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G. Mannina

G. Viviani

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Uncertainty of a biological nitrogen and phosphorus removal model

A. Cosenza, G. Mannina, G. Viviani

*Dipartimento di Ingegneria Idraulica ed Applicazioni Ambientali, Università di Palermo,
Viale delle Scienze, 90128 Palermo, ITALY. Corresponding Author (tel. +39 0916657756;
fax: +39 0916657749; E-mail: mannina@idra.unipa.it)*

Abstract: In the last few years, the use of mathematical models in wastewater treatment plant (WWTP) processes has become a common way to predict WWTP behaviour. However, mathematical models generally demand advanced input for their implementation that must be evaluated by an extensive data gathering campaign, which cannot always be carried out. This fact, together with the intrinsic complexity of the model structure, leads to model results that may be very uncertain. Quantification of the uncertainty is imperative. However, despite the importance of uncertainty quantification, only a few studies have been carried out in the wastewater treatment field, and those studies only included a few of the sources of model uncertainty. This paper presents an uncertainty assessment of a mathematical model simulating biological nitrogen and phosphorus removal. The uncertainty assessment was conducted according to the Generalised Likelihood Uncertainty Estimation (GLUE) methodology. The model was based on Activated-Sludge Models 1 (ASM) and 2 (ASM2). Different approaches can be used for uncertainty analysis. In the present study, the GLUE procedure was employed. The GLUE methodology requires a large number of Monte Carlo simulations in which a random sampling of individual parameters drawn from probability distributions is used to determine a set of parameter values. Using this approach, model reliability was evaluated based on its capacity to globally limit the uncertainty. The method was applied to a full-scale WWTP for which quantity-quality data were gathered.

Keywords: activated sludge models; calibration; nitrogen phosphorus removal; uncertainty analysis; wastewater modelling

1 INTRODUCTION

During the last decades, interest in mathematical modelling of wastewater treatment plant (WWTP) processes has increased. The mathematical models have contributed to increasing knowledge in this field. The activated-sludge models (ASMs) (Henze et al., 2000) proposed by the working group of the International Water Association (IWA) have been applied several times in order to best understand how to improve plant design, how to optimise the processes and which control strategies to prefer (Jeppsson et al., 2007; Salem et al., 2002; Flores et al., 2005). The application of WWTP models makes it possible to improve designs: an overall optimization of the involved processes increases efficiency and enables better compliance with increasingly stringent regulations (Belia et al., 2009). Nevertheless, modelling activated-sludge systems is not easy because biological systems, as well as each natural environmental system, are intrinsically complex and are subject to many natural variations. The activated-sludge process cannot be considered a well-characterised process, and some activated-sludge model parameters are uncertain (Flores et al., 2008). Consequently, the application of ASMs requires a great number of assumptions concerning influent wastewater composition and model parameters. Traditionally, WWTP

process simulators assume constant rather than variable model parameters and are thus not capable of taking into account the inherent randomness of these parameters (Flores et al., 2008). Such assumptions have a significant influence on the model predictions and could lead engineers to make erroneous decisions during their design or optimization of a project. Therefore, an accurate analysis and quantification of model uncertainty is imperative. The assessment and presentation of uncertainty are widely recognised as important parts of the analysis of complex water systems (Beck, 1987). They allow modellers to identify the sources of error in the modelling process and to learn how the errors spread to the model outputs.

During the last few years, scientific research in the wastewater modelling field has focused on uncertainty issues, and some publications have appeared in the literature (among others, Neumann and Gujer, 2008; Benedetti et al., 2008; Flores et al., 2008; Sin et al., 2009; Bixio et al., 2002). Different approaches have been proposed for the assessment of uncertainty. These studies have all demonstrated that taking uncertainty into account can affect the decision-making process for a design project or in the prediction of plant behaviour. For instance, Bixio et al. (2002) suggested a methodology for quantification of the uncertainty of a WWTP model using a Monte Carlo simulation. The methodology takes into account the input and parameter uncertainties in order to evaluate how the uncertainty can improve the likelihood of meeting effluent standards without requiring above-average capital investments. Bixio et al. (2002) demonstrated that considering uncertainty can even reduce the capital investment. However, few studies yet deal with uncertainty in wastewater quality modelling. Indeed, as pointed out by Sin et al. (2009), the field of uncertainty analysis of WWTP models is still in its infancy. This conclusion was also one of the main outcomes at the recent WWTPMod2008 workshop on uncertainty (Belia et al., 2010).

