

A COMPREHENSIVE MODEL CALIBRATION PROCEDURE FOR ASM1

Britta Petersen^{1,3}, Krist Gernaey^{1,3}, Mogens Henze² and Peter A. Vanrolleghem³

¹ Department CGM, École Polytechnique de Montréal, P.O. Box 6079,
Station Centre-ville, Montreal H3C 3A7 (Canada)

² IMT, Technical University of Denmark, Building 115, DK-2800 Lyngby (Denmark)

³ BIOMATH Department, Ghent University, Coupure Links 653, B-9000 Gent (Belgium)

ABSTRACT

A systematic model calibration procedure for the Activated Sludge Model No. 1 (ASM1) was presented and evaluated on a combined municipal-industrial WWTP. A careful definition of the purpose of the model determines how to approach the model calibration. It was illustrated how additional information obtained from tests specifically designed to describe the hydraulics and the biology of the system help to decide on realistic values for the model parameters. The aim of the illustrative case study was to obtain a good description of the N removal capacity, since the model was to be applied for process optimisation in a later stage. Two of the most important parameters to calibrate were the maximum specific growth rates of heterotrophs and nitrifiers. It was found that additional information on the specific growth rates derived from respirometric lab-experiments can be very important to confirm that the calibrated parameters of the full-scale model are realistic.

INTRODUCTION

Model calibration is understood as the adaptation of a model to describe a certain amount of information obtained from a full-scale wastewater treatment plant (WWTP) under study. This task is often rather time-consuming, and typically the time needed for a model calibration is underestimated. Even though more than a decade has passed since the publication of the Activated Sludge Model No. 1 (ASM1) (Henze *et al.*, 1987), a fully developed model calibration procedure has not been defined yet. We have not been able to find a complete model calibration report in literature. There may be many reasons for this. Important to realize is that the purpose of the model is very much determining on how to approach the calibration, making it difficult to generalize (Henze *et al.*, 1995).

Considering the wide application of the activated sludge models there are surprisingly few references that contain details on the applied model calibration procedure. Often one has to collect bits and pieces of information from various sources to obtain an overview. We have tried to do this collection and summarize the information needed to achieve a successful model calibration.

The overall required information listed below was extracted and combined from different sources (Henze *et al.*, 1987; Lesouef *et al.*, 1992; Pedersen and Sinkjær, 1992; Siegrist and Tschui, 1992; Stokes *et al.*, 1993; de la Sota *et al.*, 1994; Dupont and Sinkjær, 1994; Weijers *et al.*, 1996; Xu and Hultman, 1996; Kristensen *et al.*, 1998):

1. Design data: e.g. reactor volume, pump flows and aeration capacities.
2. Operational data:
 - 2.1. Flow rates, as averages or dynamic trajectories, of influent, effluent, recycle and waste flows.
 - 2.2. pH, aeration and temperatures.

3. Characterisation for the hydraulic model, e.g. the results of tracer tests.
4. Characterisation for the settler model: e.g. zone settling velocities at different sludge concentrations.
5. Characterisation for the biological model, ASM1, of:
 - 5.1. Wastewater concentrations of full-scale WWTP influent and effluent (as well as some intermediate streams between the WWTP's unit processes).
 - 5.2. Sludge composition: e.g. SS, VSS, COD, nitrogen and/or phosphorus content.
 - 5.3. Reaction kinetics: e.g. growth and decay rates.
 - 5.4. Reaction stoichiometry: e.g. yield factors.

The required quality and quantity of information will depend very much on the purpose of the model. In case the model is to be used for educational purposes, for comparison of design alternatives for non-existing plants or in other situations where qualitative comparisons are sufficient, the default parameter values defined by Henze *et al.* (1987) can be applied. However, if the calibrated model is to be used for process performance evaluation and optimisation, it may be necessary to have a more accurate description of the actual processes under study. This especially applies for models of plants that treat industrial wastewater.

The information needed for the characterization of the biological model, listed in point 5 above, can basically be gathered from three sources:

1. Default values from literature.
2. Full-scale plant data.
 - 2.1. Average or dynamic data from grab or time/flow proportional samples.
 - 2.2. Conventional mass balances of the full-scale data.
 - 2.3. On-line data.
 - 2.4. Measurements in reactors to characterize process dynamics (mainly relevant for sequencing batch reactors (SBR's) and other alternating systems).
3. Information obtained from different kinds of lab-scale experiments with wastewater and activated sludge from the full-scale plant under study.

Depending on the intended use of the model, a choice will have to be made on the information source to be tapped from. Furthermore, the purpose will decide to which level the model has to be calibrated, since the quality of the desired model predictions will depend strongly on the quality of the calibration.

PROPOSED CALIBRATION PROCEDURE

From the above we have devised an overall model calibration procedure that is summarized in Figure 1. It should be stressed that, depending on the purpose, not all steps in the proposed model calibration procedure may have to be taken.

Steps 1-5 correspond to the initial phase of collection of the different information sources. In general design (1) and operational (2) data are always needed for a model calibration. E.g. the flow and load variations are important in the design of measuring campaigns for hydraulic, sludge settling and biological characterization of the full-scale WWTP. The hydraulics (3) are typically characterized via tracer tests at the full-scale installation (De Clercq *et al.*, 1999). The settling characteristics (4) can be

characterized via on-line or lab-scale settling tests (Vanderhasselt *et al.*, 1999). Finally, the biology can be characterized via different information sources, as indicated above. A review of the information that can be gained from different kinds of lab-scale experiments is presented in detail elsewhere (Petersen *et al.*, 2001).

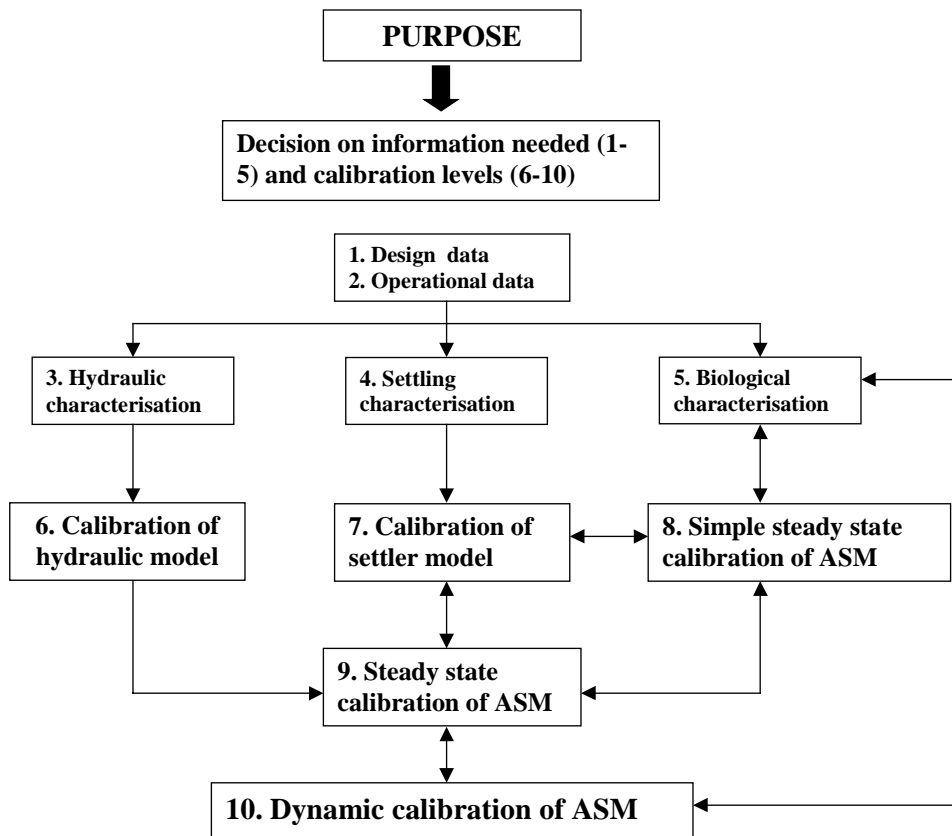


Figure 1. Schematic overview of the different steps in the proposed activated sludge model calibration procedure

Basically steps 6-10 concern different calibration levels. The calibration of the hydraulic model via tracer test results, and the settler model calibration via results from sludge settling tests are steps 6 and 7 respectively. Typically, a first level of calibration of the biological component (e.g. ASM) is a simple steady state model calibration step (8). In this phase of the model calibration the different reactors in the treatment plant are each represented, for instance, by an ideal, perfectly mixed tank, resulting in a simple treatment plant configuration. Data obtained from the full-scale WWTP are averaged, thereby assuming that this average represents a steady state, and the model is calibrated to fit to average effluent and sludge waste data. Typically, the calibration of the ASM and the settler are linked together, since the aim is most often to describe the final effluent quality. Moreover, the recycle from the settler has an influence on the activated sludge system. Thus, at this stage, there may be an interaction between the steady state calibration and the settler model calibration, indicated with the double arrow in Figure 1. Finally, the characterization of wastewater components may be adjusted according to the calibration of the full-scale model, indicated with the double arrow between (8) and (5) in Figure 1.

