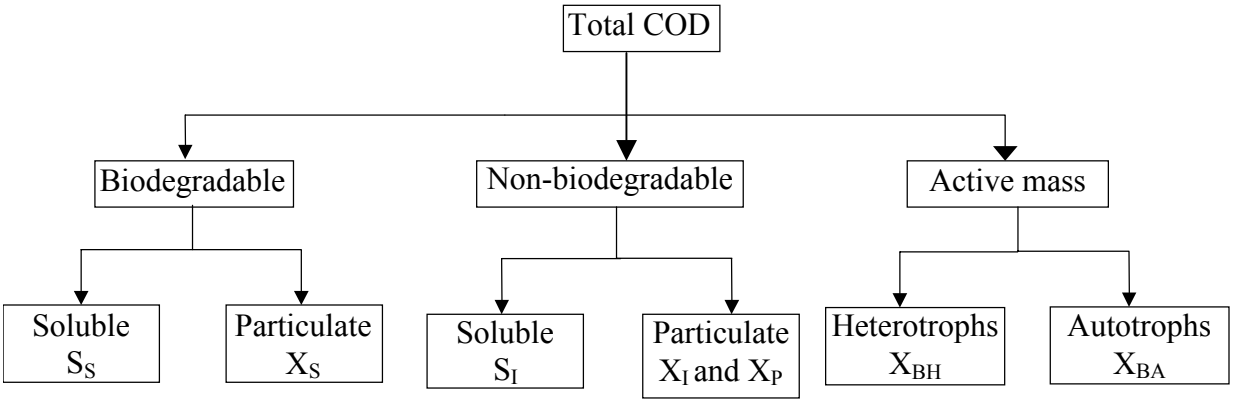

Figure 5. The COD fractionation in influent wastewater

The effluent soluble inert COD, S_I is assumed to be equal to the influent inert soluble COD of the treatment plant if it is operated at an SRT at least higher than 3 days (Ekama *et al.*, 1986a; Mamais *et al.*, 1993). In a practical way 90% of the effluent COD can be regarded as inert influent soluble COD (Siegrist and Tschui, 1992). The inert COD fractions can also be experimentally calculated via long-term COD measurements as described in Germirli *et al.* (1991). The respirometric tests also provide information on the inert fractions as described below.

Biodegradable COD fractions

The biodegradable COD fraction can be estimated via respirometry. However, the COD fractions will be dependent upon the heterotrophic yield coefficient, Y_H (Sollfrank and Gujer, 1991). The readily biodegradable COD fraction, S_S can be estimated by using one of several respirometric methods proposed elsewhere (Ekama *et al.*, (1986a); Spanjers and Vanrolleghem (1995); Sollfrank and Gujer (1991); Sperandio and Paul, 2000; Insel *et al.* (2003a). These respirometric tests are usually carried under following conditions:

- Addition of nitrification inhibitor
- Biomass yield, Y_H is a priori known
- Appropriate initial substrate to biomass S_0/X_0 ratio

In addition to readily biodegradable COD (S_S), slowly biodegradable COD, (X_S) fraction can be estimated from the same respirometric test (see Figure 6) under an appropriate selection of substrate to biomass ratio, S_0/X_0 (Insel *et al.,* 2003a). On the other hand, care should be taken not to exercise high initial substrate to biomass ratio S_0/X_0 during batch experiments, since it may alter the history (physiology) of the activated sludge culture thereby causing a biased characterization of biomass and the wastewater (Chudoba *et al.*, 1992; Novak *et al.*, 1994; Grady *et al.,* 1996).

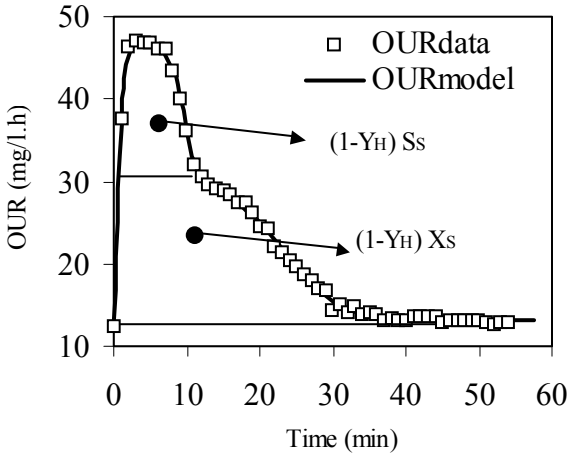

Figure 6. Estimation of biodegradable COD fractions from respirograms

An alternative approach for the estimation of X_I is the comparison of the measured and predicted sludge concentration and sludge production. In most modelling efforts, the X_I concentration is typically used as a "tuning component" in the model calibration of the sludge balance (Nowak *et al.*, 1999) or can be determined by the measurement of residual COD after a long term BOD test (Lesouef *et al.*, 1992). However, X_I, b_H and Y_H are inherently correlated parameters in terms of sludge production. The effect of the increase in one parameter can be compensated with the other. To break this correlation, first it is proposed to determine the b_H from long term batch experiments and therefore fixed it (see section decay rate determination). Second, oxygen consumption (or requirement) of the plant may be used to provide information on the average yield. Moreover, the influent X_S concentration has a large influence on the oxygen levels in the compartments (Daigger and Nolasco, 1995) since X_S accumulates with increasing sludge age, and its degradation time is much longer than that for S_S. Additionally, X_S incorporates organic nitrogen and phosphorus as well. The degradation of this component releases nitrogen and phosphorus into the bulk liquid.

Nitrogen fractions

For the nitrogen fractions a similar approach to the COD fractionation is proposed both for influent and effluent nitrogen characterisation. It is assumed that the influent contains negligible concentrations of nitrate nitrogen. With the assumption that there is no or negligible biomass in the influent wastewater, the total Kjeldahl-nitrogen can be fractionated according to Eq1 (Henze *et al*., 1987).

$$TKN = X_{NI} + X_{ND} + S_{NI} + S_{ND} + S_{NH} \qquad \text{(Eq1)}$$

The analytically measured NH_4-N concentration is considered to be equal to S_{NH} (APHA, Standard Methods, 1998). This component is expected to be available in the monitoring data of most wastewater treatment plants. It is assumed that the ratio of soluble to total TKN is proportional with the ratio of COD_{sol} to COD_{total}. Thus, the Soluble Kjeldahl Nitrogen (SKN) can be approximated via Eq2, and by assuming that the nitrogen content of inert soluble organic matter (i_{NSI}) equals 1.5% (Henze *et al*., 1995) the concentration of S_{ND} can be determined via Eq3. Alternatively, SKN can be determined analytically from the filtered sample as well.

$$SKN = \frac{CODsol}{CODtot} \cdot TKN = S_{NI} + S_{ND} + S_{NH} \qquad \text{(Eq2)}$$

$$S_{ND} = SKN - i_{NSI} \cdot S_I - S_{NH} \quad \text{(Eq3)}$$

The nitrogen content of inert suspended organic matter (i_{NXI}) is initially assumed to be 1% (Henze *et al*., 1995) resulting in Eq4 for the determination of X_{ND}.

$$X_{ND} = TKN - i_{NXI} \cdot X_I - SKN \quad \text{(Eq4)}$$

Determination of Kinetic Parameters

The following methodology is advised for the determination of key kinetic parameters of the activated sludge processes included in ASM1, i.e. those related to heterotrophic and autotrophic activity.

Maximum specific growth rates

Regarding the determination of maximum specific growth rates for heterotrophs and nitrifiers a respirometric batch test is proposed. This experiment is a good example where the Optimal Experimental Design (OED) methodology can be applied. Indeed, in one batch experiment proper addition of wastewater and ammonium (S_0/X_0) as determined by OED allows simultaneous determination of nitrification and COD degradation kinetics as applied successfully in Petersen (2000). The design of these experiments is described in more detail elsewhere (Petersen, 2000), but consisted of simultaneous addition of wastewater and an optimal dose of ammonium. The exogenous oxygen uptake rate for substrate degradation, $r_{O,ex}$, resulting from the addition of wastewater and wastewater with extra addition of ammonium, respectively, is given in Figure 7. In this case the data can be described by the following equation (Eq5):

$$r_{O,ex} = (1 - Y_H) \cdot \frac{\mu_{\max H} X_H}{Y_H} \cdot \frac{S_S}{K_S + S_S} + (4.57 - Y_A) \cdot \frac{\mu_{\max A} X_A}{Y_A} \cdot \frac{S_{NH}}{K_{NH} + S_{NH}} \quad \text{(Eq5)}$$

Using model-based parameter estimation and assuming the yield coefficients are known, the maximum growth rates for heterotrophs and nitrifiers together with the Monod affinity constants K_S and K_{NH} can be determined. If the aim is only to determine the maximum growth rates for the heterotrophic and nitrifying biomass then the Monod affinity constants and as well as yield coefficient could simply be fixed to their ASM1 default values. The reader is advised to consult the IWA task group report on ASM1 for default parameter values for municipal wastewater treatment plants (Henze *et al.,* 1987).