Manifold sources of uncertainty in the model predictions have been identified and, as suggested by the literature, can be classified as follows (Belia et al., 2009): 1) uncertainty in external influence factors (e.g., the measurement errors that affect the observed input data), which can have significant effects on model predictions; 2) uncertainty in the model structure, which is attributable to an inappropriate model that is too simple compared with the complexity of the real system that it tries to represent (e.g., inadequate selection of processes algorithms); 3) uncertainty in model parameter values (e.g., wrong estimation of parameter values); and 4) uncertainty in the numerical calculations used to solve the model algorithms (e.g., programming errors).

Bearing these considerations in mind, this study presents an uncertainty analysis of a mathematical model for the simulation of biological nitrogen and phosphorus removal processes. The uncertainty analysis is assessed by means of the Generalised Likelihood Uncertainty Estimation (GLUE) methodology (Beven and Binley, 1992). This methodology is one of the most widely used methods for investigating uncertainties in hydrology, and is now spreading into other research fields. The goal of the study was to test the suitability of such a methodology for WWTP modelling in order to provide an easy and useful tool for uncertainty assessment, a topic that is still only rarely addressed compared with other research fields.

2 MATERIALS AND METHODS

2.1 Uncertainty assessment

As outlined in the introduction, in the present study, the GLUE methodology was used for uncertainty quantification (Beven and Binley, 1992). The GLUE methodology is a non-formal Bayesian methodology that facilitates an easy assessment of uncertainty. On the other hand, in formal Bayesian methodology, a formal description of the likelihood function is always required. This is extensively discussed in the literature. For example, Mantovan and Todini (2006) reported incoherencies of the GLUE methodology with Bayesian inference. Beven et al. (2007) replied that formal Bayesian inference is a special case of GLUE when a formal likelihood description is used. Regardless of this discussion, Freni et al. (2009b) also demonstrated that both methods perform similarly when the GLUE methodology is based on the same assumptions as the Bayesian approach. To apply the GLUE methodology, the model was run using a uniform randomly sampled parameter sets.

By means of a likelihood measure, E, parameter sets can be classified; sets with poor likelihood weights with respect to a user-defined acceptability threshold (Tr) are discarded as “non-behavioural”. All parameter sets coming from the behavioural simulation runs are retained, and their likelihood weights are rescaled so that their cumulative total sum is equal to one. The likelihood measure E represents the ability of the model to fit real data. On the other hand, the acceptability threshold Tr represents a user-defined critical value indicating the minimum value of E that each modelling simulation should have in order to be representative of the model behaviour with respect to the analysis aim. Tr is usually set equal to zero.

In the present study, the following equation was employed as a likelihood measure (Freni et al., 2009a):

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

where θ_i represents the i^{th} set of model parameters (randomly generated), $\sigma^2_{M_j-O_j}$ is the variance of the residuals between model and observations of the j^{th} simulated model output and $\sigma^2_{O_j}$ is the variance of observations for the period under consideration.

Treating the distribution of likelihood values as a probabilistic weighting function for the predicted variables, it is possible to assess the uncertainty associated with the predictions (conditioned on the definition of the likelihood function) of the input data and model structure. A method of deriving predictive uncertainty bands from the behavioural simulations using the likelihood weights has been shown by Beven and Binley (1992). The uncertainty bands are calculated using the 5th and 95th percentiles of the predicted output likelihood weighted distribution. Wider bands mean higher uncertainty in the estimation of the modelling output and thus lower confidence in the model results.

