

A practical protocol for calibration of nutrient removal wastewater treatment models

Giorgio Mannina, Alida Cosenza, Peter A. Vanrolleghem and Gaspare Viviani

ABSTRACT

Activated sludge models can be very useful for designing and managing wastewater treatment plants (WWTPs). However, as with every model, they need to be calibrated for correct and reliable application. Activated sludge model calibration is still a crucial point that needs appropriate guidance. Indeed, although calibration protocols have been developed, the model calibration still represents the main bottleneck to modelling. This paper presents a procedure for the calibration of an activated sludge model based on a comprehensive sensitivity analysis and a novel step-wise Monte Carlo-based calibration of the subset of influential parameters. In the proposed procedure the complex calibration issue is tackled both by making a prior screening of the most influential model parameters and by simplifying the problem of finding the optimal parameter set by splitting the estimation task into steps. The key point of the proposed step-wise procedure is that calibration is undertaken for sub-groups of variables instead of solving a complex multi-objective function. Moreover, even with this step-wise approach parameter identifiability issues may occur, but this is dealt with by using the general likelihood uncertainty estimation (GLUE) method, that so far has rarely been used in the field of wastewater modelling. An example from a real case study illustrates the effectiveness of the proposed methodology. Particularly, a model was built for the simulation of the nutrient removal in a Bardenpho scheme plant. The model was successfully and efficiently calibrated to a large WWTP in Sicily.

Key words | ASM, calibration protocol, GLUE, identifiability, sensitivity analysis, wastewater treatment modelling

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INTRODUCTION

In recent years, the use of mathematical modelling of wastewater treatment processes has gained increased interest, largely due to the great benefits furnished from its employment during plant design phases as well as during operational management. The integration of knowledge by means of mathematical models is useful for several reasons: (i) such models make it possible to test hypotheses on functional interactions in the system; (ii) they are compact and transparent archives of knowledge about a system that facilitate communication among engineers and scientists; and (iii) they

can be used for predicting future states of the system or its responses to assumed or expected changes in driving conditions (Reichert & Vanrolleghem 2001). Indeed, several models have been developed to aid the design, operation and research of wastewater treatment plants (WWTPs). In 1987, a Task Group of the International Water Association (IWA) introduced the Activated Sludge Model no. 1 (ASM1) for the description of biological chemical oxygen demand (COD) and nitrogen removal (Henze *et al.* 2000). Following the development of the ASM1 model, this Task Group developed

the ASM2 model to also include phosphorus removal, and, to compare results, the assumptions underlying ASM1 were re-used as much as possible.

As with every model, for a correct and reliable application, ASMs need to be calibrated. Due to the fact that ASMs are complex environmental models, model calibration is a very challenging task. Indeed, complex environmental models are generally characterized by several parameters to be assessed and also several model outputs to be fitted with the measured data. Further, especially for the quality aspects limited data are generally available due to the fact that they require large economic as well as human resources. Owing to these aspects, complex environmental models are generally over-parameterized and identifiability issues have to be faced (among others, Reichert & Omlin 1997; Weijers & Vanrolleghem 1997; Dochain & Vanrolleghem 2001; Freni *et al.* 2011). In the past three decades, the model calibration issue has been the object of numerous publications among the scientific literatures and different model calibration approaches and optimization techniques were proposed or discussed according to the modelling focus (e.g. Van der Molen & Pintér 1993; Wang *et al.* 1995; Petersen *et al.* 2003). In the field of WWTP modelling the problem of model calibration and the issue of the identification, estimation and control of processes was first discussed by Beck in 1986 underlying the important role of model uncertainty in the model calibration (Beck 1986, 1987, 1991). The problem has also been undertaken by applying the ASM models. As a matter of the fact, several applications of ASM models are present in the literature concerning both pilot and full-scale plants, but only a few deal with effective model calibration to real WWTPs (Van Veldhuizen *et al.* 1999; Brdjanovic *et al.* 2000; Petersen 2000; Makinia *et al.* 2006; Vandekerckhove *et al.* 2008; Mannina & Viviani 2009). All these applications, while highlighting both the benefits and difficulties encountered, have mainly served to show how laborious the implementation of ASMs can be. Numerous applications of ASMs have demonstrated, for example, that the ASM parameters are not universal in the sense that not all systems can be modelled using the same parameter values (Weijers & Vanrolleghem 1997; Brun *et al.* 2002). Site-specific model parameters must be obtained by calibration with experimental data. Dedicated measurement campaigns consisting

of intensive sampling and measurements of influent and effluent variables, every few hours over a period of a few days to a week, are typically used to capture the dynamics in a WWTP (Sin *et al.* 2005; Freni *et al.* 2010). As a consequence, model application to a full-scale WWTP can be a major challenge. Moreover, the large number of parameters of ASMs in comparison to the limited amount of data means that not all parameters can be uniquely estimated (Weijers & Vanrolleghem 1997; Brun *et al.* 2002).

With the objective of aiding modellers during such complex calibration studies, different systematic calibration protocols have been proposed in recent years: the STOWA protocol (Hulsbeek *et al.* 2002), BIOMATH (Petersen *et al.* 2002; Vanrolleghem *et al.* 2003), the WERF (Water Environment Research Foundation) protocol (Melcer *et al.* 2003) and HSG (Hochschulgruppe) (Langergraber *et al.* 2004). An important characteristic of these protocols is that they do not have the ambition to estimate all parameters, but rather they estimate only a subset of them. The way these subsets are obtained is quite different throughout the different protocols (expert-based, prior sensitivity analysis, etc.). Sin *et al.* (2005) made an initial evaluation of these four protocols.

Importantly, in view of the approach developed in this paper, Insel *et al.* (2006), proposed a step-wise methodology for model calibration of nutrient-removing SBRs. The methodology considered four iterative steps, sequentially calibrating to $\text{NH}_4\text{-N}$, O_2 , $\text{NO}_3\text{-N}$ and $\text{PO}_4\text{-P}$ profiles. Corominas *et al.* (2008) integrated this approach into the BIOMATH protocol. As another important step forward, more recently, Sin *et al.* (2008) proposed a Monte Carlo-based calibration method for ASMs, similarly to Ruano *et al.* (2007) where instead the Monte Carlo method was used to define identifiable parameter subsets. Recently, Mannina & Viviani (2010a) and Mannina (2011) applied the step-wise methodology proposed by Insel *et al.* (2006) for the model calibration of a river water quality model. Although the number of model parameters was lower compared with the ASMs, the methodology was very effective providing satisfactory results.

These calibration protocols tried to tackle the rather complex calibration issue of ASMs, but this phase still remains the weakest link in the overall modelling of activated sludge systems (Sin *et al.* 2005; Hauduc *et al.* 2009). Moreover, each calibration study published in the literature

has followed its own procedure in choosing the type of laboratory experiments for the influent characterization and the kinetic/stoichiometric parameter estimation, the definition of parameter subsets to be calibrated, the hydraulic characterization and the settling characterization. This variability in approaches makes it difficult to compare the results (Sin et al. 2005; Hauduc et al. 2009) and, unfortunately, the point made by Sin et al. (2005) that a standard approach in performing a calibration study for a WWTP model is lacking, still holds.

Bearing in mind the considerations discussed above and knowing that the calibration is still considered one of the main bottleneck/time-demanding tasks in a modelling study (Hauduc et al. 2009), the aim of the present work was to propose a useful, flexible and simple procedure for model calibration. The peculiarity of the proposed procedure is that the combination of issues connected to the model complexity, the lack of data and the large number of parameters involved is solved by making a previous screening of the most influential model parameters, the grouping of outputs and subsequently estimating the parameters in a step-wise manner. The procedure will be illustrated with a full-scale case study of a WWTP with a Bardenpho scheme.

PROPOSED PROCEDURE

In this study, a sensitivity analysis and model calibration methodology is proposed. The methodology consists of different steps in two major phases. In the first phase a preliminary sensitivity analysis is carried out with the aim of reducing the number of model parameters to be calibrated. A novel feature is that rather than pursuing a single subset of different parameters, different subsets are selected, each focusing on a different group of output variables to be described by the model under study. In the second phase the model calibration is performed by means of a group-wise Monte Carlo technique. In Figure 1, the sensitivity analysis and the model calibration flow-chart are shown.