The parameter estimation can also be applied in a two step protocol for heterotrophic and nitrifying biomass characterization. In the first step, heterotrophic parts can be identified from an experiment with ATU addition (by inhibiting the nitrification). The resulting respirogram will provide the information necessary to determine the parameters for COD degradation kinetics. In the second step, an experiment without ATU addition can be performed and the resulting OUR data can be used to determine the nitrification kinetics by fixing the heterotrophic parameters determined in the first experiment. Either approach can be expected to yield the same results for heterotrophs and nitrifiers. It is quite important to note that if a storage phenomenon is observed (Henze *et al.*, 2000), the ASM1 model presented in Eq5 will fail to model the OUR data obtained from the experiment. This means that the method proposed will fail to determine the kinetic parameters. In order to model the system, a more suitable mathematical model such as ASM3 should be applied to describe the storage processes (Koch *et al.,* 2000).

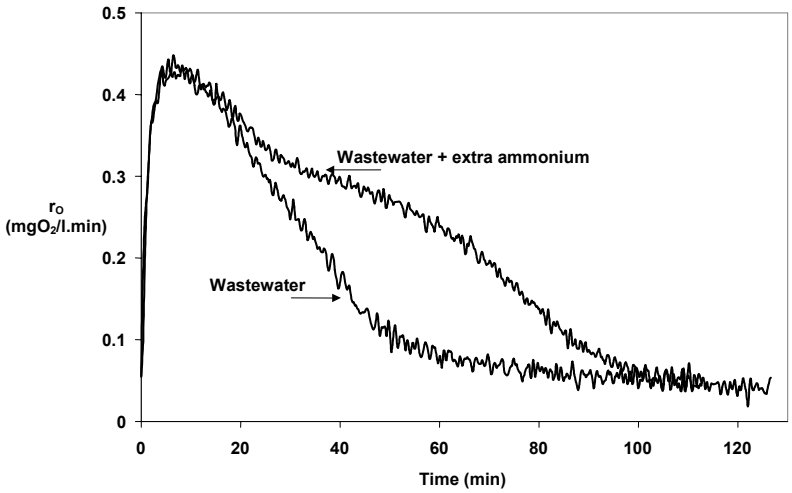

Figure 7. Example of respirograms obtained from respirometric tests with wastewater and wastewater mixed with ammonium (Petersen, 2000)

Another point is the selection of the identifiable parameters (or combinations) from the measurements, i.e. the respirometry. The experiments should contain adequate information about the parameter(s) to be estimated. In the literature, several methods for the identification of model parameters have been proposed (Dochain and Vanrolleghem, 2001). An application for the identifiable parameter extracted from respirograms can be found in Dochain *et al.* (1995). Recently, Petersen et al. (2003a) showed that identifiability results could be generalised by applying a set of ASM1 matrix based generalisation rules. The identifiable parameter combinations could be predicted directly based on the knowledge of the process model under study (in ASM1-like matrix representation), the measured variables and the biodegradable substrate considered. This generalisation procedure reduces the time-consuming task of deriving the structurally identifiable model parameters significantly, and helps the user to obtain these directly without the necessity to go too deeply into the mathematical background of structural identifiability. The results of the studies of Dochain *et al.* (1995) and Petersen *et al.* (2003a) are summarized in Table 1.

The sensitivity analysis is the most commonly used method for visualizing the effect of parameter(s) on the measurement output. From the batch experiments (oxygen uptake rate test) discussed above, it is difficult to identify the maximum growth rate of active biomass. In this case the active heterotrophic biomass fraction can be approximated using the mass balance over the plant according to Eq6. The active heterotrophic biomass concentration in a continuous system in steady state can be calculated as:

$$X_H = \frac{Y_H}{1 + b_H \theta_X} \frac{\theta_X}{\theta_H} COD_{Degraded} \qquad \text{(Eq6)}$$

Where θ_X is the sludge age, θ_H is the hydraulic retention time, $COD_{Degraded}$ is the total amount of COD removed, b_H the decay rate and Y_H the yield coefficient (Orhon and Artan, 1994; Petersen *et al.*, 2003b). In the same way, the concentration of active nitrifying biomass can be determined by (Eq7):

$$X_A = \frac{Y_A}{1 + b_A \theta_X} \frac{\theta_X}{\theta_H} f_{aer} N_{Nitr.} \qquad \text{(Eq7)}$$

Where f_{aer} is the aerobic fraction of the reactor; N_{nitr} the amount of nitrified nitrogen; b_A the autotrophic decay rate coefficient and Y_A the autotrophic yield coefficent (Dupont and Sinkjær, 1994).

Hydrolysable COD and hydrolysis kinetics

The hydrolysis mechanism incorporated in the ASM models is expressed with a surface saturation type of equation. Generally speaking, this equation is governed by the maximum hydrolysis rate, K_h, and the half saturation constant for hydrolysis, K_X (Henze *et al.*, 1987). In the literature, some researchers suggest that the hydrolysis kinetics can also be expressed by a first order equation (Kappeler and Gujer 1992; Sollfrank and Gujer, 1991; Spanjers and Vanrolleghem, 1995; Sperandio and Paul, 2000). In this report, the experimental procedures suggested by Ekama *et al.* (1986a) and Insel *et al.* (2003a) are proposed for surface saturation type hydrolysis model. According to the method proposed by Ekama *et al.* (1986a), the determination of the parameters for hydrolysis is carried out by a "cyclic square wave feed" experiment in a continuous flow pilot plant experiment. To determine the hydrolysis parameters the data obtained after the drop in respiration rate are important. For details the reader is referred to the paper of Ekama *et al.* (1986a).

The second method is the batch method proposed by Insel *et al.*, (2003a) as illustrated in Figure 5. The user should however be aware of the difficulties for the accurate determination of the initial readily biodegradable, S_{S0} and slowly biodegradable substrate, X_{S0} if the respirogram is not informative resulting in a sudden peak in oxygen uptake rate during the growth phase (Brouwer *et al.*, 1998). Then, high S_0/X_0 ratios can be applied to the wastewater (Sperandio and Paul, 2000) or multiple experimental designs can be proposed (Dochain and Vanrolleghem, 2001).

Table 1. Structurally Identifiable parameter combinations for growth and hydrolysis kinetics.

Growth Dochain *et al*. (1995) Petersen *et al. (2003a)*		Hydrolysis Insel *et al.* (2003)	
No biomass growth	Biomass growth	No biomass growth	Biomass growth
$(1-Y_H)\frac{\hat{\mu}_H X_{H0}}{Y_H}$	$(1-Y_H)\frac{X_{H0}}{Y_H}$	$(1\text{-}Y_H)\ k_h\ X_{H0}$	$(1\text{-}Y_H)\ K_x\ X_{H0}$
$(1\text{-}Y_H)\ S_{S0}$	$(1\text{-}Y_H)\ S_{S0}$	$(1\text{-}Y_H)\ K_x\ X_{H0}$	$(1\text{-}Y_H)\ X_{S0}$
$(1\text{-}Y_H)\ K_S$	$(1\text{-}Y_H)\ K_S$	$(1\text{-}Y_H)\ X_{S0}$	$(1\text{-}Y_H)\ X_{H0}$
	$\hat{\mu}_H$		k_h

Indice "0" indicates the initial value

The parameter combinations that are identifiable from a batch experiment with inhibited nitrifiers are listed in Table 1. As an example, in the second column of Table 1, the parameter combinations regarding the Monod kinetics can be estimated using only the OUR profile. The initial concentration of active heterotrophic biomass, X_{H0} and the initial concentration of readily biodegradable substrate, S_{S0}, are identifiable from the respirogram together with the kinetic constants, $\hat{\mu}_H$ and K_S (Petersen *et al.,* 2003a). The same procedure is also applicable for the hydrolysis kinetics proposed by Insel *et al.*(2003a). The advantage of this method is that it allows the user to estimate the kinetic parameters and the COD fractions, simultaneously. However, expectedly, the initial S_0/X_0 plays a crucial role in the estimation of the parameters. As a result, parameter correlation problems should be taken into account within the modelling context as part of the practical parameter identifiability problems.

