18th World IMACS / MODSIM Congress, Cairns, Australia 13-17 July 2009
http://mssanz.org.au/modsim09

Parameter estimation and sensitivity analysis of a nitrogen and phosphorus biological removal model

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Abstract: Stringent water quality standards imposed by the Water Framework Directive 2000/60 have motivated world-wide needs to protect surface water bodies against eutrophication.

In the last years research has moved on different fronts: (1) optimization of nutrients removal processes in many full scale Wastewater Treatment Plants (WWTPs); (2) development of new technologies to achieve more stringent limits for total nitrogen and total phosphorus; (3) setting up modeling tools useful to predict, control and assess nitrogen and phosphorus biological removal processes. In this context, the processes modeling for different system configurations is undoubtedly a common key point of the different fronts. Indeed, thanks to model approach is possible to assess the response of a system in different operating conditions and with different technologies. Nevertheless, with respect to modeling of biological phosphorus removal that is notoriously one of the more difficult processes to control at full scale Waste Water Treatment Plants (WWTPs) (Ingildsen et al, 2006), practical use is still limiting (Meijer et al., 2002). In this context, an integration of the procedure for the parameter estimation, based on Monte Carlo simulations is presented. The procedure has been applied to a model for the simulation of nitrogen and phosphorus biological removal processes (according to the Bardenpho scheme). The model was calibrated and validated to a Sicilian (Italy) full scale WWTP. The main purpose of this work was to define a clear and effective approach both on identifiability of sensible model parameters and on parameter estimation.

The model calibration has been carried out considering an ad-hoc field data gathering campaign to a full scale WWTP. The model calibration has been performed considering a preliminary sensitivity analysis of the main model parameters in order to identify the most sensitive parameters to be calibrated as well as the best goal seek to be optimized. At this aim, several Monte Carlo runs have been carried out considering both simultaneously and single model parameter variation assuming a uniform distribution. During the calibration of the sensitive model parameters, the reduction of the ranges of parameter values after each Monte Carlo simulation (one simulation comprising 10,000 runs each with a different randomly generated parameter set) has been executed. The objective of reducing the range has been to approximate the region of best values of the parameters, and also to increase the likelihood of achieving a better performance of the model on the next Monte Carlo simulation (von Sperling, 1993). In the first simulation the parameter sets which provided efficiency values, for all state variables, greater than or equal to zero have been retained and the respectively simulations have been considered behavioral. All other sets have been rejected. The narrowing of the parameter range at each simulation has been performed thanks to the visual inspection of the relative frequency histogram of the parameter value that enables us the identification of the range where the frequency of the behavioral simulations is more dominant. The procedure has been repeated until the performance of the model has been judged satisfactory. In particular, the procedure gives us a good result at the 2nd run in which the sum of the variable efficiencies results maximum and the error of each variable is acceptable. Simulation results showed a good adaptation with experimental data demonstrating that the calibrated model was able to describe the behavioral of the WWTP in a reliable way.

Keywords: *Monte Carlo simulation; sensitivity analysis; calibration; parameter estimation*

1. INTRODUCTION

Stringent water quality standards imposed by the Water Framework Directive 2000/60 have motivated world-wide the needs to protect surface water bodies against eutrophication.

In the last years the research has moved on different fronts: (1) optimization of nutrients removal processes in many full scale Waste Water Treatment Plants (WWTPs); (2) development of new technologies to achieve more stringent limits for total nitrogen and total phosphorus; (3) setting up modeling tools useful to predict, control and assess nitrogen and phosphorus biological removal processes. In this context, the processes modeling for different system configurations is undoubtedly a common key point of the different fronts. Indeed, thanks to model approach it is possible to assess the response of a system in different operating conditions and with different technologies. The integration of knowledge in the form of mathematical models is useful for various reasons: (i) such models make possible testing of 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 and Vanrolleghem, 2001).

