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The GSA-GLUE approach for uncertainty assessment of an integrated MBR model

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Abstract: In the recent literature, the uncertainty of wastewater treatment plant (WWTP) modelling has had relevant interest both for designers and operators. Indeed, the frequent data lacking and the need to improve process knowledge, in case of innovative technologies, make the use of mathematical models more uncertain. Therefore, the need to make model uncertainty more explicit is warmly recommended. However, only few applications of uncertainty analysis in the wastewater field have been carried out. In this work, the combination of the global sensitivity analysis (GSA) and the Generalized Likelihood Uncertainty Estimation (GLUE) is applied for the uncertainty assessment of a WWTP model, in order to discuss and verify its applicability. In particular, the GSA-GLUE approach is applied to an integrated membrane bioreactor (MBR) model able to simulate the biological nutrient removal processes occurring in a University Cape Town (UCT)-MBR system. The model under study is also able to simulate the physical processes of cake layer formation on membrane surface and the particle retention inside the cake layer. The GSA-GLUE approach has been applied by using quantity-quality data acquired in a UCT-MBR pilot plant. The results have demonstrated that the GSA-GLUE approach can be a valuable tool for designing and managing WWTP.

Keywords: Uncertainty analysis; wastewater modelling; global sensitivity analysis.

1 INTRODUCTION

In the last decade the use of membrane bioreactor (MBR) technology for treating municipal wastewater has considerably increased (Judd and Judd, 2010). At the same time, the need to improve the MBR process understanding has grown. In this context, mathematical modelling of MBR systems has had an important role as useful support for "*MBR knowledge upgrading*". Several MBR models have been proposed in literature adapting or integrating, with physical module, the activated sludge models (ASMs) (Henze et al., 2000) originally developed for conventional activated systems (Fenu et al., 2010; Mannina et al., 2011). However, even if the application of MBR models represents an useful support, model complexity is quite often a critical issue that has to be faced by modellers for model application. Indeed, in order to represent the peculiarities of MBR systems, a great number of new processes and, consequently, of new parameters have to be added adapting or integrating the ASM models. The frequent data and knowledge lacking often imposes to make a considerable number of assumptions on the model structure and on the values of parameters and input variables. Such assumptions and the intrinsic uncertainty of biological processes could make model predictions extremely uncertain (Mannina et al., 2012). Uncertainty analysis is therefore essential in MBR modelling as in any environmental modelling field. An accurate assessment of models' uncertainty provides more effective models as decisional supports. Making uncertainty more explicit as well as the adoption of a lager safety factors during designing process can be also possible (Vanrolleghem et al., 2011).

In the field of wastewater modelling, during the last years, models' uncertainty issue has had peculiar interest among researchers. They have tried to reach the same high knowledge level acquired in other environmental modelling fields such in the case of hydrology field (Belia et al., 2009). Several uncertainty studies have been conduced in order to improve knowledge. The uncertainty methodologies, previously used in other research fields, have been lately investigated and compared in order to discuss their applicability to wastewater treatment plant (WWTP) models (Martin et al., 2010; Mannina et al., 2012). However, only few studies have been conduced on integrated MBR complex models and on filtration models (Mannina et al., 2010; Yuan and Sin, 2011). Recently, several authors have demonstrated the ability of global sensitivity analysis (GSA) in quantifying uncertainties (Flores-Alsina et al., 2009; Sin et al., 2011). Furthermore, very recently the applicability of the Generalized Likelihood Uncertainty Estimation (GLUE) proposed by Beven and Binley (1992), most widely used for investigating uncertainties in hydrology, has been critically discussed by Mannina et al. (2010).
However, the possibility to transfer in the wastewater modelling field the combination of the GSA and GLUE (see, Ratto et al., 2001) for assessing the uncertainty has never been discussed. Indeed, the GSA-GLUE, for the first time proposed by Ratto et al. (2001) and recently applied by Vezzaro and Mikkelsen (2012), has twofold main advantages: 1) provide a quantitative assessments of that model parameters which mainly influence the behavioural model runs by means of GSA; 2) by using GLUE and defining a likelihood measure the performance of GSA conditioned to the observations is allowed.
In order to fill this gap the main objective in this study is to discuss the applicability of the GSA-GLUE approach, never used in wastewater modelling field, for uncertainty analysis of activated sludge models (ASMs). Specifically, the standardized regression coefficient (SRC) method has been employed. In particular, the GSA-GLUE approach has been applied to an integrated MBR model, previously developed by Cosenza et al. (2011), able to describe the biological processes occurring in a University Cape Town (UCT)–MBR pilot plant.

