

Evaluation of an ASM1 model calibration procedure on a municipal–industrial wastewater treatment plant

Britta Petersen, Krist Gernaey, Mogens Henze and Peter A. Vanrolleghem

ABSTRACT

The purpose of the calibrated model determines how to approach a model calibration, e.g. which information is needed and to which level of detail the model should be calibrated. A systematic model calibration procedure was therefore defined and evaluated for a municipal–industrial wastewater treatment plant. In the case that was studied it was important to have a detailed description of the process dynamics, since the model was to be used as the basis for optimisation scenarios in a later phase. Therefore, a complete model calibration procedure was applied including: (1) a description of the hydraulics in the system via a tracer test, (2) an intensive measuring campaign and (3) supporting lab-scale experiments to obtain and confirm kinetic parameters for the model. In this paper the model calibration procedure for this case study is described step by step, and the importance of the different steps is discussed. The calibrated model was evaluated via a sensitivity analysis on the influence of model parameters and influent component concentrations on the model output. The sensitivity analysis confirmed that the model output was sensitive to the parameters that were modified from the default parameter values. The calibrated model was finally reduced from a 24 tanks-in-series configuration to a 12 tanks-in-series configuration, resulting in a 50% reduction of the simulation time.

Key words | nitrification, denitrification, ASM1 model, calibration procedure, sensitivity analysis, model reduction

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INTRODUCTION

Implementation of biological nutrient removal on wastewater treatment plants (WWTPs) resulted in an increased knowledge of the biological degradation processes. This resulted in the development and use of more advanced dynamic mathematical models that may be able to describe the biological nutrient removal processes. These activated sludge models allow us to study and to further increase our understanding of the influence of process modifications on treatment process efficiency. The dynamic models are, for example, increasingly used for scenario evaluations aiming at the optimisation of activated sludge processes (Stokes *et al.* 1993; de la Sota *et al.* 1994; Coen *et al.* 1997, among many others). The Activated Sludge Model No. 1 (ASM1) presented by the IAWQ Task

Group on Mathematical Modelling for Design and Operation of Biological Wastewater Treatment Processes (Henze *et al.* 1987) is generally accepted as the state-of-the-art. ASM1 was primarily developed for municipal activated sludge wastewater treatment plants to describe the removal of organic carbon substances and nitrogen with simultaneous consumption of oxygen and nitrate as electron acceptors, and to yield a good description of the sludge production. ASM1 has been extended to include a description of biological phosphorus removal, resulting in ASM2 and ASM2d (Henze *et al.* 1995, 1999). Recently, some of the model concepts behind ASM1 have been altered in ASM3 (Gujer *et al.* 1999), a model that also focuses on the degradation of carbon and nitrogen but

allows the introduction of processes describing the storage of biopolymers under transient conditions.

In this study model calibration is understood as the adaptation of the model to fit a certain set of information obtained from the full-scale 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 ASM1, a fully developed model calibration procedure has not yet been defined. We have not been able to find a complete model calibration report in the literature. There may be many reasons for this. It is important to realise that the purpose of the model is very much in determining how to approach the calibration, making it difficult to generalise (Henze *et al.* 1995). Still, considering the wide application of these 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 from various sources to obtain an overview.

In this study we have attempted to gather and summarise the information needed to achieve a successful model calibration. The set of information listed below was extracted and combined from different sources (Henze *et al.* 1987; Lesouef *et al.* 1992; Pedersen & Sinkjær 1992; Siegrist & Tschui 1992; Stokes *et al.* 1993; de la Sota *et al.* 1994; Dupont & Sinkjær 1994; Weijers *et al.* 1996; Xu & 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 mixed liquor suspended solids 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 unit processes), as averages or dynamic trajectories, e.g. suspended solids (SS), chemical oxygen demand (COD), Kjeldahl nitrogen (TKN), ammonium nitrogen ($\text{NH}_4\text{-N}$), nitrate nitrogen ($\text{NO}_3\text{-N}$), orthophosphate ($\text{PO}_4\text{-P}$), etc.

- 5.2. Sludge composition, e.g. SS, volatile suspended solids (VSS), COD, nitrogen and/or phosphorus content.
- 5.3. Reaction kinetics, e.g. growth and decay rates.
- 5.4. Reaction stoichiometry, e.g. yields.

As mentioned above, the required quality and quantity of the information will depend very much on the purpose of the model. In cases when the model is to be used for educational purposes (e.g. to increase basic understanding of the processes), for comparison of design alternatives for non-existing plants or in other situations where qualitative comparisons are sufficient, the default parameter values defined by Henze *et al.* (1987) can be applied. A reasonably good description can most often be obtained with this default parameter set for typical municipal cases without significant industrial influences (Henze *et al.* 1997). However, if the calibrated model is going 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. Some processes may need a more adequate description than others, again depending on the purpose of the study. This may especially apply for models that are supposed to describe the processes in an industrial or combined municipal and industrial treatment plant.

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

1. Default values from literature (e.g. Henze *et al.* 1987).
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.

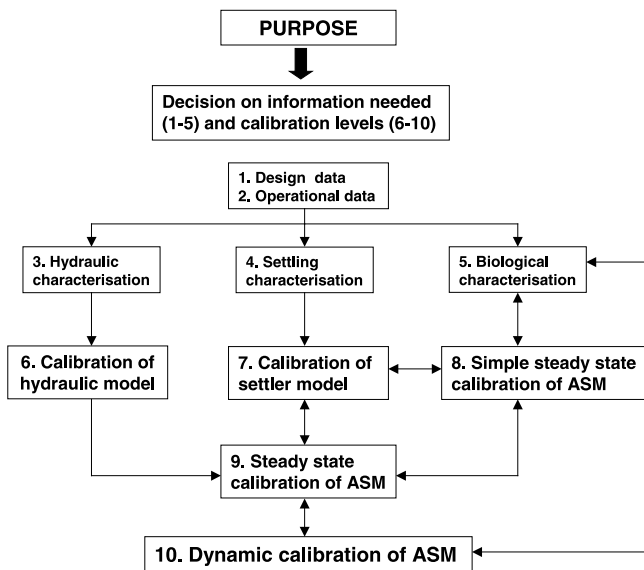


Figure 1 | Schematic overview of the different general steps in an activated sludge model calibration procedure.

2.3. On-line data.

2.4. Measurements in reactors to characterise process dynamics (mainly relevant for sequencing batch reactors (SBRs) 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.

Again, the intended use of the model will determine which information source to choose for the characterisation of the different biological processes in the model. In addition, 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 model calibration. Figure 1 illustrates the different general steps in a model calibration procedure. It should be stressed that, depending on the purpose, not all steps may have to be taken.

Steps 1–5 in Figure 1 indicate the collection of information. Design (1) and operational (2) data are in general always needed for a model calibration. For example, the flow and load variations are important in the design of measuring campaigns for hydraulic, sludge

settling and biological characterisation of the full-scale WWTP. The hydraulics (3) are typically characterised via tracer tests at the full-scale installation. The settling characteristics (4) can be characterised via on-line or lab-scale settling tests (Vanderhasselt *et al.* 1999). Finally, the biology can be characterised via different information sources, as indicated above. A review of the information that can be obtained from different kinds of lab-scale experiments is presented in detail elsewhere (Petersen 2000), and for information especially obtained from respirometric tests the reader is referred to Vanrolleghem *et al.* (1999).

In Figure 1 steps 6–10 illustrate 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 indicated in steps 6 and 7, respectively. A first ASM calibration level is typically 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 by an ideal perfectly mixed tank, resulting in a simple treatment plant configuration. Here 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 by the double arrow. Finally, the characterisation 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 that includes the hydraulic model (9). In general, with a steady state model calibration, only parameters responsible for the long-term behaviour of the WWTP can be determined, i.e. Y_H , f_p , b_H and X_I in the influent (Henze *et al.* 1999; Nowak *et al.* 1999). These parameters are correlated to a certain degree, meaning that a modification of one parameter value can be compensated by a modification of another parameter value. In

the study of Nowak *et al.* (1999) on mass balances of full-scale data, it was therefore chosen to fix Y_H and f_p , leaving X_1 in the influent and b_H to be determined from the steady state data. In the study of Lesouef *et al.* (1992) two WWTP models were calibrated via steady state calibration only, and this calibrated model was applied to simulate dynamic process scenarios. However, if one relies entirely on a steady state calibration to dynamic data, some problems may be encountered since the real input variations are usually faster than the slow process dynamics that were focused upon during the steady state calibration. In other words, the process does not operate in steady state but one still attempts to fit a steady state simplification of the model to an unsteady situation. A steady state calibration may, however, be very useful for the determination of initial conditions prior to a dynamic model calibration and for the initiation of a first parameter estimation (e.g. Pedersen & Sinkjær 1992; Stokes *et al.* 1993; Dupont & Sinkjær 1994; Xu & Hultman 1996; Kristensen *et al.* 1998).