Nowadays, modeling of the pollutants (usually COD, N and P) removal processes from an activated sludge system using activated sludge models (ASMs) is widely accepted (Henze et al., 2000). Nevertheless, with respect to modeling of biological phosphorus removal that is notoriously one of the most difficult processes to control at full scale WWTPs (Ingildsen et al, 2006), its practical use is still limited (Meijer et al., 2002). This is partly due to the complexity of the process in carrying out data gathering campaign, but also to a limited practice. Among all the applications of ASM models present in the literature and concerning both pilot plants and full scale ones only few are effectively calibrated to real WWTP (Peterson et al., 2002 and Makinia et al., 2006). All these applications, even though highlight both advantages and difficulties encountered, have showed how plodding is the ASMs employment. Numerous applications of ASMs have been demonstrated, for example, that the ASMs parameters are not universal (Henze et al., 2000). Calibration of ASMs is strictly required prior to application of dynamic models for a WWTP. Identification and estimation of parameters are major issues in the modeling of activated sludge systems. The high number of parameters of the ASMs makes it difficult to identify which parameters for calibration. Moreover, the non-linear model algorithms, the large number of state variables involved and the usual data scarcity contribute to the complexity of the problem.

In addition, it is striking to observe that nowadays a standard procedure for calibration of ASMs does not exist. In the last years, different systematic calibration protocols have been proposed: the WERF protocol (Melcer et al., 2003), the STOWA protocol (Hulsbeek et al., 2002), HSG guidelines (Langergraber et al., 2003) and the BIOMATH calibration protocol (Vanrolleghem et al., 2003) whose objective is to aid modelers during calibration study. These calibration protocols have attempted to tackle the rather complex calibration issue of ASMs, but still remains to be the weakest link in the overall modeling of activated sludge systems (Sin et al., 2005).

In this context, an integration of the procedure for the parameter estimation, based on Monte Carlo simulations is presented. The procedure has been applied to a model for the simulation of nitrogen and phosphorus biological removal processes (according to the Bardenpho scheme). The model was calibrated and validated to a Sicilian (Italy) full scale WWTP. The main purpose of this work was to define a clear and effective approach both on identifiability of sensitive parameters and their estimation.

2. MATERIAL AND METHODS

2.1. Model Structure

In order to simulate the nitrification-denitrification and enhanced biological phosphorus removal (NDEBPR) processes occurring in a full scale WWTP characterized by a Bardenpho scheme, a model built on the ASM concept has been used (Henze et al., 2000). In the model the complexity of ASM2d has been reduced by omitting processes that do not play significant roles and components which do not have a dominant effect upon the kinetics of the processes. In order to improve the model performance, some of the ASM1 processes and components have been considered. In particular, regarding the processes involving nitrogen, the ammonification process according to ASM1 has been employed in order to describe the release of ammonium (S_{NH4}) from soluble biodegradable organic nitrogen (S_{ND}). According to such employed assumption, the fermentable readily biodegradable organic substrate (S_F) do not contain a constant fraction

of nitrogen and phosphorus. Further, in analogy to ASM1, the hydrolysis of particulate biodegradable organic nitrogen (X_{ND}) has been included as a separate process. Then a constant fraction of nitrogen and phosphorus in the slowly biodegradable substrates (X_S) has not been considered. The model defines 17 variables and 20 processes and has a total of 45 parameters. The model has been used to simulate the dynamic conditions in a NDEBPR scheme modeling the following variables: ammonia ($N\text{-}NH_4$), nitrate ($N\text{-}NO_3$), total soluble phosphate (P_{Stot}), total COD (COD_{tot}) and total soluble COD (COD_{fil}). Definitions of all model state variables, biological processes, stoichiometry and kinetics are available elsewhere Cosenza et al., 2008; Henze et al., 2000.