2 MATERIAL AND METHODS

2.1 Uncertainty assessment

In the following, the key elements of both GSA and GLUE will be discussed the reader is referred to the literature for details (Beven and Binley, 1992; Ratto et al., 2001; Saltelli et al., 2004).
The GSA is able to provide information on how the model outputs are influenced by the simultaneous variation of the input factors (Saltelli et al., 2004). In this study the GSA has been performed by applying SRC method. Such method consists of performing a multivariate linear regression between the model outputs (y) and inputs (x) by using Monte Carlo simulations (with random sampling of inputs). The standardised regression slopes (β_i), computed according to equation 1, represent a valid measure of sensitivity (Saltelli et al., 2004):

$$SRC(x_i) = \beta_i = b_i \cdot \sigma_{x_i} / \sigma_y \qquad (1)$$

where σ_{xi} and σ_y represent respectively the factor and the model output standard deviation. The goodness of SRC as measure of sensitivity is indicated by the coefficient of determination R^2, which represents the portion of total variance explained by the regression model; this value has to be greater than 0.7 (for linear model R^2 is close to 1). The sign of β_i indicates its positive (sign +) or negative (sign -) effect (Sin et al., 2011) on the model output variation. The SRC method generally requires a number of MC in the order of 500 – 1000 in the case of random sampling.
The GLUE method (Beven and Binley, 1992) allows the estimation of model uncertainty on the basis of equifinality concept. The GLUE method is based on making a large number of model runs by using different sets of model parameters

randomly generated from a specific prior distribution. By comparing predicted and observed data, for each set of model parameters, the goodness of the model run is assigned. Such goodness is expressed by the value of an assigned likelihood measure. A subjective threshold is employed for the likelihood measure in order to distinguish between behavioural and no behavioural simulation runs.
The GSA-GLUE approach has the peculiarity to consider the likelihood response surface as a further model output to take into account during GSA application. In this way it is possible to select parameters that are important for the likelihood surface and un-influential for the simulated model outputs (Vezzaro and Mikkelsen, 2012). These latter parameter will be included in the uncertainty analysis.
The GSA-GLUE approach consists on the following steps: 1) definition of model outputs to analyse; 2) definition of the prior parameters distribution; 3) choice of likelihood measures to investigate; 4) sampling of parameter sets, model running for each parameter sets and evaluation of likelihood measure on the basis of measured data; 5) definition of a weighted model likelihood; 6) application of the GSA, on the runs performed during point 4), by selecting the important model parameters; 7) definition of posterior distribution for the important model parameters conditioned to the measured data; 8) GLUE application 9) calculation of uncertainty bands.

2.2 Model description and case study

The integrated ASM2d-SMP-P model under study has been developed during a previous study (Cosenza et al., 2011). The model is divided into two sub-models (biological and physical) and involves 19 biological state variables and 79 parameters (kinetics, stoichiometry, physical parameters and fractionation coefficients). For the variables, process and parameter descriptions the reader is referred to the literature (Jiang et al., 2008; Cosenza et al., 2011; Mannina et al., 2012). The biological sub-model is able to simulate the biological nutrient removal processes occurring in a UCT-MBR system and the soluble microbial products (SMPs) formation/degradation. The physical sub-model is able to simulate the cake layer formation on membrane surface. In particular, it is able to evaluate the rate of sludge attachment and detachment on the membrane surface throughout the suction and backwashing phase, the solid mass deposited on the membrane surface and the cake layer thickness. Moreover, the physical sub-model describes the permeate COD profile inside the cake layer. Indeed, particles are retained inside the cake layer which contribute to the reduction of total COD concentration in the effluent (Mannina et al., 2011). The model has been applied to a pilot plant having an UCT-MBR scheme. The pilot plant consists of three reactors in series, anaerobic (section 1), anoxic (section 2) and aerobic (section 3) respectively, followed by an aerobic tank (section 4) where two submerged hollow fibre membrane modules (Zenon Zeeweed, ZW 10) are submerged and a tank in which permeate is collected (section 5). In order to maintain the desiderated biomass concentration recycled fluxes are considered from membrane tank to aerobic tank, from aerobic to anoxic tank and from anoxic to anaerobic tank. The pilot plant has been operated for 165 days feeding with 40 L/h of municipal wastewater. During this period samples of composite influent wastewater (section 0), grab mixed liquor in sections 1-4 and the permeate (section 5) were collected three times per week. Samples were analysed for total and volatile suspended solids (TSS and VSS), total and soluble COD, NH_4-N, NO_2-N, NO_3-N, N_{TOT}, P_{TOT} (APHA, 1998).