Decay rate of biomass

The endogenous respiration rate, r_{Oend}, can be measured simply as a function of time in a long term (e.g. 10-12 days) aerated batch test without substrate supply. The heterotrophic endogenous decay rate, b_H', can be determined as the slope of the curve consisting of ln [OUR(t)] data points plotted as function of time (Ekama *et al*., 1986a). This decay rate can be transformed into the model decay rate based on the death regeneration concept via Eq8 (Henze *et al*., 1987), where Y_H and f_p can be assumed known (e.g $Y_H = 0.67$ and $f_p = 0.08$ according to the ASM1 default parameters).

$$b_H = \frac{b'_H}{1 - Y_H(1 - f_p)} \qquad \text{(Eq8)}$$

If the collected r_O data are fluctuating with time, a similar but an extended procedure suggested by Avcioglu *et al.* (1998) can be used. Another method for the determination of b_H was proposed by Spanjers and Vanrolleghem (1995). The model for carbon oxidation and nitrification is applied to the respiration rate data resulting from acetate/ammonium mixtures addition to activated sludge samples in batch experiments. According to this method, the heterotrophic and autotrophic endogenous decay rate can be found by curve fitting. Generally, the sludge is sampled from the main reactor and kept aerated without any feed during the experiment. Then a known amount of a readily biodegradable substrate (eg. acetic acid/ammonium mixture) is spiked into the sludge at different times. The respirograms are plotted versus time (Figure 8). The decrease over time of the maximum respiration rate of heterotrophs and nitrifiers allows to estimate the parameters b_H and b_A. Again, the selection of the S_0/X_0 ratio is crucial for the estimation of decay rates.

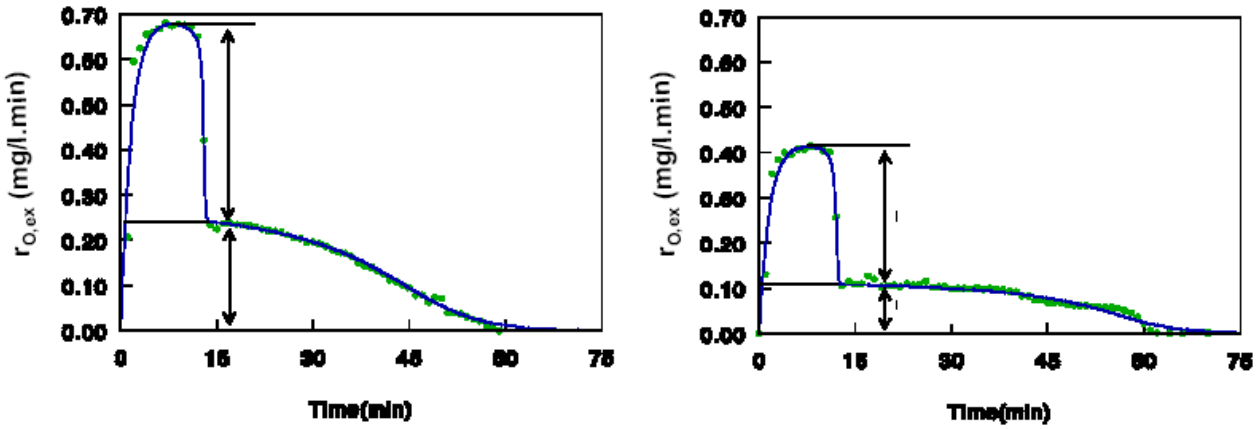

Figure 8. Determination of the r_{omax} of a sludge sample after an incubation time of 1 day (left) and 7 day (right) (Spanjers and Vanrolleghem, 1995)

<u>Influent wastewater characterization for EBPR models</u>

- Fermentation product (acetic acid), S_A: The acetic acid component can be determined directly by GC, High Performance Liquid Chromatography (HPLC) and/or the titration procedure proposed by De Haas and Adam (1995). Chemical Oxygen Demand (COD) measurements are not recommended due to the volatility of acetate.

- Fermentable substrate (acetic acid), S_F: The definition of readily biodegradable substrate, according to the ASM1 and ASM2d model is the sum of acetic acid, S_A and the fermentable substrate, S_F fractions.

The fermentable COD fraction, S_F can be calculated with Eq9 if the S_A fraction is determined previously:

$$S_F = S_S - S_A \qquad \text{(Eq9)}$$

- Particulate COD components: The particulate components different from the ASM1 in influent wastewater are the phosphorus accumulating organisms (X_{PAO}), the stored polyphosphate (X_{PP}) and the organic storage products (X_{PHA}). The COD concentration values of these components in the influent can be regarded as negligible compared to the total influent COD.

- In the ASM2(d) model, the phosphorus is represented by 2 fractions. The first one is the ortho-phosphate fraction available in the bulk liquid not only as a nutrient for the ordinary heterotrophs and autotrophs but also for the PAOs. The second one is the organic phosphate fraction incorporated in the influent components (S_F, X_I, X_S, X_H). As a result, the total phosphorus content of the wastewater is the sum of ortho-phosphate and organically bound phosphate. The phosphorus components can be determined from filtered (0.45 μm) and raw wastewater using the APHA Standard Methods (1998).

EBPR activity test

The magnitude of P uptake is strongly linked to the phosphorus release under anaerobic conditions (Wentzel *et al*., 1985). The phosphorus content of biomass (Bio-P sludge) can be calculated according to the method proposed by Wentzel *et al.* (1985). The anaerobic batch test should be performed with the addition of acetate (or sewage) to the mixed liquor sampled from the EBPR plant. However, the nitrate already present in the mixed liquor should be taken into consideration (Comeau *et al.,* 1990) since ordinary heterotrophs consume part of the acetate for denitrification if nitrate is present. Therefore, an excessive amount of acetate has to be injected or the sludge should be rinsed. In addition, the pH value of the mixed liquor should be kept constant during the experiment since the P release is influenced by the external pH (Smolders *et al.*, 1994) (See Figure 9).

Aerobic (or anoxic) batch tests with oxygen (or nitrate) and orthophosphate measurements allow to estimate the kinetic parameter combinations and the initial states of Table 2. Basically, the proposed method (Vanrolleghem *et al.*, 2002) is based on a batch experiment conducted with the sludge sampled from a bio-P treatment plant. The sludge is first subjected to anaerobic conditions with the addition of an excess amount of acetate as described below. In the following stage the sludge is washed and aerated with the addition of certain amount of phosphate. During the aeration phase, respirometric data (nitrate in anoxic experiments) together with the filtered orthophosphate measurements are collected. The initial phosphate concentration at the start of the experiments can be adjusted using OED techniques to achieve optimal parameter accuracy. The other parameters have to be taken as default or should be calibrated using full- scale treatment plant data.