Proposed parameter subsets selection procedure

Sensitivity analysis is a decisive procedure to identify the parameters that can have significant effects on modelled

process behaviour. It should be applied prior to numerical parameter optimization (Brun et al. 2002; Petersen et al. 2002). The influence of parameters can be affected by operating conditions, the parameter values of the model, influent composition and type of sensitivity index (Saltelli et al. 2000).

The proposed parameter subset selection procedure is based on the methodology proposed by Weijers & Vanrolleghem (1997). In particular, the sensitivity analysis proposed here is divided into six connected sequential steps (Figure 1).

The sensitivity analysis begins by considering the set of model outputs of interest to the modeller (Step 1 of Figure 1). More specifically, the experiments may be planned according to the pursued objective in order to collect as much information as possible. The sensitivity of these representative model outputs will then be evaluated. However, to accomplish the sensitivity analysis, *a priori* assumptions on the model parameter values must be made. In particular, default values drawn from the modeller's experience as well as from the relevant literature are employed. The *a priori* values of the model parameters are used as initial guesses for carrying out the sensitivity analysis (Step 2 of Figure 1).

In Step 3 of Figure 1 the variation range of the model parameters and the type of distribution that will be used in the Monte Carlo simulations are defined. The variation range for each parameter should be the broadest range drawn from the relevant literature (Hauduc et al. 2010). Using a Monte Carlo sample, one model parameter is varied at a time (OAT), in order to evaluate the influence of the parameter on the model output (Step 4 of Figure 1). To quantify the influence on the model outputs, the likelihood measure of each model output and the corresponding sensitivity coefficient are calculated (Step 5 of Figure 1). In the present study the following equation was employed as a likelihood measure

$$L(\theta_i/Y_j) = \exp\left(\frac{-\sigma^2_{M_j-O_j}}{\sigma^2_{O_j}}\right) \quad (1)$$

where θ_i , represents the *i*-th set of (randomly generated) model parameters and $\sigma^2_{M_j-O_j}$ is evaluated as

$$\sigma_{M_j-O_j} = \sum_i^K (M_{j,i} - O_{j,i})^2 \quad (2)$$

which is the sum of squared errors between model output ($M_{j,i}$) and observation ($O_{j,i}$) of the j -th variable, while $\sigma^2_{O_j}$ is evaluated as

$$\sigma_{O_j} = \sum_i^K (O_{j,i} - \bar{O}_j)^2 \quad (3)$$

which is the sum of squared errors between the observations ($O_{j,i}$) and the average value of the observations (\bar{O}_j) for the period under consideration.

The likelihood measure according to Equation (1) varies between zero and one, with a likelihood of one corresponding to a perfect fit (Nash & Sutcliff 1970). As for large errors, as the ratio goes to infinity, the likelihood becomes zero. Because the model is characterised by more than one output, it is suggested to use an overall model efficiency according to the following equation

$$E_i = \sum_j^n \alpha_j L(\theta_i/Y_j) \quad (4)$$

where E_i represents the weighted sum of the likelihood measures of the n model outputs computed on the i -th selected parameter set (θ_i) and α_j is a normalizing constant that represents the weight of the j -th model output. For each model output j , it is proposed to compute the weight α_j by dividing the maximum value of the likelihood measure of the model output j by the sum of the maximum values of the likelihood measures of the other $n - 1$ model outputs. This weighting is of course performed after all Monte Carlo simulations have been completed.

The sensitivity analysis is now finalised by calculating so called sensitivity coefficients according to the following expression

$$s_{i,j} = \left| \frac{(E_{max,j} - E_{min,j})/E_j}{(K_{max,i} - K_{min,i})/K_i} \right| \quad (5)$$

where j and i , respectively, represent the model output and the model parameter, $K_{max,i}$, $K_{min,i}$ and K_i , are respectively, the maximum, the minimum and the average values of the i th parameter while $E_{max,j}$, $E_{min,j}$ and E_j are the maximum, the minimum and the average values of the efficiencies.

Following the evaluation of the sensitivity coefficients, the set of the most influential parameters for each representative output is defined (Step 6 of Figure 1). To achieve this important step, first the sensitivity coefficients for each model output are scaled to the maximum sensitivity coefficient for that output, obtaining the scaled sensitivity coefficients ($s_{s,i}$). Thereafter, the scaled sensitivity coefficients ($s_{s,i}$) are sorted in decreasing order. According to the adopted procedure a model parameter was considered influential if its average scaled sensitivity coefficient was larger than 0.1. This procedure is basically established to ensure that at least one parameter will be selected for each output available (Weijers & Vanrolleghem 1997).

Following Insel et al. (2006), the idea to group the model parameters to be calibrated has been adopted. In contrast, in this case parameters were not grouped according one output variable, but rather different groups of model outputs and corresponding influential model parameters were selected. The groups were formed by putting together all variables related to TSS, COD, N and P respectively. Subsequently, an appropriate calibration hierarchy must be established on the basis of interdependency of state variables (Step 6i of Figure 1). For each group of outputs, for example, the nitrogen outputs (NH₄-N, NO₃-N, TKN) the influential parameters will be identified. In this way it becomes possible to establish the order in which the step-wise procedure of the model calibration will be carried out (see below). It is important to note that it can happen that some parameters belong to more than one model output. This is due to the fact that those parameters influence more than one process. For the calibration of these parameters one should choose the optimized parameter value on the basis of multiple model outputs, as explained below.

Proposed calibration procedure

Following the sensitivity analysis, the set of model parameters to be calibrated has been reduced to the set of influential ones grouped according to a number of related model outputs. For the calibration, our experience is very good with the generalized likelihood uncertainty estimation (GLUE) methodology (Beven & Binley 1992). GLUE is based on Monte Carlo simulations: a large number of model parameter sets are generated from the multidimensional parameter space, each

with random parameter values selected from uniform probability distributions for each parameter in order to explore the whole confidence region (among others, Freni & Mannina 2010). No correlation between parameters was assumed. The acceptability of each set is assessed by comparing predicted to observed data throughout a chosen likelihood measure/efficiency. This leads to a division of all parameter set in two categories: parameters sets that allows acceptable description of the data and set that are unacceptable. The Monte Carlo sample dimension was selected, verifying that the analysis had converged. Convergence was evaluated by analyzing statistics and variations and changing the sample dimensions between 1000 and 10000 simulations (Bertrand-Krajewski *et al.* 2002; Freni *et al.* 2009a, 2009b; Mannina & Viviani 2010b).

The proposed model calibration is composed of four steps, as shown in the bottom part of Figure 1. The procedure begins with the selection of the first group of representative model outputs and the corresponding model parameter subset (*iii* of Figure 1) previously identified by the sensitivity analysis procedure (i.e., Step 6*ii* Figure 1). The model parameter subset is calibrated according to the model outputs and the objective function (Equation (4)) by carrying out the necessary Monte Carlo simulations. For each Monte Carlo run, the likelihood with respect to each representative model output (Equation (1)) is calculated. After the Monte Carlo simulation has been carried out, the overall model efficiency is determined (Equation (4)) and the best parameter values selected according to the maximum value of $E_{m,i}$ (Step 8 in Figure 1).

Once the parameter subset values are evaluated, it is checked whether all model parameters corresponding to the first group are also influential for the next group of model outputs. If all model parameters are influential for the next group they will all be included in the following *i-th* step (Step 9a of Figure 1) and the procedure returns to Step 7 of Figure 1. Instead, if only a part of the model parameters corresponding to the first group are also influential for the next group, the non-influential parameters are fixed at their calibrated values (Step 9b of Figure 1) before returning to Step 7 of Figure 1 and the remaining parameters are included in the following *i-th* step (Step 9c of Figure 1). The procedure including Step 7–9a or c is repeated for the N groups of model outputs by using the same parameter evaluation described above. It is important to stress that if at least one parameter

corresponding to the first group is influential for the next group all model outputs of the first group will also be included in the next group. The final set of calibrated model parameter values is obtained by combining the values of the parameters that were fixed in previous steps (Step 10 of Figure 1).