The GLUE methodology can also be used to analyse the impact of each parameter on modelling outputs. Plotting the cumulative likelihood distributions for the set of behavioural simulations ($E \geq \text{Tr}$) and the set of unconditioned cumulative distributions, respectively, it is possible, by comparing the deviation between the two, to determine if the model output in question is sensitive to changes in the parameter values. If little difference between the two cumulative distribution functions (CDFs) is found, the parameter is considered insensitive with regard to the model output. Conversely, if a great difference is found, the parameter is considered to be sensitive. Applying the nonparametric Kolmogorov–Smirnov d-statistic (maximum distance between the two CDFs), a measure of sensitivity is introduced, i.e., $d = 1$ is the most sensitive and $d = 0$ is non-sensitive (Hornberger and Spear, 1981; Beven et al., 2008; Freni et al., 2009a). This sensitivity analysis is used to determine the relative importance of each parameter in the model structure. It is evident that the GLUE results can be affected by the definition of parameter variation ranges. This definition can influence the analysis because it defines the domain where the model uncertainty is evaluated. The selection of the parameter variation ranges can be accomplished by considering the physical meaning of the parameters, but this approach cannot be used for conceptual parameters that have a weak link to the physical system. In addition, this approach can produce variation intervals that are too wide, thereby leading to the problems described above.

2.2 The case study

The municipal activated-sludge WWTP under study was located in Sicily, Italy, and had an outflow to the Mediterranean Sea. The plant was designed for a design capacity of 40,000 inhabitant equivalents (IE). The influent of the WWTP, with average and maximum values of 400 m³/h and 600 m³/h respectively, consisted of domestic and non-industrial wastewater produced by a nearby refinery. After the pretreatment step (coarse grit removal, fine grit removal, filtration with a rotating panel, sand and grease removal), the influent was introduced into an equalisation tank with a volume of 1,700 m³ in which the wastewater was discontinuously aerated (3 h/d). The effluent of the equalisation tank flowed to the biological activated-sludge treatment area, which consisted of an activated-

sludge reactor designed according to a Bardenpho scheme and a secondary clarifier (with a volume of 2,885 m³) where the COD, N and P removal was accomplished. More specifically, the activated-sludge reactor was composed of three completely mixed compartments of different sizes. The first compartment operated as an anaerobic zone, the second as an anoxic zone and the third as an aerobic zone, with volumes (V) of 900, 1,140 and 5,800 m³, respectively. Returned activated sludge (RAS) from the bottom of the secondary clarifier and internal mixed-liquor recirculation (MLR) from the end of the aerobic zone were pumped to the anaerobic and anoxic zones, respectively. Aeration was supplied by 900 fine bubble diffusers positioned on the bottom of the aeration zone.

The influent flow rate (Q_{INF}) under normal operating conditions was approximately 400 m³/h; the MLR flow rate (Q_{MLR}) and the RAS recirculation (Q_{RAS}) were generally set to 3 and 1.5 Q_{INF} , respectively. The waste activated sludge (WAS) was simply dewatered by a belt-press filter.

2.3 Model description

The model adopted in this study was able to reproduce the nitrification-denitrification/enhanced biological phosphorus removal processes occurring in a full-scale WWTP characterised by a Bardenpho scheme. The model was built on ASM concepts; in particular, the complexity of the ASM2 model was reduced by omitting processes that did not play a significant role and components that did not have a dominant effect upon the kinetics of the processes (Henze et al., 2000).

The model describes the following variables: ammonia (NH₄-N), nitrate (NO₃-N), total soluble phosphate (P_{Stot}), total COD (COD_{TOT}), particulate material (X_{TSS}) and total soluble COD (CODsol). The model did not take into account the solid-liquid separation in the secondary clarifier. Accordingly, the concentrations of the soluble components in the returned activated sludge were assumed to be equal to the effluent concentrations from the aerobic reactor.

The model was calibrated using the design and operational data of a real WWTP and chemical-physical data collected during an ad hoc field data-gathering campaign carried out during the period from 01 March 2006 to 12 April 2006 in the same plant. In particular, total suspended solids (TSS), total and soluble COD (COD_{TOT} and CODsol), orthophosphate (P-PO₄), total soluble phosphorus (P_{Stot}), NH₄-N, NO₃-N, dissolved oxygen, temperature, pH and air flow rate were monitored in different sections of the plant. The samples were withdrawn from the effluent of the anaerobic, the anoxic and the aerobic tank (sections 1, 2, 3 and 4) and from the RAS channel (section 5). For further details on the model calibration and the gathering campaign, the reader is referred to Cosenza et al. (2008). In the following section, the model parameters are reported according to the ASM notation (Henze et al., 2000).