2.2. Case Study

The model calibration has been carried out considering an ad-hoc field data gathering campaign to a Sicilian (Italy) municipal full scale WWTP (Cosenza et al., 2008). The WWTP secondary treatment processes consists of an activated sludge reactor, according to a Bardenpho scheme, and secondary clarifiers as shown in Figure 1. Returned activated sludge (RAS) from the bottom of the secondary clarifier and internal mixed liquor recirculation (MLR) from the end of aerobic zone are respectively pumped to anaerobic zone and anoxic one. Aeration is supplied by 900 fine bubbles diffusers positioned on the bottom of aeration zone. Further, regarding the influent flow rate (Q_{inf}), under normal operating conditions, it is equal to approximately 400 m^3/h. On the other hand, the mixed liquor recirculation flow rate (Q_{MLR}) and the returned activated sludge recirculation (Q_{RAS}) are normally set, respectively, to 3 and 1.5 Q_{inf}. An extensive ad-hoc gathering campaign has been carried out during the period from 01 March 2006 to 12 April 2006 During the field campaign Total Suspended Solids (TSS), referring to total COD (COD_{tot}), soluble flocculated COD (COD_{fil}), Ortophosfate ($P\text{-}PO_4$), total soluble Phosforus (P_{Stot}), $N\text{-}NH_4$, $N\text{-}NO_3$, dissolved oxygen, temperature, pH and air flow rate were monitored in different sections of the plant (Figure 1). The samples of wastewater were withdrawn from the effluent of each zone (sections 1-4) and from RAS channel (section 5) and analyzed for the components showed in Figure 1 according to analytic methods proposed by IRSA. The samples were withdrawn according to the hydraulic retention time. To accurately characterize the wastewater influent, a specific ad-hoc sampling scheme was carried out for such a purpose. During this process, samples were withdrawn only from influent channel every 2 h between 8:00 am (19/06/2006) and 8:00 am (20/06/2006). The data was used to obtain daily patterns of WWTP influent pollutants employing Fourier series analysis.

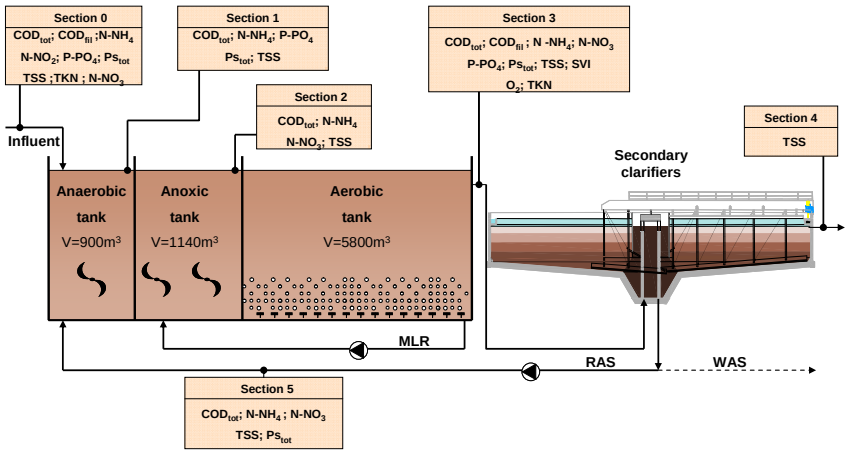

Figure 1. Flow sheet of WWTP with locations of sampling points.

2.3. Procedure for the Simultaneous Parameter Estimation and Sensitivity Analysis

In Figure 2 a flow chart of the step-wise procedure adopted for simultaneous parameter estimation and sensitivity analysis using Monte Carlo simulation, is showed. The procedure is divided into two blocks: preliminary steps and iterative steps.

The preliminary steps: The preliminary steps are divided into five sub-steps each strictly connected to the other. The first step (1. of Figure 2) is the definition of the model representative outputs. To accomplish such an object, an *a priori* assumption on parameter values has to be made. In particular, default values drawn from modeller's experience or relevant literature have to be decided. Thereafter, these values have to be adjusted through a trial and error calibration obtaining a first set of the model parameters. During this step, chose the model outputs on the basis of research goal as well as model responses. Thereafter, define the variation ranges of the model parameters (2. of Figure 2). The variation range for each parameter should be the broadest range drawn from relevant literature. Following the definition of the variation range of the

model parameters, chose a parameter distribution for the Monte Carlo simulations of the subsequent step (i. of Figure 2). More specifically, a pre-selection of the most influential parameters is recommended in order to limit the model parameters and identify the most sensitive ones to be calibrated. To accomplish such a step, a sensitivity coefficient is required ($s_{i,j}$) according to the procedure proposed by Weijer and Vanrolleghem (1997). In particular, consider the variation of each model parameter at time by running several Monte Carlo simulations. From each Monte Carlo analysis calculate a sensitivity coefficient according to the following equations:

$$s_{i,j} = \left| \frac{\left(E_{max,i} - E_{min,i} \right) / E_i}{\left(K_{max,j} - K_{min,j} \right) / K_j} \right| \quad (1)$$