The next step in the calibration procedure is a steady state model calibration in which this time the hydraulic model is included (9). In general, with a steady state model calibration, only parameters affecting the long-term behaviour of the WWTP can be determined, i.e. the yields (e.g. Y_H), the fraction of inerts produced in decay f_p , decay rates (e.g. b_H) and the influent inert fraction X_I . A steady

state calibration is also very useful for (i) the determination of the initial conditions of the state variables of the model prior to a dynamic model calibration and (ii) for the initiation of a first parameter estimation.

If it is the aim to describe and predict more short-term and dynamic situations, a model calibration to dynamic data will be needed since such data contain more information than steady state data, especially on fast dynamic behaviour. The important point in model calibration based on dynamic data is to obtain a more reliable estimation of the maximum specific growth rates $\mu_{\max H}$ and $\mu_{\max A}$, which are the most important parameters in predicting dynamic situations.

MEASUREMENT CAMPAIGNS: SOME GUIDELINES

At WWTP's data are most often collected routinely with a daily or weekly sampling frequency. This sampling frequency may, however, not be high enough, and for more accurate modeling it may therefore be required to run special measuring campaigns. The sampling frequencies should be chosen in relation to the time constants (related to the time frame over which variables change) of the process and influent variations. For instance, one of the important time constants of the process is the hydraulic retention time. Various lengths of measuring campaigns are recorded in literature. Ideally, one should choose to sample about five times faster than the hydraulic retention time and have a test duration of 3 - 4 times this key time constant (Ljung, 1987). However, since measurements on full-scale WWTP's are relatively expensive these recommendations may not always be completely fulfilled.

Data from the full-scale installation alone may be insufficient for a dynamic model calibration since the reaction kinetics can not be readily obtained from such data, except for specific designs like SBR's and alternating systems (Vanrolleghem and Coen, 1995). For a dynamic model calibration on a full-scale WWTP the modeller is therefore typically aiming at combining more information rich results derived from lab-scale experiments (carried out with sludge and wastewater from the full-scale installation) with data obtained from measuring campaigns on the WWTP under study (Dupont and Sinkjær, 1994; Xu and Hultman, 1996; Kristensen *et al.*, 1998).

CASE STUDY

In this paper the calibration procedure presented in Figure 1 is concretized for the combined municipal-industrial activated sludge WWTP of Zele, Belgium (Figure 2). Despite a step-wise renovation process with the aim of complying with the Flemish effluent standard for total N (15 mg N/l as yearly average), the effluent total N concentration remained too high. For the period January 1997 - November 1998 an average total N concentration of 19.6 mg/l was calculated (average of 53 effluent samples). The absence of a denitrification compartment in the WWTP is believed to be the main reason for the high effluent total N concentrations. In view of this, a modeling study was initiated, the purpose of which was to obtain a good description of the nitrogen removal process and its limitations. The model was to be applied for process optimization of the nitrogen removal, results of which have been reported by Gernaey *et al.* (2000).

The plant

Figure 2 gives a schematic overview of the process layout of the Zele WWTP with a design capacity of 50000 IE. Important for the sequel is that the influent of the WWTP is a mixture of 40 % household and 60 % industrial wastewater (slaughterhouses, industrial laundry, textile cleaning, textile painting etc.). The influent is divided over two parallel rectangular primary clarifiers after the pretreatment step. The activated sludge tank consists of one plug flow aeration tank that is divided into 6 lanes of about

400 m³ each. The mixed liquor flows to two secondary clarifiers (diameter 33 m and volume 2050 m³) through an open aerated channel of about 200 m³. The underflow from the secondary clarifier flows back to the aeration tank through an aerated sludge recycle channel with a volume of 400 m³.

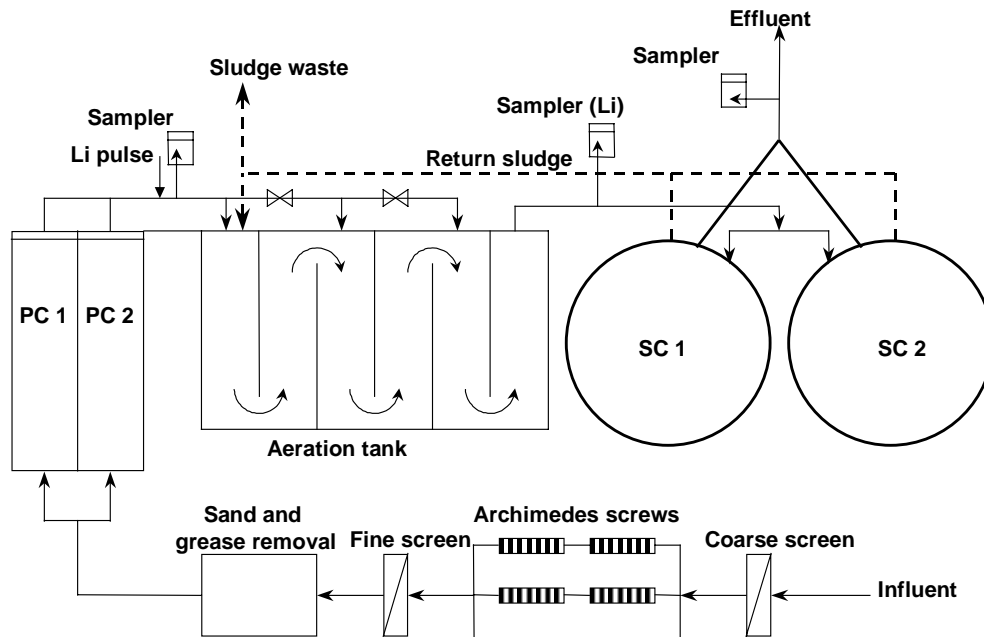


Figure 2. Schematic overview of the process layout of the Zele wastewater treatment plant (PC = primary clarifier; SC = secondary clarifier)

Calibration strategy

When the purpose of the model is known, the necessary information set and calibration strategy are defined. A tracer test was carried out first, to have an adequate description of the hydraulic flow pattern. The sludge at the Zele WWTP is settling reasonably well, and it was therefore found adequate to describe the settler with a simple point-settler model. Hence, no specific tests had to be carried out to characterize the settling properties, and step 4 of the calibration procedure (see Figure 1) could be eliminated. With respect to the wastewater characterisation an intensive measuring campaign was designed to obtain sufficient dynamic data. The variation in readily biodegradable organic substrate was characterized, since the model was to be applied later on for optimisation of N removal. The chemical composition of the sludge was analyzed to support the calibration of the sludge balance. Moreover, lab-scale experiments were planned for the determination of the sludge kinetics related to nitrification and COD degradation, and a decay experiment was carried out to support the description of biomass decay in the treatment plant. No specific experiments were carried out for the determination of stoichiometric coefficients. It was finally investigated whether the calibrated model could be reduced, allowing to increase simulation speed while maintaining the accuracy of the full model.

Measuring Campaign

In November 1998 an intensive measuring campaign was carried out. To test the carefully planned strategy, a 1-day test campaign was done some time before, as was a tracer test that allowed to identify the hydraulic characteristics of the plant. The “dry run” test campaign allowed to evaluate whether the planned measurement frequency of one sample every two hours was high enough to observe the dynamics, and to check if the installed measuring/sampling equipment worked properly. Only afterwards a detailed one-week measuring campaign was carried out.

Two automatic samplers with built-in refrigerator (4°C) were installed on the treatment plant. Time proportional samples (100 ml every 6 minutes) were taken every second hour on the effluent of the primary clarifier (= influent to activated sludge tank) and on the effluent of the secondary clarifier (see Figure 2). The influent samples were analyzed for the following parameters via standard methods: Suspended solids (SS), ammonium nitrogen (NH₄-N), total Kjeldahl nitrogen (TKN), total and soluble chemical oxygen demand (COD_{tot} and COD_{sol}). The effluent samples were analyzed for SS, NH₄-N, nitrate nitrogen (NO₃-N), nitrite nitrogen (NO₂-N), COD_{tot} and COD_{sol}. In addition, mixed liquor and return sludge were sampled at regular times (once or twice per day) to measure the COD, TKN, SS and volatile suspended solids (VSS) content of the sludge.

Effluent flow data were collected with a data logger that was temporarily connected to the effluent flow sensor. Sludge waste flows were obtained from treatment plant operation logbooks. Temperature and pH of the activated sludge in the aeration tank were measured daily.

