

Global sensitivity analysis in ASM applications: comparison of the SRC and Extended-FAST method for a UCT-MBR model

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Abstract

In this study global sensitivity analysis is performed to identify influential as well as non-influential parameters in a model of a University Cape Town Membrane Bioreactor (UCT-MBR). In particular, the Standardised Regression Coefficients (SRC) and Extended-FAST sensitivity analysis methods are applied. The sensitivity of model variables towards parameter variation is analysed for COD_{TOT}, S_{NH4}, S_{NO3}, S_{PO}, and MLSS along five reactor compartments. Both methods indicate that the parameters identified as being influential differ from section to section due to the different processes involved. Moreover, the relevant influence of the membrane filtration parameters is detected in the first plant section due to the influence of the recycled sludge. It is found that the computationally less expensive SRC method is applied outside its range of applicability with $R^2 = (0.3-0.6) < 0.7$. Nevertheless, the ranking obtained with the SRC method for the influential parameters is very similar to that of the Extended-FAST method, except for MLSS. However, to obtain reliable quantitative information on variance decomposition and to detect and quantify (in some cases considerable) interactions present among parameters the use of the computationally more expensive Extended-FAST is found to be necessary in this case study.

Keywords

Wastewater treatment; MBR modelling; global sensitivity analysis

Introduction

Over the past 40 years, the knowledge acquired in the field of wastewater treatment has increased considerably. The better understanding of the main processes that take place in wastewater treatment, has allowed developing innovative technologies such as membrane bioreactors (MBR), to improve the design approaches and to optimize the operation of wastewater treatment plants (WWTPs). Indeed, MBR employment provides high effluent quality and compact plant configurations (Judd and Judd, 2010). In this context, mathematical modelling has played a key role. By means of mathematical models it has been possible, for example, to test hypotheses on functional interactions in the system or predict future states of the system or its responses to assumed or expected changes in driving conditions. Nowadays, WWTP models, more specifically activated sludge models (ASMs) (Henze *et al.*, 2000), are widely used for applications such as design, control and optimization. However, these models are complex and generally characterized by several parameters to be assessed in view of the frequent lack of data limiting their employment. On account of this, WWTP modelling requires a considerable number of assumptions about the model structure, the values of parameters and the input variables. One may ask whether and how these model assumptions influence the outputs of the model. In this context sensitivity analysis represents a very powerful tool as it is able to provide information about how the variation in the

outputs of the model can be apportioned to the variation of the input factors (Saltelli, 2000). As summarised in Saltelli (2000) one may perform a sensitivity analysis for several reasons such as: (1) to evaluate if the model structure is able to describe the processes under study; (2) to select the most influential or non-influential input factors for the model output; (3) to evaluate the input factors interactions; (4) to select the region in the space of input factors on which focus attention during the model calibration. This last reason has a fundamental role when the model is over-parameterised.

Several sensitivity analysis methods have been applied in the past. According to Saltelli (2000) they can be grouped into three main classes: screening methods, local methods and global methods. The first one represents an economical and qualitative method. The local sensitivity analysis (LSA) provides a measure of the local effect on the model output by a one-factor-at-a-time variation of the model input factors. Finally, the global sensitivity analysis (GSA) provides information on how the model outputs are influenced by the simultaneous variation of the input factors. In this way it is also possible to identify the factor interactions (Homma and Saltelli, 1996; Saltelli *et al.*, 2004).

In the field of environmental sciences most previous studies using GSA have been conducted in hydrology or water resources and only few applications exist for water and wastewater treatment plants (Brockmann and Morgenroth, 2007, Neumann *et al.* 2007, Benedetti *et al.*, 2008, Neumann *et al.* 2009, Flores-Alsina *et al.*, 2010, Sin *et al.*, 2010; Sin *et al.*, 2011). GSA may help the modeller to identify influential parameters (*factors prioritization*) as well as non-influential parameters (*factors fixing*) («factors» is a term widely used in the sensitivity analysis literature and is a synonym for «model parameters»). By applying the «Extended Fourier Amplitude Sensitivity Testing» (Extended-FAST) (Cukier *et al.*, 1973; Schaibly and Shuler, 1973, Saltelli *et al.* 1999) information is obtained about i) which factors, if known, are expected to reduce output variance the most (*factors prioritization*) and ii) which factors can be fixed anywhere, in their range of uncertainty, without significantly reducing output variance (*factors fixing*).

This paper presents a comparison between two GSA methods, namely the Standardized Regression Coefficients (SRC) method (Saltelli *et al.*, 2008) and the «Extended - Fourier Amplitude Sensitivity Testing» (Extended-FAST) method, on an extended ASM model to detect influential and non-influential factors. The methods have been applied to a UCT-MBR pilot plant located at Acqua dei Corsari WWTP.

Materials and Methods

Standardized Regression Coefficients (SRC)

The SRC method consists of running a Monte Carlo simulation (with random sampling of inputs) and performing a multivariate linear regression between the model outputs and inputs (eq. 1):

$$y = b_o + \sum_{i=1}^n b_i \cdot x_i + \varepsilon \quad (1)$$

where y represents the model output, x_i the i th factor, n the number of factors, b_i the regression slopes, and ε the random error of the regression model. The SRC's are the standardised regression slopes:

$$SRC(x_i) = \beta_i = b_i \cdot \sigma_{x_i} / \sigma_y \quad (2)$$

where σ_{x_i} and σ_y represent respectively the factor and the model output standard deviation.

