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# SYSTEMATIC CALIBRATION OF ACTIVATED SLUDGE MODELS

# *SYSTEMATISCHE CALIBRATIE VAN ACTIEF SLIB MODELLEN*

door

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# Summary

There is a good deal of experiences/reasons accumulated over the past decade concerning the full-scale application of mechanistic models (e.g. Activated Sludge Models (ASM) of Henze *et al.* (2000)) that stimulate and encourage further investment/research in this field. First of all, these ASMs are objective and represent the state-of-the-art in understanding of the complex activated sludge processes ongoing in wastewater treatment plants (WWTPs). Second, they have been successfully applied worldwide on many cases for the optimisation of full-scale operation of WWTPs, e.g. for cost reduction, control, improving effluent quality etc. Third, modelling of WWTPs further increases the in-depth understanding of complex activated sludge processes, which in turn is used to further develop the existing models (an interactive/constructive cycle). Last but not least, they enable dynamic simulation of WWTPs, which is valuable to cross check existing designs of WWTPs based on steady-state approaches and/or rules of thumb.

Because the parameters of the ASMs are not universal, model calibration is strictly required prior to full-scale application. This step critically determines the overall quality of the model application. The research carried out in this thesis is, therefore, situated in the quest to further develop the systematic calibration of Activated Sludge Models (ASMs) and particularly to improve and standardize the quality of the calibration of ASMs for nitrogen removing WWTPs.

In Chapter 2 therefore, a previously proposed calibration methodology (Petersen *et al.*, 2003a) is further improved on the basis of rigorous scientific and engineering experiences with the systematic calibration of activated sludge models. The main motivation of the so-called BIOMATH protocol was to systematize the calibration exercise such that different model calibration studies can be compared and the quality of the calibration study itself can be checked. The two distinctive properties of the BIOMATH protocol are the respirometry based influent characterisation procedure and the incorporation of the Optimal Experimental Design (OED) methodology. From the systematic calibration protocol it becomes clear that lab-scale batch experiments are very much important and are mostly used in full-scale model calibrations (i) to improve the identifiability of the complex ASMs, e.g. by providing estimates to the kinetic and stoichiometric parameters of the model and (ii) for the influent wastewater characterisation. However, the use of batch experiments has so far been limited to aerobic conditions because an appropriate sensor to collect data under anoxic conditions was lacking.

Keeping that in mind, in Chapter 3.1, an integrated sensor was developed by combining the aerobic set-up of Gernaey *et al*. (2002a) and the anoxic set-up of Petersen *et al*. (2002a) in one single unit. The integrated sensor provides an information rich matrix of data consisting of oxygen uptake rate (OUR), nitrate production (NP), nitrate uptake (NU) and proton production (Hp), and was successfully used to sequentially monitor aerobic and anoxic activated sludge activities in BNR plants. In Chapter 3.2, the ion selective electrode (ISE) used for nitrate measurements in the integrated sensor was replaced with a novel nitrate biosensor (Larsen *et al*., 2000). The anoxic set-up developed in Chapter 3.2 successfully provided for the first time high quality and high frequency nitrate uptake rate (NUR) measurements of activated sludge, i.e. every 3 secs. This high quality NUR data allowed to compare the anoxic activity of biomass with the aerobic activity in detail. This was also shown to be essential for model development purposes (see Chapter 4.3).

A complementary step to the use of batch experiments is the *accurate* interpretation of the resulting data in view of parameter estimation for full-scale models of WWTPs. Therefore, the in-depth/mechanistic understanding and the model-based interpretation of the results obtained from the short-term batch experiments were the prime focus of the second part of the thesis. In Chapter 4.1, the titrimetric model of Gernaey *et al*. (2002a) was successfully extended to model the time-varying $CO_2$ transfer rate (CTR) observed in the titrimetric data resulting from aerobic carbon source degradation. This extension made it possible to apply the Gernaey model to adequately interpret titrimetric data collected under a wider range of experimental conditions.

In Chapter 4.2 the oxygen uptake rate (OUR) data collected under aerobic carbon source degradation process were analysed in depth in view of mechanistic interpretation/modelling. In Chapter 4.2.1, it was shown that neither ASM1 nor ASM3 were able to mechanistically describe OUR data collected with biomass from different full-scale WWTPs. This failure was

hypothesised to be due to the conceptual basis of both models: ASM1 assumes that in feast phase substrate is only used for growth while in the endogenous phase biomass only decay. ASM3 assumes that substrate is used only for storage in the feast phase while it grows on the stored substrate in the endogenous/famine phase. This hypothesis was supported by the numerous results obtained elsewhere with the research on storage phenomena by activated sludge. To improve the mechanistic description of activated sludge activity, a simultaneous storage and growth model was successfully developed using a new approach. In this new approach, (i) the substrate uptake kinetics was explicitly separated from the growth kinetics of biomass and (ii) degradation of storage products was modelled using a second order model. This new model was successfully evaluated using OUR data and validated using independent PHB measurements. The model was shown to provide realistic and mechanistically more meaningful parameter estimates. For example, the yield of heterotrophic growth was estimated to be around 0.59, which is much lower than the estimate of ASM1, e.g. 0.75 mgCOD/mgCOD.