3 RESULTS AND DISCUSSION

3.1 Methodology application

In order to reduce the number of parameters, a preliminary local sensitivity analysis was carried out before the model uncertainty analysis (details are discussed in Cosenza et al., 2008). Following this preliminary model parameter analysis, the number of sensitive model parameters was 29. These 29 parameters were allowed to vary during Monte Carlo simulations, while 12 were held constant. In this way, the impact of such a reduction on the reported uncertainty outputs was quantified. In particular, for each sensitive model parameter, a uniform distribution was considered, and the broadest variation range—drawn from the relevant literature (Henze et al., 2000; Weijer and Vanrolleghem, 1997; Petro Alfonso and Maria da Conceição Cunha, 2002; Iacopozzi et al., 2007; Sin et al., 2009; Flores Alsina et al., 2008) was selected in order to explore the overall confidence region. It is important to emphasise that the parameter variation ranges considered during the uncertainty analysis were equal to the ranges that were used during the sensitivity analysis and the model calibration steps.

To apply the GLUE methodology, the defined parameter space for each sensitive parameter was randomly sampled with the Monte Carlo technique. In particular, 1 000 behavioural simulations (approximately 440 000 simulations) were run on randomly sampled parameter sets. This number of simulations has been found to be consistent with the objectives of the present study. Specifically, a sample dimension was selected, verifying that the uncertainty analysis was not affected by any bias linked to the number of Monte Carlo simulations. This study was carried out by analyzing the statistics and variations and changing the sample dimensions between 100 and 1 000 behavioural simulations (Bertrand-Krajewski et al., 2002). For each parameter set, the uncertainty was spread by running the model simulation, and a likelihood measure was computed for each model variable in order to evaluate the ability of the model to fit real data. At the end of this step, we had 1 000 likelihoods and 1 000 respective dynamic profiles for each model variable. According to Equation (1), the likelihood measure varies between 0 and 1, with a likelihood of 1 corresponding to a perfect fit. For large errors, the likelihood becomes 0 as the ratio goes to infinity. In order to evaluate how the parametric uncertainty was spread in the model output variables (owing to the sensitive model parameters), the nonparametric Kolmogorov–Smirnov d-statistic (d K-S) was assessed (Smirnov, 1948).

As outlined in the previous paragraph, in order to evaluate how the uncertainty of the sensitive model parameters was spread in each model output variable and in the global model response, the d K-S was calculated for each model output. Therefore, the cumulative likelihood distribution of the 1 000 likelihoods was computed and compared with the cumulative density function of the uniform distribution (CDFu) for each model output variable and sensitive parameter. Regarding the global model response, the cumulative likelihood of the model (E_{MOD}) was computed by considering the weighted sum of the efficiencies of the n model outputs for each model run and then comparing it with the CDFu. In particular, the d K-S represents the maximum absolute value of the distance between the cumulative likelihood distributions and the CDFu, and it is generally used as a measure of parameter sensitivity. Values of d close to 1 indicate a very high sensitivity, whereas a d -value close to 0 indicates low sensitivity (Thorndahl et al., 2008).

3.2 Model parameter uncertainty results and model uncertainty bands

In Figure 1, the d K-S values of some model variables are shown. The results show a different response in terms of the spread level of parametric uncertainty, depending on the model output variable considered. The COD showed the highest values of d K-S for the different parameters (Figure 1a, b and c). Indeed, the d K-S of the rate constant for the lysis of heterotrophic biomass (b_H) had the maximum absolute value, equal to 0.9 for $COD_{TOT,2}$. The $COD_{sol,3}$ (Fig. 1c) is the model variable for which the parametric uncertainty was more evident. In this case, 42% of the model parameters had a d K-S value higher than 0.2.