SRCs are valid measures of sensitivity when, as suggested by Saltelli (2004), the coefficient of determination R^2 , which indicates the portion of total variance explained by the regression model, is greater than 0.7. For linear models $\sum(\beta_i) = 1$, otherwise this sum which represents the model coefficient of determination R^2 is lower than 1 (Saltelli *et al.*, 2008). A high absolute value of β_i indicates a relevant effect of the related i -th model parameter on the model output. The sign of β_i indicates its positive (sign +) or negative (sign -) effect (Sin *et al.*, 2011). The required number of simulations found in literature is generally between 100 and 1000 (Neumann, submitted).

Extended-FAST

The Extended-FAST method belongs to the variance decomposition methods. It is founded on the variance decomposition theorem which states that the total variance of the model output ($Var(Y)$) may be decomposed into conditional variances. This method does not require any assumptions on model structure (linearity, monotonicity etc.). In particular, for each factor i two sensitivity indices are defined: the first order effect index (S_i) and the total effect index (S_{Ti}). S_i measures how the i -th factor contributes to $Var(Y)$ without taking into account the interactions among factors. It is expressed as:

$$S_i = \frac{Var_{x_i}(E_{x_{-i}}(Y|x_i))}{Var(Y)} \quad (3)$$

where E indicates the expectancy operator and Var the variance operator. According to the notation used by Saltelli *et al.* (2004) the subscripts indicate that the operation is either applied “over the i th factor” X_i , or “over all factors except the i -th factor” X_{-i} .

On the other hand, S_{Ti} allows evaluating the interactions among factors. It is expressed as:

$$S_{Ti} = 1 - \frac{Var_{x_{-i}}(E_{x_i}(Y|x_{-i}))}{Var(Y)} \quad (4)$$

The Extended-FAST method requires an $n \cdot N_{MC}$ simulations, where n is the number of factors and N_{MC} the number of MC simulations per factor ($N_{MC} = 500 - 1000$ according to Saltelli *et al.* (2005)).

It is important to underline that in the context of *factors fixing* the analysis of S_{Ti} has to be performed. If the S_i value is small it doesn't mean that the parameter may be fixed anywhere within its range because a high S_{Ti} value would indicate that the parameter is involved in interactions.

The MBR model and case study

The two methods were applied to an integrated ASM2d-SMP-P model (Cosenza *et al.*, 2011). The model couples the ASM2d-SMP model (first introduced by Jiang *et al.* (2008)) with a physical model derived from Di Bella *et al.* (2008) and Mannina *et al.*, 2010. It is able to simulate the biological nutrient removal (BNR) processes, the soluble microbial products (SMPs) formation/degradation and the cake layer formation which occur in a plant characterized by a UCT-MBR scheme. It involves 19 model state variables and 79 parameters (kinetic, stoichiometric, physical and fractionation related). The analysis is conducted for a pilot plant, which was operated at a feed inflow of 40 L/h of municipal wastewater during 165 days. Until day 76 it was operated with complete sludge retention while after day 76, the sludge was regularly withdrawn, maintaining the sludge age near to 37 days. During the entire experimental period composite influent wastewater samples were taken (section 0), grab mixed liquor samples in each tank (sections 1-4), mixed liquor samples in the oxygen depletion reactor (section 6) and in the permeate (section 5). This was done three times per week and the 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). Further details about the pilot plant and sampling campaign can be found in Cosenza *et al.* (2011) and Di Trapani *et al.* (2011).

Simulations were run using continuous input time series which were obtained by employing a truncated Fourier series calibrated on discrete measured input data (Mannina *et al.*, in press). Four different sections of the UCT-MBR plant were considered. In particular, the anaerobic (section 1), anoxic (section 2), aerobic (section 3) and permeate (section 5) tanks were considered. For the calculation of the sensitivity according to each method, the average value of the simulated time series was considered. The variables taken into account were: COD_{TOT} , S_{NH_4} , S_{NO_3} , S_{PO} , MLSS, for each section, COD_{SOL} (COD soluble) for section 3, and TN (total nitrogen) for section 5.

In the following the results for $COD_{TOT,1}$, $S_{PO,1}$, $S_{NO_3,2}$, $S_{PO,3}$ and $COD_{TOT,5}$ are analysed and compared (the subscript indicates the plant section). These variables have been selected as

representative of the main processes occurring in each reactor. Moreover, a synthesis of the results for all model variables for each method is presented.

Comparison of the sensitivity methods

The results were analysed by comparing the values of the sensitivity coefficients. In particular, as suggested in literature (Saltelli *et al.*, 2008) the β_i^2 were compared to the S_i values and the rankings of influential parameters were compared.

Results and Discussion

Standardised Regression Coefficients (SRC)

In order to apply the SRC method a parameter matrix (800×79) was generated using Latin Hypercube Sampling (LHS) (convergence was tested and found to be satisfactory with 800 simulations). In Table 1 SRCs (β_i 's), the linear model determination coefficients (R^2) and the sum of the squares of the standardized regression coefficients ($\Sigma\beta_i^2$) are reported. The results analysis was performed as in Sin *et al.* (2011) where $abs(\beta_i)$ with values greater than 0.1 were selected as being influential.