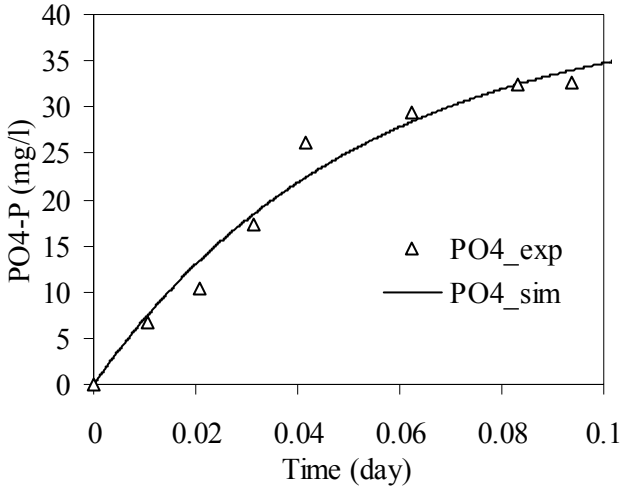

Figure 9. Phosphorus release test result

The maximum phosphorus concentration can be calculated with the formula given below:

$$P(t) = P_{max}\left(1 - \frac{P_{max} - P_{t=0}}{P_{max}} e^{-kt}\right)$$

where;
P(t) = phosphorus concentration at time t, mgP/l
P_{max} = the maximum potential phosphorus concentration, mgP/l
and $P_{t=0}$ = initial phosphorus concentration, mgP/l
k= first order rate constant

Table 2. Identifiable parameter combinations for PAOs for ASM2d

Anaerobic Condition	Aerobic Condition
$-q_{PHA}X_{PAO}$	$(\frac{1-Y_H}{Y_H}\hat{\mu}_{PAO}X_{PAO} + Y_{PHA}q_{PP}X_{PAO})$
Y_{PO4}	$-q_{PP}X_{PAO}$

III. Stage-3. Steady state calibration of the selected model

In this phase, the different reactors in the treatment plant are represented by an ideal perfectly mixed tank as a simple treatment plant configuration (Figure 1-Module 8). The data of full-scale wastewater treatment plant are averaged assuming that this average represents a steady state, and the model is calibrated to fit to average effluent concentration and sludge waste data. The calibration of the activated sludge model and the settler are linked to each other in order to describe the final effluent quality. At this stage, the interaction between the steady state calibration and the settler model calibration is taken into consideration. Another advantage is the characterization of wastewater components that can be adjusted by changing model parameters (i.e. Y_H, b_H etc.) during calibration using the full-scale data.

After the combination of the sub-models, a steady state calibration of the overall activated sludge plant is carried out with the collected data in Stage II (and/or using available long term data). The steady state calibration is done for each of the sub-models, i.e. the calibration of mass transfer model, the settling model and the biological model. Depending on the objectives and/or conditions of the treatment plant, these sub-models can be omitted or considered as a sub-model in the general steady state calibration task

(Module 9). In the steady state calibration of the model the controllers (aeration, return and internal recycle rates etc.) are incorporated in the model. The main idea is to estimate the appropriate biomass composition in the reactors or settler. It should be noted here that the biomass composition obtained from the steady state calibration is used in the dynamic model calibration as the initial biomass composition.

Influent wastewater characterization is essential for the simulation of the activated sludge plant. Therefore, the wastewater characterization has to be performed carefully. After that the sub-models should be selected based upon the objectives of the modelling study. Then, the overall steady state simulation of the model is carried out using the default parameters and the flux based average influent characterization of the wastewater. Here, the mass balance of the sludge and the sludge production of the activated sludge plant should be fitted to the actual measurements.

If the simulated steady state performance is in good agreement with the data collected in Stage II or with the long-term data the dynamic calibration of the general model can be performed. The steady-state simulation (calibration) results can be compared on the basis of averaged effluent COD, N and P concentrations, oxygen consumption and sludge production.

IV. Stage-4. Dynamic calibration and evaluation of the results

In Stage IV, the dynamic calibration of the activated sludge model is aimed. Before proceeding into more details of the dynamic calibration, the sludge production must be modeled and must be in good agreement with the real situations (this is expected to be achieved in Stage III). As an initial guess, the biomass composition resulting from the steady state calibration as described in Stage III is taken as the starting point. The dynamic calibration of the model necessitates the availability of dynamic influent concentration profiles. A larger amount of data and optimized sampling both provide sufficient information on the understanding of the system behavior and allow a precise estimation of parameters, which should be considered in Stage II. Now, the decision has to be made on the parameters to be estimated (i.e. Kinetic or stoichiometric constants for the biological model).

The sensitivity analysis is necessary and uses the dynamic influent data and the parameters obtained in Stage III. The output variables again, have to be selected upon the objectives of the modelling study or the availability and the quality of the data. For instance, if the effluent nitrate concentration is measured or the objective is the optimization of the effluent nitrate concentration, the sensitivity functions of the parameters should be carried out with respect to effluent nitrate. In this way, one may conclude which parameters are more influential to the available effluent nitrate data. Then, the calibration of the model can be done by fine-tuning the parameters on the basis of fitting the model to dynamic data obtained from the measurement campaign. After the dynamic calibration, if the standard deviations are still quite high for the most sensitive parameters, additional lab experiments could be performed. In this respect, one should refer to Stage II and Stage III for the experimental study.

The calibration can be performed manually or using the optimizer (or parameter estimation) module available in the various wwtp simulators. The first approach is expert-knowledge driven and requires a sound insight into the system. Whereas the latter approach requires a priori information about model structure and quality of the available information obtained from the measurement campaign. In other words, it usually requires a system identification (structural and/or practical) (Weijers and Vanrolleghem, 1997; Reichert and Vanrolleghem, 2001; Brun *et al.,* 2003) where the parameter sub-sets that can be estimated under available measurement campaign data are determined. From practical application point of view, this approach is usually not preferred due to the over-parameterized nature of

the ASM models with respect to availability of the dynamic data (Reichert and Vanrolleghem, 2001). It is therefore not surprising to see that almost all of the calibration studies dealing with ASMs are done manually.

Following the calibration of the AS model, a final evaluation should be performed within the context of the objectives to be reached. The success of the calibrated model should be judged. If it is found that the calibrated activated sludge model does not mimic the dynamic behavior of the system, solutions have to be investigated by re-evaluation of the plant data, the sub-models or even the targets defined in the first step. Additionally, it can be proposed that the existing model needs to be modified or that an alternative activated sludge model is used in the calibration. However, in this situation, the protocol must be followed again for the new activated sludge model.

A CASE STUDY-Calibration of a carrousel type activated sludge treatment plant

The application of this methodology is illustrated with a model calibration case study for a carrousel plant. On the basis of available data gathered from previous measurement campaign, the methodology shown in Figure 1 is followed. According to Stage 1in Figure 1, the ***target*** in this case study is to model the plant with the aim of decreasing the effluent nutrient (N, P) concentrations via model-based scenario analysis (Insel *et al.*, 2003b). It should be noted here that there was no opportunity to carry out mass transfer, settling characterization and a biological characterization using the sludge. With the assumptions provided, the characterization steps in Stage II had to be skipped. However, plant survey and data analyses could be performed with the available data.

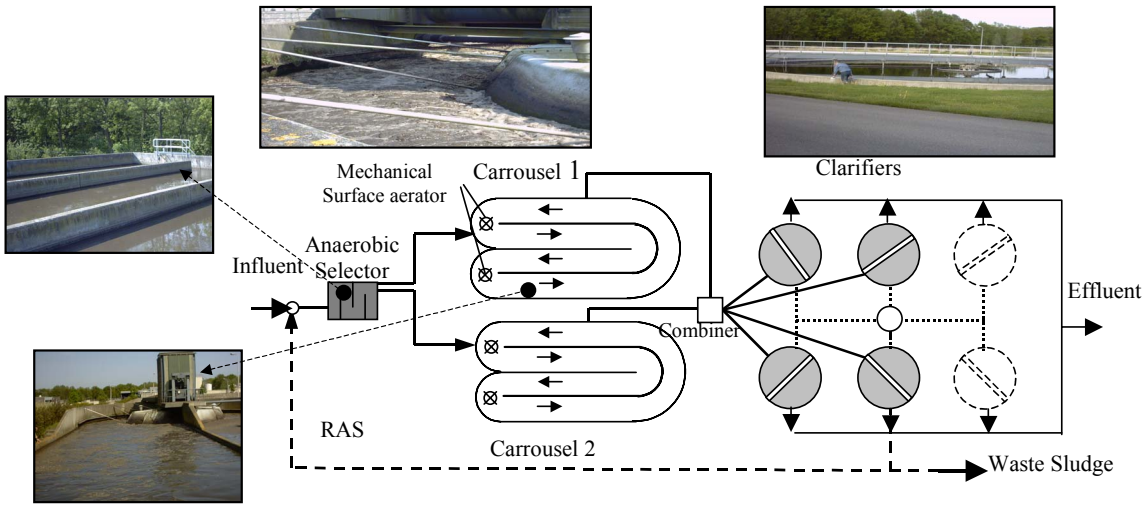

Figure 10. General plant layout

Brief description of the plant

General information

The treatment plant under study is located in the Netherlands (see Figure 10) and is a carrousel type plant receiving the wastewater of 50,000 PE. The average daily influent flow rate of the plant was recorded in the range of 5800-6000 m^3/day. The carrousel plant consists of one anaerobic reactor (selector), 2 carrousels and 4 clarifiers. In case of high hydraulic loadings, the influent flow bypasses the

anaerobic selector and is equally distributed to the carrousels. The sludge recycle is controlled in order to avoid sludge overflow from the weirs of the clarifiers. The volumes for the anaerobic compartment (1), carrousels (2) and the clarifiers (4), are given in total as 1400 m^3, 10000 m^3 and 2460 m^3 respectively. The flow rates according to the plant records are illustrated in Figure 11.