Respirometric lab-scale experiments with wastewater and activated sludge were carried out during the measuring campaign. Experiments were performed in a RODTOX (Vanrolleghem *et al.*, 1994) and hybrid respirometer (Gernaey *et al.*, 2001). As mentioned, the purpose of these experiments were two fold, i.e. wastewater and sludge kinetic characterisation.

STEP 1-2: DESIGN AND OPERATIONAL DATA

In the description of the plant above, the most important design data have been mentioned. Table 1 lists the operational data as they were observed during the intensive measuring campaign conducted at the plant.

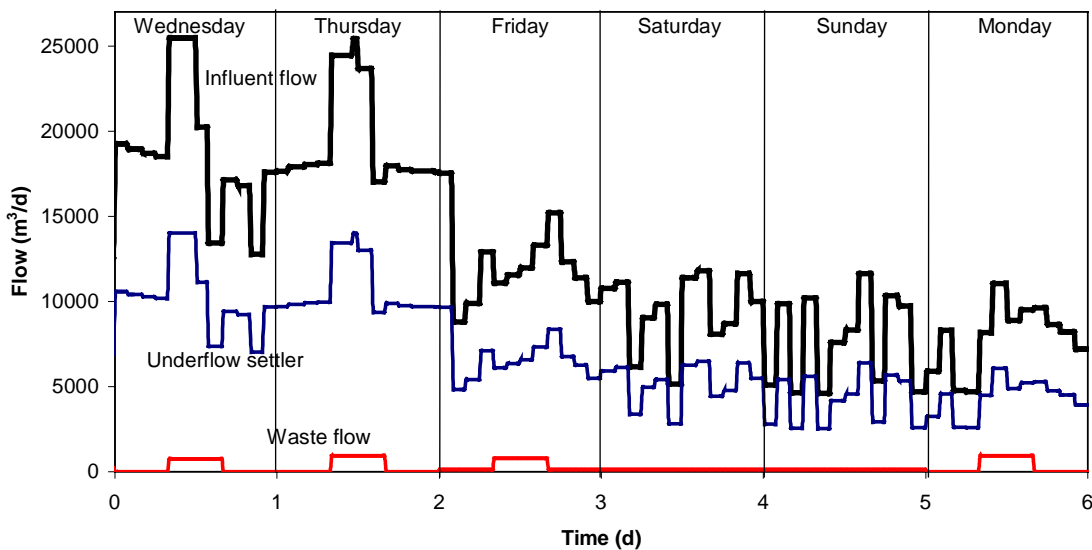


Figure 3. Flow rates during the measuring campaign: 2 hour average influent flow rates were collected at the treatment plant. Settler underflow rates are obtained as $0.55 \cdot$ influent flow (proportional recycle flow controller). The discontinuous waste flow rates were obtained from treatment plant operation logbook data.

As can be seen from Figure 3, the data contain a rain event on the first day. Key parameters reported in Table 1 were therefore calculated both including and excluding the data obtained during the rain event. The data show that the daily COD load, and thereby the sludge load, increased significantly during the rain period. Although the sludge age seems low for a nitrifying WWTP, it is the experience at the

WWTP that it is difficult to maintain a higher sludge age during winter due to a decrease in sludge settleability and a concomitant risk for sludge wash-out. The observed yield is also slightly higher than expected (Henze *et al.*, 1997).

Table 1. Operational data of the Zele WWTP obtained during the intensive measuring campaign

Variable	Unit	Value (incl. rain period)	Value (excl. rain period)
Influent flow average	m ³ /d	12559	10255
Waste flow average	m ³ /d	248	241
Temperature	°C	10.5	10.5
PH		7.2	7.2
Sludge concentration average*	g SS/l	4.0	3.9
COD load	kg COD/d	5607	3730
TKN load	kg TKN/d	342	258
Sludge load	kg COD/kg SS.d	0.48	0.32
Sludge production	kg SS/d	2394	2300
Sludge age	d	6.2	8.6
Observed yield	kg SS/ kg COD	0.42	0.62

*See also Table 2

STEPS 3 AND 6: CHARACTERISATION AND CALIBRATION OF HYDRAULICS

A tracer test was carried out with lithium chloride (LiCl) to characterize the hydraulics of the activated sludge tank. The tracer was added as a pulse at the beginning of the aeration tank (indicated on Figure 2). During the test mixed liquor samples were taken at the point where the activated sludge flows over into the secondary clarifiers (see Figure 2). The sampling frequency took into account the worst case scenario (with respect to obtaining detectable Li concentrations) of an ideally mixed situation, although the expectation in view of the design was plug-flow mixing behaviour. Thus, frequent sampling (one sample every 5 to 10 minutes) was undertaken for 0 - 1.5 times the hydraulic retention time.

Figure 4 shows the pulse response obtained. A sharp peak was recorded with a maximum tracer concentration after a retention time of 0.1 d with a second, smaller peak after approximately 0.27 d. This secondary peak is due to tracer being recycled internally in the treatment plant with the sludge recycle.

After normalising the data, a simple data interpretation was applied first. The N tanks-in-series pulse response equation,

$$C_{Nt} = \frac{N}{(N-1)!} * (N * \theta_t)^{(N-1)} * e^{(-N\theta_t)}$$

was fitted via the solver function in MSExcel and N = 19 was found to give the best fit. This simple approach however assumes constant flow rate and, thus, does not include flow variations that occur

during a tracer test. Moreover, the sludge recycle (including the tracer that is recycled via the underflow of the settlers, e.g. leading to the second peak after 0.27 d in Figure 4) and the residence time of the recycle liquid flow in the secondary clarifiers are not considered in this simplified approach.

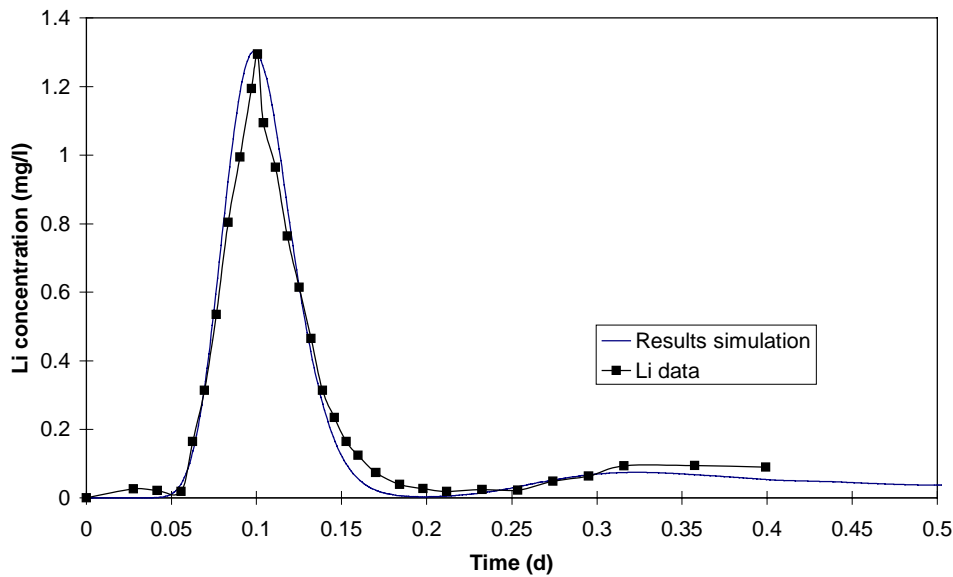


Figure 4. Tracer test results at the Zele WWTP, together with the best model fit

To obtain a better hydraulic description different configurations were simulated in the WEST modelling and simulation environment (Hemmis NV, Kortrijk, Belgium, www.hemmis.com). The value of $N = 19$ obtained from the simple data interpretation was used as a starting point for this more detailed model-based interpretation. The resulting plant configuration that gave the best description of the tracer test data consisted of (i) 24 tanks in series (6 lanes, each consisting of 4 tanks in series, where each tank has a volume of 100 m^3) describing the activated sludge reactors, (ii) two 100 m^3 tanks to describe the sludge channel between aeration tank and secondary clarifiers, (iii) an ideal point-settler with a “buffer tank” of 1000 m^3 to represent the residence time for the liquid that is recycled through the settler underflow, (iv) a lane of 5 tanks (80 m^3 each) describing the recycle channel between the secondary clarifiers and the aeration tank. The resulting hydraulic scheme is illustrated in Figure 5 in the process configuration for the dynamic model.