Table 1. Results of SRC application for each model output. The results refer to the parameters that are influential at least for one variable. $\Sigma\beta_i^2$ refer to the total sum. For the parameters' meaning refer to Henze *et al.* (2000), Jiang *et al.* (2008) and Di Bella *et al.* (2008)

Parameter	VARIABLES SECTION 1					VARIABLES SECTION 2					VARIABLES SECTION 3					VARIABLES SECTION 5					
	COD _{TOT}	S _{NH4}	S _{NO3}	S _{PO}	MLSS	COD _{TOT}	S _{NH4}	S _{NO3}	S _{PO}	MLSS	COD _{TOT}	COD _{SOL}	S _{NH4}	S _{NO3}	S _{PO}	MLSS	COD _{TOT}	S _{NH4}	S _{NO3}	CTN	S _{PO}
R^2	0.35	0.44	0.42	0.49	0.28	0.35	0.44	0.42	0.49	0.28	0.36	0.36	0.42	0.51	0.23	0.27	0.45	0.39	0.49	0.47	0.23
	SRC																				
K_H	-0.05	0.10	-0.06	0.13	-0.29	-0.04	0.08	-0.04	0.12	-0.22	-0.06	-0.06	-0.03	-0.02	0.01	-0.28	0.14	-0.04	-0.01	0.00	0.01
η_{FE}	-0.03	0.08	-0.03	0.15	0.01	-0.02	0.06	-0.02	0.14	0.01	-0.03	-0.03	-0.03	-0.02	-0.08	0.02	-0.01	-0.03	-0.01	-0.05	-0.09
K_O	0.00	0.01	0.00	0.08	-0.02	0.00	0.01	0.00	0.08	-0.01	0.00	0.00	-0.02	-0.19	-0.03	-0.01	0.03	-0.02	-0.19	-0.16	-0.02
K_{NO3}	0.09	0.04	0.07	-0.05	0.10	0.07	0.03	0.05	-0.05	0.07	0.09	0.08	0.02	0.04	-0.10	0.10	-0.03	0.01	0.05	0.05	-0.09
μ_H	-0.35	0.05	-0.43	0.06	-0.22	-0.26	0.04	-0.32	0.06	-0.17	-0.34	-0.34	0.02	-0.25	0.17	-0.22	-0.39	0.02	-0.25	-0.36	0.17
$\eta_{NO3,H}$	0.03	-0.04	-0.08	0.01	-0.05	0.02	-0.03	-0.06	0.01	-0.04	0.03	0.03	-0.05	-0.08	0.00	-0.05	-0.02	-0.04	-0.08	-0.12	0.00
b_H	0.15	-0.23	0.30	-0.35	0.00	0.11	-0.19	0.22	-0.35	0.00	0.16	0.16	-0.01	0.26	-0.05	-0.01	0.27	0.00	0.25	0.29	-0.04
$K_{NH,H}$	0.07	0.03	0.03	0.04	0.04	0.05	0.02	0.03	0.04	0.03	0.07	0.07	0.04	-0.02	-0.04	0.03	0.18	0.05	-0.03	0.11	-0.05
q_{PHA}	-0.02	0.03	0.00	0.32	0.00	-0.01	0.02	0.00	0.31	0.00	-0.01	0.00	0.03	-0.02	-0.01	0.00	0.02	0.03	-0.02	0.03	-0.02
q_{PP}	0.03	0.00	-0.02	0.24	0.07	0.02	0.00	-0.02	0.23	0.05	0.04	0.04	0.01	-0.03	0.03	0.07	-0.05	0.02	-0.03	-0.01	0.02
μ_{PAO}	0.01	-0.06	0.02	-0.13	0.01	0.01	-0.05	0.02	-0.13	0.01	0.01	0.01	-0.07	0.04	-0.12	0.01	0.04	-0.07	0.04	-0.02	-0.11
b_{PAO}	-0.03	0.07	0.01	0.02	-0.02	-0.02	0.06	0.01	0.02	-0.01	-0.03	-0.03	0.07	-0.03	0.12	-0.02	0.00	0.07	-0.03	0.04	0.11
μ_{AUT}	0.13	-0.52	0.10	-0.06	0.07	0.10	-0.43	0.08	-0.06	0.06	0.13	0.13	-0.59	0.38	-0.07	0.07	0.18	-0.56	0.35	-0.19	-0.08
b_{AUT}	0.03	0.03	0.02	0.00	0.01	0.03	0.03	0.02	0.00	0.01	0.03	0.03	0.02	0.00	-0.02	0.01	0.01	0.02	0.01	0.04	-0.01
Y_H	-0.03	-0.12	0.22	-0.14	0.01	-0.02	-0.10	0.16	-0.14	0.01	-0.01	-0.02	-0.03	0.27	-0.06	0.01	0.11	-0.04	0.28	0.21	-0.04
f_{XI}	-0.06	-0.10	0.08	-0.19	-0.12	-0.04	-0.09	0.06	-0.19	-0.09	-0.04	-0.06	0.01	0.07	-0.13	-0.12	0.01	0.01	0.08	0.07	-0.13
Y_{PAO}	0.00	0.02	0.04	0.11	-0.01	0.00	0.02	0.03	0.11	-0.01	0.01	0.01	0.02	0.03	-0.03	-0.01	0.03	0.02	0.03	0.06	-0.02
F_{SA}	-0.02	0.00	-0.06	0.08	-0.05	-0.02	0.00	-0.04	0.08	-0.04	-0.03	-0.03	0.01	-0.11	-0.06	-0.05	0.03	0.00	-0.10	-0.07	-0.05
β	-0.05	0.00	0.00	0.01	-0.04	-0.03	0.00	0.00	0.01	-0.03	-0.04	-0.04	0.01	0.00	-0.03	-0.04	0.10	0.01	0.00	0.04	-0.04
f	-0.34	-0.02	0.10	-0.03	0.04	-0.25	-0.02	0.08	-0.03	0.03	-0.34	-0.34	-0.01	0.07	-0.06	0.04	0.24	-0.02	0.08	0.10	-0.05
$i_{N,XI}$	0.00	0.06	-0.05	0.05	0.01	0.00	0.05	-0.04	0.05	0.01	0.00	0.00	0.06	-0.12	-0.02	0.01	-0.04	0.05	-0.12	-0.06	-0.01
$i_{N,XS}$	-0.03	0.00	0.01	-0.04	-0.01	-0.02	0.00	0.01	-0.04	0.00	-0.03	-0.03	0.00	0.16	0.00	-0.01	-0.02	-0.01	0.17	0.12	0.01
$i_{P,XI}$	-0.04	0.02	-0.03	-0.05	-0.03	-0.03	0.01	-0.02	-0.05	-0.03	-0.04	-0.04	0.01	-0.01	-0.11	-0.04	0.01	0.02	-0.02	0.00	-0.13
$i_{P,XS}$	0.04	-0.03	0.02	0.07	-0.01	0.03	-0.02	0.01	0.06	0.00	0.04	0.04	-0.03	0.03	0.23	-0.01	-0.03	-0.03	0.03	-0.01	0.23
$i_{P,BH}$	-0.06	-0.05	0.03	0.00	-0.03	-0.04	-0.04	0.02	0.00	-0.03	-0.06	-0.06	-0.06	0.06	0.12	-0.03	0.06	-0.06	0.06	0.01	0.12
$\Sigma\beta_i^2$	0.39	0.46	0.42	0.50	0.28	0.22	0.31	0.23	0.48	0.16	0.39	0.40	0.44	0.52	0.25	0.27	0.47	0.41	0.50	0.45	0.25