2.3 Method application

The GSA-GLUE approach was applied by taking into account model simulations and data of the last 65 days of plant managing. In order to employ SRC, Monte Carlo simulations have been conduced, propagating uncertainty from inputs to outputs, and then a linear regression on Monte Carlo simulations have been performed. In performing the linear regression each variable of interest was considered as a multivariate linear function of the model inputs. A prior uniform distribution was considered for each parameter. The variation range of each model parameter, according to previous studies (Sin et al., 2011), has been obtained by varying of +/-5% the calibration parameter value (Cosenza et al., 2011). The SRC method has been applied taking into account as model outputs the average value of fifteen simulated time variables, the respective likelihood (E_j) and the overall model efficiency (E_m). In particular the average value of $S_{NH4,1}$, $S_{PO,1}$, $MLSS_{,1}$, $COD_{TOT,2}$, $S_{NH4,2}$, $S_{NO3,2}$, $S_{PO,2}$, $MLSS_{,2}$, $COD_{TOT,3}$ (soluble COD) $COD_{SOL,3}$, $S_{NH4,3}$, $MLSS_{,3}$, $COD_{TOT,5}$, $S_{NH4,5}$ and (total nitrogen) $C_{TN,5}$ were considered. Concerning the E_j the following expression was employed (Mannina et al., 2011):

$$L(\theta_i/Y) = E_j = \exp\left(\frac{-\sigma^2_{Mj-Oj}}{\sigma^2_{Oj}}\right) \qquad (2)$$

where θ_i represents the ith set of model parameters (randomly generated), σ^2_{Mj-Oj} is the variance of the residuals between model and observations of the jth simulated model output and σ^2_{Oj} is the variance of observations for the period under consideration. Moreover, for each *ith*-set of model parameters, $E_{m,i}$ was computed as the weighed sum of the likelihood of the fifteen simulated variables taken into account. The weight of each variable was computed by dividing the maximum value of the likelihood measure of this variable by the sum of the maximum values of the likelihood measures of the other variables. Model parameters were selected as important whenever the normalized (respect to the maximum absolute value) absolute value of β_i ($|\beta_{I,n}|$) was greater that 0.2, at least for one of the fifteen variables and E_m. Un-important parameters were fixed at their value in correspondence of the maximum value of $E_{m.}$ For the important model parameters a posterior distribution, conditioned to measured data, was computed on the basis of the cumulated likelihood distribution of $E_{m.}$

Subsequently, in order to apply the GLUE, Monte Carlo simulations were performed varying only the important parameters. For each model parameter set a likelihood measure of each variable was computed. The number of the required Monte Carlo simulations was selected according to previous studies (Dotto et al., 2012). In particular, the uncertainty analysis was carried out in several steps in which starting from 500 Monte Carlo simulations from time to time the number of simulations was increased of 500. Step by step the cumulated likelihood distributions were compared to those of the previous step. The number of Monte Carlo simulations for which the difference between the distributions was lower than 0.01, in terms of Kolmogorov – Smirnov maximum distance, was considered appropriate for the analysis. The uncertainty bands were calculated by using the 5th and 95th percentiles of the model cumulative likelihood distributions. The ratio between the maximum band width (computed as difference between the value at 95th percentile and that at 5th) and the average band width have been considered to evaluate the degree to which model accounts uncertainty.