where *i* and *j*, respectively, represent the selected model outputs and the model parameter, $K_{max,j}$, $K_{min,j}$ and $K_{,j}$ are, respectively, the maximum, minimum and average values of the jth parameter, $E_{max,i}$, $E_{min,i}$ and $E_{,i}$ represent the maximum, minimum and average values of the efficiency. This latter is calculated according to Nash and Sutcliffe (1970). After the evaluation of the sensitivity coefficients for each model parameters and for each model outputs, define the first set of the most sensitive parameters by means of the procedure suggested by Weijer and Vanrolleghem (1997). More specifically, scale the sensitivity coefficients for each model output by maximal sensitivity coefficient for that output and chose the sensitive parameters as the ones which show a scaled mean output sensitivity larger than 0.2 in at least one of the model output. As aforementioned, at the end of this first block (preliminary step), the first set of the most sensitive parameters along with the variation range are established.

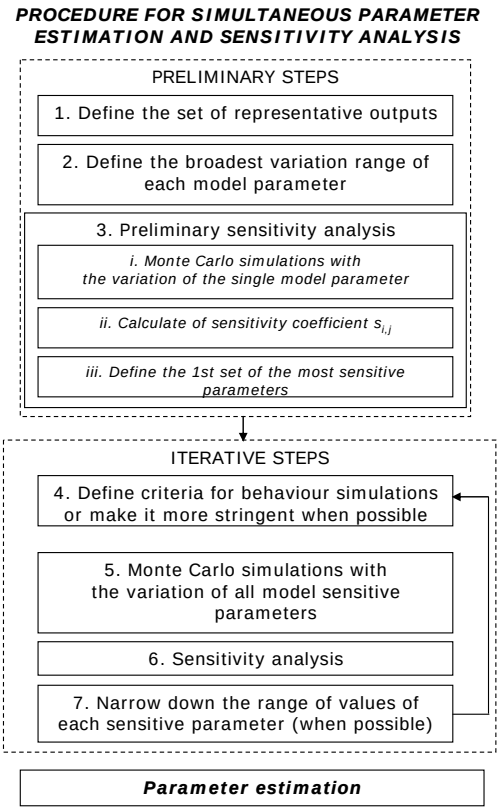

Figure 2. Flow chart of the proposed procedure for parameter estimation.

Iterative steps: This second block is made up of four steps that are repeated until the best model outputs are obtained. More specifically, the simultaneous sensitivity analysis and parameter estimation begins with the definition of the criteria for defining and assessing the behavioral simulations (4 of Figure 2). In the first run the parameter sets which provided efficiency values, for all state variables, greater than or equal to a user defined threshold (Tr) are retained. These simulations, i.e. simulations characterized by an efficiency greater to a defined Tr, are considered behavioural (BS) and are retained for the following steps, all the others are rejected and considered non behavioural (NBS). In the next step (5 of Figure 2) run a large number of Monte Carlo simulations according to the Generalised Likelihood Uncertainty Estimation (GLUE) methodology (Beven and Binley, 1992). For each Monte Carlo run vary each model parameter simultaneously in the variation range and according to a parameter distribution defined in the previous steps. Actually, the variation ranges of the model parameters is equal to the preliminary steps block ones (Figure 2) only for the first run. Indeed, for the other runs the ranges is narrowed as explained in the following. According to the established criteria, in the step (5) all the BSs are retained and the remained simulations are considered as NBS. As a result of this step, a new model output is obtained as well as a new set of model parameters. Such a new model output should be characterized by a model efficiency higher respect to the preliminary steps one. Starting from the new set of model parameters gained from the 5 step, consider a new sensitivity analysis in order to reduce the model parameters as well as redefine the model parameter ranges. More specifically, consider N Monte Carlo runs changing one parameter at time and calculate the sensitivity coefficients according to the equation (1). It is striking to observe that in the first run of the iterative steps block, the sensitivity analysis gives the same result of the preliminary sensitivity analysis. After assessing the sensitivity coefficients, calculate the parameter frequencies in order to narrow the parameters variation ranges (7 of Figure 2). The objective of reducing the range has been to approximate the region of best values

Table 3. Tr, No. *BS*., upper and lower bounds of the sensitive parameter subset for each run, (the colored space indicates the insensitive parameter).