The following parameters, ranked according to decreasing importance, were found to have a significant impact on $COD_{TOT,1}$: $\{\mu_H, f, b_H, \mu_{AUT}\}$. The influence of the parameters μ_H and μ_{AUT} seems to be in contradiction with the anaerobic conditions in section 1. The influence of the parameter f (f represents the substrate fraction below the critical molecular weight able to be retained by the membrane) on $COD_{TOT,1}$ is ascribable to the recycled sludge. Its negative value (-0.33) (see Table 1) means that with increasing f a decrease in $COD_{TOT,1}$ concentration takes place.

The parameters $\{b_H, q_{PHA}, q_{PP}, f_{XI}, \eta_{FE}, Y_H, \mu_{PAO}, K_H, Y_{PAO}\}$ were found to be the most influential in determining $S_{PO,1}$. Among these parameters, q_{PHA} is certainly the most important from a process point of view since it influences the storage processes of X_{PHA} (poly-hydroxy alkanoates and organic storage polymer) which is fundamental for the aerobic phosphate uptake; an increasing value of q_{PHA} causes an increasing value of S_{PO} in the anaerobic section, which is confirmed by the

positive value of SRC (0.32) (see Table 1). The parameter sub-set $\{q_{PP}, \mu_{PAO}, Y_{PAO}\}$ influences the aerobic and anoxic kinetics of PAOs which may indirectly (by means of the recycled sludge) influence the $S_{PO,1}$ concentration. The parameter sub-set $\{b_H, f_{XI}, \eta_{FE}\}$ influences the lysis of PAO and of slowly biodegradable substrate and therefore indirectly influences the $S_{PO,1}$ concentration.

The parameters $\{\mu_H, \eta_{NO3,H}, Y_H\}$ were found to have a significant impact on $S_{NO3,2}$. These parameters are directly connected to the anoxic growth of heterotrophic organisms (denitrification) on S_A (acetate) and S_F (fermentable substrate) so they are highly correlated to the S_{NO3} concentration in the anoxic tank. In particular, regarding the most influential parameter (μ_H) the negative value of SRC (-0.32) (see Table 1) means that an increase of its value causes a decrease of $S_{NO3,2}$. The parameters $\{i_{P,XS}, \mu_H, b_{PAO}, i_{P,BM}\}$ were found to have a significant impact on $S_{PO4,3}$. This shows a high affinity with the biological process of phosphorus uptake which occurs in the aerobic tank. The parameter $i_{P,XS}$ (phosphorus content of X_S) influences the aerobic hydrolysis as well as the X_{PAO} lysis, which reduce the S_{PO4} content in the aerobic tank. The parameter $i_{P,BM}$ (phosphorus content of biomass) influences the $S_{PO4,3}$ concentration through the aerobic growth of heterotrophic PAO (*luxury uptake*) and non-PAO organisms. Regarding the parameter μ_H it doesn't directly influence the aerobic growth of PAO, however it influences the $S_{PO4,3}$ concentration through the heterotrophic aerobic growth on S_F and S_A ; also, the parameter b_{PAO} indirectly influences the *luxury uptake* process by means of X_{PAO} lysis.

The parameters $\{b_H, f, K_{NH,H}, \mu_{AUT}, k_H, Y_H, \beta\}$ were found to have a significant impact on $COD_{TOT,5}$. The importance of these parameters is consistent with the modeller's experience. Indeed, this parameter set shows the impact of the heterotrophic biomass activity and of the membrane separation. It is important to underline that the parameter f has an important influence on the $COD_{TOT,5}$ concentration (SRC=0.24), justified by the physical filtration processes; the positive sign is also in accordance with the physical meaning of the parameter.