Aeration control

The dissolved oxygen concentration is simultaneously controlled in both carrousels. The control strategy is different for day and night operation. During the day period, the 2 aerators in each carrousel are manipulated to keep the dissolved oxygen concentrations in the range between 0.9 mg/l and 1.2 mg/l. In the course of the night period, the carrousels are operated as an alternating plant by turning the aeration on/off in so-called intermittent aeration to stimulate denitrification. In this alternating aeration period, the total cycle time, T_C is set to 110 minutes. The aeration is off during 80 minutes and turned on for 30 minutes. In each 30 minutes aeration period, the aerators are operated as during the day period and the dissolved oxygen is controlled in the range of 0.9-1.2 mgO/l. It should be noted that during the intermittent aeration one of the aerators was kept at its maximum level (low O_2 transfer) to keep the MLSS in suspension. The average internal mixed liquor recycle rate in the carrousel is calculated as 635,040 m^3/day leading to a typical flow velocity of 0.3 m/s. The average sludge recirculation rate (Q_R) through the anaerobic selector is calculated as 8434 m^3/day.

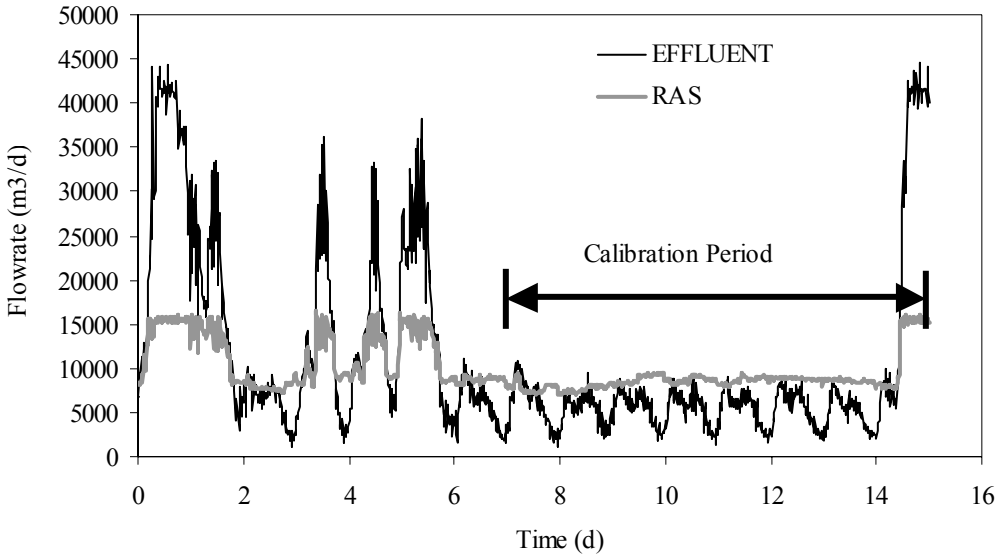

Figure 11. Influent, effluent and sludge recycle flowrates

The measurement campaign data include dissolved oxygen, NO_3-N (both on-line); effluent orthophosphate and TSS concentrations (lab analyses) in the carrousel for a period starting from 17/07/2000 till 25/07/2000, corresponding to day 7 and 14 in Figure 11, respectively. The total/filtered (0.45 μm) COD, VFA, BOD_5, total/filtered TKN, NH_4-N, total/filtered phosphate and TSS measurements were performed on the influent, with a sampling interval of 4 hrs between grab samples during the measurement campaign period (for the influent wastewater characterization consult Insel *et al.*, 2003b). The temperature of the mixed liquor was around 18 ^{0}C. The nitrate and the dissolved oxygen concentrations were measured in Carrousel 1 with a sampling interval of 15 and 5 minutes, respectively. The orthophosphate analyses were performed daily on the effluent of the clarifier. The dissolved oxygen, TSS and the nitrate measurements were performed in the carrousel reactor. Only the phosphate samples are available for the effluent.

The second step comprises the simulation of the system with simplified layout to check the mass balances on the sludge and to acquire a rough estimation of the plant removal efficiency as described in Stage III (Figure 1). It should be stressed here that a rain event just before the measurement campaign carried a high concentration of TSS to the system, which makes it more difficult to get an accurate estimate on the MLSS concentrations. This in turn makes it difficult to have a good idea on the influent X_I, since there is uncertainty about the sludge age. It also affected the phosphate mass balance over the system adversely. No parameter adjustments were done at the simple steady state calibration level (Module 8). The layout for the simulation is shown in Figure 12.

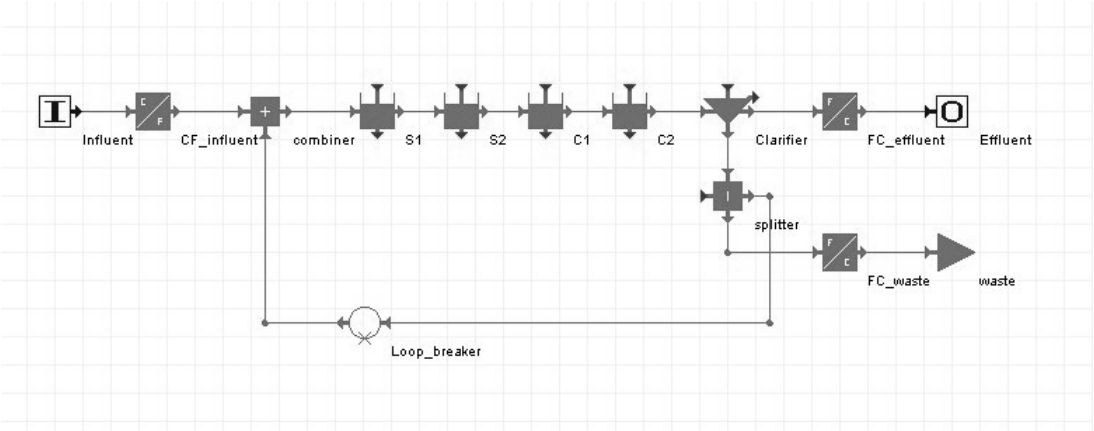

Figure 12. Plant layout for simple steady state calibration (WEST)

The second part of Stage III-Module 9 is concerned with the estimation of the parameters using the real layout presented in Figure 13. The steady state calibration using the flux based (averaged) influent wastewater characterization is used for the estimation of the parameters using the plant layout in Figure 13. The most sensitive parameters adjusted in the calibration are given in Table 3. To keep it simple and to decrease the simulation time for each run, the two identical carrousels were combined together and the settler was regarded as a point settler. The dissolved oxygen is controlled in the 1st and the 4th reactor. The oxygen control strategy was active during the calibration period.

It is worth mentioning here that the number of parameters modified during the calibration was kept at a minimum level by selecting the most sensitive parameters with respect to the measurement output (NO_3, NH_4 and PO_4). In short, the hydrolysis parameters, endogenous parameters for X_{PAO} and the oxygen half saturation constants for autotrophs and heterotrophs were found to be the most sensitive parameters.

Table 3. ASM2d parameters after calibration (Insel *et al.*, 2003c)

Parameters	**Symbol**	**Unit**	**Default (ASM2d)**	**Calibrated**
Anaerobic hydrolysis reduction factor	η_{fe}	-	0.1	0.8
Anoxic hydrolysis correction factor	η_{NO3hyd}	-	0.6	0.8
Half saturation constant for oxygen	K_O	mgO/l	0.2	0.15
Endogenous decay rate for X_{PAOs} X_{PP} X_{PHA}	b_{PAO}, b_{PP}, b_{PHA}	day^{-1}	0.2	0.12
Half saturation constant for hydrolysis	K_X	mgCOD/mgCOD	0.1	0.03
Half saturation constant for O_2 (X_{AUT})	K_{OAUT}	mgO/l	0.5	0.2

The validation simulation using the dynamic influent file shows that the calibrated model gave a reasonable description for the measurement outputs (see Figure 14 and 15). In stage IV, the dynamic calibration of the model can be done or improved using the dynamic influent file. A buffer tank was introduced to the layout (not shown in Figure 13) for mimicking the smoothing effect of the clarifier.