MATERIALS AND METHODS

Case study – plant description

The municipal activated sludge WWTP under study is located in Sicily (Italy), with its effluent discharged in the Mediterranean Sea. The plant was designed for a capacity of 40,000 inhabitant equivalents (IE). The influent of the WWTP consists of domestic and the non-industrial part of wastewater produced by a nearby refinery. After the pretreatment step (coarse grit removal, fine grit removal, screen with rotating panel, sand and grease removal) the influent is introduced into an equalization tank with a volume of 1700 m³ in which the wastewater is discontinuously aerated (3 h/d). The effluent of the equalization tank flows to the biological nutrient removal activated sludge plant (Figure 2) that consists of an activated sludge reactor, according to a Bardenpho scheme, and a secondary clarifier (with a volume of 2885 m³). The activated sludge reactor is composed of three completely mixed compartments of different sizes. The first compartment operates as an anaerobic zone, the second as an anoxic zone and the third as an aerobic zone, with volumes (V) of 900, 1140 and 5800 m³, respectively. Return activated sludge (RAS) from the bottom of the secondary clarifier and internal mixed-liquor recirculation (MLR) from the end of the aerobic zone are, respectively, pumped to the anaerobic and anoxic zones. The influent flow rate (Q_{inf}) is an average 400 m³/h; the mixed-liquor recirculation flow rate (Q_{MLR}) and the return activated sludge recirculation (Q_{RAS}) are generally set, respectively, to 3 and 1.5 Q_{inf} . The waste activated sludge (WAS) is simply dewatered by a belt-press filter. The sludge retention time (SRT) during the period under study was around 20–25 days.

Measurements

All necessary design and operational data, such as zone volumes, pump flows, Q_{inf} , Q_{MLR} , and Q_{RAS} were initially

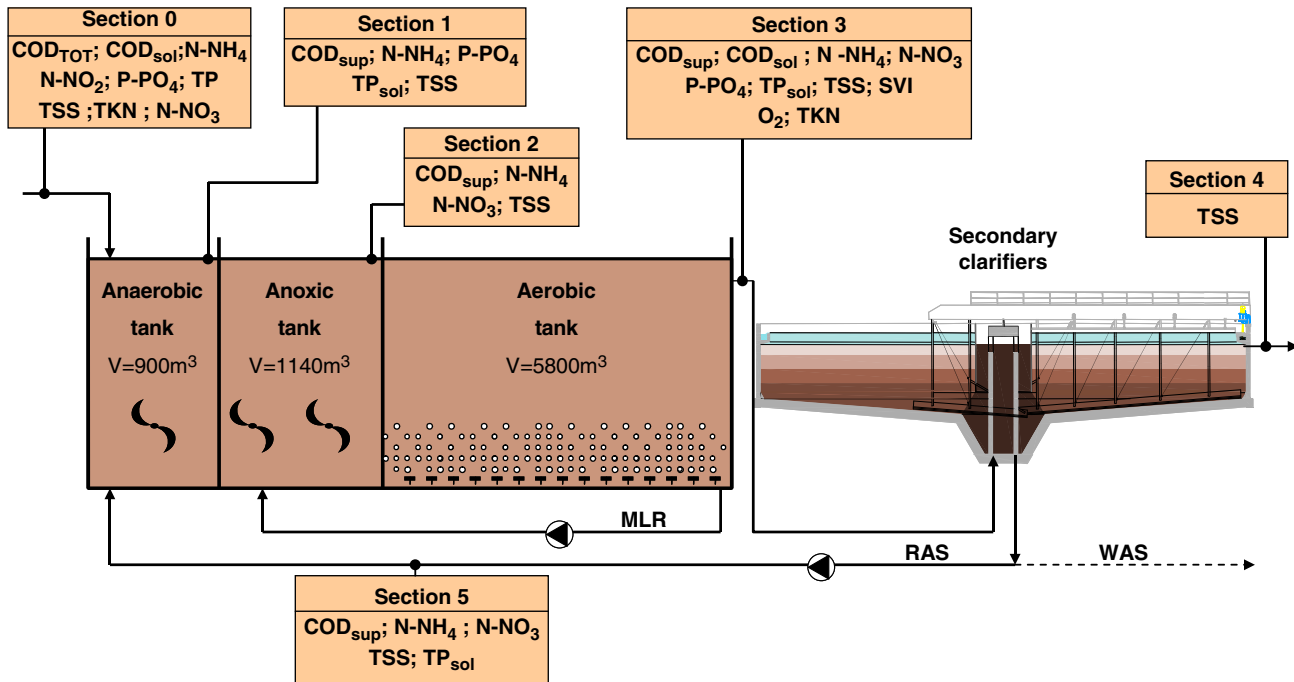


Figure 2 | Flow sheet of WWTP with locations of sampling points.

recorded. An intensive dedicated measurement campaign was carried out from 01 March 2006 to 12 April 2006. The grab wastewater samples were withdrawn from the effluent of each zone (sections 1–4 in Figure 2) and from the RAS channel (section 5). It is important to underline that the samples were not withdrawn simultaneously. Indeed, between samples at one and a subsequent section, a lag time was set according to the hydraulic retention time (HRT) of the corresponding tank. The HRT of each tank was computed by dividing the volume of the tank to the inflow for the tank, also taking into account the recycle flow.

The following characteristics of the samples were analyzed according to IRSA methods (Istituto di Ricerca Sulle Acque 1994): total suspended solids (TSS), (COD_{sup}), COD_{sol} , NH_4 -N, NO_3 -N, NO_2 -N, orthophosphate (PO_4 -P), TP, total kjeldahl nitrogen (TKN), sludge volume index (SVI), dissolved oxygen (O_2) and air-flow rate. The measure of COD_{sup} was performed on supernatant samples (the supernatant samples were taken from the surface after 2–3 minutes of decantation), whereas the measures of COD_{sol} and TP_{sol} were performed on filtrate samples (through a $0.45 \mu m$ GF/C filter). In Table 1 the average values of the measured variables are reported. It is important to precise that the high average

effluent TSS concentration is due to the abnormal functioning of the secondary settling which sometimes occurred during the measurement campaign.

As discussed above, six sampling sections were considered; the collected data were all used for the model calibration, while the average values for each component and section were adopted as initial conditions.

Another 1-day sampling campaign was conducted, during which samples were withdrawn only from the influent channel every 2 hours between 8:00 am (19/06/2006) and 8:00 am (20/06/2006). The data were used to determine the daily pattern of several influent pollutants necessary for the implementation of the long-term WWTP simulation.

Influent characterization

Influent characterization is one of the dominant factors in WWT modelling (Roeleveld & van Loosdrecht 2002). This influent characterization consists of translating data available from the WWTP into data that can be used in the model (Vandekerckhove et al. 2008). In this study influent characterization was carried out by means of data collected during the measurement campaigns.