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 $\mu_{\max A}$ (Henze *et al.* 1999), which are the most important parameters in predicting dynamic situations.

At WWTPs, data are most often collected routinely at a daily or weekly sampling frequency. This sampling frequency may, however, not be high enough, and for more accurate modelling it may therefore be required to run special measuring campaigns (e.g. Pedersen & Sinkjær 1992; de la Sota *et al.* 1994; Dupont & Sinkjær 1994; Xu & Hultman 1996; Coen *et al.* 1997). The sampling frequencies should be chosen in relation to the time constants of the process and influent variations. One of the important time constants of the process is the hydraulic retention time. Various lengths of measuring campaigns are recorded in the 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 WWTPs are relatively expensive these recommendations may not always be completely fulfilled.

Furthermore, data from the full-scale installation alone may be insufficient for a dynamic model calibration since the reaction kinetics cannot readily be obtained from such data, except for specific designs like SBRs and alternating systems (Vanrolleghem & 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 & Sinkjær 1994; Xu & Hultman 1996; Kristensen *et al.* 1998).

In this paper the model calibration procedure presented in Figure 1 is concretised for the combined municipal–industrial activated sludge WWTP in Zele, Belgium. The purpose of the model calibration was to obtain a good description of the nitrogen removal capacity and, to a lesser extent, of the COD removal. In a second phase the model was to be applied for process optimisation of nitrogen removal (Gernaey *et al.* 2000). Based on this purpose the necessary information set and calibration strategy were defined. A tracer test was carried out first, to have an adequate description of the hydraulic flow pattern, which is especially important if dynamic situations are to be predicted. 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. Thus, no specific tests were carried out to characterise the settling properties, i.e. step 4 of Figure 1 is not included in this study. 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 characterised, since the model was to be applied later on for optimisation of nitrogen removal, including the start-up of denitrification. The sludge composition was analysed 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

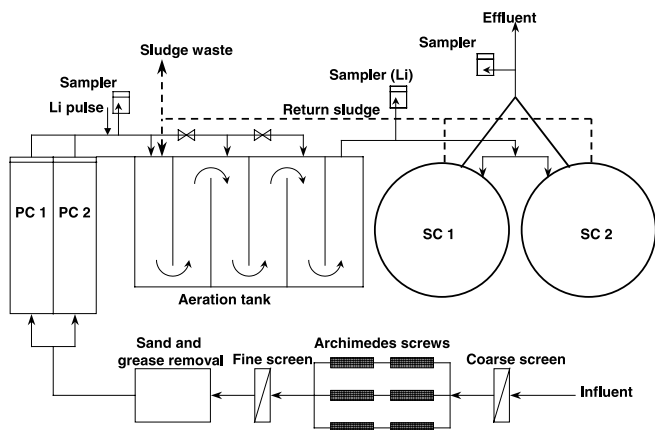


Figure 2 | Schematic overview of the process layout of the Zele wastewater treatment plant (Aquafin NV, Aartselaar, Belgium).

plant. No specific experiments were carried out for the determination of stoichiometric coefficients. A sensitivity analysis was carried out on the calibrated model to check whether the parameters that were modified during the model calibration procedure were indeed influencing the model output. It was finally investigated if the calibrated model could be reduced, to increase simulation speed while maintaining the same accuracy of the full model.

CASE STUDY

The municipal activated sludge WWTP at Zele (Aquafin NV, Aartselaar, Belgium) was constructed in 1983 for a design capacity of 50,000 inhabitant equivalents (IE). Figure 2 gives a schematic overview of the process layout. The influent of the WWTP consists of 40% household wastewater and 60% industrial wastewater (slaughterhouses, industrial laundries, textile cleaning, textile painting, etc.). The influent is divided over two parallel rectangular primary clarifiers after the pretreatment step (coarse grit removal, fine grit removal, sand and grease removal). The effluent of the primary clarifier flows to the biological activated sludge treatment, where it is mixed with recycled sludge. 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 through an open

aerated channel of about 200 m³. The clarifiers each have a diameter of 33 m and a volume of 2050 m³. The final effluent is discharged into a nearby stream. The underflow from the secondary clarifier flows back to the aeration tank through an aerated sludge recycle channel with a volume of 400 m³. The primary and secondary sludge are thickened prior to anaerobic digestion.

The Zele WWTP is going through a stepwise renovation process with the aim of obtaining an effluent quality that complies with the Flemish effluent standard for total nitrogen (15 mg total nitrogen per litre as a yearly average). A first step in the renovation process was the installation of a fine bubble aeration system in 1997. This had an immediate positive effect on the nitrification capacity, resulting in a decrease of the effluent NH₄-N concentration. However, the effluent total nitrogen concentration remained too high to comply with the effluent standard. An average total nitrogen concentration of 19.6 mg/l was calculated for the period January 1997 to November 1998 (the 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 nitrogen concentrations.

MATERIALS AND METHODS

Tracer test

A tracer test with lithium chloride (LiCl) was carried out to characterise the hydraulics of the activated sludge tank. The tracer was added as a pulse at the beginning of the aeration tank, where presettled influent is mixed with return sludge (indicated in 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 5–10 minutes) was undertaken for 0–1.5 times the hydraulic retention time.

Measuring campaign

The measuring campaign was carried out in November 1998. First, a 1-day campaign was done to test the planned strategy, e.g. 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 was a detailed one-week measuring campaign carried out. Two automatic samplers with built-in refrigerator (4°C) were installed on the treatment plant. Time proportional samples (100 ml every 6 min) 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 analysed for the following parameters via standard methods: SS, NH₄-N, TKN, total and soluble chemical oxygen demand (COD_{tot} and COD_{sol}). The samples for COD_{sol} were filtered through 0.45 µm filters prior to analysis. The effluent samples were analysed for SS, NH₄-N, 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 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.

Lab-scale experiments

Respirometric lab-scale experiments with wastewater and activated sludge were carried out during the measuring campaign. Experiments were performed in the RODTOX (Vanrolleghem *et al.* 1994) and the hybrid respirometer (Gernaey *et al.* 2001). The purposes of these experiments were two-fold.

Wastewater characterisation—determination of readily biodegradable COD

The first purpose was to measure the short-term biochemical oxygen demand (BOD_{st}) to determine the readily

biodegradable COD (COD_{st}) of the influent. The BOD_{st} was determined as the area under the oxygen uptake rate profile related to substrate degradation (a respirogram). Only unfiltered influent samples were subjected to respirometric analysis. Some of the samples (typically the ones with a high COD concentration) were also analysed after inhibiting nitrification with allylthiourea (ATU). The measured BOD_{st} values were converted to COD units via an assumed yield factor Y_H of 0.67 (Henze *et al.* 1987):

$$\text{COD}_{\text{st}} = \frac{\text{BOD}_{\text{st}}}{(1 - Y_H)} \quad (1)$$

For the case when BOD_{st} was available from experiments in the presence of ATU, the value was immediately used as an estimate for the COD_{st} concentration. For the case when the BOD_{st} value resulted from an experiment in which no ATU was added, the COD_{st} concentration was determined according to (2). The BOD_{st} requirement for the oxidation of NH₄-N (BOD_{st,NH4}) was determined using the NH₄-N concentrations obtained from the chemical analyses of the wastewater (3). The value of Y_A was set to 0.24 (Henze *et al.* 1987), thereby neglecting the amount of NH₄-N consumed for biomass growth during the tests. The latter is a reasonable and common assumption in short-term respirometric experiments such as the ones carried out in this study:

$$\text{BOD}_{\text{st}} = \text{BOD}_{\text{st,total}} - \text{BOD}_{\text{st,NH4}} \quad (2)$$

$$\text{BOD}_{\text{st,NH4}} = (4.57 - Y_A)\text{NH}_4 - \text{N} \quad (3)$$

Activated sludge kinetics—maximum specific growth rates

Experiments were carried out to obtain data to estimate the kinetic parameters related to nitrification. The design of these experiments is described in more detail elsewhere (Petersen 2000), but consisted of simultaneous addition of wastewater and ammonium, thus allowing us to estimate the nitrification kinetics and the degradation of COD in a single experiment. The exogenous oxygen uptake rate, $r_{O,\text{ex}}$, caused by the wastewater and ammonium addition can be described by (4). Note that in (4) one biomass X is

used for the interpretation of respirometric data derived from short-term respirometric tests. This is done on purpose, since it is not known which fraction of the particulate COD corresponds to X_{BH} and X_{BA} :

$$r_{O,ex} = (1 - Y_H) \frac{\mu_{max} H^X}{Y_H} \frac{S_S}{K_S + S_S} + (4.57 - Y_A) \frac{\mu_{max} A^X}{Y_A} \frac{S_{NH}}{K_{NH} + S_{NH}} \quad (4)$$

Decay rate

The endogenous respiration rate, $r_{O,end}$, was measured as a function of time in a long term (5 days) aerated batch experiment without substrate supply. The observed endogenous decay rate, b'_H , was determined as the slope of the curve consisting of $\ln(r_{O,end}(0))/\ln(r_{O,end}(t))$ data points plotted as a function of time (Ekama *et al.* 1986). This decay rate was transformed into the model decay rate based on the death regeneration concept via (5) (Henze *et al.* 1987), where Y_H was set equal to 0.67 and f_p to 0.08 according to the ASM1 default parameters

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

Temperature correction of the parameters determined from the lab-scale experiments (18°C) was carried out according to standard procedures (Henze *et al.* 1997).