In Chapter 4.3 the simultaneous storage and growth model developed in Chapter 4.2.2 was adapted to anoxic conditions and called ASM3e. The ASM3e includes the pH effect of denitrification process since titrimetry was shown to be positive on improving the identifiability of complex models. It was shown here that the ASM3e model could better describe the NUR data collected in Chapter 3.2 and provides more realistic parameter estimates compared to the ASM1e model (the ASM1 model extended with the pH effect of denitrification). Moreover, it was observed that it was possible to estimate the nitrate affinity constant of denitrifiers, $K_{NO3}$, in experiments with nitrate as limiting substrate, thanks to the high frequency and high quality NUR data. The $K_{NO3}$ was estimated to be in the order of 0.015 mgN/l which is low compared to the default values in ASMs (Henze *et al*., 2003). Both models were shown to adequately describe the anoxic titrimetric data but the identifiability of both models when using the titrimetric data should be further studied to eliminate parameter correlation problems. The initial substrate to biomass ratio, $S_0/X_0$, was studied in detail here and observed to be a key factor influencing the response of heterotrophic biomass in anoxic batch experiments. It is advised to keep this ratio low (below 0.1 mgCOD/mgCOD) to obtain representative “extant” parameter estimates for full-scale models. Increasing this ratio in batch experiments was shown to change the estimates of the kinetic parameters of denitrifiers due to physiological adaptation of biomass. A hypothesis complementary to the hypothesis of

Chudoba *et al*. (1992) was developed to explain the physiological adaptation of biomass occurring in response to increasing the $S_0/X_0$ level in anoxic batch experiment.

In Chapter 4.4 the fast transient phenomena often observed in high frequency respirometric measurements obtained under both aerobic (OUR) and anoxic (NUR) conditions were addressed in detail. Referring to dynamic metabolic network modelling of pure cultures (e.g. Chassagnole *et al*., 2002), it appears that this fast transient phenomenon (which takes 2-5 minutes) results from the substrate metabolism at the cellular level, i.e. it takes some time until the electrons of the substrate reach the electron acceptor (e.g., oxygen, nitrate, etc.) reduction sites in the cell. This is reflected as a first order response in the (oxygen or nitrate) measurements obtained in the external environment. This phenomenon could therefore be modelled using a first order model. The first order time constants observed in both OUR and NUR profiles were higher than those of the titrimetric data which appear to reflect the substrate uptake dynamics. These results further support the abovementioned hypothesis. Moreover, it was shown that it is necessary to account for this transient in model-based parameter estimation using respirometric data, otherwise it will induce error into the separate (unique) parameter estimates (e.g. in $\mu_{maxH}$ and $K_S$ parameters). It is also expected that this fast transient occurs regularly in particular WWTPs (e.g., carrousel, SBRs with short cycles of intermittent aeration, anaerobic selectors in WWTPs etc.) and should be studied in detail.

In the third part of the thesis the focus was turned to the evaluation of the BIOMATH systematic calibration protocol. In Chapter 5.1, the BIOMATH protocol was evaluated using the ASM2dN model of a lab-scale nutrient removing SBR (80 L). The BIOMATH protocol was extended with a step-wise calibration procedure for different biological processes in the ASM2dN model. This was possible because the SBR operates batch-wisely thereby providing information relevant for each process under anaerobic, aerobic and anoxic conditions. The calibrated ASM2dN model was also used for the systems analysis to understand in-depth the contributions of each process to the overall N and P removal in the SBR. This type of analysis is important to find out the key degrees of freedom of the system to be used in the process optimisation which is studied in detail in Chapter 6.

A very important aspect of mechanistic modelling of WWTPs is the model validation. In other words, once a model is calibrated to a WWTP, how long does this calibrated model remain valid in terms of adequately representing the WWTP? To answer this question, in

Chapter 5.2 the ASM2d model calibrated 3 years ago to the Haaren WWTP (50,000 PE, The Netherlands) was validated using a new measurement campaign reflecting the recent behaviour of the Haaren WWTP. The BIOMATH calibration protocol was followed for both designing the measurement campaign and performing the validation exercise. The validation results were in general quite positive, i.e. it was still possible to adequately predict the dynamic trends observed in the MLSS and $NO_3$-N measurements but a few parameters needed to be calibrated slightly to better fit the dynamic trends in $PO_4$-P and $NH_4$-N data. This positive outcome of the validation study implies that the lifetime of a calibrated model may be compatible with the lifetime of the WWTP. This certainly reinforces confidence into full-scale mechanistic modelling of WWTPs. However, since the model calibration and validation were performed in the summer period, it will be quite relevant and useful to validate the model under different periods, e.g. spring or winter.

In the final part of the thesis, the attention was focused on the application of calibrated models. Within this frame, in Chapter 6 an iterative systematic protocol was developed and evaluated on a lab-sale SBR (80 L). The particular aim of this protocol was to systematize the model-based search for an optimal operation scenario for activated sludge systems. The application of this protocol to the lab-scale SBR in view of improving both effluent quality and robustness of the SBR operation revealed that it was possible to improve the existing N and P removal by 54% and 74% respectively. However, this protocol can be and should be further improved by incorporating the change in settling properties of activated sludge when different operation scenarios are considered in the systematic search.