Table 1 | Average measured values during the campaign from 01/03/2006 to 12/04/2006

No. Section ↓	Average measured values [mg/L]												
	COD _{sup}	COD _{TOT}	COD _{sol}	O ₂	P-PO ₄	TP	TP _{sol}	N-NO ₂	N-NO ₃	N-NH ₄	TKN	TSS	SVI
0	–	422	78.5	–	1.5	2	–	–	0.5	32.5	33.5*	190	–
1	239	–	–	–	2.26	–	2.64	–	–	22	–	6667	–
2	120.5	–	–	–	–	–	–	–	1.3	15	–	6800	–
3	54	–	11.5	2.5	0.64	–	1	–	18.8	0.09	20*	9400	80
4	–	–	–	–	–	–	–	–	–	–	–	180	–
5	173	–	–	–	–	–	0.75	–	7.8	0.08	–	10550	–

(*only two measures)

Regarding the influent organic matter fractions, four components were considered: the soluble biodegradable COD (S_S , the sum of S_F and S_A), the non-biodegradable soluble COD (S_I), the biodegradable particulate COD (X_S) and the non-biodegradable particulate COD (X_I). Heterotrophic and autotrophic biomasses were considered negligible in the influent. With the aim of defining an appropriate set of fractionation coefficients, exclusively connected to the COD_{sup} , the procedure as indicated by Makinia *et al.* (2005) was preliminarily employed. Since the volatile fatty acid (VFA) and BOD_5 concentrations were not measured, the following assumptions were made by drawing upon the relevant literature (Henze *et al.* 2000; Makinia & Wells 2000; Meijer *et al.* 2002; Ferrer *et al.* 2004): the VFA fraction (S_A) was set equal to 8 per cent of the COD_{sup} and the BOD_5 equal to 45 per cent of COD_{TOT} . The fractional coefficients derived according to Makinia *et al.* (2005) as well as the employed hypotheses are: $F_{SF} = 0.25$, $F_{SA} = 0.08$, $F_{SI} = 0.02$, $F_{XS} = 0.55$ and $F_{XI} = 0.1$ (Table 2). These values were considered as parameters in the calibration procedure and were then adjusted to obtain the best fit between the measured and simulated values.

Regarding the nitrogen components, it was assumed that the measured values for NH_4-N and NO_3-N were equal to S_{NH4} and S_{NO3} , respectively. The ratio between S_{NH4} and TKN was assumed equal to 70 per cent in order to cope with the absence of specific data on such concentration values.

Accordingly, S_{ND} and X_{ND} were taken as 20 and 10 per cent of the indirectly derived TKN, respectively (Henze *et al.* 2000). Concerning the phosphorus model components, the measured values of PO_4-P were considered as inorganic

soluble phosphorus (S_{PO4} model component) and TP was considered as the sum of PO_4-P and the other phosphorus fractions.

Model description and assumptions

The previously described sensitivity analysis and model calibration methodology has been applied to calibrate a model able to describe the nitrogen and phosphorus removal processes on the basis of data collected at a real municipal activated sludge WWTP.

In order to simulate the nitrification-denitrification/enhanced biological phosphorus removal processes occurring in the studied full-scale WWTP, the ASM2 was selected similarly to Amano *et al.* (2002). The model was used to simulate the following variables: ammonia (NH_4-N), nitrate (NO_3-N), total soluble phosphorus (TP_{sol}), supernatant COD (COD_{sup}), dissolved oxygen (SO_2), particulate material (X_{TSS}) and soluble COD (COD_{sol}).

The COD_{sup} , COD_{sol} , X_{TSS} and TP_{sol} were assessed as follows from the ASM2 state variables

$$COD_{sup} = S_F + S_A + S_I + f_{NS} \cdot (X_I + X_S + X_H + X_{AUT} + X_{PAO} + X_{PHA}) \quad (6)$$

where f_{NS} represents the non-settleable fraction of the particulate organic variables and has been computed subtracting the COD_{sol} from the COD_{sup} and by dividing by the sum of the particulate organic variables.

$$COD_{sol} = S_F + S_A + S_I \quad (7)$$

Table 2 | (continued)

Description	Symbol	Unit	Default	Calibrated	Range	Reference	COD _{sup,1}	COD _{sup,2}	COD _{sol,3}	X _{rss,1}	X _{rss,2}	X _{rss,3}	S _{NH4,1}	S _{NH4,2}	S _{NH4,3}	S _{NO3,2}	S _{NO3,3}	S _{PO4,1}	S _{PO4,3}	TP _{sol,1}	TP _{sol,3}		
Saturation/inhibition coefficient for nitrate	K _{NO}	gN/m ³	0.5	0.34	0.1–0.55	Weijers & Vanrolleghem 1997 (*)	X									X	X						
Rate constant for lysis	b _H	d ⁻¹	0.192	0.264	0.02–1.44	Jeppsson 1996 (*)	X	X		X	X							X				X	
Hydrolysis rate constant	K _H	d ⁻¹	3	2.76	0.96–3	Jeppsson 1996 (*)	X	X		X	X					X							
Maximum rate for fermentation	q _{FE}	gS _p /(gX _H *d)	3	2.928	1.5–3	Henze <i>et al.</i> 2000	X									X	X					X	
Saturation coefficient for O ₂ heteroorgan.	K _{OH}	gO ₂ /m ³	0.2	0.29	0.01–0.5	Jeppsson 1996 (*)	X						X					X	X		X	X	
Rate constant for storage of PP	q _{PP}	gX _{pp} /(gX _{PAO} *d)	1.5	1.34	1–1.5	Henze <i>et al.</i> 2000																	
Ammonification coefficient	K _{AMM}	m ³ COD/(g*d)	0.04	0.04	0.04–0.08	Jeppsson 1996																	
Saturation coefficient for O ₂ autotorgan.	K _{OA}	gO ₂ /m ³	0.4	2.5	0.4–3	Jeppsson 1996 (*)				X			X					X	X		X	X	
Rate constant for lysis of X _{PHA}	b _{PHA}	d ⁻¹	0.2		0.1–0.2	Henze <i>et al.</i> 2000																	
Decay rate of nitrifiers	b _{AUT}	d ⁻¹	0.15		0.05–0.2	Jeppsson 1996																	
Saturation coefficient for S _A	K _A	gCOD/m ³	4	3.52	3.5–4.5	Henze <i>et al.</i> 2000 (*)	X									X			X			X	
Saturation coefficient for polyphosphate	K _{PP}	gX _{pp} /(gX _{PAO}	0.01	0.017	0.01–0.02	Henze <i>et al.</i> 2000 (*)																	
Yield coefficient of heterot. organisms	Y _H	gCOD/gCOD	0.625	0.45	0.38–0.75	Jeppsson 1996 (*)				X	X		X			X	X	X	X		X	X	

Table 2 | (continued)

Description	Symbol	Unit	Default	Calibrated	Range	Reference	COD _{sup,1}	COD _{sup,2}	COD _{sol,3}	X _{TSS,1}	X _{TSS,2}	X _{TSS,3}	S _{NH4,1}	S _{NH4,2}	S _{NH4,3}	S _{NO3,2}	S _{NO3,3}	S _{PO4,1}	S _{PO4,3}	TP _{sol,1}	TP _{sol,3}	
Saturation coefficient for growth on S _F	K _F	gCOD/m ³	4	7.55	4–14	Henze et al. 2000	X		X													
PP requirement for PHA storage	Y _{PO4}	gP/gCOD	0.4	0.11	0.1–0.6	Henze et al. 2000 (*)		X										X			X	
Rate constant for lysis of X _{PAO}	b _{PAO}	d ⁻¹	0.1		0.1–0.2	Henze et al. 2000																
Oxygen mass transfer coefficient	K _{1a}	d ⁻¹	240		84–360	Iacopozzi et al. 2007																
Fraction of X _S in influent total COD	F _{Xs}	gCOD/gCOD	0.55	0.616	0.5–0.72	(**)																

$$X_{TSS} = i_{TSS,XI} \cdot X_I + i_{TSS,XS} \cdot X_S + i_{TSS,BM} \cdot (X_H + X_{AUT} + X_{PAO}) + i_{TSS,XPP} \cdot X_{PP} + i_{TSS,XPHA} \cdot X_{PHA} \quad (8)$$

where $i_{TSS,XI}$, $i_{TSS,XS}$, $i_{TSS,BM}$, $i_{TSS,XPP}$ and $i_{TSS,XPHA}$ represent, respectively, the TSS contents of X_I, X_S, of the sum of X_H, X_{AUT} and X_{PAO}, of X_{PP} and X_{PHA}.

$$TP_{sol} = S_{PO4} + i_{PSF} \cdot S_F + i_{PSI} \cdot S_I \quad (9)$$

where i_{PSF} and i_{PSI} are respectively the P contents of soluble substrate S_F and the P content of inert soluble COD S_I.