RESULTS

The results of the different model calibration steps, outlined in Figure 1, are described for the example that was studied.

Steps 1–2: design and operational data

The volumes are repeated in Table 1, and Table 2 lists the operational data during the 6 day measuring campaign (18–23 November 1998). The data include a rain event on

Table 1 | Design data from Zele WWTP

Design parameter	Unit	Value
Volume activated sludge tank	m ³	2,600
Volume of recycle channel	m ³	400
Volume of secondary clarifier	m ³	2 × 2,050

the first day of the measuring campaign, as can be seen from the flow data (2 hour averages) in Figure 3. Therefore some key parameters were calculated both including and excluding the data obtained during this rain event (Table 2). Table 2 clearly shows that the daily COD load, and thereby the sludge load, increased significantly during the rain period. The sludge age seems low for a nitrifying WWTP. It is the experience at the WWTP, however, that it is difficult to maintain a higher sludge age during winter due to a decrease in sludge settleability and thereby an increased risk for sludge washout. The observed yield is also slightly higher than expected according to the sludge load (Henze *et al.* 1997) but is probably related to the low sludge age (young sludge).

Steps 3 and 6: characterisation of hydraulics and calibration of hydraulic model

The data resulting from the tracer test are shown in Figure 4. A sharp peak was recorded with a maximum Li concentration of 1.2 mg/l at $t = 0.1$ d. The increase of the Li concentration around $t = 0.27$ d is due to the Li that is recycled internally in the treatment plant with the sludge recycle.

The tracer test data were normalised by C_O (6), where M is the total mass of Li added at $t = 0$, and the time was normalised by the average hydraulic residence time (θ_H) during the test, which was 2.6 h. First, a simple data interpretation was applied. The N tanks-in-series model (7) was fitted to the normalised Li data via the solver function in MS Excel and $N = 19$ gave the best fit:

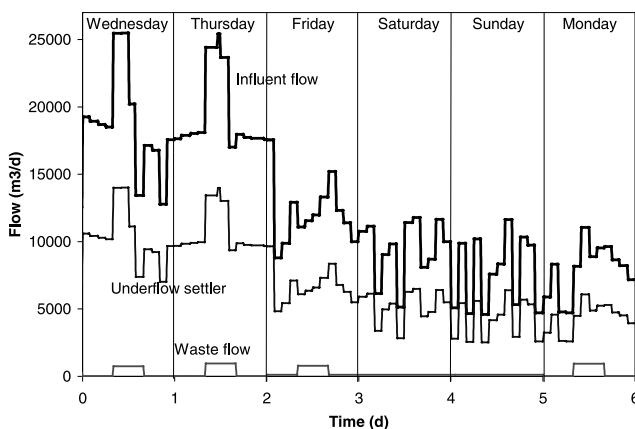
$$C_O = \frac{M}{V} \quad (6)$$

Table 2 | Operational data from Zele WWTP obtained during the measuring campaign

Variable	Unit	Value (incl. rain period)	Value (excl. rain period)
Influent flow average	m ³ /d	12,559	10,255
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	5,607	3,730
TKN load	kg TKN/d	342	258
Sludge load	kg COD/kg SS. d	0.48	0.32
Sludge production	kg SS/d	2,394	2,300
Sludge age	d	6.2	8.6
Observed yield	kg SS/kg COD	0.42	0.62

*See also Table 3.

$$C_{Nt} = \frac{N}{(N-1)!} (N\theta_t)^{(N-1)} e^{-N\theta_t} \quad (7)$$

**Figure 3** | Simulated flow rates during the measuring campaign ($t=0$ corresponds to the beginning of the measuring campaign). Influent flow rates (2 h averages) were collected at the treatment plant. Settler underflow rates are obtained as 0.55 × influent flow (proportional recycle flow controller). The discontinuous waste flow rates were obtained from treatment plant operation logbook data.

This simple approach, however, assumes a constant flow rate and thus does not include the flow variations that occurred during the tracer test. Moreover, the sludge recycle (including the LiCl that is recycled via the underflow of the settlers) and the residence time of the recycle liquid flow in the secondary clarifiers were not considered in this simplified approach. Thus, to obtain a better hydraulic description different configurations were simulated in the WEST++ modelling and simulation environment (Hemmis NV, Kortrijk, Belgium). 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 consisted of the following components:

- A plug-flow aeration tank consisting of 24 tanks in series (6 lanes, each consisting of 4 tanks in series, where each tank has a volume of 100 m³).
- The sludge channel that transports the sludge from the aeration tank to the secondary clarifiers consists of two tanks in series of 100 m³ each.

- An ideal point-settler and a ‘buffer tank’ of 1000 m³ to take the residence time into account for the liquid that is recycled together with the recycle sludge (settler underflow).
- The recycle channel that transports the recycle sludge from the secondary clarifiers to the aeration tank consists of five tanks in series of 80 m³ each.

The model fit on the Li tracer data for this configuration is shown in Figure 4, and the hydraulic scheme is illustrated in Figure 14 in the process configuration for the dynamic model.

Step 5: biological characterisation

Wastewater characterisation

Figures 5, 6 and 7 show the chemical analysis results for the influent samples (presettled wastewater). The influent COD_{tot}, TKN and SS concentrations were highest on Wednesday afternoon and Thursday morning as a result of the rain event. The COD_{sol} and NH₄-N concentrations were, however, not higher during the rain event compared to the other working days, indicating that the increase of COD_{tot} and TKN concentrations during the rain event were related to the extra SS load. The high SS content of the presettled wastewater during the rain event indicates that the primary clarifiers are overloaded when the influent flow is high, e.g. due to rainfall.

For both COD (Figure 5) and nitrogen (Figure 6) a diurnal pattern can be distinguished, with lower concentrations during the night and higher during daytime. The concentration variations are much lower at the weekend due to the absence of industrial discharges. The start-up of industrial activity after the weekend again caused an increase of the influent pollutant concentrations. In Figure 5 it can furthermore be seen that the COD_{st}, obtained via BOD_{st} from respirometric tests (1), is related to COD_{sol}. Moreover, the COD_{st} seems to be related to the industrial discharges since there is hardly any COD_{st} present in the influent during the weekend.

The results of the chemical analyses on the effluent are shown in Figures 8, 9 and 10. Effluent COD and N concentrations show a diurnal pattern but, as expected,

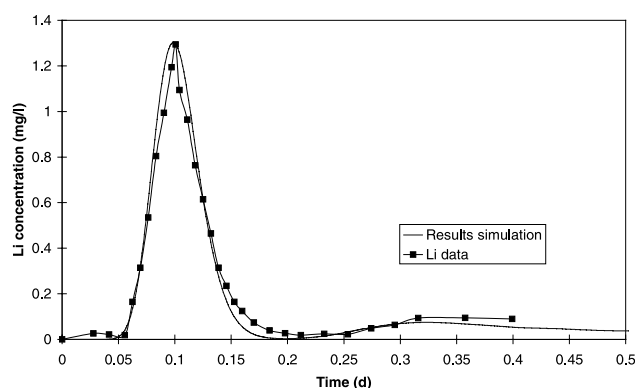


Figure 4 | Data resulting from the tracer test on the aeration tank of the Zele WWTP, together with the best model fit that was obtained. See text for explanation of the model.

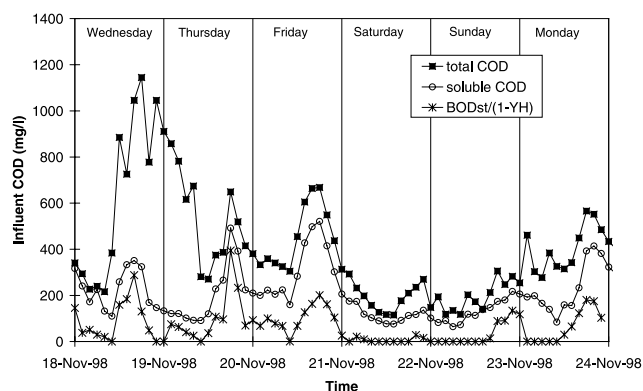


Figure 5 | COD_{tot} and COD_{sol} concentrations measured on the influent of the Zele WWTP during the measuring campaign. COD_{st} values were calculated using the BOD_{st} values resulting from respirometric experiments with unfiltered wastewater (see (1)).