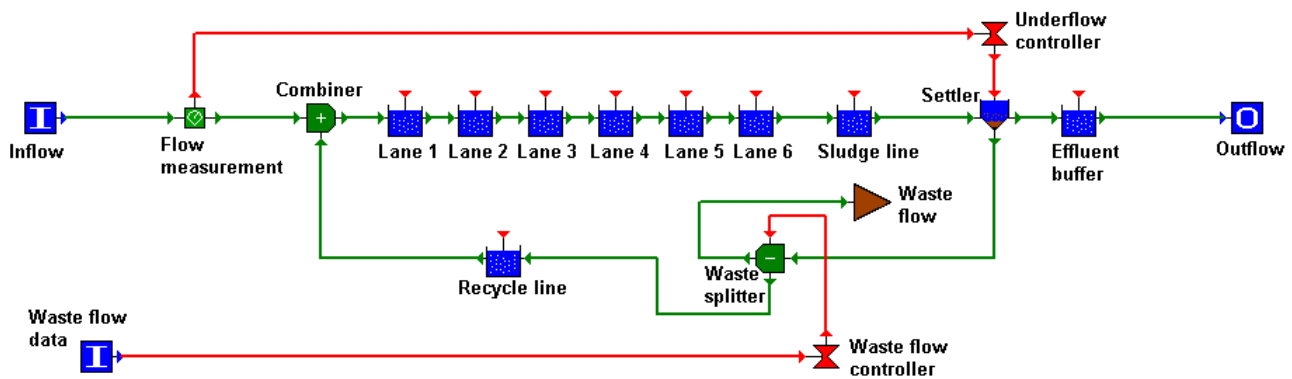


Figure 5. Implementation of the Zele wastewater treatment plant in the WEST simulator

STEP 5: BIOLOGICAL CHARACTERISATION

It would lead too far to discuss all the experimental data recorded during the intensive measuring campaign. Some interesting features are discussed though. For instance, due to the rain event on the first day of the measuring campaign, high influent COD, TKN and SS concentrations are clearly visible. As the soluble fractions are not increased compared to the other days, it can be concluded that the rain event induces a considerable particulate load that cannot be retained by the primary clarifiers.

A diurnal pattern can be distinguished in dry weather. The concentration variations are much lower in the weekend due to the absence of industrial discharges during daytime. The fact that the readily biodegradable COD is present only during the week may also be an effect of the industrial discharge.

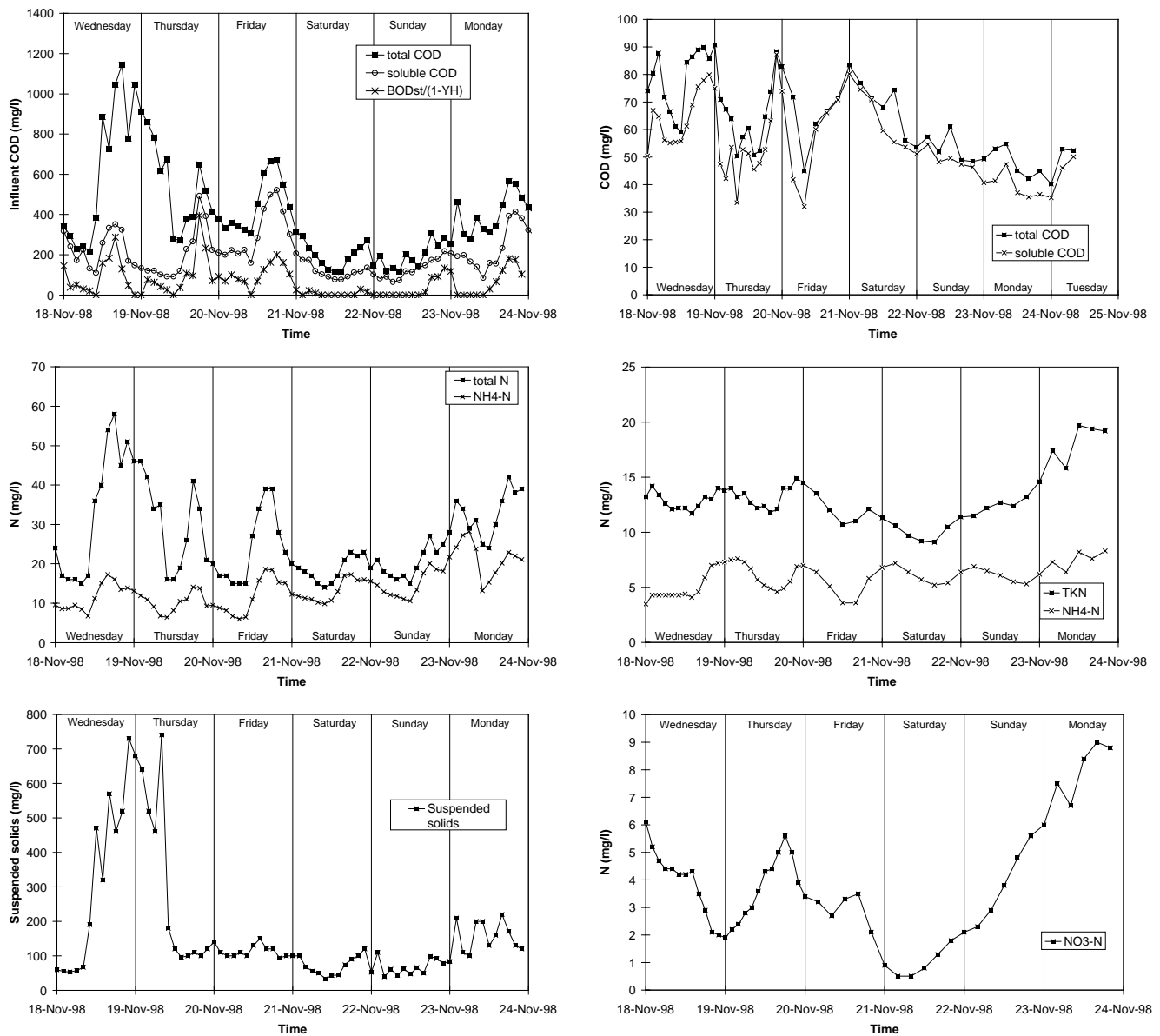


Figure 6. Data set collected during the intensive measuring campaign at the Zele WWTP. Left: influent; Right effluent. Top: COD fractions (total, soluble and (only for influent) readily biodegradable); Middle: Total Kjeldahl and $\text{NH}_4\text{-N}$; Bottom left: Suspended Solids; Bottom right: $\text{NO}_3\text{-N}$.

Effluent quality too shows a diurnal pattern (right column of Figure 6). Evidently, the variations are much smaller than the concentration variations measured in the presettled influent. During the measuring campaign the effluent total N concentration was, in general, lower than the 15 mg/l total N effluent standard. However, on Monday, a day with normal dry weather flow, the effluent total N concentration exceeded the 15 mg/l total N standard. The data also show that full nitrification was not reached. Besides $\text{NH}_4\text{-N}$, $\text{NO}_3\text{-N}$ contributed significantly to the effluent total N concentrations during the measuring campaign.

Translation of wastewater data into ASM1 fractions

An essential step in the wastewater characterisation is the translation of the available data from the measuring campaign into a data set that can be used as input to the ASM1. First of all, it is assumed that the oxygen concentration (S_O) in the incoming wastewater is zero and the conversion of alkalinity (S_{ALK}) is not considered to be limiting in this study. Thus, the ASM1 wastewater components to consider are related to the organic carbon (COD) and nitrogen components.

COD components

The total COD in the model includes the components described in the following equation:

$$\text{COD}_{\text{tot}} = S_S + S_I + X_S + X_I$$

The presence of heterotrophic and autotrophic biomass (X_{BH} and X_{BA}) in the influent wastewater was not considered in the ASM1 report (Henze *et al.*, 1987). Activated sludge may, however, be inoculated significantly by X_{BH} in the influent, especially in cases where no primary settling is present. As an initial approximation X_{BH} and X_{BA} were assumed to be zero in this study. The methods used to characterize the organic wastewater components are summarized in Figure 7.