3 RESULTS AND DISCUSSION

3.1 Influential model parameters

In order to apply SRC method, 800 Monte Carlo simulations for each model parameter have been performed. The linear model determination coefficients (R^2), obtained by applying SRC method, were always >0.7 for the variables taken into account, with a mean value equal to 0.79, except for $E_{CODTOT,2}$, $E_{SNO3,2}$, $E_{CODTOT,5}$, $E_{SNH4,5}$, $MLSS_3$. Such result demonstrates that the averaged simulated variables, the efficiency of each variable and the model efficiency could be linearized and that β_i may be used as a valuable measure of sensitivity. The low R^2 values for $E_{CODTOT,2}$, $E_{SNO3,2}$, $E_{CODTOT,5}$, $E_{SNH4,5}$, $MLSS_{,3}$ are mainly due to the interactions among the parameters involved in describing such variables. Since the mean value of R^2 is greater than 0.7 the individual contribution of each model parameter to the total variance of the variables taken into account may be calculated by means β_i^2. That parameters which are selected as non-important by means $|\beta_{I,n}|$ may also fixed without influencing the model's predictions. In Figure 1 the $|\beta_{I,n}|$ values of the important model parameters for some model variables are shown.

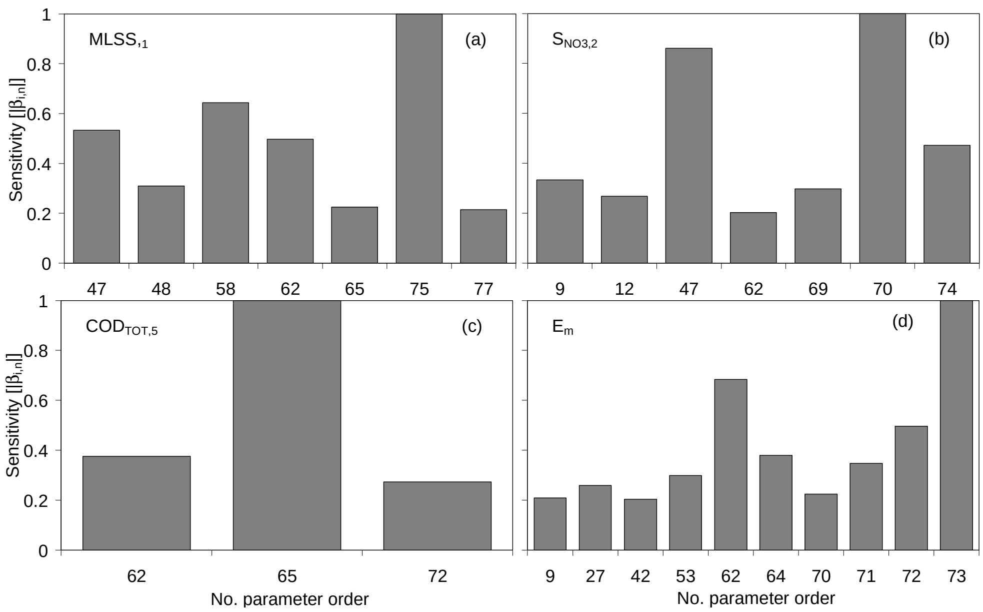

Figure 1 Important model parameters for $MLSS_{,1}$ (a), $S_{NO3,2}$ (b), $COD_{TOT,5}$ (c) and for E_m (d)