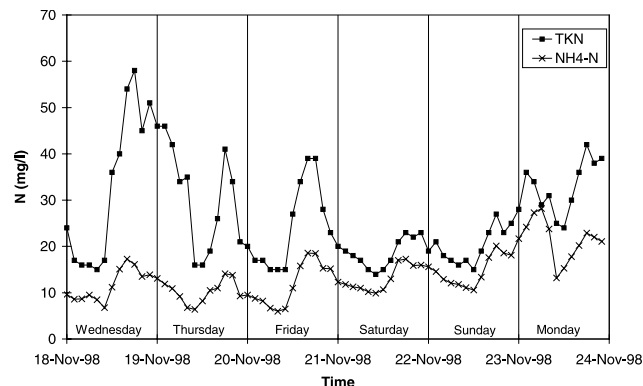


Figure 6 | TKN and NH₄-N concentrations measured on the influent of the Zele WWTP during the measuring campaign.

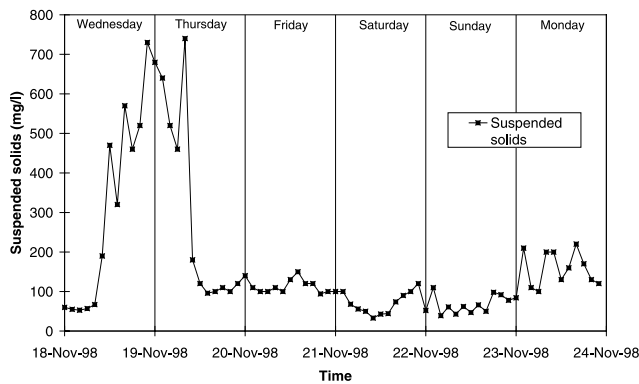


Figure 7 | SS concentration measured on the influent of the Zele WWTP during the measuring campaign.

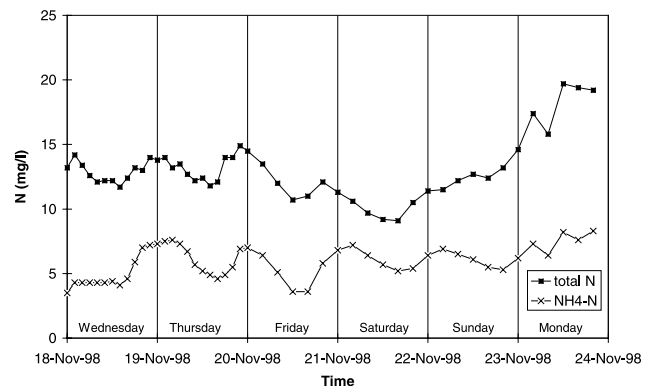


Figure 9 | Total nitrogen and $\text{NH}_4\text{-N}$ concentrations measured on the effluent of the Zele WWTP during the measuring campaign.

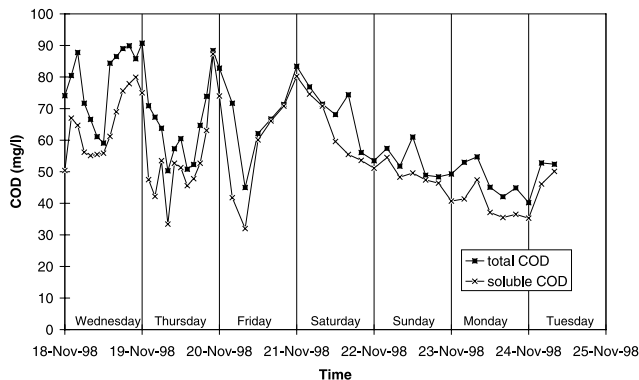


Figure 8 | COD_{tot} and COD_{sol} concentrations measured on the effluent of the Zele WWTP during the measuring campaign.

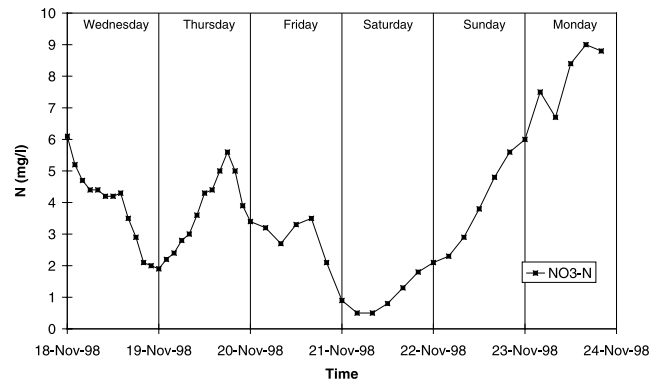


Figure 10 | $\text{NO}_3\text{-N}$ concentrations measured on the effluent of the Zele WWTP during the measuring campaign.

the variations were rather small compared to the concentration variations measured in the presettled influent. During the measuring campaign the effluent total nitrogen concentration was, in general, lower than the 15 mg N/l effluent standard (Figure 9). However, on Monday, a day with normal dry weather flow, the effluent total nitrogen concentration exceeded the 15 mg N/l standard. Also, in Figure 9 it can be seen that full nitrification was not reached. Besides $\text{NH}_4\text{-N}$, $\text{NO}_3\text{-N}$ contributed significantly to the effluent total nitrogen concentrations during the measuring campaign (Figure 10).

The next step in the wastewater characterisation is the conversion of the available data from the measuring campaign into a data set that can be used as input for the ASM (in this case ASM1). It is assumed that the oxygen

concentration (S_{O}) in the incoming wastewater is zero. Furthermore, the conversion of alkalinity (S_{ALK}) is not considered in this study, since influent S_{ALK} is not inhibiting nitrification at the treatment plant. The plant indeed has no problems in reaching full nitrification during summer time, when the temperatures are considerably higher compared to winter. The ASM1 wastewater components to consider in the wastewater characterisation are thus related to the organic carbon (COD) and nitrogen components.

COD components

The total COD in the model includes the components described in (8) (Henze *et al.* 1987):

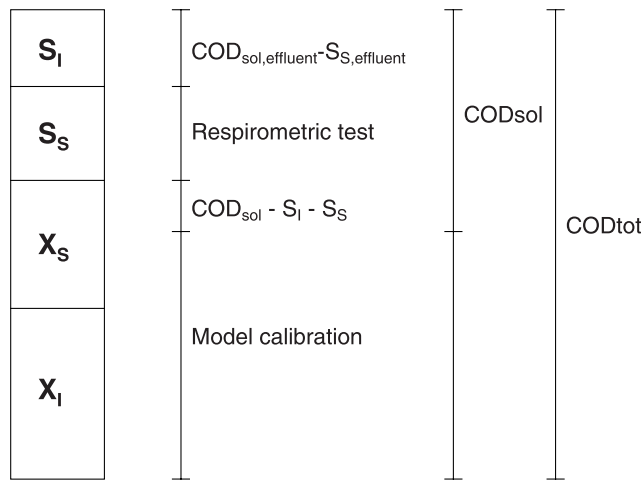


Figure 11 | Summary of influent characterisation methods for organic wastewater components.

$$\text{COD}_{\text{tot}} = S_S + S_I + X_S + X_I \quad (8)$$

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. However, it can be difficult to determine the amount of biomass in the wastewater, and the biomass fraction is therefore often lumped into X_S (Henze *et al.* 1995). This does not influence the modelling significantly but it may affect the value of the biomass yield. Contrary to the heterotrophic biomass, the presence of autotrophic biomass (X_{BA}) can be important to keep sufficient nitrification in the system in cases where the sludge retention time is too low to sustain the nitrifying biomass. Model results may reveal whether this is the case. As an initial approximation X_{BH} and X_{BA} were assumed to be zero in this study. The methods for characterisation of the organic wastewater components are summarised in Figure 11.

- Inert soluble organic matter (S_I), influent and effluent.
Influent S_I was determined via effluent data (Henze 1992). The weekly BOD_5 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 BOD_5 concentration of 6.2 ± 3.0 mg/l had been measured, and an average $\text{BOD}_5/\text{COD}_{\text{tot}}$ ratio of $7 \pm 3\%$ 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 (9). The choice of this low BOD yield is due to the fact that significant biomass decay takes place during a BOD measurement. The influent S_I was obtained by combining (9) and (10):

$$S_{S,\text{effluent}} = \frac{0.07\text{COD}_{\text{tot}}}{(1-Y)} = 0.0875\text{COD}_{\text{tot,effluent}} \quad (9)$$

$$\begin{aligned} S_{I,\text{effluent}} &= S_{I,\text{influent}} \\ &= (\text{COD}_{\text{sol,effluent}} - S_{S,\text{effluent}}) \end{aligned} \quad (10)$$

- Readily biodegradable substrate (S_S), influent. Based on the results of the respirometric tests, the influent readily biodegradable COD (1) is set equal to the model component S_S .
- In the next step, the mass balance for influent COD_{sol} ($\text{COD}_{\text{sol,influent}}$) was checked (11):

$$\text{COD}_{\text{sol,influent}} = S_S + S_I + S_{\text{rest}} \quad (11)$$

For the case when $\text{COD}_{\text{sol,influent}}$ in (11) is higher than $S_S + S_I$, S_{rest} can be added to the slowly biodegradable substrate, X_S . In contrast, if $\text{COD}_{\text{sol,influent}}$ is lower than $S_S + S_I$, part of the measured BOD_{st} may be considered to originate from X_S . For the wastewater under study it appeared that $\text{COD}_{\text{sol,influent}} > (S_S + S_I)$; thus S_{rest} was added to the X_S component.