Figure 1 summarizes the influential model parameters clustered with respect to each sub-group of model outputs. It is important to underline, that for each sub-group of model outputs the parameters influence changes from section to section due to the different processes involved. This demonstrates the usefulness and advantage of performing the sensitivity analysis considering different plant sections. For example, considering S_{NH} , the parameter μ_{AUT} is the only influential parameter for each section (Figure 1 b). While the COD relevant (Figure 1 a) parameters μ_H, b_H and f were influential for each section it was shown that the kinetic parameters have the highest influence for $COD_{TOT,5}$. Contrary to the modeller's expectation the parameter f was more influential for the intermediate sections than for the permeate section. This result is most likely due to the recycled sludge fluxes. Among the influential model parameters for the MLSS sub-group only the parameter f_{xi} appears to be non-influential (Figure 1 e). The P sub-group (Figure 1 d) presents the highest number of influential model parameters showing a clear distinction, in relation to the section, between the parameters involved in the phosphorus release process and in the phosphorus uptake one.

Important to note is that the R^2 values (0.23 – 0.49) found to be < 0.7 , which means that this technique is being applied outside its application range.

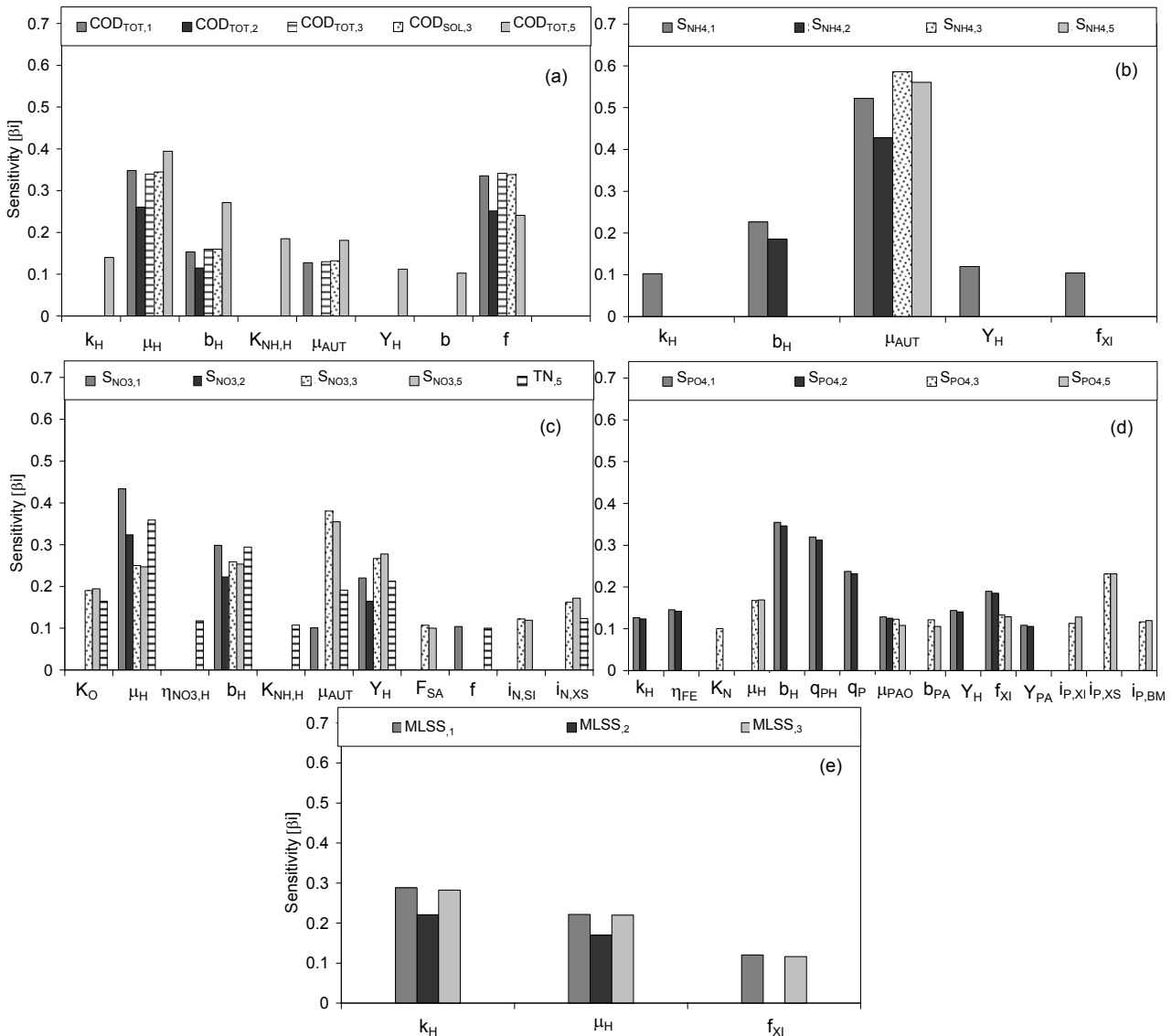


Figure 1. Influential model parameters for each model output according to the SRC method

Extended-FAST

In order to apply the Extended-FAST method 39,500 model runs were conducted corresponding to 500 simulations for each model parameter; factors with S_i and greater than 0.01 were defined as being influential. The results of the most influential parameters obtained by applying Extended-FAST method for the variables of the section 1, are summarized in Table 2 (the summary of all influential parameters is reported in Appendix 1).

The following parameters were found to have a significant impact on $COD_{TOT,1}$ on the basis of S_i : $\{\mu_H, f, b_H, K_H, C_E\}$. A high degree of interaction occurs for influential parameters indicated by the sum of S_{Ti} for this variable (11.42). The sum of the first order indices explains 57% of the total variance indicating that the model is non-linear and/or non-additive. The following parameters were found to have a significant impact for $S_{PO4,1}$: $\{b_H, q_{PHA}, q_{PP}, Y_H, k_H, f_{XI}, \eta_{FE}, \mu_H, \mu_{AUT}, F_{SF}, K_O, \mu_{PAO}, F_{XI}, F_{SA}, i_{N,XS}, K_{NH,H}\}$ (see Table 2). The sum of the first order indices explains 99% of the total variance indicating that the model is almost linear and/or additive contrasting the SRC result ($R^2=0.42$) which doesn't show a linear model.