Run	Tr	No.*B.S*	Parameter→ / Range ↓	k_h [h^{-1}]	k_O [gO2/m^3]	k_{NO} [gN/m^3]	μ_H [h^{-1}]	η_{NO3} [-]	k_F [gCOD/m^3]	k_{NH4} [gN/m^3]	μ_{AUT} [h^{-1}]	b_{AUT} [h^{-1}]	μ_{PAO} [h^{-1}]	f_{SI} [gCOD/gCOD]	Y_H [gCOD/gCOD]	f_{SF} [gCOD/gCOD]	F_{XI} [gCOD/gCOD]	F_{SI} [gCOD/gCOD]
1	*Ei* >0	25	Upper	0.17	1	0.6	0.3	0.85	12	2	0.05	0.34	0.042	0.2	0.75	0.25	0.15	0.07
			Lower	0.021	0.1	0.35	0.025	0.4	4	0.14	0.0083	0.0017	0.0292	0	0.58	0.15	0.1	0.02
2	*Ei* >0.01	338	Upper	0.16	0.4	0.6	0.135				0.05	0.2723	0.0408	0.0667	0.75		0.15	
			Lower	0.03	0.16	0.45	0.025				0.0139	0.0017	0.0292	0	0.58		0.103	
3	*Ei* >0.01	5542	Upper	0.117	0.256	0.6	0.0617				0.0428	0.2182	0.037	0.0267	0.6367		0.1407	
			Lower	0.0309	0.16	0.5	0.025				0.0163	0.0017	0.0292	0	0.58		0.103	
4	*Ei* >0.03	2962	Upper			0.6	0.0544				0.0393	0.1893	0.037	0.00168	0.6367		0.1307	
			Lower			0.533	0.029				0.0163	0.0594	0.0163	0	0.58		0.103	

of the parameters, and also to increase the likelihood of achieving a better performance of the model on the next Monte Carlo simulation (von Sperling, 1993). More specifically, the range of parameters narrowing at each run is performed thanks to the visual inspection of the frequency histogram of the parameter values NBS. An unambiguous narrow range parameter criterion has been defined. More specifically, for each simulation, consider as range limits the first and the last value for which the relative frequency value is greater than or equal to the medium relative frequency.

The block of the iterative steps is repeated several runs until the performance of the model is judged satisfactory; each run is characterized by different ranges of parameter values, sensitive parameters involved and criteria for the definition of behavioural simulations. It is important to underline that from one run to another the criteria for the definition of behavioural simulations (4 of Figure 2) becomes more restrictive if the number of the sensitive parameters decreases due to the narrowing of the variation ranges. Chose as set of model parameters the one that provides the maximum value (EM) of the sum of the efficiencies for the model outputs.

3. RESULTS

3.1 Evolution of the Procedure

As described above, the parameters estimation as well as the sensitivity analysis have been performed following the specific procedure showed on Figure 2. The procedure consists of a series of steps divided in two blocks: preliminary and iterative steps.

Preliminary steps: First, a parameter set has been obtained by considering a trial and error calibration. The set obtained from the try and error calibration has been used thereafter for the following iterative steps. More specifically, the default values (obtained from literature) have been opportunely modified through visual comparison of the results to the available data. Among the model outputs, only a subset has been chosen as representative: S_{NH4} in the section 1 and 2, COD_{TOT} in the section 1 and S_{NO3} in the section 3. The chosen outputs showed the excellent fitting between simulated and measured data. From now on, the simultaneous parameter estimation and sensitivity analysis procedure have been performed referring only to such outputs. In order to perform the *preliminary sensitivity analysis*, for each parameter, a uniform distribution was chosen since the statistical distribution of these parameters in activated sludge models is not available. The upper and lower bounds of the uniform distributions of the model parameters were defined according to the broadest range found in relevant literature (Henze et al., 2000; Weijer and Vanrolleghem, 1997). In the *preliminary sensitivity analysis*, 1,500 Monte Carlo simulations for each parameter have been carried out considering the variation of a single model parameter at a time. Consequently the Nash and Sutcliffe index has been calculated using equation (1). The 1st sensitive parameter subset for dynamic calibration has been selected following the above mentioned procedure where the scaled sensitivity coefficient ($s_{i,j}$) plays the discriminating role for the choice. Due to the preliminary sensitivity analysis, the number of model parameters to be calibrated was considerably reduced (from 45 to 15). During the dynamic calibration only the most sensitive parameters have been analyzed. The remaining parameters have not been changed and their values have been set to the literature ones.