- Slowly biodegradable substrate (X_S), influent. Contribution to the X_S concentration partly came from the mass balance in (11) as S_{rest} , but was also partly determined from the steady state model evaluations (see also X_I).
- 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, 1995). The

Table 3 | Analysis of results on activated sludge and recycle sludge (average and 95% confidence interval, resulting from 10 measurements)

	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

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 of (12) (assuming that influent X_{BH} and X_{BA} are negligible, see above):

$$\text{COD}_{\text{tot}} - \text{COD}_{\text{sol}} = X_S + X_I \quad (12)$$

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

Nitrogen 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 (13) (Henze *et al.* 1987):

$$\text{TKN} = X_{NI} + X_{ND} + S_{NI} + S_{ND} + S_{NH} \quad (13)$$

- 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}). Only TKN measurements were available. It was assumed that the ratio of soluble to total TKN was proportional with the ratio of COD_{sol} to COD_{tot} . Thus, the soluble Kjeldahl nitrogen (SKN) can be approximated via (14), 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 (15):

$$\text{SKN} = \frac{\text{COD}_{\text{sol}}}{\text{COD}_{\text{tot}}} \text{TKN} = S_{NI} + S_{ND} + S_{NH} \quad (14)$$

$$S_{ND} = \text{SKN} - i_{NSI}S_I - S_{NH} \quad (15)$$

- Slowly biodegradable organic nitrogen (X_{ND}). The nitrogen content of inert suspended organic matter (i_{NXI}) is initially assumed to be 1% (Henze *et al.* 1995) resulting in (16) for the determination of X_{ND} :

$$X_{ND} = \text{TKN} - i_{NXI}X_I - \text{SKN}. \quad (16)$$

Sludge composition

The average results of the sludge composition analysis, based on ten measurements of the COD, SS and VSS content of the activated sludge and recycle sludge, are given in Table 3. The measured COD/VSS ratio is slightly higher than typical values, although Stokes *et al.* (1993) observed similar values. The high content of reduced matter could be due to industrial discharges (e.g. discharge of fat from the slaughterhouses).

Kinetic characterisation

In Figure 12 a typical respirogram of a wastewater and a respirogram obtained after addition of wastewater plus extra ammonium are illustrated. It is obvious that the wastewater respirogram cannot 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, the wastewater respirogram alone

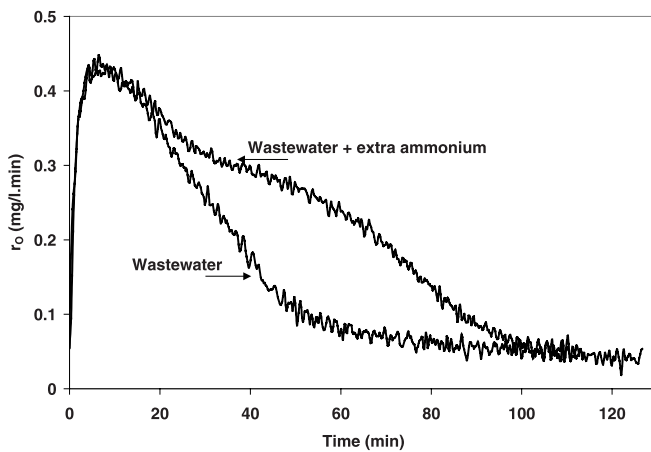


Figure 12 | Example of respirogram obtained from respirometric tests with wastewater and wastewater mixed with ammonium.

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 where extra ammonium was added together with the wastewater to simultaneously identify 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).

The respirogram were in general not informative enough to describe the degradation of COD in the wastewater via Monod kinetics, as described in (4) (no zero-order respiration rate plateau was reached in the experiment). Consequently, the degradation of COD was instead described via a first-order model (17), where the first-order rate constant k replaces the Monod parameter combination $\mu_{\max H}/K_S$:

$$r_{O,ex} = \frac{1 - Y_H}{Y_H} k X_{BH} S_S(t) \quad (17)$$

Step 7–9: steady state model calibration

For the steady state model calibration a simple WWTP configuration was constructed in WEST ++ (Figure 13). The steady state configuration consists of an aeration tank ($V = 2,600 \text{ m}^3$), a point-settler, an internal recycle line

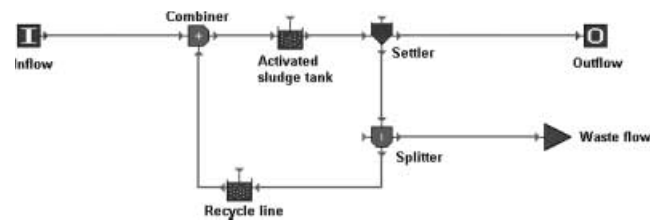


Figure 13 | Treatment plant configuration used for the steady state model calibration.

($V = 400 \text{ m}^3$), and a constant average sludge waste flow from the recycle line.

As mentioned above, the main aim of the steady state model is to fit the modelled sludge production to the sludge production calculated from plant data collected during the measuring campaign (based on waste flow data and sludge concentration measurements). This is done by adjusting parameters responsible for long-term behaviour, i.e. the decay rates b_H and b_A , together with the influent concentration of X_I . Furthermore, for the point-settler model the parameter that describes the fraction of suspended solids going to the final effluent (f_{NS}) was adjusted to fit the average measured effluent suspended solids concentration (in this case 11 mg SS/l).

The experimental value of the decay rate determined based on the lab-scale test was 0.41 d^{-1} (value corrected for temperature and transformed to the death regeneration concept, as described in (5)). This value was used as a guideline for the model calibration. The influent for the steady state model was obtained by averaging the dynamic influent data. Initially, these averages were calculated using only the dry weather flow data (influent data from 19 November 1998 at 10.00 a.m. until the end of the measuring campaign, and with the wastewater characterisation as described above). For this period of the measuring campaign the waste sludge production was calculated to 10,342 kg SS, with an average waste flow rate of 241 m^3/d . Converting into COD units, using the SS to COD conversion factor of 1.38 resulting from the COD analyses done on the recycle sludge samples, the waste sludge production was calculated to be equivalent to 14,065 kg COD. However, during the initial calibration of the steady state model only about half of this waste sludge production could be predicted no matter what the values applied for

Table 4 | The average COD composition of the influent during the measuring campaign

COD component	%
S_I	12
S_S	16
X_S	22
X_I	50

b_H and b_A were. Adjustment of the specific growth rates did not solve the sludge balance problem either. The simulated average sludge concentration in the aeration tank and the recycle line were much lower than the measured concentrations. It was tried to increase the model waste sludge production by assuming that all particulate COD consisted of X_I (instead of 50% as initially assumed), but the sludge balance did not improve sufficiently to solve the problem.

The resulting distribution of the different COD components in the influent is summarised in Table 4. Initially, X_I consisted of 25% of the total COD and X_S of 47%, assuming that X_S consisted of S_{rest} plus 50% of the particulate COD, as described above.

We then tried to find other reasons for the imbalance in the waste sludge production. As mentioned above (Figure 5 and 7) the COD and SS concentrations, together with the influent flow (Figure 3), were very high during the first two days of the measuring campaign due to the rainfall. This indicates that the primary clarifiers did not retain the solids sufficiently during the rain event. This high load during the rain event could be due to a flush effect in the sewers. This extra load of COD and SS during the rain event 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 for the sludge balance during the model calibration it was therefore decided to include the data measured during the rain event for the calculation of the average influent composition.

The waste sludge production too was recalculated to include the data of the rain event. A total waste sludge

production of 14,364 kg SS (19,535 kg COD) was obtained, with an average waste flow rate of 248 m³/d. A new series of steady state simulations now resulted in a waste sludge production of 19,177 kg COD, which was comparable to the waste sludge production measured at the WWTP (with the wastewater composition of Table 4).

The value of the f_{NS} parameter of the point-settler model was adjusted to 0.23% to describe the measured average SS concentration in the final effluent.

The final calibrated value of b_H was 0.5 d⁻¹ which is higher than the default value for 10°C (Henze *et al.* 1987) but in accordance with the experimental value of 0.41 d⁻¹. Furthermore, initial adjustments of the maximum specific growth rates, μ_{maxA} and μ_{maxH} , were carried out. However, it should be stressed that final values can only be assigned to these parameters in the dynamic model calibration, which is the last part of the model calibration procedure (Figure 1).