For $MLSS_{,1}$ (Figure 1a) $i_{TSS,XI}$ (no. order 75) and F_{XI} (no. order 58) which respectively represent the factor for converting the inert biomass concentration into total suspended solid and the fraction of inert biomass in the inlet wastewater have the highest influence. Indeed, $i_{TSS,XI}$ and F_{XI} are respectively responsible for 57% and 24% of the total variance of $MLSS_{,1}$. The positive value of β_i for $i_{TSS,XI}$ and F_{XI} indicates that increasing the value of these two parameters an increasing of the $MLSS_{,1}$ occurs. Regarding to $S_{NO3,2}$ the parameters $i_{N,BM}$ (no. order 70) and Y_H (no. order 47), which respectively represent the nitrogen content of biomass and the yield coefficient of heterotrophic biomass growth, have the highest absolute influence (Figure 1b). The influence of Y_H, which contribute with the 42% to the total variance of $S_{NO3,2}$, is strongly related to the denitrification process which occurs inside the anoxic tank. As well known, denitrification occurs by means of heterotrophic biomass; increasing Y_H the nitrate concentration inside the anoxic tank decreases (as confirmed by the negative value of β_i related to Y_H for $S_{NO3,2}$). For $COD_{TOT,5}$ (Figure 1c) parameters γ (no. order 62) and C_E (no. order 65), which represent the compressibility of cake layer on the membrane surface and the efficiency of backwashing for membrane cleaning respectively, have the highest influence. As demonstrated by the positive value of β_i related to γ and C_E for $COD_{TOT,5}$, increasing these two parameters the ability of cake layer to hold particles and consequently reduce the permeate total COD concentration increases. In terms of global model response (Figure 1d) it is evident that E_m is mainly influenced by γ and $i_{P,XS}$ (no. order 73). This latter parameter represents the phosphorus content of particulate biodegradable organics. The influence of γ and $i_{P,XS}$, which respectively contribute with the 15% and 33% to the total variance of E_m, represents the importance of the presence of membrane and the high weight of phosphorus removal for global model efficiency. In general, among the 79 model parameters investigated only 31 parameters reported were important. Thus, the number of parameters to be considered in the following GLUE analysis has been substantially reduced.

3.2 Uncertainty assessment - uncertainty bands

For the GLUE application 900 Monte Carlo simulations were performed by changing, inside their variation range, the value of the 31 important model parameters.

In Figure 2 the uncertainty bands of some model variables considered for the GSA-GLUE application are reported. In particular, uncertainty bands of $S_{PO,2}$ (Figure 2a), $COD_{SOL,3}$ (Figure 2b), $COD_{TOT,5}$ (Figure 2c) and $C_{TN,5}$ (Figure 2d) are shown.
From a visual inspection of Figure 2 one may observe that the uncertainty bands width changes considerably from variable to variable. Such results is mainly due to the fact that among the modelled processes some of them result to be more sensitive than others (e.g. phosphorus removal process). Moreover, as also demonstrated in previous uncertainty analysis and sensitivity analysis, conduced on ASM models, the uncertainty changes from plant section to section due to the different processes involved (Mannina et al., 2012; Cosenza et al., 2011). Such consideration has peculiar interest in case uncertainty analysis is conduced with the aim to optimize the WWTP plant behaviour. In other words by conducing the uncertainty analysis section by section modeller may also have information about the uncertainty of the intermediate processes which are relevant in uncertainty propagation of effluent variables. This demonstrates the usefulness and advantage of performing the analysis considering different plant sections.
Analyzing in details the results showed on Figure 2 it is possible to observe that for $S_{PO,2}$ (Figure 2a) the patterns related to calibrated model, 5% and 95% percentiles are almost overlapped for the first period of simulation (until the 17th day of simulation). Such result was likely due to the fact that before this day the orthophosphate concentration in the influent wastewater, and consequently in the anoxic tank, was too low. This circumstance has inhibited the phosphorus release process which occurs in anaerobic conditions. Therefore, until the 17th day of simulation the model uncertainty propagation generated by applying GLUE doesn't provide any model response in terms of $S_{PO,2}$. During the days 18-27 a K_2PO_4 dosing was done, inside the anaerobic tank, in order to increase the influent P-PO_4 concentration. After the dosing period, the model uncertainty propagation causes an evident response of the model even in terms of uncertainty. Globally for the $S_{PO,2}$ the average value of the width is equal to 4.2 mg/L which represents the 39% of the average simulated value by means of the calibrated model. For COD variables a good robustness of the model is shown on Figure 2 despite the complexity of the processes (both biological and physical) involved. Indeed, for $COD_{SOL,3}$ (Figure 2b) and for $COD_{TOT,5}$ (Figure 2c) the 97% and 98% respectively of measured data lay inside the bands. For COD variables the average widths of the bands are equal to 53 mg/L and 33 mg/L respectively for $COD_{SOL,3}$ and for $COD_{TOT,5.}$ The wide widths of the bands for $COD_{SOL,3}$ and for $COD_{TOT,5}$ is mainly due to the high influence of the parameter C_E as discussed above. A little variation of C_E value provide an high variation in terms of $COD_{SOL,3}$ and $COD_{TOT,5.}$