For the sake of conciseness, in the following, the differences between the developed model and the ASM1 and ASM2 models are outlined, referring the reader to the literature for the definitions of all model state variables, biological processes, stoichiometry and kinetics (Henze et al. 2000).

Similarly to ASM2, the developed model includes cell internal storage compounds. However, to improve model performance, some of the ASM1 processes and components were considered for addition to ASM2. In particular, the ammonification process was employed to describe the release of ammonium (S_{NH4}) from soluble biodegradable organic nitrogen (S_{ND}). In further analogy to ASM1, the hydrolysis of particulate biodegradable organic nitrogen (X_{ND}) was included as a separate process.

In contrast to ASM2, chemical precipitation of phosphorus was not included in the model because no chemical flocculants were added.

As in most WWTPs the nitrite and nitrate inflow concentration were assumed to be zero, so the influent soluble nitrogen only consists of ammonium and biodegradable organic nitrogen. Besides, the measured values of the temperature and pH, respectively close to 20°C and neutrality, were not strongly varying during the simulation period. The latter two considerations enabled further simplification of the model equations and therefore a reduction in the number of model parameters to be considered for the calibration. The kinetic parameters' temperature dependency did not have to be taken into account during calibration and the alkalinity of the wastewater was not introduced as a model component.

Nevertheless, whenever the model is used at other temperatures than 20°C, the developed model uses the temperature correction term according to van't Hoff- Arrhenius, in line with the ASM models (Henze et al. 2000).

WWTP influent model

To carry out WWTP simulations, a continuous input series in terms of quantity and quality data is needed. To compose such a long-term dynamic time series starting from discrete measured input data, a truncated Fourier series was employed (Mannina & Viviani 2009). Indeed, such series, after the evaluation of the input characteristics on the basis of the measured data, enables the simulation of a continuous WWTP inflow. In this study, the Fourier series used is just a sum of three superimposed sinusoids that is multiplied with the daily measured concentration to make up a long-term dynamic time series. Accordingly, the generic input variable, Y , can be modelled by the following equation

$$Y(t) = \mu \cdot (1 - (\beta_1 \cdot \sin(\omega_1 \cdot t + \phi_1) + \beta_2 \cdot \sin(2\omega_2 \cdot t + \phi_2) + \beta_3 \cdot \sin(3\omega_3 \cdot t + \phi_3))) \quad (10)$$

where β_1 , β_2 , β_3 , ω_1 , ω_2 , ω_3 , ϕ_1 , ϕ_2 and ϕ_3 are the series parameters, t is the time and μ is the daily average value of the simulated variable.

As shown in Figure 3(a) the Fourier series moves through-out a line that generally coincides with the horizontal line whose value is the average of the variable being modelled. To generate a long term series, since μ value is generally not constant from day to day, a linear relationship was considered to avoid discontinuities (see Figure 3(b)). More specifically, a line connecting the first average parameter value to the following one was used. In order to evaluate the average value, for the generation of a long term series, the simulated variable is computed by using the following equation

$$\mu(t) = \left(\frac{\mu(t_+) - \mu(t_-)}{t_+ - t_-} \right) \cdot (t - t_-) + \mu(t_-) \quad (11)$$

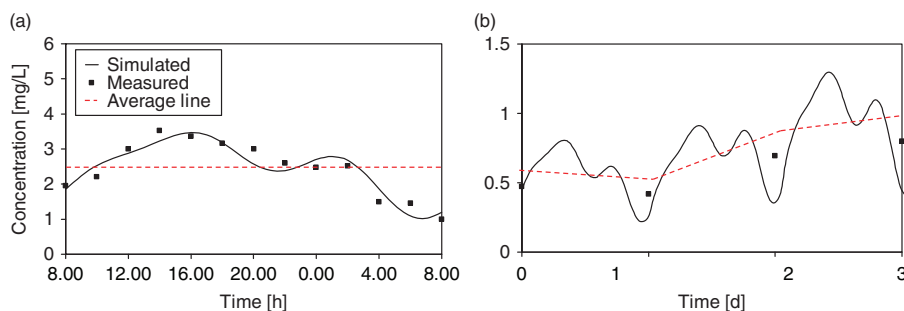


Figure 3 | Example of Fourier series pattern for a day with measurements every two hour (a) and for three days obtained by coping the (a) pattern into (b).

where $\mu(t_+)$ and $\mu(t_-)$ are respectively the measured mean value at the time $t + 1$ and $t - 1$.

WWTP hydraulics model

In the present study no WWTP flow propagation modelling has been performed. Indeed, as usual in WWTP modelling, an instantaneous flow propagation was considered through the plant, neglecting any flow attenuation due to storage effects. However, in term of mixing regime, only three CSTRs were considered, assuming each one to be perfectly mixed.

Settler model

Concerning the settler, an ideal point settler was implemented and the concentrations of the soluble components in the return activated sludge were assumed to be equal to the effluent concentrations from the aerobic reactor. The concentrations of the particulate components were computed by means of the mass balance in the clarifier, as suggested by Qian (2008).

RESULTS AND DISCUSSION

WWTP influent model

Starting from the collected data base, the measured data were modelled according to the Fourier series Equation (10) by adjusting the parameter values of the Fourier series to minimize the sum of squared errors. Figure 4 compares the daily patterns of the modelled input data according to the Fourier series with the measured profiles.

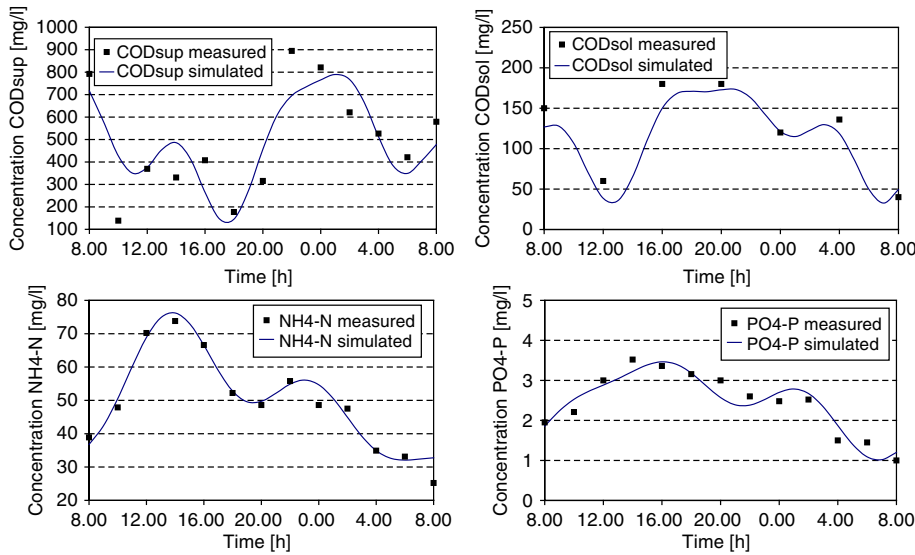


Figure 4 | Measured and simulated values during 19–20/06/2006 in section 0.

Once the Fourier parameters were estimated, a long input time series for the overall simulation period (1 March to 12 April) was created starting from the measured daily values of the influent concentrations (Figure 5). This pattern was determined by copying the daily pattern (19–20 June 2006) described by the truncated Fourier series to the full simulation period on the basis of Equation (10). It is worthy to mention that the forecasting of diurnal influent profile by means of the

Fourier series or other similar methods can induce bias into data. Indeed, the uncertainty associated to the data of the diurnal influent profile can propagate throughout the model leading to poor results. Indeed, the uncertainty in the model input could be higher than the model parameters uncertainty. In view of this fact, it is advisable to reduce the input uncertainty by gathering new data before carrying out model calibration assessing the kinetic parameters.