Iterative steps: As explained above, this phase involves the iterative developing of several steps. In the present work the iterative steps have been repeated four times, each of them characterized by: different range of

parameter values, sensitive parameters involved and criteria for the definition of behavioural simulation.

Table 3 summarizes all relevant information of each run. It is important to note that the threshold for the assessment of the BS becomes more and more stringent if the number of sensitive parameter decreases. This criteria have to be simultaneously fulfilled for the four variables. The number of behavioural simulations (No. *BS*.) depends both on the variation range of parameters and on the Tr. More precisely, although the narrowing of the parameter variation range involves an increase of the No. *B.S.*, as an effect of the selection of the region of best values for parameters, on the other hand the more stringent Tr arranges a decrease of the No. *B.S.* as shown in Table 3 between the third and the fourth run.

The narrowing of the range of parameters at each run has been performed thanks to the visual inspection of the frequency histogram of the parameter values non behavioural. Firstly, the variation range of each parameter has been divided into 15 variation classes, each one with the same size. Then, for each class, the relative frequencies of occurrence of the behavioural simulations have been identified. For each simulation run, the range limits have been chosen considering the first and the last value for which the relative frequency value is greater than or equal to the medium relative frequency one. In the example given in Figure 3, it can be seen that the values of kh greater than 0.12 have less chance of producing behavioural simulations and therefore can be excluded from the next run. For each run the set of the model parameters, which provides the maximum value of the sum of the efficiencies for the four variables, was chosen for the next simulation run. More specifically, in the new run the values of the insensitive parameters are maintained equal to the set values of the maximum efficiency.

3.2 Statistical Criteria for Evaluating Model Fit

The statistical evaluation of model performance for each run focuses on the mean absolute error (MAE) and root mean squared error (RMSE). The MAE is simply the average of the absolute errors between the simulated and observed values. Hence, if the MAE is zero that says the mathematical model is perfectly able to reproduce the physical one and the value increases proportionally with the discrepancies. The RMSE is useful since it is thought of as a typical magnitude for model errors. It has been spotlighted that the maximum value (E_M) of the sum of the efficiencies for the four variables increased up to the 2nd run, see Figure 4 [a]. Through the analysis of MAE and RMSE (Figure 4 [b] and [c]) values, it was been possible to evaluate the model error for each variable, confirming that the global minimum error occurs in the 2nd run. The procedure gives us good results in terms of behavioural simulations and global model efficiencies (computed as sum of the efficiencies for the four variables) until 2nd run. It is evident that the range narrowing and the iterative procedure could be stopped to the 2nd run. However, the set of model parameters which provides the maximum value (E_M) of the sum of the efficiencies for the four variables was chosen for calibration (estimated parameter set), this set corresponds to the 2nd run where the values of RMSE and MAE for each variable are globally acceptable. Inherently the