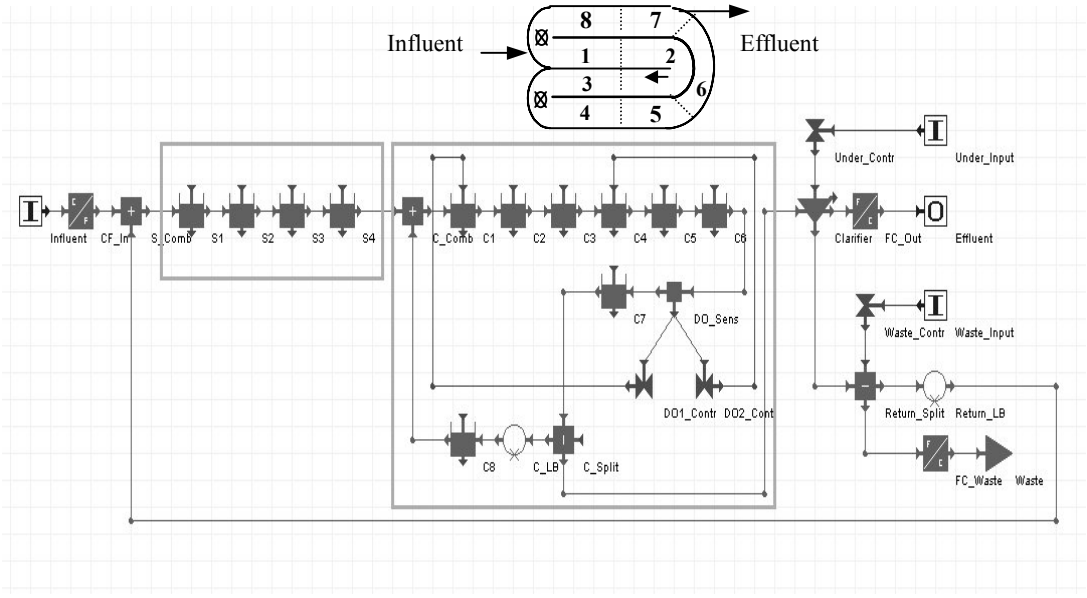

Figure 13. Plant layout for the steady state and dynamic calibration (Insel *et al.,* 2003b)

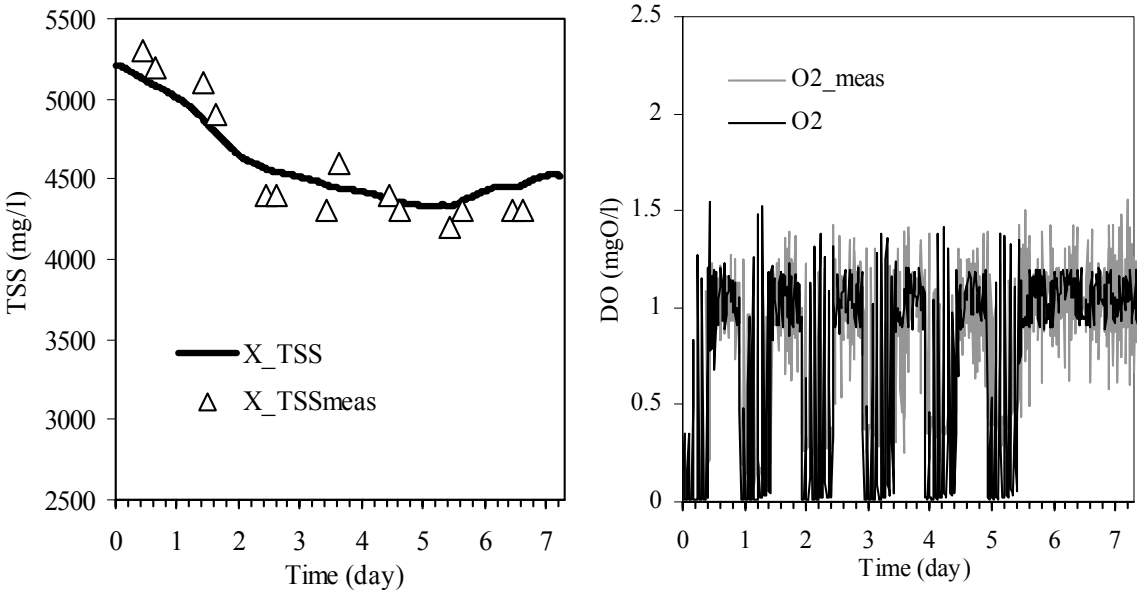

Figure 14. Simulated and measured TSS (left) and dissolved oxygen (right) profiles

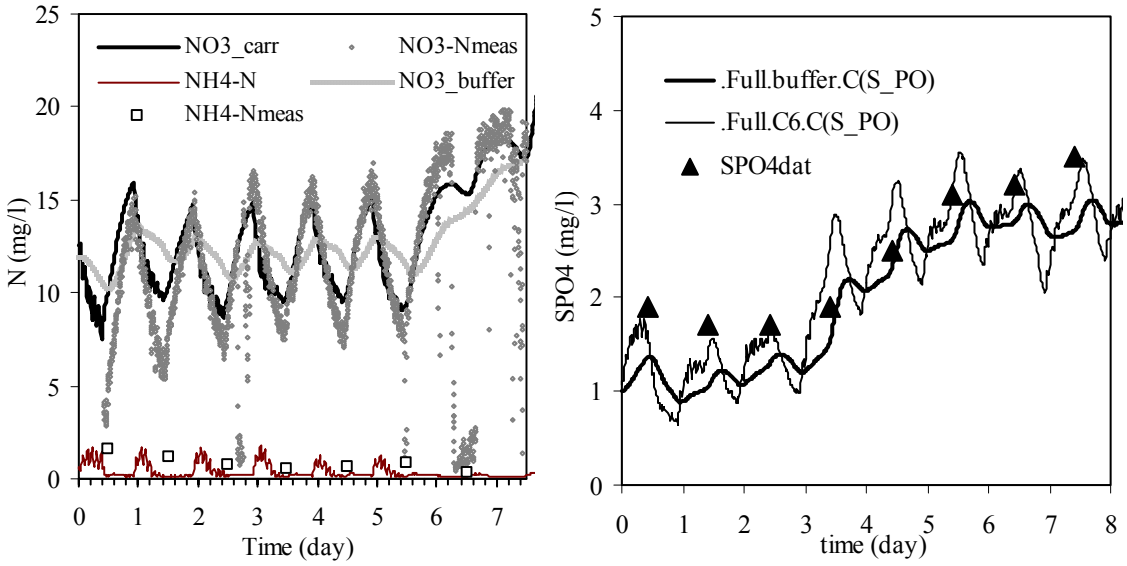

Figure 15. Simulated and measured nitrogen (left) and phosphate (right) profiles

DISCUSSIONS

The proposed method for activated sludge model calibration combines modules for hydraulic characterization, settling characterization and biological characterization of the treatment plant under study. The crucial points in this procedure are the definition of the target of the modelling study, and the selection of further necessary steps within the proposed model calibration framework. As discussed in the presentation of the procedure, the selection of those modules is dependent on the assumptions made. In addition, depending on the targets of the modelling study or the problems experienced during the data collection the relative importance of the modules may change. Although each module is regarded as an individual section they are interrelated to each other. Thus, these interactions have to be considered to predict the general behavior of the system. For instance, if there is a problem with the sludge settleability, the settling characterization should be linked to the characterization of the biological compartment. The same holds for the hydraulic characterization, i.e. large bioreactors may necessitate dispersion models.