The autotrophic biomass fraction (f_{BA}) in the activated sludge of the full-scale installation can be approximated by (18) (Sinkjær *et al.* 1994):

$$f_{BA} = Y_A \frac{\theta_X}{1 + b_A \theta_X} \frac{N_{NIT}}{MLVSS \times V} \quad (18)$$

The calculated fraction became 0.0085 mg COD_{NIT}/mg COD. This value is comparable with the steady state model calibration that yielded an autotrophic biomass fraction of 0.0086 mg COD_{NIT}/mg COD. The fraction of heterotrophic biomass was calculated similarly and a value of 0.217 mg COD_{HET}/mg COD was obtained, comparable to a model value of 0.182 mg COD_{HET}/mgCOD.

Step 10: dynamic model calibration

The configuration of the dynamic model (see Figure 14) consists of a plug-flow reactor (6 times 4 reactors in series of 100 m³ each), a sludge line (2 reactors in series of 100 m³ each), a point-settler, an effluent buffer tank ($V = 3,500$ m³), and a recycle line (5 reactors in series of 80 m³ each). The effluent buffer tank was added to the configuration to simulate the liquid retention time in the settlers. However no reactions were assumed to take place there.

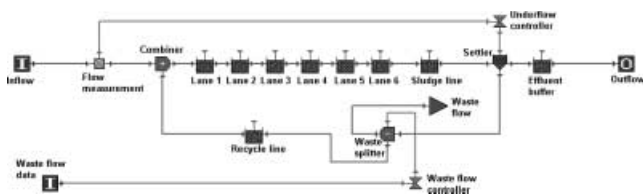


Figure 14 | Model configuration for the calibrated model.

The recycle flow was controlled at 55% of the influent flow rate, to simulate the behaviour of the full-scale WWTP. For this purpose an influent flow measurement coupled to a proportional underflow controller was included in the model. Furthermore, a waste flow controller (see Figure 14) was implemented in the model to simulate the discontinuous sludge waste from the recycle line. This on/off controller was fed with a data flow that indicated the sludge waste rate (data obtained from plant operation logbook).

A problem with the nitrogen balance appeared during the rain period, since a rather high effluent S_{NH} peak resulted from the simulations (20–25 mg NH_4-N/l). This peak was not observed in the data. To solve the problem, it was assumed that the nitrogen content of the high X_I load during the rain period was higher than the assumed 1%. By adjustment of i_{NXI} to 3% during the rain weather period the problem of the nitrogen balance could be solved, because less nitrogen was thus released by hydrolysis and ammonification. Note that a fraction of inert nitrogen of 3% is considerably higher than the typical value of 0.5–1% (Henze *et al.* 1995).

The maximum specific growth rates μ_{maxH} and μ_{maxA} were calibrated to be $2.8 d^{-1}$ and $0.31 d^{-1}$ respectively and the K_S was adjusted to 15 mg COD/l.

The parameter combination involving μ_{maxA} identifiable from the lab-scale experiments is given by

$$(4.57 - Y_A) \frac{\mu_{maxA} X_{BA}}{Y_A}$$

(Petersen *et al.* 2000), which in fact is equal to the maximum oxygen uptake rate for nitrification, assuming no substrate limitations. 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 value of the above mentioned parameter combination. With a μ_{maxA} of $0.31 d^{-1}$ and an average simulated X_{BA} of about 40 mg COD/l, the simulated maximum oxygen uptake rate becomes 225 mg/l.d. This is in very good agreement with the parameter combination derived from lab-scale experiments, with an average of 237 mg/l.d ($n = 21$) and a 95% confidence interval of 175–300 mg/l.d. 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 9). Thus, in this case the influence of the half saturation coefficient, K_{NH} , is insignificant.

In the lab-scale experiments the heterotrophic substrate degradation was described with a first-order expression since the data were not informative enough to be described with the Monod model, as explained above. An evaluation of the calibrated parameters of the full-scale model versus the lab-scale parameters can still be carried out. The substrate degradation rate was calculated based on both the lab-scale model and its parameters on the one hand (17), and the Monod model and its parameters on the other hand (19):

$$r_S = \frac{\mu_{maxH} X_{BH}}{Y_H} \frac{S_S(t)}{K_S + S_S(t)} \quad (19)$$

The calculated profiles can be seen in Figure 15. The lab-scale parameters are estimated on 16 different lab tests and the corresponding 95% confidence interval is given in Figure 15 as well. For the Monod model the average simulated biomass concentration was used for X_{BH} . In the lab-scale experiments the identifiable parameter combination was kX_{BH}/Y_H , and the estimated parameter combinations were adjusted for the differences in sludge concentrations between the different experiments. It is clear from (16) that, as S_S increases, the model result based on the lab-scale parameters deviates from the Monod model. However, it is important to notice that, for the smaller S_S concentrations 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 values of $2.8 d^{-1}$ for μ_{maxH} and 15 mg/l for K_S are reasonable. The simulated S_S concentrations in the main part of

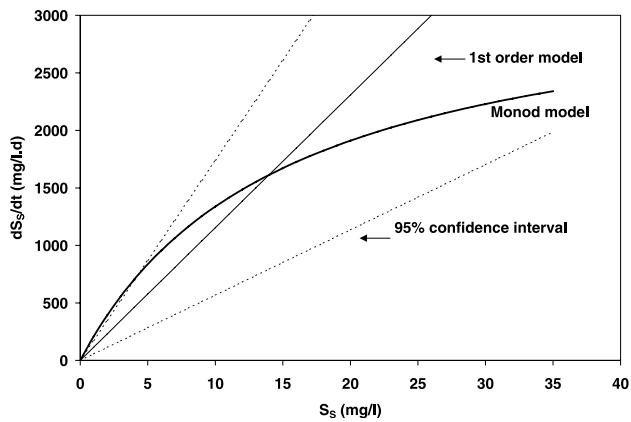


Figure 15 | Substrate removal rate (dS_s/dt) plotted as a function of the substrate concentration for the Monod model (used in the calibrated model) and the first-order model (used for the interpretation of respirometric data).

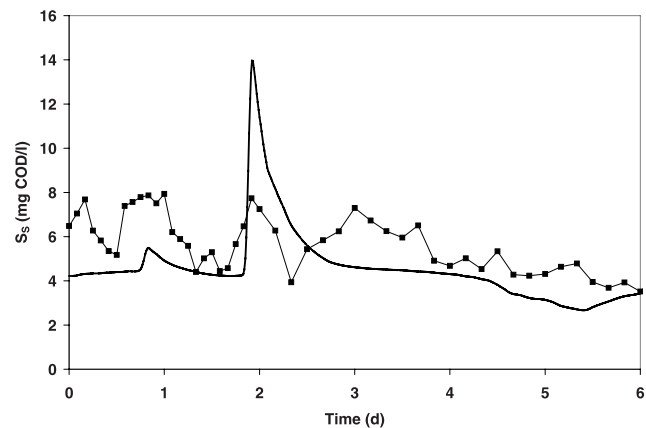


Figure 17 | Effluent S_s data (squares) and model effluent S_s predictions.

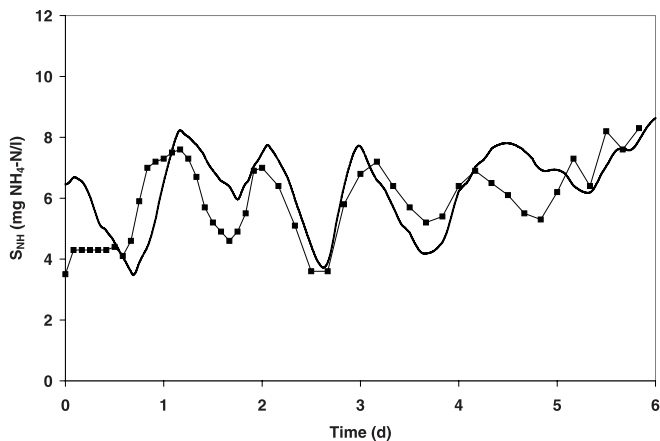


Figure 16 | Effluent S_{NH} data (squares) and model effluent S_{NH} predictions.

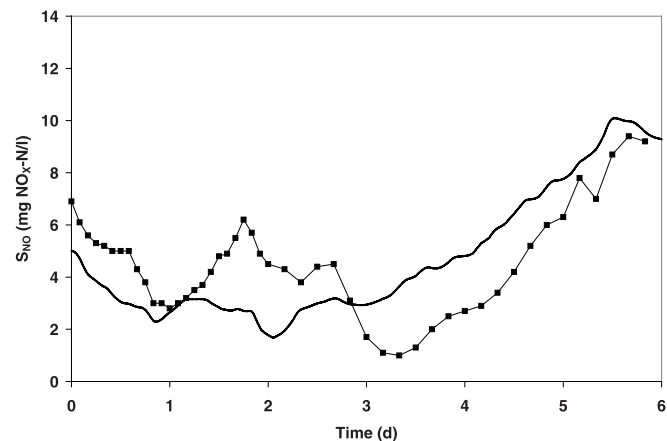


Figure 18 | Effluent S_{NO} data (squares) and model effluent S_{NO} predictions.

the aeration tanks were indeed below the value of K_S . Thus, the experimental first order description of the S_S removal is realistic.