The following parameters were found to have a significant impact on $S_{NO3,2}$: $\{\mu_H, Y_H, b_H, k_H, f_{XI}, \eta_{NO3,HYD}, F_{SF}\}$ (see Appendix 1); $\{\mu_H, Y_H\}$ are highly connected with the denitrification process. In this case the sum of S_i is equal to 0.83 (83% of model variance) and the sum of S_{Ti} is equal to 3.14.

Table 2 Results of influential model parameters for the variables of section 1 obtained by applying the Extended-FAST method

Parameter	MLSS,1		COD _{TOT,1}		S _{NH4,1}		S _{NO3,1}		S _{PO,1}		Parameter	MLSS,1		COD _{TOT,1}		S _{NH4,1}		S _{NO3,1}		S _{PO,1}	
	S _i	S _{Ti}	S _i	S _{Ti}	S _i	S _{Ti}	S _i	S _{Ti}	S _i	S _{Ti}		S _i	S _{Ti}	S _i	S _{Ti}	S _i	S _{Ti}	S _i	S _{Ti}	S _i	S _{Ti}
K _H	0.16	0.75	0.02	0.33	0.05	0.37	0.04	0.15	0.08	0.19	K _{NO3,PAO}	0.00	0.10	0.00	0.13	0.01	0.36	0.00	0.02	0.00	0.11
η _{NO3,HYD}	0.00	0.09	0.00	0.12	0.02	0.43	0.02	0.06	0.01	0.11	K _{NH,PAO}	0.00	0.09	0.00	0.12	0.00	0.38	0.00	0.02	0.00	0.09
η _{FE}	0.00	0.07	0.00	0.11	0.05	0.36	0.00	0.01	0.06	0.16	μ _{AUT}	0.00	0.11	0.00	0.16	0.36	0.75	0.00	0.04	0.03	0.19
K _O	0.00	0.09	0.00	0.13	0.02	0.48	0.00	0.02	0.02	0.11	K _{P,A}	0.00	0.14	0.00	0.15	0.01	0.31	0.00	0.05	0.00	0.14
K _{NO3}	0.00	0.09	0.00	0.10	0.00	0.37	0.00	0.02	0.00	0.07	K _{H,BAP}	0.00	0.11	0.00	0.13	0.00	0.29	0.00	0.01	0.00	0.14
μ _H	0.17	0.63	0.20	0.61	0.01	0.19	0.36	0.74	0.05	0.27	K _{H,UAP}	0.00	0.12	0.00	0.14	0.00	0.32	0.00	0.01	0.00	0.15
b _H	0.17	0.68	0.09	0.57	0.11	0.32	0.09	0.36	0.19	0.41	Y _H	0.01	0.22	0.00	0.13	0.03	0.27	0.18	0.33	0.11	0.28
K _A	0.00	0.09	0.00	0.10	0.00	0.41	0.00	0.02	0.00	0.06	f _{XI}	0.01	0.08	0.00	0.11	0.02	0.24	0.02	0.09	0.07	0.20
K _{NH,H}	0.00	0.14	0.01	0.17	0.01	0.35	0.01	0.08	0.01	0.17	Y _{PAO}	0.00	0.07	0.00	0.11	0.00	0.36	0.01	0.05	0.01	0.18
q _{PHA}	0.00	0.07	0.00	0.10	0.01	0.26	0.00	0.02	0.16	0.37	Y _A	0.00	0.07	0.00	0.12	0.01	0.38	0.00	0.01	0.00	0.06
q _{PP}	0.00	0.08	0.00	0.10	0.01	0.27	0.00	0.04	0.16	0.38	f _{BAP}	0.00	0.06	0.00	0.11	0.01	0.33	0.00	0.01	0.00	0.06
μ _{PAO}	0.00	0.07	0.00	0.11	0.00	0.28	0.00	0.03	0.01	0.10	F _{SF}	0.00	0.06	0.00	0.12	0.01	0.31	0.01	0.04	0.02	0.10
b _{PHA}	0.00	0.07	0.00	0.12	0.00	0.33	0.00	0.02	0.00	0.06	F _{SA}	0.00	0.07	0.00	0.12	0.00	0.26	0.01	0.04	0.01	0.08
K _{PHA}	0.00	0.12	0.00	0.13	0.01	0.35	0.00	0.04	0.00	0.08	F _{XI}	0.00	0.10	0.00	0.13	0.01	0.32	0.00	0.02	0.01	0.12
K _{O,PAO}	0.00	0.15	0.00	0.14	0.01	0.45	0.00	0.02	0.00	0.11	i _{N,XS}	0.00	0.08	0.00	0.12	0.00	0.21	0.00	0.02	0.01	0.08

The following parameters were found to have a significant impact on S_{PO4,3}: {i_{P,XS}, μ_H, q_{PP}, b_{PAO}, i_{P,SF}, i_{P,XI}, q_{PHA}, f_{XI}, b_H, F_{SA}, k_H} (see Appendix 1). In this case the model sum of S_i is equal to 0.63 (63% of model variance) and the sum of S_{Ti} is equal to 3.5.