The application of the methodology is dynamic in such a way that it can be used for designing the measurement campaign or modelling the wastewater plant on the basis of the available short or long term data provided. The lab-scale, pilot scale or on-site experiments dedicated to the assessment of certain parameters decrease the uncertainty on the parameter estimates, especially when OED techniques are used. From a modelling point of view, the steady state calibration of the model has to mimic the activated sludge performance on the long run by disregarding the sudden process disturbances. Thus, long-term data is important in terms of understanding the plant performance. On the other hand, a short-term intensive measuring campaign reflects the responses under dynamic variations (e.g. diurnal load variations). As an example, it should be noted here that some disturbances such as temperature changes have to be considered during long-term simulations since they might directly affect the aeration transfer and the biological reactions etc. However, short-term disturbances can be inhibition, aeration controller failure, etc. These factors should also be taken into consideration. The lack of knowledge on the operational changes (mostly manually controlled AS plants) introduce large uncertainties in

understanding the system behavior, which are difficult to interpret and to consider in the final plant model.

The most important factors in modelling are the accurate influent wastewater characterization and the exact mass balance calculation over the sludge in the system. Basically, these two components are known to be highly correlated. In the case of calibrating an activated sludge plant using the full scale data, the uncertainty will be on the particulate COD components, (X_I and X_S) if the sludge age can not be determined exactly using the phosphate balance or else. One should consider the release of N and P entrapped in the X_S during hydrolysis, as well. In this respect, a respirometric determination (based on biological characterization) is proposed for each modelling case. The sampling type and frequency depend on the needs (2 hrs–24 hrs composite).

A sensitivity analysis can be performed in the steady state and the dynamic calibration stage to figure out which parameter groups should be selected for the calibration of the model. The results of the sensitivity analysis vary depending on the plant configuration and controller strategy. Another important point in this step is that the sensitivity of the model outputs to controller parameters is often higher than for activated sludge parameters. The sensitivity of a parameter can be determined by increasing and decreasing its value and by observing the resulting changes in the simulation output. Dynamic simulations can be used for fine-tuning the parameters or can serve as a verification step by itself. The main issue in the verification step is to test the model by using an independent data set, which was not used in the calibration. In case the calibrated model fails to predict the new dynamic data "reasonably" good, it is then advised to iterate the calibration modules (see Figure 1). In the second iteration, the following should be considered:

- Modification of the model structure. For example, addition of specific components and or processes to the model (two-step nitrification/denitrification, etc.)
- Apply in-depth calibration level for each module in the calibration protocol
    - Perform tracer studies for accurate hydraulic characterization,
    - Implement a more complex settler model e.g. takacs for a better prediction of the settlers
- Perform dedicated lab-scale experiments (preferably designed by OED principles) for quantification of the biomass activity under anoxic, aerobic and anaerobic conditions.

Upon "successful" calibration and verification of the model, the calibrated model can finally be used to achieve the modelling objectives e.g. decreasing the aeration demand, the effluent N and P concentrations of the plant.

CONCLUSIONS

- A calibration protocol based on consolidated scientific and engineering experience is presented for modelling wastewater treatment plants. The protocol is composed of a set of interactive and independent modules for the calibration of hydraulic, settling and biological characterization of the treatment plant.
- The protocol is designed to provide guidelines for the new modelers in this field. The major features of the protocol are highlighted as follows:
    - Object-oriented flexible calibration protocol: The targets of modelling and the availability of the data for calibration determines the overall procedure/steps to be executed during the calibration
    - Data collection and quality is of crucial importance for a reliable calibration, hence data quality should be checked e.g. via mass balances.
    - The influent wastewater characterization and the solids mass balance of the system (SRT) are essential to a successful calibration.

- Influent wastewater characterization is based on respirometric methods in contrast to physico-chemical methods.
- The OED principle is incorporated in the design of experiments (lab-scale as well as full-scale). In this way, uncertainty of the estimates of the model parameters is reduced as well as the required number of experimental works.
- The calibration is based on iterative approach until reaching a "reasonable" good agreement between model results and measurements.

- The calibration protocol is applied successfully to a carrousel type plant treating municipal wastewater. The calibration study showed that the operating parameters of the plant i.e. controllers, internal recirculation, sludge recycles are more sensitive than the ASM model parameters.
- Finally, the calibration protocol has a dynamic structure, which can be updated straightforwardly with the new developments (new experimental methodologies etc.) in the field of activated sludge modelling.

REFERENCE

APHA (1998) Standard Methods for the Examination of Water and Wastewater, 20th ed. American Public Health Association, Washington, DC.

Avcioglu E, Orhon D and Sözen S (1998). A new method for the assessment of heterotrophic endogenous respiration rate under aerobic and anoxic conditions, *Wat. Sci. Tech.*, 38 (8-9), 95-103.

Barker PS and Dold PL (1997) General model for biological nutrient removal activated-sludge systems: model presentation, *Wat. Env. Res.*, 69(5), 969-984.

Barker PD and Dold PL (1995) COD and nitrogen mass balances in activated sludge systems, *Wat. Res.*, 29(2), 633-643.

Boyle WC and Campbell HJJr (1984) Experiences with oxygen transfer testing of diffused air systems under process conditions, *Wat. Sci. Tech.*, 16 (Vienna), 91-106.

Brouwer H, Klapwijk A and Keesman KJ (1998) Identification of activated sludge and wastewater characteristics using respirometric batch experiments, *Wat. Res.*, 32(4), 1240-1254.

Brun R, Kuhni M, Siegrist H, Gujer W and Reichert P (2002) Practical identifiability of ASM2d parameters - systematic selection and tuning of parameter subsets, *Wat. Res.*, 36(16), 4113-4127

Capela S, Gillot S and Héduit A (1999) Oxygen transfer under process conditions: Comparison of measurement methods. In: Proceedings 72nd Annual WEF Conference and Exposition. New Orleans, USA, October 9-13 1999.

Carucci A, Rolle E and Smurra P (1999) Management optimization of a large wastewater treatment plant, *Wat. Sci. Tech.,* 39(4), 129-136.

Chambers B (1992) Design methodology for optimisation of aeration efficiency in activated sludge plants. *In: Proceedings 6th Forum Applied Biotechnology. Med. Fac. Landbouww. Univ. Gent*, 57, 1631-1642.

Chudoba P, Capdeville B and Chudoba J (1992) Explanation of biological meaning of the So/Xo ratio in batch cultivation, *Wat. Sci. Tech.* 26(3-4) 743-751.

Coen F, Vanderhaegen B, Vanrolleghem PA and Van Meenen P (1997) Improved design and control of industrial and municipal nutrient removal plants using dynamic models, *Wat. Sci. Tech.,* 35(10), 53-61.

Comeau Y, Hall KJ and Oldham WK (1990). Indirect polyphosphate quantification inactivated sludge, *Wat. Pollut. Res. J. Canada.,* 25(2)*,* 161-174.

Daigger GT and Nolasco D (1995) Evaluation and design of full-scale watewater treatment plants using biological processes models, *Wat. Sci Tech*, 31(2), 245-255.

Daigger GT and Roper RE (1985) The relationship between SVI and activated sludge settling characteristics, *J. Wat. Pollut. Cont. Fed.*, 57(8), 859-866.

De Clercq (2003) Computational fluid dynamics of settling tanks: development of experiments and rheological, settling and scrapers submodels, PhD Thesis, Ghent University, Faculty of Agricultural and Applied Biological Science, Belgium.

De Clercq B, Coen F, Vanderhaegen B and Vanrolleghem PA (1999) Calibrating simple models for mixing and flow propagation in wastewater treatment plants, *Wat. Sci. Tech.*, 39(4), 61-69.

De Haas DW and Adam N (1995) Use of simple titration procedure to determine H_2CO_3 alkalinity and volatile fatty acids for process control in wastewater treatment, *Water SA*, 21(4), 307-318.

De Pauw D, Sin G, Insel G, Van Hulle S, Vandenberghe V and Vanrolleghem PA (2003) Discussion of 'Assessing Parameter Identifiability of Activated Sludge Model No. 1' by Pedro Afonso and Maria da Conceicao Cunha, *Journal of Environmental Engineering*. (accepted).

Dochain D and Vanrolleghem PA (2001) Dynamical Modelling and Estimation in Wastewater Treatment Processes, *IWA Publishing*, London.

Dochain D, Vanrolleghem PA and Van Daele M (1995) Structural identifiability of biokinetic models of activated sludge respiration, *Wat. Res*., 29(11), 2571-2579.

Dupont R and Sinkjaer O (1994) Kinetic constants of nitrification, *Wat. Sci. Tech.,* 30(4), 181-190.

Ekama GA, Dold PL and Marais, GvR (1986a) Procedures for determining influent cod fractions and the maximum specific growth-rate of heterotrophs in activated-sludge systems, *Wat. Sci. Tech.* 18(6) 91-114.