Both the description of the effluent S_{NH} and S_S data are good (Figures 16 and 17). Only on one occasion do the simulations result in a S_S peak that is not present in the data. This S_S peak results from a high influent concentration together with a high flow rate, which could not be modelled adequately. One explanation could be that degradation of S_S could have continued for a while in the secondary clarifiers, while the model assumes that no degradation reactions take place in the clarifiers. 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 example, the NO_3-N effluent concentration decreased to about 1 mg N/l on Friday evening and Saturday morning. This was probably due to an increased residence time in the aeration tank (lower flow) combined with the availability of sufficient readily biodegradable carbon for denitrification entering the WWTP on Friday afternoon (see Figures 3 and 5). The effluent NO_3-N concentration increased again on Sunday and Monday (Figure 10) due to a lack of readily biodegradable COD (see Figure 5).

Table 5 | List of the main parameters for the 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
$\mu_{\max H}$	3.0	2.8	d^{-1}
$\mu_{\max A}$	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

The saturation coefficient for oxygen, K_{OH} , was increased slightly to 0.5 mg O₂/l to decrease the inhibition of denitrification by O₂, and the fraction of denitrifiers, η_g , was decreased to 0.6, to make the simulated S_{NO} concentration in the effluent approach the measured values. The resulting description of effluent S_{NO} is not perfect but follows the trend of the data reasonably (Figure 18). Table 5 shows the complete parameter list for the dynamic model.

Finally, the removal efficiencies for COD_{tot}, COD_{sol}, TKN and NH₄-N have been calculated based on the actual measured and averaged data on the one hand, and based on averaged results of the dynamic simulation including the whole measuring campaign on the other hand. From these results, it has been calculated how close the model describes the removal of COD_{tot}, COD_{sol}, TKN and

NH₄-N (see Table 6). As can be seen from Table 6 the model describes 94–100% of the actual removal, which can be considered to be very satisfactory.

Sensitivity analysis

The parameter values of the calibrated model given in Table 5 did not seem very different from the default parameter set. Therefore, it was investigated if the parameters that were modified during the model calibration were indeed influencing the model outputs significantly. To this purpose a sensitivity analysis was carried out with the calibrated model, to check the sensitivity of the model output (effluent S_S , S_{NH} and S_{NO} concentrations) and the predicted biomass concentration (X) to changes in the

Table 6 | Removal efficiency based on measurements and simulation, expressed as percentage of the observed removal that is described by the model

Removal efficiency	COD _{tot}	COD _{sol}	TKN	NH ₄ -N
Measurements	84%	73%	68%	58%
Simulation	83%	72%	67%	54%
Model description	99%	100%	99%	94%

model parameters and influent pollutant concentrations. The sensitivity was evaluated using relative sensitivity functions, RSF (see (20)). The calibrated model was used as the reference simulation, and the model output obtained after increasing the value of a specific parameter with 1% was used to obtain the relative sensitivity functions (20):

$$\text{RSF} = \frac{\Delta y}{y} \frac{p}{\Delta p} \quad (20)$$

The value of the relative sensitivity function at the beginning of the period with dynamic data was used for the evaluation (=output corresponding to the end of the steady state simulation). One can comment that this leads to a steady state sensitivity analysis. However, it should be added here that a similar sensitivity analysis was done for the period with dynamic data (calculation of the average model deviation Δy based on the simulation data obtained for the period with dynamic data), and that the results of this analysis were rather similar to the results of the steady state analysis presented here. The results of this evaluation are shown in Table 7. The influence of a parameter on the model output was interpreted as proposed by Julien (1997). For $\text{RSF} < 0.25$, a parameter is considered to have no significant influence on a certain model output; if $0.25 \leq \text{RSF} < 1$, the parameter is considered to be influential; if $1 \leq \text{RSF} < 2$, the parameter is considered to be very influential; and if $2 \leq \text{RSF}$, the parameter is considered to be extremely influential. When the value of a parameter and the output change in the same direction, this is indicated with a positive sign in Table 7; when they move in the opposite direction this is indicated with a negative sign.

The sludge concentration is only significantly influenced by the value of Y_H and by the influent X_1 concentration. The latter confirms that a modification of the influent fractionation (the fraction of X_1 was increased) was indeed one of the most appropriate things to do to increase the sludge concentration in the system (and consequently also the sludge production) during the steady state model calibration. Besides the sludge concentration, Y_H also influences the output S_S , S_{NO} and S_{NH} concentrations. However, at the beginning of the calibration it was decided not to change Y_H (and Y_A). The sensitivity analysis shows furthermore that all but one (η_g) of the parameters that were modified from their default values in the final calibrated model ($\mu_{\max H}$, $\mu_{\max A}$, b_H , b_A , K_S , K_{OH} , η_g) influence one or several of the simulated effluent concentrations. This confirms (at least for six out of the seven parameters: $\mu_{\max H}$, $\mu_{\max A}$, b_H , b_A , K_S , K_{OH}) that a modification of these parameter values resulted in a considerable change in the simulated model output. Finally, it should be stressed that both $\mu_{\max H}$ and $\mu_{\max A}$ are very influential on effluent S_S and extremely influential on effluent S_{NH} and S_{NO} concentrations respectively. In other words, this confirms that even a slight modification of the value of these parameters, as in the presented model calibration, can have an important effect on the model output.

Model reduction

It was investigated whether the number of tanks could be reduced in the hydraulic model to increase the calculation speed of the model. To evaluate the effect of model reduction, the quality of the fit between simulated values and available data was evaluated by calculating the average relative deviation (ARD) between model predictions of S_{NH} and available data points (21):

$$\text{ARD} = \frac{1}{n} \sum_{i=1}^n \left(\frac{|X_{i\text{obs}} - X_{i\text{sim}}|}{X_{i\text{obs}}} \right) \times 100\% \quad (21)$$

For the calibrated model ARD was 16.5% when considering the effluent S_{NH} concentration. For a reduction of the number of tanks from 24 to 12 in the activated sludge lanes, and from 5 to 3 in the recycle channel, the same

Table 7 | Results of sensitivity analysis with the calibrated model of the Zele WWTP. (+, -=influential; ++, --=very influential; +++, ---=extremely influential). See text for a further explanation of the results

Parameter	X	Effluent S_S	Effluent S_{NO}	Effluent S_{NH}
Y_H	+	--	+	--
Y_A				
μ_{maxH}		--		
μ_{maxA}			+++	----
b_H		+++		
b_A			-	+
K_S		++		
K_{NH}			-	+
K_{OH}				-
K_{OA}			-	+
k_a				
k_h		--		+
K_X				
η_g				
Influent component				
S_S			-	+
S_{NH}			++	+
X_I	+			
X_S		+	--	+

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 of 73.5%. Although the dynamics of the effluent S_{NH} data could still be described, the simulated S_{NH} concentrations were in general higher than the measured data with the

last model. The reason for this is simply that the mixing patterns are more approaching an ideally mixed situation compared to the original model. In general, except for the case of zero-order degradation kinetics, an ideally mixed tank results in a lower substrate removal efficiency in comparison with an ideal plug-flow tank when the same reactor volume is available. Conclusively, the model reduction resulted in a model that needed about 50%

less calculation time for a simulation than the original calibrated 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 $S_{\text{NH}}(0)$. Thus, this means that a ‘wrong’ hydraulic characterisation could be compensated by a change of parameter values.

DISCUSSION

In this study it was stressed that the purpose of the model should determine how the model is calibrated, e.g. which information is needed and to which level the model should be calibrated. A systematic and general model calibration procedure was proposed, and concretised for a combined municipal–industrial WWTP. ASM1 was applied in the case under study, but the proposed general model calibration procedure is applicable for any activated sludge model.

The purpose of the case study was to obtain a good description of the biological N removal, since the model was to be used for process optimisation focusing on an improvement of the N-removal capacity, including start-up of denitrification (Gernaey *et al.* 2000). Therefore, it was also important to describe the variation in readily biodegradable COD. Biodegradation of COD will influence the N components in the activated sludge system, e.g. because S_{NH} is incorporated into new biomass and S_{NO} is consumed during denitrification. It was observed that the presence of readily biodegradable COD in the influent was mainly related to industrial activity, resulting in a lack of biodegradable COD during the weekend. For future implementation of denitrification in the WWTP this may cause problems in maintaining the denitrification efficiency during weekends. This weekend effect was reported previously for another Flemish municipal WWTP (Coen *et al.* 1997).