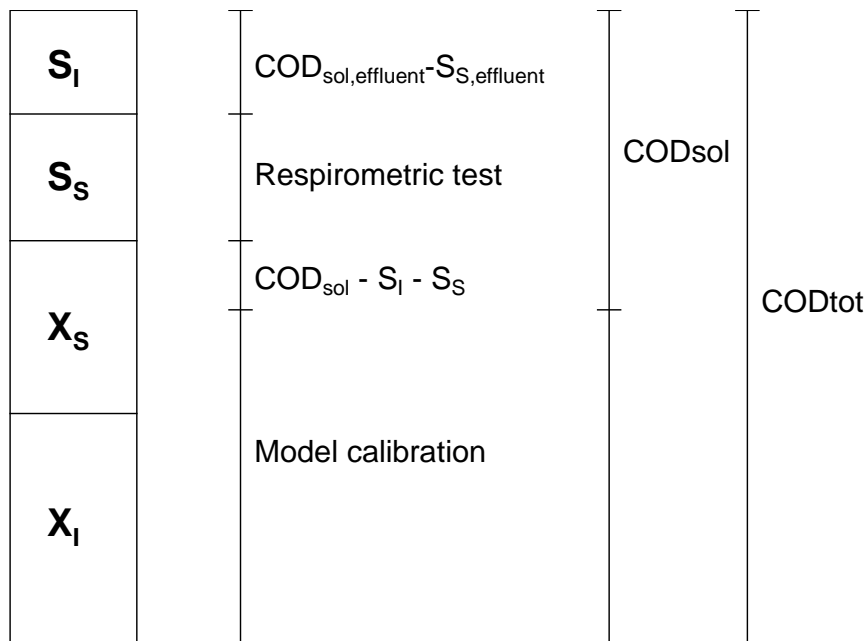


Figure 7. Summary of influent characterisation methods for organic wastewater components

Inert soluble organic matter (S_I), influent and effluent

Influent S_I was determined via effluent data (Henze, 1992). The weekly BOD₅ results of the effluent (available from samples that are routinely taken on the effluent of the WWTP) were used to determine the effluent S_S concentration. An average effluent BOD₅ concentration of 6.2 ± 3.0 mg/l had been measured, and an average BOD₅/COD_{tot} ratio of 0.07 ± 0.03 was calculated for the effluent data. Assuming a BOD yield (Y) of 0.20 (STOWA, 1996), the corresponding effluent S_S concentrations were calculated according to the equations below. The influent S_I was then obtained by combining both equations.

$$S_{S,\text{effluent}} = \frac{0.07 * \text{COD}_{\text{tot}}}{(1 - Y)} = 0.0875 * \text{COD}_{\text{tot,effluent}}$$

$$S_{I,\text{effluent}} = S_{I,\text{influent}} = (\text{COD}_{\text{sol,effluent}} - S_{S,\text{effluent}})$$

Readily biodegradable substrate (S_S), influent

Using respirometric tests (Vanrolleghem *et al.*, 1999), the influent readily biodegradable COD is set equal to the model component S_S .

In the next step, the mass balance for influent COD_{sol} (COD_{sol,influent}) was checked:

$$\text{COD}_{\text{sol,influent}} = S_S + S_I + S_{\text{rest}}$$

In case the measured COD_{sol,influent} is higher than $S_S + S_I$, a solution may be to add S_{rest} to the slowly biodegradable substrate, X_S . On the contrary, if COD_{sol,influent} is lower than $S_S + S_I$, part of the measured BOD_{st} may be considered to be originating from X_S . For the wastewater under study it appeared that COD_{sol,influent} > ($S_S + S_I$), thus S_{rest} was added to the X_S component.

Slowly biodegradable substrate (X_S), influent

Part of the X_S concentration came from the above mass balance as S_{rest} . However, X_S was also partly determined from the steady state model evaluations as the remainder of the particulate COD that was not considered X_I (see below).

Inert suspended organic matter (X_I), influent

The best estimate for X_I is obtained by comparing the measured and predicted sludge concentration and sludge production (Henze *et al.*, 1987; Henze *et al.*, 1995). The X_I influent concentration is typically used as a “tuning component” in the model calibration of the sludge balance (Henze *et al.*, 1995; Nowak *et al.*, 1999), and the X_S concentration is adjusted accordingly via the mass balance below (assuming that X_{BH} and X_{BA} are negligible in the influent, see above).

$$\text{COD}_{\text{tot}} - \text{COD}_{\text{sol}} = X_S + X_I$$

Initially X_I was assumed to be 50 % of the particulate COD. However, this was adjusted during the steady state model calibration (see Steps 7-9 below).

N components

For the nitrogen fractions a similar approach was used for both influent and effluent characterisation. It was assumed that the influent contains negligible concentrations of nitrate (S_{NO}). The total Kjeldahl nitrogen could then be fractionated according to (Henze *et al.*, 1987):

$$\text{TKN} = X_{\text{NI}} + X_{\text{ND}} + S_{\text{NI}} + S_{\text{ND}} + S_{\text{NH}}$$

Ammonia nitrogen (S_{NH})

The analytically measured $\text{NH}_4\text{-N}$ concentration was considered to be equal to S_{NH} .

Soluble biodegradable organic nitrogen (S_{ND})

Since only TKN measurements were available, an assumption had to be made on the soluble fraction. It was considered that the ratio of soluble to total TKN was equal to the ratio of COD_{sol} to COD_{tot} . The soluble Kjeldahl nitrogen (SKN) was therefore approximated via

$$\text{SKN} = \frac{\text{COD}_{\text{sol}}}{\text{COD}_{\text{tot}}} \cdot \text{TKN} = S_{\text{NI}} + S_{\text{ND}} + S_{\text{NH}}$$

and by assuming that the nitrogen content of the inert soluble organic matter (i_{NSI}) equals 1.5% (Henze *et al.*, 1995) the concentration of S_{ND} can be determined via:

$$S_{\text{ND}} = \text{SKN} - i_{\text{NSI}} \cdot S_{\text{I}} - S_{\text{NH}}$$

Slowly biodegradable organic nitrogen (X_{ND})

For the determination of X_{ND} an assumption must be made concerning the nitrogen content of inert suspended organic matter (i_{NXI}). With a value of 1% for i_{NXI} (Henze *et al.*, 1995), X_{ND} becomes:

$$X_{\text{ND}} = \text{TKN} - i_{\text{NXI}} \cdot X_{\text{I}} - \text{SKN}$$

Sludge composition

Based on ten measurements of the COD, SS and VSS content in the mixed liquor and the recycle sludge (Table 2), it can be concluded that this activated sludge has a slightly higher COD/VSS ratio than typical values, perhaps due to the industrial origin of part of the wastewater.

Kinetic characterization

Respirometric experiments were conducted to obtain data from which kinetic parameters related to nitrification and COD degradation could be estimated. The design of these experiments is described in more detail elsewhere (Petersen, 2000), but consisted of simultaneous addition of wastewater and ammonium, thus allowing to estimate the nitrification kinetics and the degradation of COD in a single experiment. The exogenous oxygen uptake rate, $r_{\text{O,ex}}$, caused by the wastewater and ammonium addition can be described by :

$$r_{\text{O,ex}} = (1 - Y_{\text{H}}) \cdot \frac{\mu_{\text{max H}} X}{Y_{\text{H}}} \cdot \frac{S_{\text{S}}}{K_{\text{S}} + S_{\text{S}}} + (4.57 - Y_{\text{A}}) \cdot \frac{\mu_{\text{max A}} X}{Y_{\text{A}}} \cdot \frac{S_{\text{NH}}}{K_{\text{NH}} + S_{\text{NH}}}$$

Table 2. Sludge composition analysis (average and 95% confidence interval)

	SS (g/l)	VSS/SS	COD/SS	COD/VSS	TKN/COD (%)
Activated sludge	4.01 ± 1.20	0.70 ± 0.02	1.38 ± 0.26	1.99 ± 0.36	3.90 ± 1.31
Recycle sludge	10.05 ± 5.27	0.69 ± 0.02	1.37 ± 0.12	1.98 ± 0.17	3.45 ± 1.38

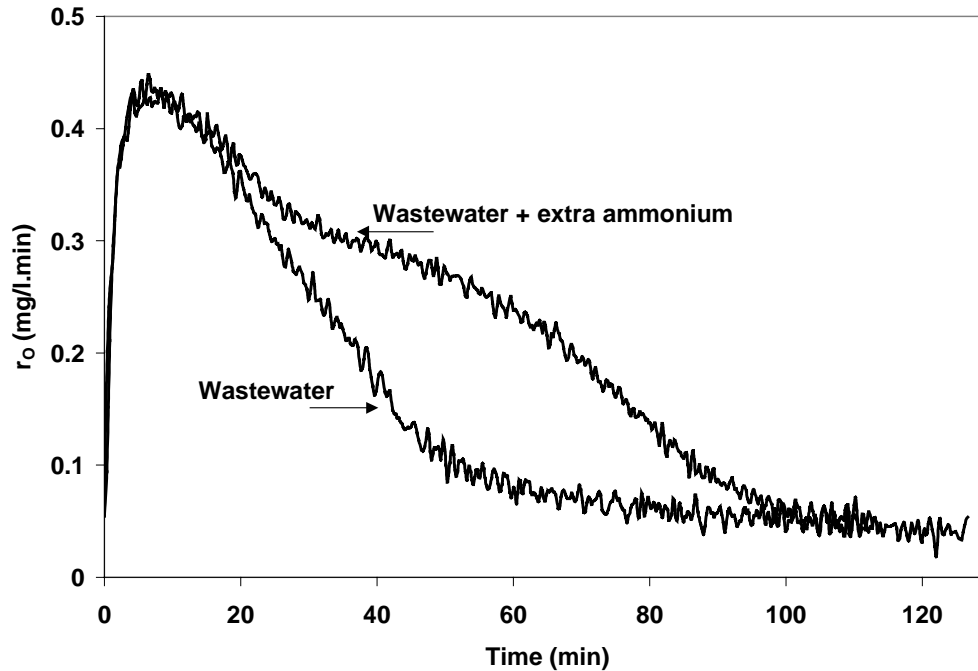


Figure 8. Example of respirometric tests with wastewater and wastewater mixed with ammonium

In Figure 8 a typical respirogram of a wastewater sample (lower line) and a respirogram obtained after addition of wastewater plus extra ammonium (top line) are illustrated. It is obvious that the first respirogram obtained when only wastewater is added to the sludge can not be separated clearly into two parts, i.e. one part that describes the oxygen consumption due to COD degradation and one part that describes the nitrification. Thus, it can be concluded that such respirogram is not informative enough for the identification of both the nitrification kinetics and the degradation kinetics related to COD removal. Therefore optimal experiments were designed by Petersen (2000) where an optimal dose of additional ammonium was added together with the wastewater. In this way it became possible to simultaneously and reliably identify the kinetic parameters of both processes from one set of experimental data. For a complete description of the lab-scale experiments and their interpretation, including the estimation of kinetic parameters, the reader is referred to Petersen (2000) and Gerney *et al.* (2001).