The following parameters resulted to be influential for COD_{TOT,5} concentration {f, μ_H, b_H, K_{NH,H}, μ_{AUT}, k_H, C_E} (see Appendix 1). Again, the influence of physical filtration process is present (f, C_E). Similarly to the SRC method the influence of the model parameters changes with respect to the section of the pilot plant taken into account. The changing influence is more evident for the parameter μ_{AUT} which appears to be the most influential parameter for S_{NH4,3}. Another example is the parameter f which has a S_i for COD_{TOT} which is three times higher for section 5 than in the other sections.

To give an example, Figure 2 shows the S_i and S_{Ti} (S_{Ti} = S_i + interaction) for S_{NH4,2}. Important to note is that the parameters K_A, K_{NH,H}, K_{O,PAO}, K_{NO3,PAO} and K_{NH,PAO} cannot be considered non-influential due to their high S_T values.

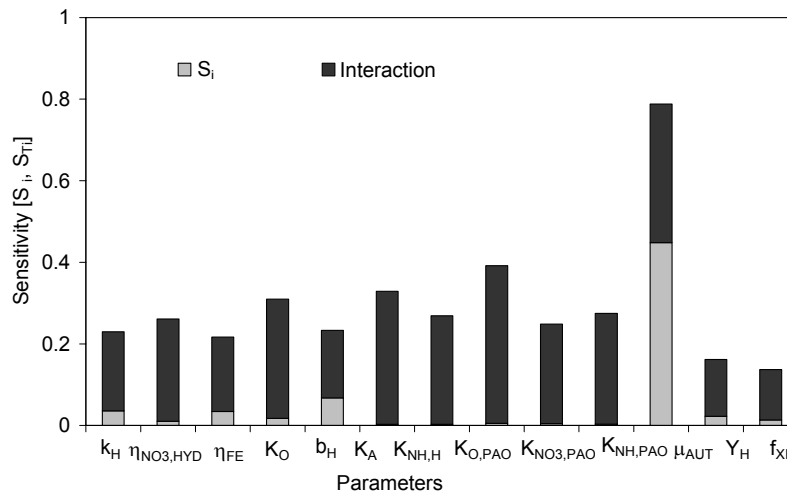


Figure 2. First order effect S_i and total effect S_{Ti} indices for S_{NH4,2} obtained with the Extended-FAST method

Comparison of SRC and Extended-FAST

Although the SRC method is found to be outside its range of applicability (R² is always < 0.7) the high correlation between β_i² and S_i indicates that SRC and Extend-FAST detect the same parameters as being influential and lead to a similar ranking (Table 3). The exception of MLSS is probably due to the interaction among parameters and variables involved in the MLSS expression.

Table 3. Results of methods comparison: comparison between β_i^2 and S_i , values of the sum $\Sigma\beta_i^2$ and S_i for each variable

	Section 1					Section 2					
Variables	COD _{TOT,1}	S _{NH4,1}	S _{NO3,1}	S _{PO,1}	MLSS ₁	COD _{TOT,2}	S _{NH4,2}	S _{NO3,2}	S _{PO,2}	MLSS ₂	
R ² (β_i^2 versus S_i)	0.9	0.96	0.91	0.83	0.53	0.9	0.99	0.87	0.8	0.53	
$\Sigma\beta_i^2$	0.39	0.45	0.42	0.5	0.27	0.22	0.31	0.23	0.48	0.16	
ΣS_i	0.57	0.99	0.78	1.1	0.61	0.57	0.86	0.83	0.98	0.6	
	Section 3					Section 5					
Variables	COD _{TOT,3}	COD _{SOL,3}	S _{NH4,3}	S _{NO3,3}	S _{PO,3}	MLSS ₃	COD _{TOT,5}	S _{NH4,5}	S _{NO3,5}	CTN ₅	S _{PO,5}
R ² (β_i^2 versus S_i)	0.9	0.9	0.99	0.81	0.64	0.52	0.66	0.9	0.81	0.88	0.66
$\Sigma\beta_i^2$	0.39	0.4	0.44	0.51	0.24	0.27	0.47	0.41	0.5	0.45	0.24
ΣS_i	0.56	0.57	0.66	0.91	0.64	0.6	0.9	0.64	0.9	0.95	0.66

Conclusions

- A comparison of two global sensitivity analysis methods (SRC and Extended-FAST) was presented with the aim to identify influential (*factors prioritization*) and non-influential model parameters (*factors fixing*). The methods were compared for a complex integrated MBR model with 21 output variables and 79 parameters.
- It was found that, although the SRC method was applied outside its range of applicability ($R^2 < 0.7$), the ranking of influential model parameters (*factors prioritization*) was very similar to the results obtained with Extended-FAST, except for the MLSS variables.
- To obtain reliable quantitative estimates of the variance contributions it was necessary to compute first order effect indices S_i with the computationally much more expensive method Extended-FAST, as the SRC method was outside its range of applicability.
- For some variables significant interactions among parameters were revealed by computing the total effect indices S_{Ti} using Extended-FAST e.g. for $S_{NH4,2}$.