In general, μ_{AUT} and K_{NH} showed the highest sensitivity. The calibrated value of the nitrifying growth rate, $\mu_{AUT}=1.08\text{ d}^{-1}$, was in agreement 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 was 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 because of a lower diffusion limitation related to the higher turbulence and smaller flocs in comparison with full-scale plants (Henze et al., 2000). Regarding the calibrated value of $Y_{PO_4}=0.11\text{ gP/gCOD}$, this value was not close to the default value (Henze et al., 2000). Similar results were obtained by Machado et al. (2009), which the authors explained by the presence of glycogen-accumulating organisms (GAOs) not considered by ASM2. Indeed, under anaerobic conditions, PAOs and GAOs can alternatively store fermentation products, SA. While PAOs utilise the energy obtained from the hydrolysis of polyphosphate and from glycogen degradation, GAOs use only the energy from glycogen degradation. This fact justifies the decreases of the Y_{PO_4} value with the increase in the GAO population (Ferrer et al., 2004). Nevertheless, despite agreement with the aforementioned parameter values, it has to be stressed that with respect to their level of sensitivity, the parameter significance levels may differ from one plant to another because of changes in the process scheme and available data (among others, Ruano et al., 2007).

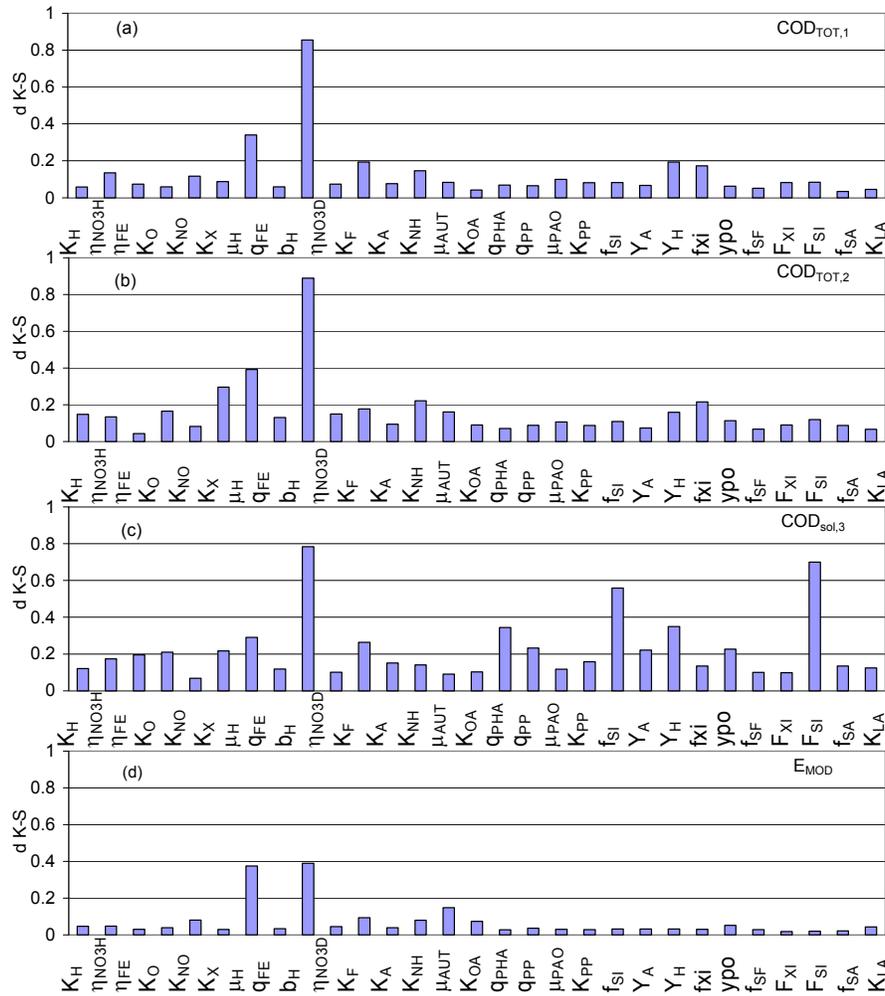


Figure 1. d K-S values for COD_{TOT,1} (a), COD_{TOT,2} (b), COD_{sol,3} (c) and for the total model response computed considering E_{MOD} (d)

In terms of global model response (Figure 1d), it is worthwhile to observe that the parametric uncertainty is flatter because it is computed on the weighted sum of the efficiencies of the *n* model outputs. However, the global model response, like the single model variable, was still the most sensitive model output and was sensitive to the parameters b_H , μ_H and μ_{AUT} . In Figure 2, the cumulative likelihood of b_H , μ_H and μ_{AUT} are reported. The results show that in terms of the global model response, despite the higher compensation effect among the parameters, the model outputs were strongly influenced by such parameters.