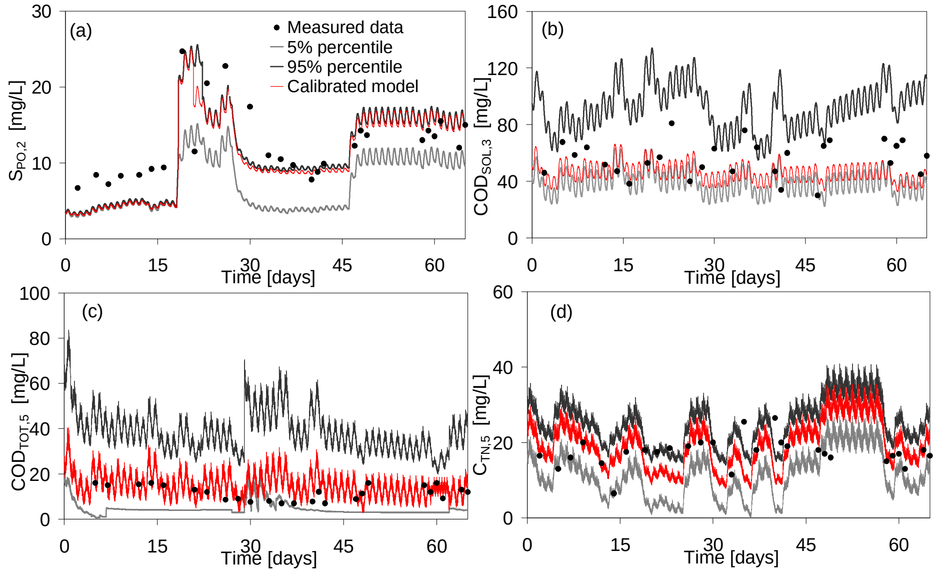

Figure 2 Uncertainty bands, measured data, 5% and 95% percentiles for $S_{PO,2}$ (a), $COD_{SOL,3}$ (b), $COD_{TOT,5}$ (c) and $C_{TN,5}$ (d).

Even for the $C_{TN,5}$ (Figure 2d) the uncertainty bands contain a great part (97%) of the measured data, showing an high ability of the model in reproducing such variable. Moreover, for $C_{TN,5}$ the average value of the width of the bands is equal to 13.7 mg/L which represents the 70% of the calibrated model showing a lower width than other variables.

4 CONCLUSIONS

In this study, GSA-GLUE approach has been applied for the first time in order to assess the uncertainty of an integrated MBR model. The study was aimed to verify the applicability of such approach even for complex integrated MBR models. The GLUE methodology has been applied by considering only the important model parameters with a posterior distribution conditioned to the measured data. The conditioned parameter space was investigated by performing Monte Carlo simulations. For each model simulation the simulated variable values were compared with the measured values. The goodness of this comparison was provided by the likelihood measure of each variable. The global model behaviour has been evaluated by means of a weighted sum of the likelihood of the variables taken into account.

The 5^{th} and 95^{th} percentiles of the cumulative model likelihood distributions for each simulation instance of time were used for calculating uncertainty bands for each model output variable.

From GSA-GLUE application, the following conclusion can be drawn:

- The GSA-GLUE approach may be applied also considering a regression method for important parameters selection instead of more complicated and computational demanding variance based GSA methods;
- The SRC method application has demonstrated that for the considered variation range of the model parameters the model behaviour is highly linear; such implication enabled to also quantify the variance associated to each model parameter;
- A substantial reduction of model parameters (from 79 to 31) to be involved in the GLUE application has been possible by mean of SRC results;
- The uncertainty bands show that the model presents a satisfactory agreement with measured data. Regarding to the $S_{PO,2}$ the influence of the inhibition of the biological releasing process has influenced the uncertainty bands in the first period of simulation. Despite the complexity of the processes involved in COD removal in a MBR process the uncertainty bands have demonstrated high robustness of the model in reproducing such variables.
- In view of its high potentiality the GSA-GLUE approach should be further investigated in the field of WWTP modelling in order to improve results in uncertainty assessment.

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