An interesting finding for this treatment plant was that the respirometric tests were in general not informative enough to describe the degradation of COD in the wastewater via Monod kinetics, as described in the equation above (i.e. the respiration rate was not saturated at a certain constant maximum value in the experiment corresponding to an absence of zero order kinetics). Consequently, the COD degradation was instead described with a simpler model, i.e. a first order model, where the first order rate constant k replaces the Monod parameter combination $\mu_{\max H} / K_S$, leading to the following model for the respiration rate:

$$r_{O,ex} = (1 - Y_H) \cdot \frac{kX}{Y_H} S_S + (4.57 - Y_A) \cdot \frac{\mu_{\max A} X}{Y_A} \cdot \frac{S_{NH}}{K_{NH} + S_{NH}}$$

STEP 7-9 STEADY STATE MODEL CALIBRATION

The main aim of this step is to fit the sludge production to the plant data. This is done by adjusting parameters for long term behavior such as decay rates and influent inert particulates X_I . An experimental value of the decay rate was determined from a lab-scale respirometric test in which the endogenous respiration rate, $r_{O,end}$, is measured in a long term (5 days) aerated batch experiment without substrate supply. The endogenous decay rate, b_H' , is determined as the slope of the curve consisting of $\ln(r_{O,end}(0))/\ln(r_{O,end}(t))$ data points plotted as function of time (Ekama *et al.*, 1986). This decay rate can then be transformed into the model decay rate b_H via (Henze *et al.*, 1987):

$$b_H = \frac{b_H'}{1 - Y_H(1 - f_p)} \quad (5)$$

where Y_H was set to 0.67 and f_p to 0.08 according to the ASM1 default parameters (Henze *et al.*, 1987). Temperature correction of the parameters determined from the lab-scale experiments (18 °C) were carried out according to standard procedures (Henze *et al.*, 1997). The value of 0.41 d^{-1} obtained in this way was used as a starting point in the calibration.

For the steady state model calibration a simple WWTP configuration was constructed in the simulator. The steady state configuration consisted of one aeration tank ($V = 2600 \text{ m}^3$), a point-settler, an internal recycle line ($V = 400 \text{ m}^3$), and a constant average sludge waste flow from the recycle line.

Initial trials of steady state calibration of the sludge production were unsuccessful when the rainy period was not included in the evaluated period. Indeed, the extra load of COD and SS during the rain period contributed significantly to the sludge production, and this extra sludge production was most probably only wasted during the following dry weather flow days. To take this into account it was therefore decided to include the data measured during the rain event as well when calculating the average influent composition. With these loadings it was possible to calculate sludge productions that were comparable to the measured ones (19177 kg versus 19535 kg). To reach this, the decay rate had to be increased to 0.5 d^{-1} which is relatively high compared to the value reported in Henze *et al.* (1987), but in accordance with the experimental value of 0.41 d^{-1} .

In this step the fraction of nitrifiers and heterotrophs on the total biomass concentration (expressed as COD) is to be established as well. The calibrated values can be compared to values obtained from direct equations such as, for nitrifiers (Sinkjær *et al.*, 1994):

$$f_{BA} = Y_A \cdot \frac{\theta_X}{1 + b_A \cdot \theta_X} \cdot \frac{N_{NIT}}{MLVSS \cdot V}$$

For the plant under study, the above equation yielded $f_{BA} = 0.0085 \text{ mg COD}_{NIT}/\text{mg COD}$. This value is very close to the steady state model calibration that yielded an autotrophic biomass fraction (f_{BA}) of $0.0086 \text{ mg COD}_{NIT}/\text{mg COD}$.

The fraction of heterotrophic biomass (f_{BH}) was calculated in a similar way leading to a directly calculated value of $0.217 \text{ mg COD}_{HET}/\text{mg COD}$ that compares well to the steady state calibration value of $0.182 \text{ mg COD}_{HET}/\text{mgCOD}$.

STEP 10 DYNAMIC MODEL CALIBRATION

The configuration used to model the dynamics of the Zele WWTP was already presented in step 3 when the hydraulic calibration was completed (see Figure 5). It is indeed the hydraulic characterization that determines the number and location of the tanks in which the reactions take place. Some specific elements had to be added though to describe the process operation adequately. The recycle flow was controlled at 55 % of the influent flow rate, to simulate the behaviour of the full-scale WWTP. To this purpose an influent flow measurement coupled to a proportional underflow controller was included in the model (see Figure 5). Furthermore, a waste flow controller was implemented in the model to simulate the discontinuous sludge waste from the recycle line. This on/off controller was fed with a data input block that indicated the sludge waste rate (the data were obtained from the treatment plant operation logbook).

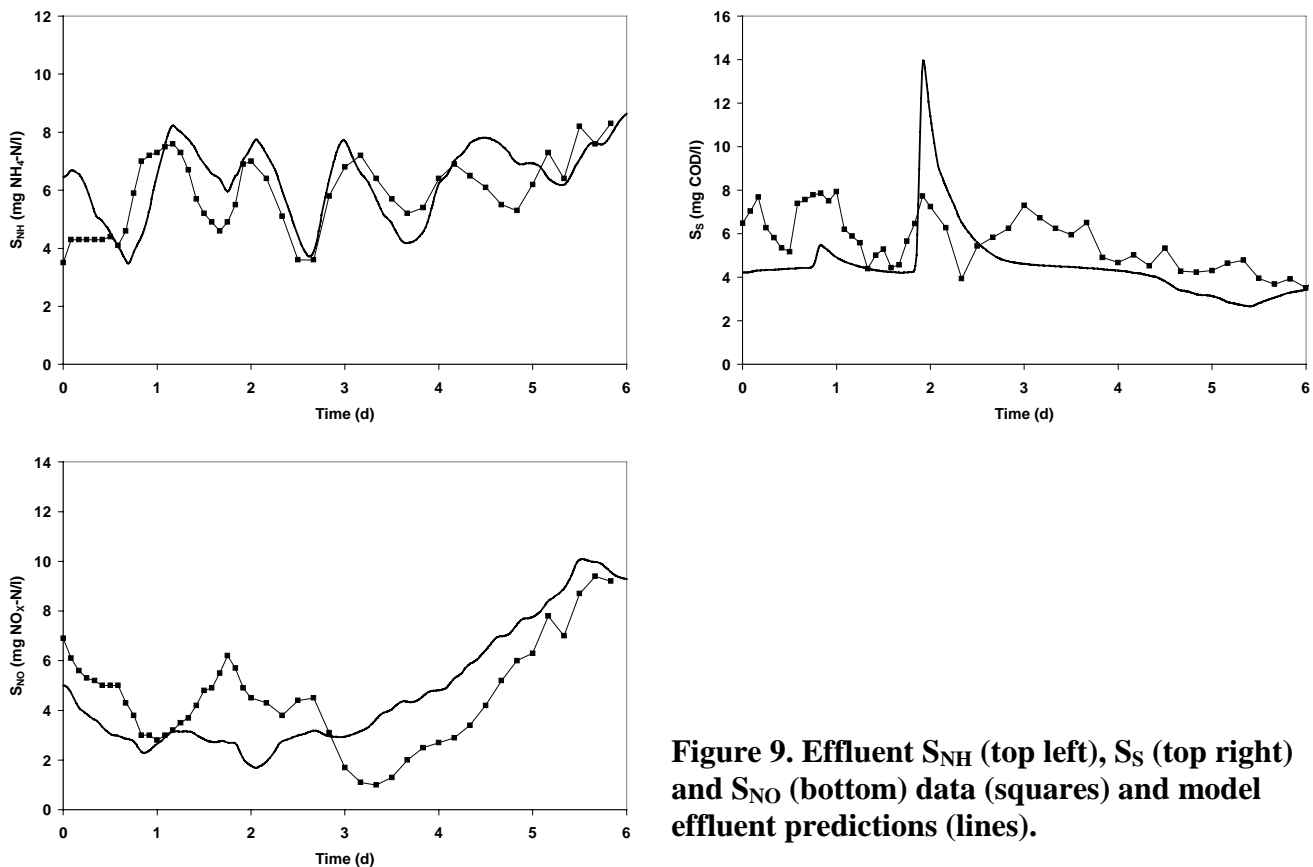


Figure 9. Effluent S_{NH} (top left), S_S (top right) and S_{NO} (bottom) data (squares) and model effluent predictions (lines).