It is worth mentioning that quantitative prioritization of the model parameter was really useful. The finding that almost half the parameters had little effect on the performance is an implicit rebuke to the architects of these models, implying the models are too complex.

The 1 000 likelihoods and the 1 000 respective dynamic profiles for each model variable were used to compute the cumulative likelihood of each variable at each simulation time. According to the GLUE procedure, the 5th and 95th percentiles of the cumulative likelihood distributions for each simulation time step and for each model output were then used for calculating uncertainty bands. In Figure 3, the uncertainty bands of some model outputs considered during the uncertainty analysis are reported.

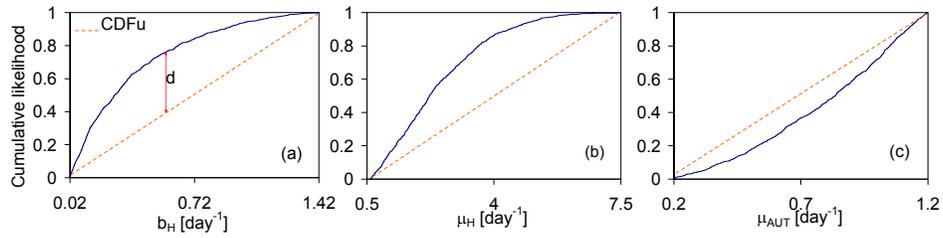


Figure 2. Cumulative likelihood of the model for b_H (a), μ_H (b) and μ_{AUT} (c)

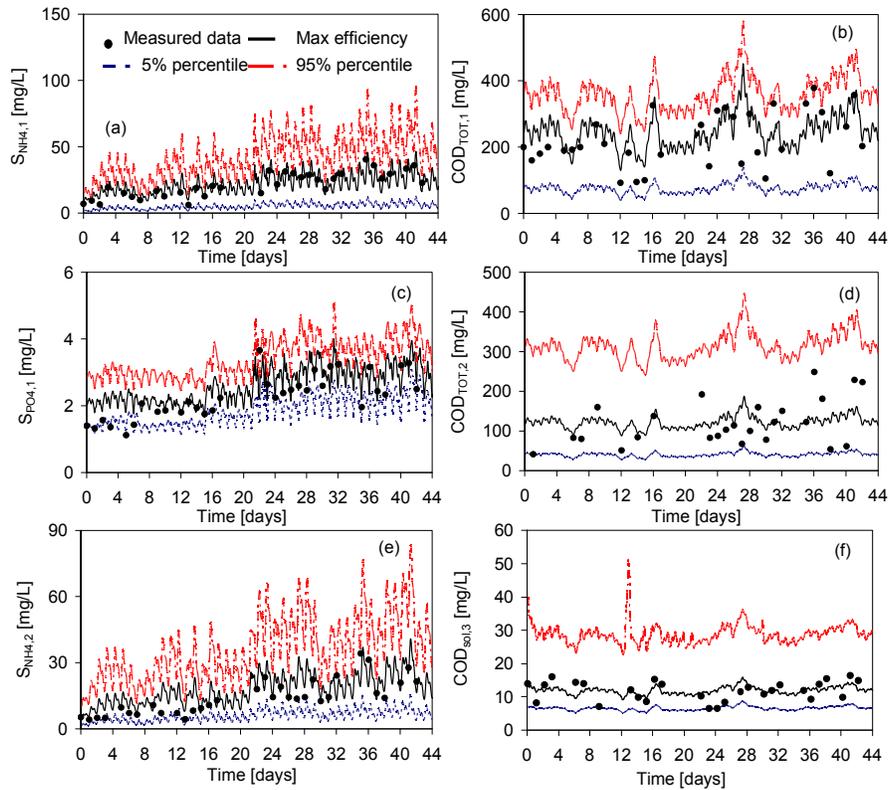


Figure 3. 5th percentile and 95th percentile.