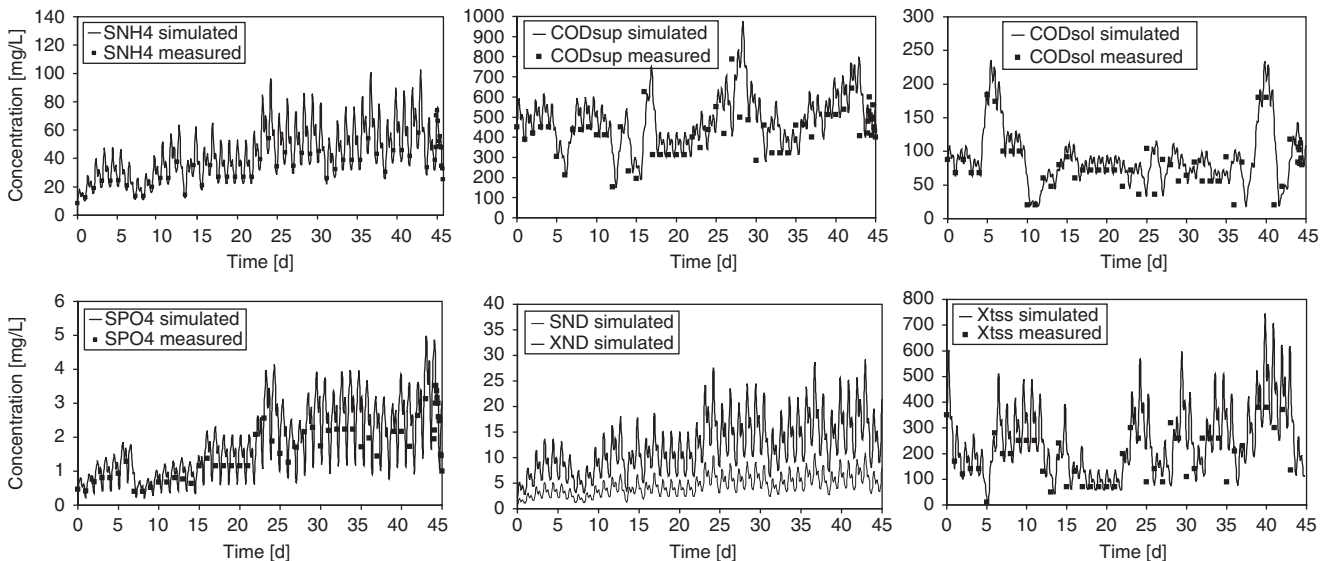


Figure 5 | Long-term series for the main model input.

Parameter subsets selection

As discussed in the previous paragraphs, the model contains 41 parameters. To avoid the problem of overparameterization and related identifiability issues a reduction of the number of model parameters was carried out by means of the sensitivity analysis shown in Figure 1. More specifically, the model parameters were changed one at a time and the importance of each model parameter was assessed for all model state variables for which we have measurements.

The modelling objective in the present work is the description of the variable concentrations in different reactors and not only in the effluent. According to this objective an appropriate experimental campaign was performed, and all relevant variables were measured. For the present study, 15 model state variables were considered, namely, $S_{NH4,1}$, $COD_{sup,1}$, $S_{PO4,1}$, $TP_{sol,1}$, $X_{TSS,1}$, $S_{NH4,2}$, $S_{NO3,2}$, $X_{TSS,2}$, $COD_{sup,2}$, $S_{NH4,3}$, $S_{NO3,3}$, $S_{PO4,3}$, $TP_{sol,3}$, $X_{TSS,3}$ and $COD_{sol,3}$. According to the flow chart in Figure 1, these variables were considered as the set of model outputs (Step 1 of Figure 1). The first model parameter values, mainly drawn from the literature, were also considered as a priori model parameter values (Step 2 of Figure 1).

To perform the sensitivity analysis a uniform distribution was chosen for each model parameter (Step 3 of Figure 1). The upper and lower bounds of the uniform distributions of the model parameters were defined according to the broadest range found in the relevant literature (Jeppsson 1996; Weijers & Vanrolleghem 1997; Henze *et al.* 2000; Afonso & da Conceição Cunha 2002; Iacopozzi *et al.* 2007; Di Bella *et al.* 2008; Flores-Alsina *et al.* 2008; Sin *et al.* 2009; Mannina *et al.* 2010) (Step 3. of Figure 1). Note that a similar study has been recently performed by Hauduc *et al.* (2010). In Table 2, the values of the default model parameters along with the variation range, their literature references and the final calibrated values are reported.

By varying one parameter at a time, a large set of parameters was obtained and the corresponding Monte Carlo simulations were carried out (Step 4 of Figure 1) for the 44 days simulation period. It is important to remark that for each simulation conducted the model was first run for the steady-state conditions and then for the dynamic ones. For each model run, the model likelihoods for each of the chosen 15 model state variables were calculated (according to Equation (1)).

The results of the Monte Carlo simulations were used to evaluate the sensitivity coefficients of each j -th model output and i -th model parameter, according to Equation (5) (Step 5 of Figure 1). Then, a set of most influential model parameters for each representative model output was selected according to the procedure described above (Step 6 of Figure 1).

In Figure 6, the results of the sensitivity analysis for four of the 15 model outputs, $COD_{sup,2}$ (a), $S_{NH4,1}$ (b), $X_{TSS,2}$ (c), and $S_{PO4,1}$ (d), as well as the total model influence of the parameters, computed as the sum of the sensitivity coefficients of all variables (e), are reported. The coloured area indicates the set of influential parameters for the corresponding model output. As can be observed, some parameters are influential for more than one model output, for example, K_x is influential both for $COD_{sup,2}$ and $X_{TSS,2}$.

In Figure 6(e), the sums of the scaled sensitivity coefficients of all representative model outputs j for each parameter i ($\sum S_{Si,j}$) are reported, revealing that F_{SF} , Y_H and μ_{AUT} are the most influential model parameters in this case study. Such a result is consistent with Ruano *et al.* (2007) who also found F_{SF} as one of the most influential model parameters in ASM2d. They also found a high sensitivity for μ_{AUT} . On the other hand, b_{aut} showed a low influence, again similar to Petersen *et al.* (2002) and Ruano *et al.* (2007).

Table 2 summarizes the results of the sensitivity analysis for each of the selected model outputs. By means of the performed analysis, that is, quantitative prioritization of the model parameters, it is possible to gain insights in the performed processes. Among the non-influential parameters, the sensitivity analysis reveals that, with the exception of K_{AMM} , b_{AUT} and K_{La} , they are all parameters related to P removal, indicating a higher relevance of the N-removal processes over these processes. This agrees with the fact that the biological phosphorus removal remained is limited during the measurement campaign. However, it has to be stressed that with respect to their level of sensitivity the parameter significance level may be different from one plant to another because of changes in process scheme and available data (among others, Ruano *et al.* 2007).

By means of the sensitivity analysis, the number of model parameters to be identified was reduced from 41 to 27, enabling a better capability for calibrating the model in the second phase of the procedure. Although the number of model parameters has been drastically reduced, not all