In the dynamic calibration, special attention was devoted to establish the parameter values of the maximum specific growth rates of heterotrophs and nitrifiers. The maximum specific growth rates μ_{maxH} and μ_{maxA} were calibrated to 2.8 d^{-1} and 0.31 d^{-1} respectively, and the K_S was adjusted to 15 mg COD/l . Since the simulated S_{NH} concentration in the aeration tanks was always higher than about 3 mg N/l (i.e. the minimum measured concentration of the final effluent, see Figure 6) the influence of the half saturation coefficient, K_{NH} , is insignificant and it does not have to (nor can it !) be estimated. With these calibrated parameters, the model predicts effluent S_{NH} and S_S data (Figure 9) reasonably well. Only on one occasion do the simulations result in a S_S peak that is not present in the data. This S_S peak corresponds to a high influent concentration that coincides with a high flow rate, which could apparently not be dealt with in an adequate way.

Initially the model predicted too high S_{NO} concentrations in the final effluent. Although the activated sludge system is fully aerated it is likely that some simultaneous denitrification can take place in the system, e.g. in the less intensively aerated recycle channel. For instance, the NO_3-N concentration decreased to about 1 mg N/l on Friday evening and Saturday morning. This can be explained by an increased residence time in the aeration tank (lower influent flow rate) combined with availability of sufficient readily biodegradable carbon for denitrification entering the WWTP on Friday afternoon (see Figure 3 and 6). The effluent NO_3-N concentration increased again on Sunday and Monday (Figure 9) probably due to lack of readily biodegradable COD (see Figure 6). To deal with this deviation, the saturation coefficient for oxygen, K_{OH} , was increased slightly to 0.5 mg $O_2.l^{-1}$ to decrease the inhibition of denitrification by O_2 . In addition, the fraction of denitrifiers, η_g , was decreased to 0.6. The resulting description of effluent S_{NO} (Figure 9) appears acceptable.

As a final evaluation of the calibration quality, the removal efficiencies for COD_{tot} , COD_{sol} , TKN and NH_4-N have been calculated on the basis of the measured data on the one hand, and on the basis of the dynamic simulation results on the other hand. Table 3 shows that the model is able to describes the actual removal very well. Table 4 summarizes the results of the calibration and gives the complete parameter list of the calibrated dynamic model of the Zele wastewater treatment plant.

Table 3. Comparison of removal efficiencies found in the data and predicted by the model

Removal efficiency	COD_{tot}	COD_{sol}	TKN	NH_4-N
Measurements	84%	73%	68%	58%
Simulation	83%	72%	67%	54%

Table 4. List of main parameters for dynamic model (10 °C)

Parameter	Default (10 °C)	Calibrated	Units
Y_H	0.67		g cell COD formed/g COD oxidized
Y_A	0.24		g cell COD formed/g N oxidized
μ_{maxH}	3.0	2.8	d^{-1}
μ_{maxA}	0.3	0.31	d^{-1}
b_H	0.2	0.5	d^{-1}
b_A	0.05	0.02	d^{-1}
K_S	20	15	g COD/ m^3
K_{NH}	1.0		g NH_4-N/m^3
K_{NO}	0.5		g NO_3-N/m^3
K_{OH}	0.2	0.5	g O_2/m^3
K_{OA}	0.4		g O_2/m^3
k_h	1.0		g slowly biodegradable COD/g cell COD.d
K_X	0.01		g slowly biodegradable COD/g cell COD
η_g	0.8	0.6	Dimensionless

Validation

Since this calibration was not using the parameter estimates obtained from the respirometric lab-experiments, a chance was available to perform a validation of the values found.

When considering the nitrification kinetics, it has to be borne in mind that, in fact, one can only estimate a parameter combination involving the maximum specific growth rate, i.e.

$(4.57 - Y_A) \cdot \mu_{\max A} \cdot X_{BA} / Y_A$ from such respirometric tests (Petersen *et al.*, 2000). This combination is in fact equal to the maximum oxygen uptake rate for nitrification assuming no substrate limitation. Thus, a way to validate the parameters of the full-scale model with the ones derived from lab-scale experiments (corrected for temperature differences) is to compare the parameter combination just described with the value found by dynamic calibration. With a $\mu_{\max A}$ of 0.31 d^{-1} and an average X_{BA} of about 40 mg COD/l , the simulated maximum oxygen uptake rate becomes $225 \text{ mg.l}^{-1}.\text{d}^{-1}$. This is in very good agreement with the parameter combination derived from 21 independent lab-scale experiments which had an average of 237 mg/l.d with a 95% confidence interval of $175\text{-}300 \text{ mg.l}^{-1}.\text{d}^{-1}$.

As mentioned above, the heterotrophic substrate degradation observed in the respirometric lab-experiments could not be described with a Monod model, but only with a first order expression. However, a validation of the calibrated parameters in the full-scale model (that does use the Monod kinetic model) versus the lab-experiment based parameters can still be carried out. Indeed, the substrate degradation rate can be calculated on the basis of both the lab-scale model and its parameters on the one hand, and the Monod model and its parameters on the other hand. The calculated substrate concentration dependent degradation rates can be seen in Figure 10. The lab-experiment based parameters were estimated on the basis of 16 different respirometric tests and the corresponding 95% confidence interval is given in Figure 10 as well.

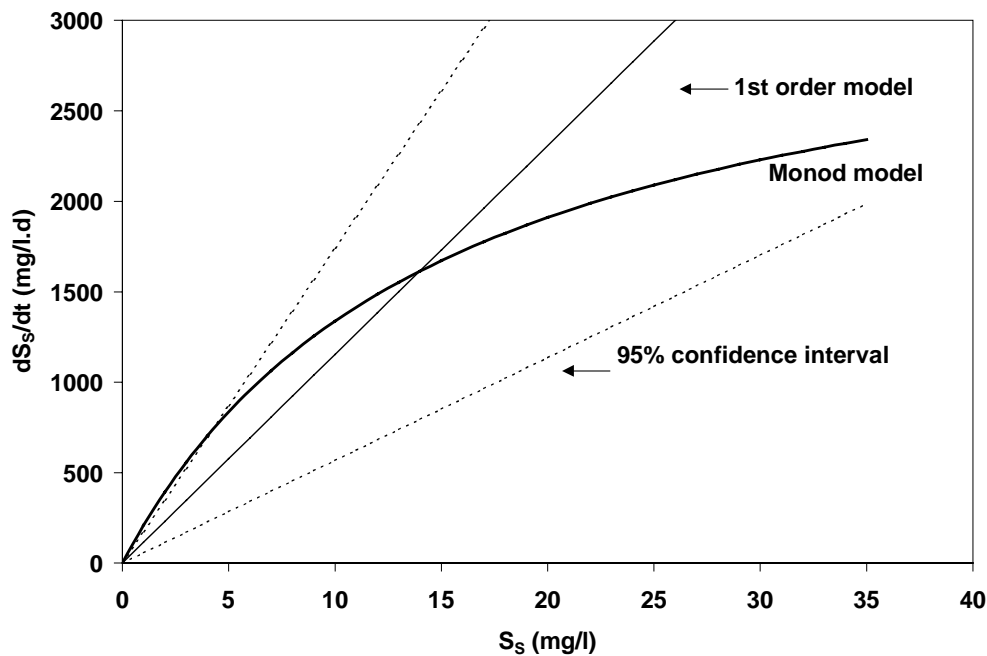


Figure 10. Substrate removal rate (dS_s/dt) plotted as a function of the substrate concentration for the Monod model (used in the calibrated model) and the 1st order model (used for the interpretation of the lab respirometric data)

For the predictions by the Monod model the average simulated biomass concentration was used for X_{BH} . It is clear that as S_S increases, the model result based on the lab-experiment based parameters deviates from the Monod model. However, important to notice is that for the smaller S_S concentrations, i.e. in the first order region of the Monod model, $S_S < K_S$, the Monod profile lies within the results of the lab-scale experiments, confirming that a value of 2.8 d^{-1} for $\mu_{\max H}$ and 15 mg/l for K_S are reasonable. The simulated S_S concentrations in the main part of the aeration tanks were indeed below the value of K_S . Thus, the experimental first order description of the S_S removal is realistic.