Analyzing the graphs reported in Figure 3, it is evident that the results of the uncertainty analysis performed in this study show different response with respect to the model output considered. Indeed, the uncertainty band widths for COD (Fig. 3b, d and f) are generally wider than the nitrogen components (Fig. 3a and e). Such a result is likely due to the different amplitude of the model parameter ranges employed. Indeed, as aforementioned, in this study in order to explore the parametric space without considering different classes of uncertainty, the broadest parameter variation range drawn from literature was employed. Such a fact affects the uncertainty band widths especially for those model outputs influenced by several sensitive parameters. Indeed, the uncertainty of $S_{PO4,1}$ (Fig. 3c) is smaller than the others because among the parameters for which the uncertainty has been studied (sensitive parameters), only three are directly connected to the phosphorus removal processes. Such results are consistent with previous studies carried out on ASMs (Sin et al., 2009). Indeed, due to the fact that ASMs are overparameterized, such models provide different responses in terms of uncertainty band widths. The uncertainty bands of X_{TSS} model outputs have not been reported because it has almost no uncertainty according to Sin et al., (2009). Indeed, in the model under study, the settling parameters are not subject to uncertainty. It is important to point out that the model uncertainty response is certainly influenced by the subjective hypotheses that have been made applying the GLUE

methodology such as the choice of the efficiency-measure. Indeed the method has many limitations as to make the results almost useless. So it would be interesting to study how the ASM model uncertainty changes changing the efficiency measure in the GLUE methodology as well addressed by Freni et al., (2009a) in the field of urban-drainage modelling. However, despite these drawbacks, the results demonstrate, according to other authors (Flores et al., 2008; Benedetti et al., 2008; Melcer et al., 2003), that when uncertainty in the ASM model inputs is considered, the results of a well structured and calibrated model might be questioned; so an accurate uncertainty analysis is important depending on the objective of the study. As a matter of the fact, although the model calibration provided acceptable results giving efficiency ranging between 0.42 and 0.75 (Cosenza et al., 2008), in terms of uncertainty a significant proportion of the measured data fall near or on the extremes of the uncertainty bands. Such a fact confirms even more the importance in the quantification of the model uncertainty. Indeed, the quantification of the uncertainty pointed out that the model structure has to be improved in order to provide a better reproduction of the simulated phenomena. The GLUE is confirmed to be a good tool for uncertainty assessment also for WWTP modelling. Such a methodology, although can be affected by subjective hypothesis, it is a valuable and easy to use tool for uncertainty. With regards to the computational time needed for the implementation, in particular with regards to the Monte Carlo simulations, the Latin hypercube sampling could be an optimum choice especially for computational demand models.

4 CONCLUSIONS

The uncertainty analysis of a mathematical model simulating biological nitrogen and phosphorus removal processes was performed using the GLUE methodology (Beven and Binley, 1992). In order to evaluate how the model parameter uncertainty can influence the response of the model, a uniform distribution of the broadest model parameter space was considered, and several Monte Carlo simulations were conducted in order to investigate this space. The output of each simulation was compared with measured data and a measure of the likelihood was created. The 5th and 95th percentiles of the cumulative likelihood distributions were then used for calculating uncertainty bands for each model output variable. From the analyses, the following conclusions can be drawn:

- The uncertainty analysis performed in this study gave different responses for several of the model outputs considered. The results were strongly dependent on the width of the parameter range and on the parameters selected during the sensitivity analysis. In addition, the correlation between the sensitive and non-sensitive parameters was ignored.
- The uncertainty assessment showed that despite the fact that the best-fit model response between the measured and simulated values was acceptable, the model approach needs to be improved in order to correctly simulate the system. Indeed, the model showed a wide band of uncertainty, with a significant proportion of the measured data results (far more than 5%) falling near or on the extremes of the uncertainty bands.
- The study demonstrated the suitability of the GLUE methodology for wastewater treatment plant modelling, although the methodology is based on some subjective choices that can affect the results. Nevertheless, as a first screening study (i.e., studies for evaluating the magnitude of the polluting emission, the classification of pollutant impacts, etc.) it could be a feasible and good solution.

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