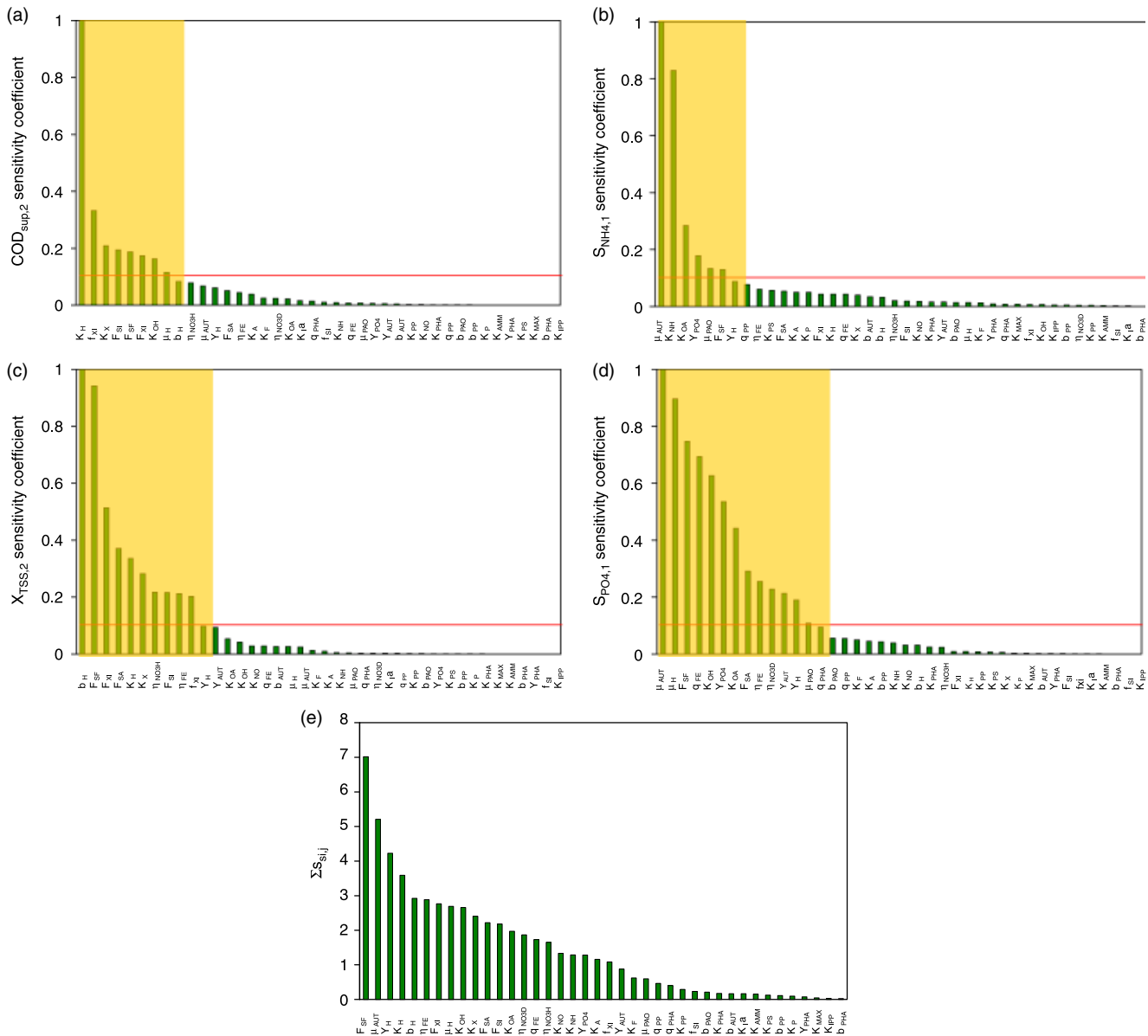


Figure 6 | Scaled sensitivity coefficients for COD_{sup,2} (a), S_{NH4,1} (b), X_{TSS,2} (c), S_{PO4,1} (d) and ΣS_{Si,lj} (e); (the coloured zone indicates influential parameters for the corresponding model output).

influential parameters can be expected to be identifiable since an OAT sensitivity analysis has been performed. In this respect, a specific investigation based on an identifiability analysis (see Weijers & Vanrolleghem 1997; Sin *et al.* 2008; Freni *et al.* 2011) should be carried out. Nevertheless, in this study we limited ourselves to single out the most influential parameters since the GLUE method for calibration can handle indirectly identifiability issues in contrast to other parameter estimation methods.

Once the influential model parameters were singled out, they were clustered into four groups according to the model output group. The selection of the groups has been done according to the objective of the study and the modeller experience. In particular the model variables of the same ‘nature’ were put together forming a group and subsequently a reasonable calibration hierarchy has been established. According to the step-wise calibration procedure, the calibration of the parameters that were influential towards X_{TSS,1},

$X_{TSS,2}$, $X_{TSS,3}$ (i.e., total suspended solid concentration in the first, second and third tank, respectively) was to be accomplished. Following this first step, the other model parameters, $COD_{sup,1}$, $COD_{sup,2}$, $COD_{sol,3}$, $S_{NH4,1}$, $S_{NH4,2}$, $S_{NH4,3}$, $S_{NO3,2}$, $S_{NO3,3}$ and finally, $S_{PO4,1}$, $TP_{sol,1}$, $S_{PO4,3}$, $TP_{sol,3}$ were assessed and included as model outputs in the parameter identification. The model parameters influential towards each group are reported in Table 2.

Calibration

Once the model parameters were defined with respect to each group of the model outputs, 10,000 Monte Carlo model runs were performed considering a uniform distribution of the parameters and simultaneously varying the influential parameters belonging to the selected model output group. The same parameter ranges as used in the sensitivity analysis were used (see Table 2) and no correlation between parameters was assumed. For each run, the simulation outputs were compared with the measured data, calculating the likelihood according to Equation (1).

The final result for each model output group was the set of values of the model parameters as selected on the basis of the maximum overall model efficiency, calculated according to Equation (4) (Step 9 of Figure 1). In this case, making a selection of the model parameters by grouping according to the proposed procedure, it was possible to obtain by the GLUE only one parameter set value in correspondence to the maximum efficiency.

In moving from one group of model calibration outputs to the next group, if a parameter was influential towards more than one model output, its value was assessed more than once and the final value adopted would be the one corresponding to the last output.

The values of the model parameters obtained in this way are consistent with previous studies (Van Veldhuizen *et al.* 1999; Brdjanovic *et al.* 2000; Henze *et al.* 2000; Rieger *et al.* 2001; Meijer *et al.* 2002; Ferrer *et al.* 2004; Makinia *et al.* 2005, 2006; Sin *et al.* 2008). However, some values of the calibrated model parameters require further discussion and it has also to be kept in mind that some differences may be due to the modified structure of the ASM2 model applied herein. As aforementioned the temperature was constant in the simulated period and set

equal to 20°C. Therefore, the kinetic model parameters refer to that temperature.

The most influential model parameters calibrated for the *N* model outputs, based on the scaled sensitivity coefficient, are μ_{AUT} and K_{NH} . The calibrated value of the nitrifiers growth rate, $\mu_{AUT} = 1.08 \text{ d}^{-1}$, is in agreements with literature values (referred to a temperature of 20°C): 1.2 d^{-1} (Makinia *et al.* 2005), 1.8 d^{-1} (Rieger *et al.* 2001), 1 d^{-1} (Henze *et al.* 2000) and 0.55 d^{-1} (Ferrer *et al.* 2004). Conversely, referring to $K_{NH} = 1.41 \text{ gN/m}^3$, there is a substantial difference with the value presented by Makinia *et al.* (2005) where the value is 0.2 gN/m^3 . However, lower values of this parameter are commonly encountered in pilot plants due to a lower diffusion limitation related to the higher turbulence and smaller flocs in comparison with full-scale plants (Henze *et al.* 2000). Among the calibrated parameter values to be discussed there is also Y_{PO4} because its calibrated value ($Y_{PO4} = 0.11 \text{ gP/gCOD}$) is not very close to the default value (Henze *et al.* 2000), see Table 2. However, similar results were obtained by Machado *et al.* (2009) that explained their result by the presence of glycogen-accumulating organisms (GAOs) not considered by ASM2.

Starting from the calibrated model parameter values, a dynamic simulation for the entire period was carried out. The results of the simulations are presented in Figure 7. Furthermore, to assess the quality of the model fits, the mean absolute error (MAE) and the root-mean-squared error (RMSE) were used as quality indices. According to Table 3, a summary of the above indices and the model efficiencies Equation (1), globally satisfactory results were obtained, as confirmed by the values of $L(\theta_i/Y_j)$ ranging between 0.12 and 0.7. For TSS and COD for the 2nd and 3rd tank, $L(\theta_i/Y_j)$ is a little lower. In addition, the values of MAE indicate that the model can be considered unbiased.