MODEL REDUCTION

Since the number of tanks in the current model of the aeration tank is 24, a considerable amount of calculations are necessary to run simulation. Indeed, in each of these tanks a full set of ASM1 differential equations must be solved. It was therefore investigated whether the number of tanks could not be reduced. To evaluate the loss in accuracy due to model reduction, the quality of correspondence between the simulated values and the available data of S_{NH} was evaluated. The criterion that was chosen is the average relative deviation (ARD):

$$ARD = \frac{1}{n} \cdot \sum_{i=1}^n \left(\frac{|X_{i_{\text{obs}}} - X_{i_{\text{sim}}}|}{X_{i_{\text{obs}}}} \right) \cdot 100\%$$

For the calibrated 24-tank model the ARD was 16.5%. When the number of tanks was reduced from 24 to 12 tanks in the aeration lane, and from 5 to 3 in the recycle channel, the same ARD (16.5%) was obtained for effluent S_{NH} . Thus, this model reduction gave the same accuracy as the full model. However a further reduction of the number of tanks to 8 in the activated sludge lanes and 2 in the recycle channel gave a significantly worse description with an ARD that increased to 73.5%. Although the dynamics of the effluent S_{NH} data could still be described, the simulated S_{NH} concentrations were in general considerably higher than the measured data with the last model. In principle, one could imagine that if the value of $\mu_{\max A}$ is increased then a similar model fit for the reduced 8 tanks in series model could be reached as for the calibrated model, since an increase of $\mu_{\max A}$ would decrease the outlet S_{NH} . Thus, this means that a “wrong” hydraulic characterisation could be compensated by a change of kinetic parameter values.

Summarising, the model reduction to 12 and 3 tanks instead of 24 and 5 resulted in a model that needed about 50% less calculation time for a simulation.

CONCLUSION

A systematic model calibration procedure was presented and evaluated for a combined municipal-industrial WWTP. It was underlined that it is very important to define the purpose of the model carefully since this will determine how to approach the model calibration. In this study it was clearly illustrated how additional information obtained from tests specifically designed to describe the hydraulics and the biology of the system help to decide on realistic model parameters during the model calibration procedure.

The aim of this study was to obtain a good description of the N removal capacity, since the model was to be applied for process optimisation in a later stage. It was thus important to have a good description of the process dynamics. Therefore, the hydraulic behaviour of the system was investigated, resulting

in a 24 tanks-in-series model to describe the plug flow aeration tank. It was shown that this hydraulic model could be reduced to a 12 tanks-in-series model, yielding a 50% reduction of the calculation time for the scenario simulations.

Two of the most important parameters to calibrate were the maximum specific growth rates of heterotrophs and nitrifiers. It was found that additional information on the specific growth rates derived from respirometric lab-experiments can be very important to confirm that the calibrated parameters of the full-scale model are realistic.

REFERENCES

- de la Sota A., Larrea L., Novak L., Grau P. and Henze M. (1994) Performance and model calibration of R-D-N processes in pilot plant. *Wat. Sci. Technol.*, **30**(6), 355-364.
- De Clercq B., Coen F., Vanderhaegen B. and Vanrolleghem P.A. (1999) Calibrating simple models for mixing and flow propagation in waste water treatment plants. *Wat. Sci. Technol.*, **39**(4), 61-69.
- Dupont R. and Sinkjær O. (1994) Optimisation of wastewater treatment plants by means of computer models. *Wat. Sci. Technol.*, **30**(4), 181-190.
- Ekama G.A., Dold P.L. and Marais G.v.R. (1986) Procedures for determining influent COD fractions and the maximum specific growth rate of heterotrophs in activated sludge systems. *Wat. Sci. Technol.*, **18**(6), 91-114.
- Gernaey K., Petersen B., Ottoy J.P. and Vanrolleghem P.A. (2001) Activated sludge monitoring with combined respirometric - titrimetric measurements. *Wat. Res.*, **35**, 1280-1294.
- Gernaey K., Petersen B., Parmentier G., Bogaert H., Ottoy J.P. and Vanrolleghem P.A. (2000) Application of dynamic models (ASM1) and simulation to minimize renovation costs of a municipal activated sludge wastewater treatment plant. Proceedings 1st World Congress of the International Water Association, 3-7 July 2000.
- Henze M. (1992) Characterization of wastewater for modelling of activated sludge processes. *Wat. Sci. Technol.*, **25**(6), 1-15.
- Henze M., Grady C.P.L.Jr., Gujer W., Marais G.V.R. and Matsuo T. (1987) Activated Sludge Model No. 1. IWA Scientific and Technical Reports No. 1. London, UK.
- Henze M., Gujer W., Mino T., Matsuo T., Wentzel M.C.M. and Marais G.v.R. (1995) Activated sludge model No. 2. IWA Scientific and Technical Report No. 3, London, UK.
- Henze M., Harremoës P., la Cour Janssen J. and Arvin E. (1997) Biological and chemical wastewater treatment. 2nd edition, Springer, Berlin.
- Kristensen H.G., la Cour Janssen J. and Jørgensen E. (1998) Batch test procedures as tools for calibration of the activated sludge model – A pilot scale demonstration. *Wat. Sci. Technol.*, **37**(4-5), 235-242.
- Lesouef A., Payraudeau M., Rogalla F. and Kleiber B. (1992) Optimizing nitrogen removal reactor configurations by on-site calibration of the IAWPRC activated sludge model. *Wat. Sci. Technol.*, **25**(6), 105-123.
- Ljung L. (1987) System Identification - Theory for the User. Prentice-Hall, Englewood Cliffs, New Jersey.
- Nowak O., Franz A., Svardal K., Muller V. and Kuhn V. (1999) Parameter estimation for activated sludge models with help of mass balances. *Wat. Sci. Technol.*, **39**(4), 113-120.
- Pedersen J. and Sinkjær O. (1992) Test of the activated sludge models capabilities as a prognostic tool on a pilot scale wastewater treatment plant. *Wat. Sci. Technol.*, **25**(6), 185-194.
- Petersen B. (2000) Calibration, identifiability and optimal experimental design of activated sludge models, Ph.D. thesis, Ghent University, Faculty for Agricultural and Applied Biological Sciences, Belgium.

- Petersen B., Gernaey K. and Vanrolleghem P.A. (2000) Improved theoretical identifiability of model parameters by combined respirometric-titrimetric measurements. A generalisation of results. In: Proceedings IMACS 3rd Symposium on Mathematical Modelling, February 2-4, 2000, Vienna University of Technology, Austria. Vol.2, 639-642.
- Petersen B., Gernaey K., Henze M. and Vanrolleghem P.A. (2001) Calibration of activated sludge models: A critical review of experimental designs. In: *Biotechnology for the Environment*. Eds. Agathos S. and Reineke W., Focus on Biotechnology, Vol. 3. Kluwer Academic Publishers, Dordrecht, The Netherlands. pp.80. (in Press)
- 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. Technol.*, **25**(6), 167-183.
- Sinkjær O., Yndgaard L., Harremoës P. and Hansen J.L. (1994) Characterisation of the nitrification process for design purposes. *Wat. Sci. Technol.*, **30**(4), 47-56.
- Stokes L., Takács I., Watson B. and Watts J.B. (1993) Dynamic modelling of an A.S.P. sewage works - A case study. *Wat. Sci. Technol.*, **28**(11-12), 151-161.
- STOWA (1996) Methoden voor influentkarakterisering - Inventarisatie en richtlijnen. STOWA Report 80-96. STOWA, Utrecht, The Netherlands. (In Dutch)
- Vanderhasselt A., Fuchs A., Vanrolleghem P., Staudinger G. and Verstraete W. (1999) Monitoring of the effects of additives on sludge separation properties by using sensors. *Water Environ. Res.*, **71**, 355-362.
- Vanrolleghem P.A. and Coen F. (1995) Optimal design of In-Sensor-Experiments for on-line modelling of nitrogen removal processes. *Wat. Sci. Technol.*, **31**(2), 149-160.
- Vanrolleghem P.A., Kong Z., Rombouts G. and Verstraete W. (1994) An on-line respirographic biosensor for the characterization of load and toxicity of wastewaters. *J. Chem. Technol. Biotechnol.*, **59**, 321-333.
- Vanrolleghem P.A., Spanjers H., Petersen B., Ginestet P. and Takacs I. (1999) Estimating (combinations of) Activated Sludge Model No. 1 parameters and components by respirometry. *Wat. Sci. Technol.*, **39**(1), 195-214
- Weijers S.R., Kok J.J., Preisig H.A., Buunen A. and Wouda T.W.M. (1996) Parameter identifiability in the IAWQ model no. 1 for modelling activated sludge plants for enhanced nitrogen removal. In: Proceedings 6th European Symposium on Computer Aided Process Engineering ESCAPE-6, Rhodos, May 1996. pp. 6.
- Xu S. and Hultman B. (1996) Experiences in wastewater characterisation and model calibration for the activated sludge process. *Wat. Sci. Technol.*, **33**(12), 89-98.