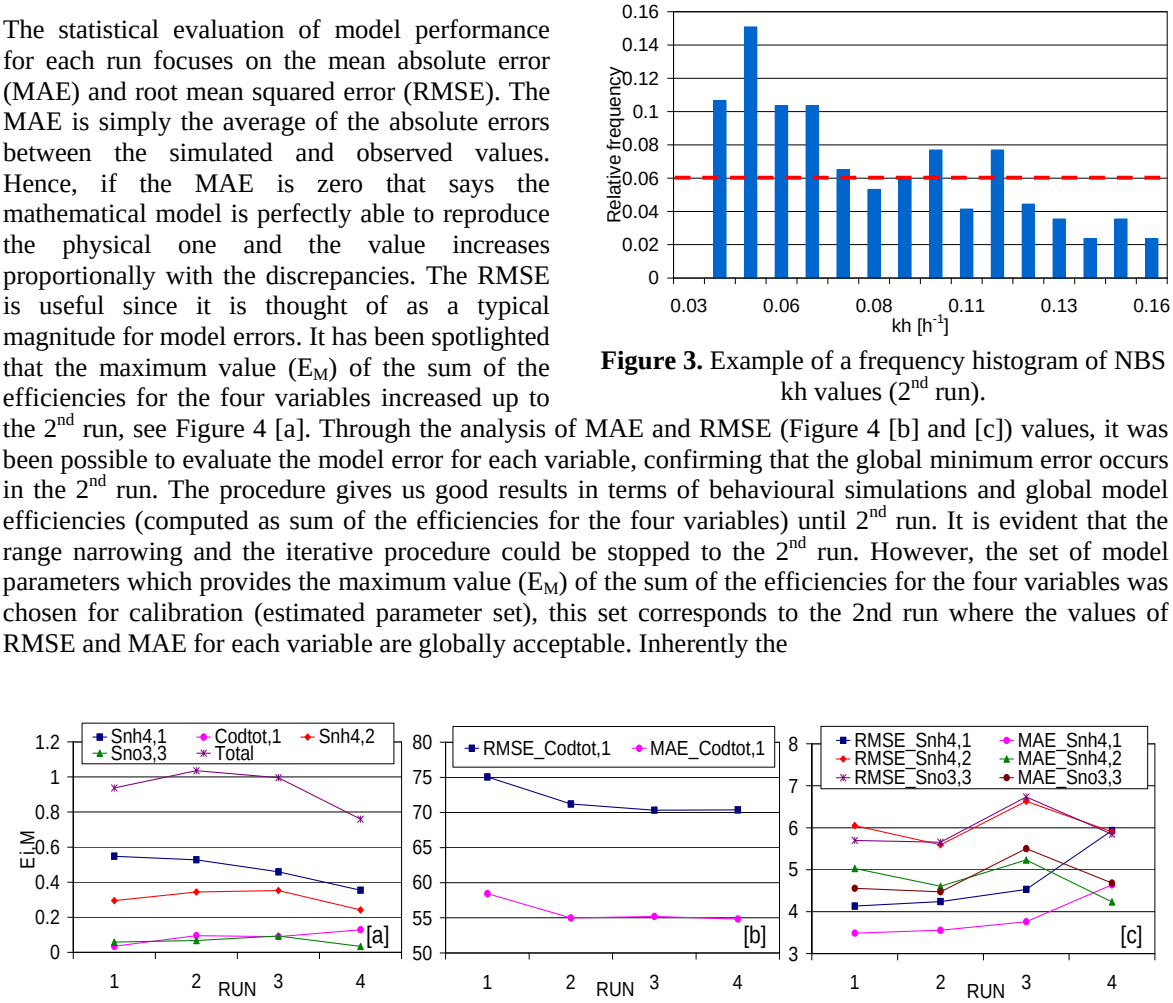

Figure 3. Example of a frequency histogram of NBS kh values (2nd run).

Figure 4. [a] Values of the efficiency of each representative variable ith which correspond to the maximum value of the sum of the efficiencies for the four variables ($E_{i,M}$); [b] RMSE and MAE of CODtot,1; [c] RMSE and MAE of Snh4 in the section 1 and 2 and Sno3,3.

parameter estimation, some deficiencies in the procedure were observed when applied to NDEBPR full scale WWTP, in which a large number of variables and parameters are involved. Although by the progressive narrowing of the parameter range in the region of best values for the parameter is identified, the reduction of the number of sensitive parameters from one run to another may give some problems. The problems are connected to the fact that only a small number of parameters (among the 45 parameters) are used for calibration, while all others remain at their default value or at their value which corresponds to the maximum sum of the variables efficiencies. Fixing parameters at inappropriate values may have serious consequences during calibration because the error of the predictions will increase considerably. Therefore, it would be useful to perform an uncertainty analysis to asses the magnitude of the prediction errors when using the wrong set of fixed parameters.

4. CONCLUSIONS

In this work an integration of the procedure for the parameter estimation, based on Monte Carlo simulations according to von Sperling (1993) was presented. The procedure concerns the simultaneous parameter estimation and a sensitive analysis. It consists of a series of steps divided in two blocks: preliminary and iterative steps in which from one run to another different ranges of parameter, criteria for behavioral definition and number of sensitive parameter are considered. The procedure has been applied to a model for the simulation of nitrogen and phosphorus biological removal processes (according to the Bardenpho scheme) and has been repeated four times. The procedure gives us a good result at the 2nd run in which the sum of the variable efficiencies results maximum and the error of each variable is acceptable.

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