A good prediction accuracy with respect to the long-term behaviour of S_{NH4} (Figure 7(b)), COD_{sup} (Figure 7(a)) and S_{PO4} (Figure 7(c)) was observed in the anaerobic zone (section 1). The simulated values show an acceptable agreement with the measured ones. Similarly, in section 2, the model fits the measured S_{NH4} values well (Figure 7(d)), although in some cases the model overpredicts. Such a disagreement is likely due to the imperfect anoxic conditions in the second tank that caused the nitrification process to occur there as well by using the recycled oxygen. Indeed, due to the recycle

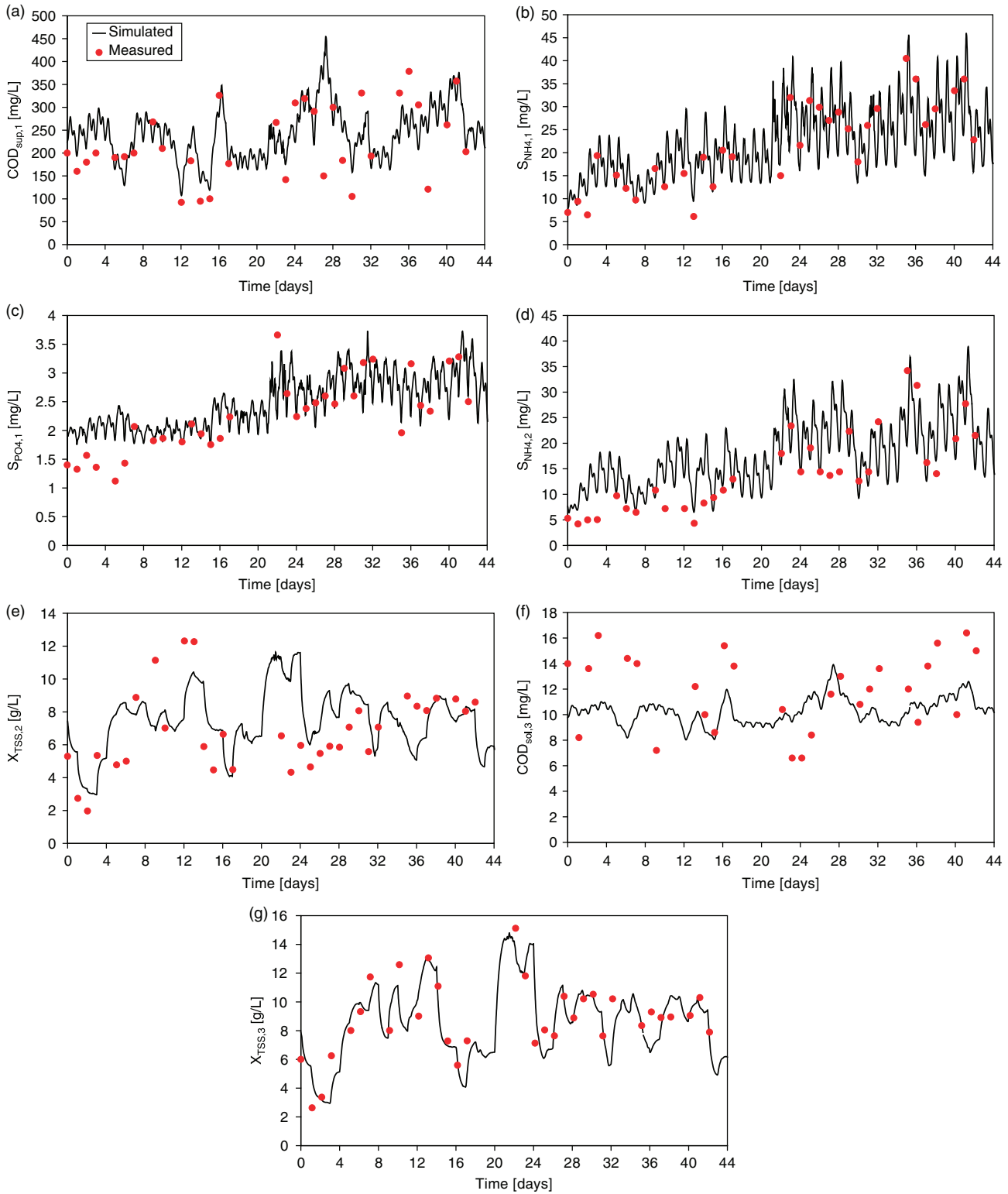


Figure 7 | Comparison of simulated and measured concentrations during the long term period.

Table 3 | Calibrated model fit

Model output	MAE [mg/L]	RMSE [mg/L]	Likelihood [-]	No.data [-]
COD _{sup,1}	52.85	71.89	0.45	31
COD _{sup,2}	48.39	58.41	0.37	33
COD _{sol,3}	3.55	4.24	0.38	27
X _{TSS,1}	1921.42	2490.62	0.33	33
X _{TSS,2}	2205.84	2610.72	0.3	33
X _{TSS,3}	1174.78	1550.09	0.7	33
S _{NH4,1}	5.90	7.33	0.54	33
S _{NH4,2}	3.99	5.18	0.65	33
S _{NH4,3}	0.90	1.10	0.21	33
S _{NO3,2}	0.75	0.99	0.13	33
S _{NO3,3}	6.28	7.52	0.28	33
S _{PO4,1}	0.37	0.46	0.6	33
S _{PO4,3}	0.59	0.79	0.15	33
TP _{sol,1}	0.53	0.64	0.4	33
TP _{sol,3}	0.94	1.14	0.12	33

of activated sludge a part of the oxygen mass is also recycled into the anoxic tank. Regarding the X_{TSS,2} the good accuracy between observed and simulated values is shown in Figure 7(e), with the exception of the first period for which a modest mismatch is also evident for the other variables. The model also shows an acceptable agreement with the measured data for X_{TSS,3} (Figure 7(g)) but it shows bias for the soluble COD in section 3, COD_{sol,3} (Figure 7(f)) (Table 3). Comparing the simulated with the measured concentrations of the overall set of selected model outputs it can be observed that the model shows a weak ability to simulate the S_{NO3,3}, as demonstrated by the low likelihood value (0.28). Furthermore, the S_{NH4} in the first tank as well as the S_{NO3} in the third tank are generally overpredicted. Such results could be due to incorrect influent ammonia concentrations that are higher than the real values. With regard to the TP_{sol,3} it presents the lower likelihood value than for the other, proving that modelling the biological phosphorus removal process does not work well. Indeed, once the parameter values of the Fourier series are evaluated, the prediction of the simulated daily influent concentrations depends on the analysis of the single measured value of the considered day. Such a value may not be representative of the daily value and this will thus affect the overall simulation of that component. In this case,

composite average values for the estimation of the daily input pattern would likely be better and could have provided a better agreement between measured and simulated values. Further, a quantification of the uncertainty associated with the model input and model parameters may help in understanding the need for gathering new data. However, it has to be stressed that uncertainty analysis in wastewater modelling field is limited to few studies (Bixio *et al.* 2002; Benedetti *et al.* 2008; Flores-Alsina *et al.* 2008; Belia *et al.* 2009; Mannina *et al.* 2010).

CONCLUSIONS

A procedure for calibration of an activated sludge model based on a comprehensive sensitivity analysis and a novel step-wise Monte Carlo-based calibration of the subset of influential parameters has been presented. A mathematical model of a nitrification/denitrification enhanced biological phosphorus-removal process was successfully used to illustrate the procedure on a full-scale plant.

The number of parameters to be calibrated was reduced thanks to an accurate sensitivity analysis, during which the influence on model response was evaluated by varying each model parameter within its variation range using the one at a time method. The model was subsequently calibrated by utilising the GLUE methodology in order to deal with any remaining the problem of model parameter ideantifiability. The model parameters were calibrated through a new step-wise procedure involving different subsets of model parameters corresponding to model outputs groups that were put together before. In the illustrative key study the iterative procedure has been applied for four model output groups using calibration hierarchy must be established on the basis of interdependency of state variables (first TSS group, second COD group, third N group and at the end the P group). At the end of the procedure, the values of the model parameters were evaluated and showed to provide a good fit between simulated and measured data.

A further development of the presented research will regard the uncertainty assessment of the model results. Such an aspect is crucial for the assessment of the model reliability and is a field that is still underdeveloped due to the fact that only a few studies have been performed until now.

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