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References

- Beck, M.B., Ravetz, J.R., Mulkey, L.A. and Barnwell, T.O. (1997). On the problem of model validation for predictive exposure assessments. *Stochastic Hydrology and Hydraulics*, 11 (3), 229-254.
- Benedetti, L., Nopens, I. and Vanrolleghem, P.A. (2008). Global sensitivity analysis of design and operational parameters of the Benchmark Simulation Model nr. 2. In: *Proceedings International Symposium on Sanitary and Environmental Engineering (SIDISA.08)*. Florence, Italy, June 24-27.
- Brockmann, D. and Morgenroth, E. (2007). Comparing global sensitivity analysis for a biofilm model for two-step nitrification using the qualitative screening method of Morris or the quantitative variance-based Fourier Amplitude Sensitivity Test (FAST). *Water Science & Technology* 56 (8), 85-93.
- Cosenza, A., Mannina, G., Neumann, M.B., Vanrolleghem, P.A. and Viviani, G. (2011). Modelling biological nitrogen and phosphorus removal with soluble microbial products (SMP) production-degradation processes: application to an UCT-MBR system. In *Proceeding of Watermatex 2011, 8th IWA Symposium on Systems Analysis and Integrated Assessment*. San Sebastián, Spain, 20-22 June 2011.
- Cukier, R.I., Fortuin, C.M., Shuler, K.E., Petschek, A.G. and Schaibly, J.H. (1973). Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients. I Theory. *The Journal of Chemical Physics*, 59 (8), 3873-3878.
- Di Bella, G., Mannina, G. and Viviani, G. (2008). An integrated model for physical-biological wastewater organic removal in a submerged membrane bioreactor: Model development and parameter estimation, *Journal of Membrane Science*, 322(1), 1-12.
- Di Trapani, D., Capodici, M., Cosenza, A., Di Bella, G., Mannina, G., Torregrossa, M. and Viviani, G. (2011). Evaluation of biomass activity and wastewater characterization in a UCT-MBR pilot plant by means of respirometric techniques. *Desalination*, 269, 190-197.

- Flores-Alsina, X., Corominas, L., Muschalla, D., Neumann, M.B. and Vanrolleghem P.A. (2010). How do initial design assumptions determine plant sizing? Assessing activated sludge process design using Monte-Carlo simulation and global sensitivity analysis. In: Proceedings IWA World Water Congress 2010. Montréal, Québec, Canada, September 19-24, 2010.
- Henze, M., Gujer, W., Mino, T. and van Loosdrecht, M. (2000). Activated sludge models ASM1, ASM2, ASM2d and ASM3. IWA Task Group on Mathematical Modelling for Design and Operation of Biological Wastewater treatment, IWA Publishing, London, UK.
- Homma, T. and Saltelli, A. (1996). Importance measures in global sensitivity analysis of nonlinear models. *Reliability Engineering and System Safety* 52, 1–17.
- Jiang, T., Myngheer, S., De Pauw, D.J.W., Spanjers, H., Nopens, I., Kennedy, M.D., Amy, G. and Vanrolleghem, P.A., (2008). Modelling the production and degradation of soluble microbial products (SMP) in membrane bioreactors (MBR). *Water Research*, 42 (20), 4955–4964.
- Judd, S.J. and Judd, C. (2010). *The MBR Book - Second Edition: Principles and Applications of Membrane Bioreactors in Water and Wastewater Treatment*. Elsevier, London, UK.
- Mannina, G., Di Bella, G., Viviani, G. (2010). Uncertainty assessment of a membrane bioreactor model using the GLUE methodology. *Biochemical Engineering Journal*, 52(2) 263–275.
- Mannina, G., Cosenza, A., Vanrolleghem, P.A. and Viviani, G. (in press). A practical protocol for calibration of nutrient removal wastewater treatment models. *Journal of Hydroinformatics*.
- Neumann, M. B. (submitted). Comparison of sensitivity analysis techniques for modelling micropollutant oxidation in water treatment.
- Neumann, M.B., Gujer, W. and von Gunten, U. (2009). Global sensitivity analysis for model-based prediction of oxidative micropollutant transformation during drinking water treatment. *Water Research*, 43, 997-1004.
- Neumann, M.B., von Gunten, U. and Gujer, W. (2007). Uncertainty in prediction of disinfection performance. *Water Research*, 41, 2371-2378.
- Saltelli, A., Ratto, M., Tarantola, S. and Campolongo, F. (2005). Sensitivity analysis for chemical models. *Chemical Reviews*, 105, 2811-2827.
- Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M. and Tarantola, S. (2008). *Global Sensitivity Analysis. The Primer*. John Wiley & Sons Ltd, The Atrium, Southern Gate, Chichester.
- Saltelli, A. (2000). *Sensitivity analysis*, John Wiley & Sons, Chichester.
- Saltelli, A., Tarantola, S., Campolongo F. and Ratto, M. (2004). *Sensitivity analysis in practice. A guide to assessing scientific models*. In: Probability and Statistics Series. John Wiley & Sons Publishers.
- Saltelli, A., Tarantola, S. and Chan, K.P.S. (1999). A quantitative model-independent method for global sensitivity analysis of model output. *Technometrics*, 41 (1), 426 39-56.
- Schaibly, J.H. and Shuler, K.E. (1973) Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients. II Applications. *The Journal of Chemical Physics*, 59 (8), 3879-3888.
- Sin, G., Ruano, M.V., Neumann, M.B., Ribes, J., Gernaey, K.V., Ferrer, J., van Loosdrecht, M.C.M. and Gujer, W. (2010). Sensitivity Analysis in the WWTP Modelling Community – New Opportunities and Applications. In: Proceedings 2nd IWA/WEF Wastewater Treatment Modelling Seminar (WWTmod2010). Mont-Sainte-Anne, Québec, Canada, March 28-30, 2010, 151-161.
- Sin, G., Gernaey, K.V., Neumann, M.B., van Loosdrecht, M. and Gujer, W. (2011). Global sensitivity analysis in wastewater treatment plant model applications: Prioritizing sources of uncertainty. *Water Research*, 45, 639-651
- Yang, J. (2011). Convergence and uncertainty analyses in Monte-Carlo based sensitivity analysis. *Environmental Modelling & Software*, 26, 4, pp. 444-457