Ekama GA and Marais GvR (1986b) Sludge settleability and secondary settling tank design procedures. *Wat. Pollut. Control*, 85(1), 101-113.

Germirli F, Orhon D and Artan N (1991) Assessment of the initial inert soluble COD in industrial wastewaters, *Wat. Sci. Tech.*, 23(4-6), 1077-1086.

Gernaey K, Vanrolleghem P and Lessard P (2001) Modelling of a reactive primary clarifier, *Wat. Sci. Tech.*, 43 (7), 73-81.

Gillot S, Deronzier G and Héduit A (1997) Oxygen transfer under process conditions in an oxidation ditch equipped with fine bubble diffusers and slow speed mixers. In: Proceedings 70th Annual WEF Conference and Exposition. Chicago, USA, October 18-22 1997. Vol. 1, 385-392.

Henze M, Gujer W, Mino T, and van Loosdrecht MCM (2000) Activated Sludge Models: ASM1, ASM2, ASM2d and ASM3, Scientific and Technical Report No:9, IWA Publishing, London.

Henze M, Gujer W, Mino T, Matsuo T, Wentzel MC and Marais GvR. (1995). Activated Sludge Model No.2. IAWPRC Task Group on Mathematical Modelling for Design and Operation of Biological Treatment, IAWQ, London.

Henze M., Dupont R., Grau, P and De la Sota A. (1993) Rising sludge in secondary settlers due to denitrification, *Wat. Res.*, 27(2), 231-236.

Henze M (1992) Characterization of wastewater for modeling of activated-sludge processes, *Wat. Sci. Tech.*, 25(6), 1-15.

Henze M, Grady, CPLJr, Gujer W, Marais GvR and Matsuo T (1987) Activated sludge model No.1, IAWPRC Sci. and Tech. Report No. 1, IAWPRC, London

Insel G, Orhon D and Vanrolleghem PA (2003a) Identification and modeling of aerobic hydrolysis mechanism-application of optimal experimental design, *J. Chem. Tech. Biotech.,* 78(4), 437-445.

Insel G, De Pauw D, Lee DS, Weijers S, Dovermann H and Vanrolleghem PA (2003b) Dynamic calibration and model based optimization of an intermittently aerated carrousel plant using the ASM2d model, (in preparation).

Kappeler J and Gujer W (1992) Estimation of kinetic parameters of heterotrophic biomass under aerobic conditions and characterization of wastewater for activated sludge modelling, *Wat. Sci. Tech.,* 25(6), 125-139.

Koch G, Kuhni M, Gujer W, Siegrist H (2000) Calibration and validation of Activated Sludge Model No. 3 for Swiss municipal wastewater. *Wat. Res.*, 34(14), 3580-3590.

Koch G, Pianta R, Krebs P and Siegrist H (1999) Potential of denitrification and solids removal in the rectangular clarifier, *Wat. Res.*, 33(2), 309-318.

Krebs P, Armbruster M, and Rodi W (2000) Numerische Nachklarbecken-Modelle. KA, *Wasserwirtchaft Abwasser Abfall*, 47(7), 985-999.

Lesouef A, Payraudeau M, Rogalla F and Kleiber B (1992) Optimizing nitrogen removal reactor configuration by onsite calibration of the IAWQ activated sludge model, *Wat. Sci. Tech.,* 25(6), 149-165.

Mamais D, Jenkins D and Pitt P (1993) A rapid physical chemical method for the determination of readily biodegradable soluble COD in municipal wastewaters, *Wat. Res.*, 27, 195-197.

Mueller J and Boyle W (1988) Oxygen transfer under process conditions, *J. Wat. Pollut. Control Fed.*, 60, 332-341.

Nowak O, Franz A, Svardal K, Müller V and Kühn V (1999) Parameter estimation for activated sludge models, *Wat. Sci . Tech*., 39(4), 113-120.

Novak L, Larrea L and Wanner J (1994) Estimation of maximum specific growth-rate of heterotrophic and autotrophic biomass - a combined technique of mathematical-modeling and batch cultivations, *Wat. Sci. Tech*. 30(11), 171-180.

Orhon D, Okutman D and Insel G (2002) Characterization and biodegradation of settleable organic matter for domestic wastewater, *Water SA*, 28(3) 299-305.

Orhon D and Artan N (1994) Modelling of activated sludge systems, *Technomic Press*, Lancaster PA.

Wanner O, Kappeler J and Gujer W (1992) Calibration of an activated-sludge model based on human expertise and on a mathematical optimization technique - a comparison, *Wat. Sci. Tech.*, 25(6) 141-148.

Petersen B., Gernaey K., Henze M. and Vanrolleghem P.A. (2003) Calibration of activated sludge models: A critical review of experimental designs. In: *Biotechnology for the Environment: Wastewater Treatment and Modeling, Waste Gas Handling.* Eds. Agathos S.N. and Reineke W., Kluwer Academic Publishers, Dordrecht, The Netherlands. 101-186.

Petersen B, Gernaey K, Henze M and Vanrolleghem P (2001) Evaluation of an ASM1 model calibration procedure on a municipal-industrial wastewater treatment plant, *J. Hydroinformatics*, 4, 15-38.

Petersen B (2000) Calibration, identifiability and optimal experimental design of activated sludge models. PhD Thesis, Ghent University, Faculty of Agricultural and Applied Biological Science, Belgium.

Reichert P, Vanrolleghem P (2001) Identifiability and uncertainty analysis of the River Water Quality Model No. 1 (RWQM1), *Wat. Sci. Tech.*, 43(7), 329-338.

Siegrist H and Tschui M (1992) Interpretation of experimental data with regard to the activated sludge model no. 1 and calibration of the model for municipal wastewater treatment plants, *Wat. Sci. Tech.,* 25(6), 167-183.

Smolders GJF, Vandermeij J, Vanloosdrecht MCM and Heijnen JJ (1994) Model of the anaerobic metabolism of the biological phosphorus removal process-stoichiometry and pH influence, *Biotech. Bioeng.*, 43(6), 461-470.

Sollfrank U and Gujer W (1991) Characterization of domestic wastewater for mathematical modelling of the activated sludge process, *Wat. Sci. Tech.,* 23(4-6), 1057-1066.

Spanjers H and Vanrolleghem P (1995) Respirometry as a tool for rapid characterization wastewater and activated sludge, *Wat. Sci. Tech.,* 31(2), 105-114.

Sperandio M and Paul E (2000) Estimation of wastewater biodegradable COD farctions by combining respirometric experiments in various So/Xo ratios, *Wat. Res*., 34(4), 1233-1244.

Sollfrank U and Gujer W (1991) Characterization of domestic wastewater for mathematical modelling of the activated-sludge process, *Wat. Sci. Tech.,* 23(4-6) 1057-1066 1991

Stamou AI (1997) Modelling of oxidation ditches using an open channel flow 1-D advection dispersion aquation and ASM1 process description, *Wat. Sci. Tech.,* 36(5), 269-276.

Takacs I, Patry G and Nolasco D (1991) A dynamic model of the clarification – thickening process, *Wat. Res.*, 25(10), 1263-1275.

Vanrolleghem PA, Insel G, Sin G, De Pauw D, Petersen B, Van Hulle S, Lee DS, De Clercq B and Gernaey K (2002) Activated sludge model calibration - The BIOMATH protocol, BIOMATH *Technical Report*, Ghent University, Applied Mathematics Biometrics and Process Control (BIOMATH) Department, Ghent, November 2002.

Vanrolleghem P, Van Daele M and Dochain D (1995) Practical identifiability of a biokinetic model of activated sludge respiration, *Wat. Res*., 29(11), 2561-2570.

Weijers SR and Vanrolleghem PA (1997) A procedure for selecting the most important parameters in calibrating the activated sludge model no.1 with full-scale plant data, *Wat. Sci. Tech.,* 36(5), 69-79.

Wouters-Wasiak K, Heduit A and Audic JM (1996) Consequences of an occasional secondary phosphorus release on enhanced biological phosphorus removal, *Water SA*, 22(2), 91-96.

Wentzel MC, Dold PL, Ekama GA and Marais GvR (1985) Kinetics of biological phosphorus release, *Wat. Sci. Tech.,* 17(11-12), 57-71.