In this study it was obviously important to have a good description of the hydraulic patterns to describe the dynamics of the system adequately. Indeed, a model

reduction study showed that the number of tanks could be halved, from 24 to 12, but still giving the same description of the effluent data with the same parameter set as the calibrated model. However, it also became clear that a further model reduction would not be possible without a compensating change in the kinetic parameters. In other words, for a further model reduction (a decrease of the number of tanks below 12) errors in hydraulics have to be compensated by ‘wrong’ biological parameters deviating from the lab-scale results, e.g. increase of $\mu_{\max A}$ to decrease the effluent S_{NH} concentration. Thus, for the case when a hydraulic model would not have been available at all, e.g. the hydraulics were described with a 4 tanks-in-series model, the calibrated parameter set might have been rather different and not corresponding at all to the results of the lab-scale experiments. This is immediately linked to the importance of evaluating the key kinetic parameters with lab-scale experiments. In this case study the decay rate and the two specific growth rates $\mu_{\max A}$ and $\mu_{\max H}$ were determined. It was illustrated how to compare these parameters obtained from lab-scale experiments with the parameters of the full-scale model, thereby verifying that the parameters of the full-scale model were realistic.

Thus, as just described above the information obtained from different tests for hydraulic, sludge settling (if needed) and biological characterisation help to frame the model calibration, and in fact reduces the apparently high degree of freedom of the model parameters significantly.

For this case study, it could be questioned, however, whether it was necessary to determine some kinetic parameters in lab-scale experiments, since the resulting calibrated parameters were not far from the ASM1 default parameter set (Henze *et al.* 1987). Still, even in this case the lab-scale results gave extra confirmation of the parameter set of the calibrated model, thereby increasing the quality and confidence of the model calibration. Moreover, the sensitivity analysis clearly showed that the calibrated model was indeed sensitive to changes of the parameters that were modified during the model calibration procedure. Two of the most influential parameters were $\mu_{\max A}$ and $\mu_{\max H}$, which confirmed that even the small deviations of these parameters from their default

values (Henze *et al.* 1987) in the calibrated model has a considerable influence on the model output. It should be stressed that such a sensitivity analysis is case specific, since the results of the analysis can be influenced by the data set that is studied. This can be illustrated with the parameter K_{NH} . The calibrated model presented here is not sensitive to a change of K_{NH} because the S_{NH} concentrations in the plant are always considerably higher than the value of K_{NH} (1 mg N/l). However, one could imagine that the influence of K_{NH} could be larger for a model that describes a treatment plant with almost complete nitrification (e.g. effluent S_{NH} concentration around 1 mg N/l).

It was clear from this study that there is an interaction between wastewater characterisation and calibration of the full-scale model to the available data (effluent and sludge wasted). For instance, the influent concentration of X_1 and X_S were adjusted during the steady state model calibration to be able to describe the sludge production data. In this phase it became clear that it was important to include the data of the rain weather period prior to the dry weather period, since a high COD load originating from the rain period contributed significantly to the sludge that was wasted during the following days.

CONCLUSIONS

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 at 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 adjust to correctly describe the dynamics were the specific growth rates, as was also evidenced by a sensitivity analysis carried out with the calibrated model. Consequently, additional information on the specific growth rates derived from lab-scale experiments is important to confirm that the calibrated parameters of the full-scale model are realistic.

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NOTATION

ARD	Average relative deviation
ASM	Activated sludge model
ATU	Allylthiourea
b_A	Autotrophic decay rate (1/min)
b_H	Heterotrophic decay rate (1/min)
b_H'	Observed endogenous decay rate (1/d)
BOD	Biochemical oxygen demand (mg O ₂ /l)
BOD ₅	5 day biochemical oxygen demand (mg O ₂ /l)
BOD _{st}	Short term biochemical oxygen demand (mg O ₂ /l)

$BOD_{st,total}$	Total short term biochemical oxygen demand (mg O_2/l)	M	Mass of Li added (g)
$BOD_{st,NH4}$	Short term biochemical oxygen demand for NH_4-N oxidation (mg O_2/l)	MLVSS	Mixed liquor volatile suspended solids
C_{Nt}	Normalized Li concentration ($= C_t/C_O$)	n	Number of experimental data points
C_O	Initial Li concentration assuming a perfectly mixed tank (g/m^3)	N	Number of tanks for an N tanks-in-series model
COD	Chemical oxygen demand (mg/l)	NH_4-N	Ammonium nitrogen (mg N/l)
COD_{HET}	Heterotrophic biomass COD (mg COD/l)	NO_2-N	Nitrite nitrogen (mg N/l)
COD_{NIT}	Nitrifying biomass COD (mg COD/l)	NO_3-N	Nitrate nitrogen (mg N/l)
COD_{sol}	Soluble COD (mg COD/l)	N_{NIT}	Amount of nitrified ammonium nitrogen (kg N/d)
$COD_{sol,effluent}$	Soluble COD in the effluent (mg COD/l)	p	Value of a parameter for the reference simulation
$COD_{sol,influent}$	Soluble COD in the influent (mg COD/l)	PC	Primary clarifier
COD_{st}	Readily biodegradable COD (mg COD/l)	PO_4-P	Orthophosphate (mg P/l)
COD_{tot}	Total COD (mg COD/l)	$r_{O,end}$	Endogenous oxygen uptake rate (mg $O_2/l.min$)
$COD_{tot,effluent}$	Total effluent COD (mg COD/l)	$r_{O,ex}$	Exogenous oxygen uptake rate (mg $O_2/l.min$)
C_t	Measured Li concentration (g/m^3)	r_s	Substrate removal rate (mg COD/l.min)
f_{BA}	Fraction of autotrophic biomass in the activated sludge	RSF	Value of relative sensitivity function
f_p	Fraction of biomass converted to X_I as a result of decay	S_{ALK}	Alkalinity concentration (meq/l)
IE	Inhabitant equivalents	SBR	Sequencing batch reactor
i_{NSI}	Nitrogen content of S_I (g N/g COD)	SC	Secondary clarifier
i_{NXI}	Nitrogen content of X_I (g N/g COD)	S_I	Inert soluble organic material concentration (mg COD/l)
k	First-order rate constant (l/mg.min)	$S_{I,effluent}$	S_I in effluent (mg COD/l)
k_a	Ammonification rate (m^3 COD/g d)	$S_{I,influent}$	S_I in influent (mg COD/l)
k_h	Maximum specific hydrolysis rate (g slowly biodegradable COD/g cell COD. d)	SKN	Soluble Kjeldahl nitrogen (mg N/l)
K_{NH}	Autotrophic half-saturation substrate concentration (mg N/l)	S_{ND}	Soluble organic nitrogen concentration (mg N/l)
K_{NO}	Half-saturation coefficient for denitrification (mg N/l)	S_{NH}	Ammonium concentration (mg N/l)
K_{OA}	Autotrophic half-saturation coefficient for oxygen (mg O_2/l)	S_{NI}	Nitrogen included in inert soluble organic material (mg N/l)
K_{OH}	Heterotrophic half-saturation coefficient for oxygen (mg O_2/l)	S_{NO}	Nitrite + nitrate nitrogen concentration (mg N/l)
K_S	Heterotrophic half-saturation substrate concentration (mg COD/l)	S_O	Dissolved oxygen concentration (mg O_2/l)
K_X	Half-saturation coefficient for hydrolysis of X_S (mg COD/l)	S_{rest}	$COD_{sol,influent} - S_{I,influent} - S_{S,influent}$ (mg COD/l)
LiCl	Lithium chloride	SS	Suspended solids (mg/l)
		S_S	Readily biodegradable soluble substrate concentration (mg COD/l)
		$S_{S,effluent}$	S_S in effluent (mg COD/l)
		$S_{S,influent}$	S_S in influent (mg COD/l)
		TKN	Kjeldahl nitrogen (mg N/l)
		V	Volume of the system (m^3)
		VSS	Volatile suspended solids (mg/l)

WWTP	Wastewater treatment plant
X	Biomass concentration (mg COD/l)
X_{BA}	Autotrophic biomass concentration (mg COD/l)
X_{BH}	Heterotrophic biomass concentration (mg COD/l)
X_I	Particulate inert organic material (mg COD/l)
$X_{i_{obs}}$	Observed values
$X_{i_{sim}}$	Simulated values
X_{ND}	Particulate organic nitrogen (mg N/l)
X_{NI}	Nitrogen included in inert particulate organic material (mg N/l)
X_S	Particulate slowly biodegradable organic material (mg COD/l)
y	Value of model output for the reference parameter set
Y	Biomass yield
Y_A	Autotrophic biomass yield (g COD biomass/g N oxidised)
Y_H	Heterotrophic biomass yield (g COD biomass/g COD substrate)
μ_{maxA}	Maximum specific growth rate of autotrophic biomass (1/min)
μ_{maxH}	Maximum specific growth rate of heterotrophic biomass (1/min)
η_g	Denitrification correction factor
Δ_p	Parameter value difference for two simulations (reference and simulation with modified parameter)
Δ_y	Difference in model output for two simulations (reference and simulation with modified parameter)
θ_H	Hydraulic residence time
θ_t	Normalized time (t/θ_H)
θ_x	Sludge age (d)

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