



Global sensitivity analysis in wastewater applications: A comprehensive comparison of different methods



Alida Cosenza^a, Giorgio Mannina^{a,*}, Peter A. Vanrolleghem^b, Marc B. Neumann^{b,c,d}

^a *Dipartimento di Ingegneria Civile, Ambientale, Aerospaziale, dei Materiali, Università di Palermo, Viale delle Scienze, 90128 Palermo, Italy*

^b *modelEAU, Département de génie civil et de génie des eaux, Université Laval, 1065 av. de la Médecine, Québec, QC G1V 0A6, Canada*

^c *Basque Centre for Climate Change, Alameda Urquijo, 4-4°, 48008 Bilbao, Spain*

^d *IKERBASQUE, Basque Foundation for Science, 48011 Bilbao, Spain*

ARTICLE INFO

Article history:

Received 22 December 2012

Received in revised form

29 May 2013

Accepted 19 July 2013

Available online

Keywords:

Calibration

Global sensitivity analysis

MBR modelling

Wastewater treatment

ABSTRACT

Three global sensitivity analysis (GSA) methods are applied and compared to assess the most relevant processes occurring in wastewater treatment systems. In particular, the Standardised Regression Coefficients, Morris Screening and Extended-FAST methods are applied to a complex integrated membrane bioreactor (MBR) model considering 21 model outputs and 79 model factors. The three methods are applied with numerical settings as suggested in literature. The main objective considered is to classify important factors (factors prioritisation) as well as non-influential factors (factors fixing). The performance is assessed by comparing the most reliable method (Extended-FAST), by means of proposed criteria, with the two other methods. In particular, similarity to results obtained from Extended-FAST is assessed for sensitivity indices, for the ranking of sensitivity indices, for the classification into important/non-influential factors and for the method's ability to detect interaction among factors and to provide results in a reasonable time.

It was found that the computationally less expensive SRC method was applied outside its range of applicability ($R^2 = (0.3-0.6) < 0.7$). Still, the SRC produced a ranking of important factors similar to Extended-FAST. For some variables significant interactions among the factors were revealed by computing the total effect indices S_{Ti} using Extended-FAST. This means that to obtain reliable variance decomposition and to detect and quantify interactions among the factors, the use of the Extended-FAST is recommended. Regarding the comparison between Morris screening and Extended-FAST a poor agreement was found. In particular, the Morris screening overestimated the number of both important and non-influential factors compared to Extended-FAST for the analysed case study.

© 2013 Elsevier Ltd. All rights reserved.

1. Introduction

In the field of mathematical modelling sensitivity analysis represents a very powerful tool as it provides information about how the variation in the outputs of the model can be apportioned to the variation of the model (input) factors (Saltelli, 2000). "Factors" is a term widely used in the sensitivity analysis literature and includes model parameters and model input variables. Saltelli (2000) singles out three main classes of sensitivity analysis methods: screening methods, local methods and global methods. Screening methods are economical and qualitative methods. Local methods provide a

measure of how the model output is affected by infinitesimal factor changes at a specific location in factor space. Global sensitivity analysis (GSA) provides information on how the model outputs are influenced by factor variation over the whole space of possible input factor values (Homma and Saltelli, 1996; Saltelli et al., 2004).

In the environmental modelling field the majority of sensitivity analysis applications are local. Moreover, often a one-at-a-time approach is used that does not allow identifying interacting factors. In recent years, several GSA techniques have been developed. Among them the most widely used are: (i) global screening methods such as the Morris screening method (Morris, 1991; Campolongo et al., 2007); (ii) variance decomposition methods such as Fourier Amplitude Sensitivity Testing (FAST), Extended-FAST and the Sobol indices method (Cukier et al., 1973; Schaibly and Shuler, 1973; Saltelli et al. 1999; Sobol, 2001); and (iii) regression-based methods such as the standardised regression coefficient (SRC) method (Saltelli et al., 2008). GSA may help the

* Corresponding author.

E-mail addresses: alida.cosenza@unipa.it (A. Cosenza), giorgio.mannina@unipa.it, mannina@idra.unipa.it (G. Mannina), Peter.Vanrolleghem@gci.ulaval.ca (P.A. Vanrolleghem), marc.neumann@bc3research.org (M.B. Neumann).

List of symbols and abbreviations

MBR	Membrane BioReactor	K_{NO_3}	Half saturation parameter for S_{NO_3} for X_H
FAST	Fourier Amplitude Sensitivity Test	K_x	Half saturation parameter for X_S/X_H
SRC	Standardised Regression Coefficient	S_F	Fermentable organic matter
GSA	Global Sensitivity Analysis	S_A	Fermentation product (considered to be acetate)
ASM	Activated Sludge Models	X_{PAO}	Phosphorus accumulating organisms model variable
UCT	University of Cape Town	X_{PP}	Stored polyphosphates in PAOs
SMP	Soluble Microbial Product	X_{PHA}	Storage compound in PAOs
TSS	Total Suspended Solids	S_{ALK}	Alkalinity (HCO_3^-)
VSS	Volatile Suspended Solids	X_{AUT}	Autotrophic nitrifying organisms
COD	Chemical Oxygen Demand	S_{BAP}	Soluble biomass associated products
NH_4-N	Ammonia nitrogen	S_{UAP}	Soluble utilisation associated products
NO_2-N	Nitrite nitrogen	S_I	Soluble undegradable organics
NO_3-N	Nitrate nitrogen	X_I	Particulate undegradable organics
N_{TOT}	Total nitrogen	$K_{O,HYD}$	Half saturation/inhibition parameter for S_{O_2}
P_{TOT}	Total phosphorus	$K_{NO_3,HYD}$	Half saturation/inhibition parameter for S_{NO_3}
COD_{TOT}	Total COD model variable	μ_H	Maximum growth rate of X_H
S_{NH_4}	Ammonia nitrogen model variable	q_{FE}	Rate constant for fermentation/Maximum specific fermentation growth rate
S_{NO_3}	Nitrate nitrogen model variable	$\eta_{NO_3,H}$	Reduction factor for anoxic growth of X_H
S_{PO_4}	Soluble inorganic phosphorus model variable	b_H	Decay rate for X_H
MLSS	Mixed liquor suspended solid	K_F	Half saturation parameter for S_F
COD_{SOL}	Soluble modelled COD	K_{FE}	Half saturation parameter for fermentation of S_F
CTN	Total nitrogen model variable	K_A	Half saturation parameter for S_A
y	Model output	$K_{NH,H}$	Half saturation parameter for S_{NH_4} for X_H
x_i	i th model factor	K_P	Half saturation parameter for S_{PO_4} for X_H
b_i	Regression slopes	$K_{ALK,H}$	Half saturation parameter for S_{ALK} for X_H
ε	Random error of the regression model	q_{PHA}	Rate constant for S_A uptake rate
σ_{x_i}	i th factor standard deviation	q_{PP}	Rate constant for storage of polyphosphates
σ_y	Model output standard deviation	μ_{PAO}	Maximum growth rate of X_{PAO}
β_i	i th factor sensitivity index	$\eta_{NO_3,PAO}$	Reduction factor for anoxic growth of X_{PAO}
EE	Elementary Effect	b_{PAO}	Endogenous respiration rate of X_{PAO}
p	Sampling level of Morris screening method	b_{PP}	Rate constant for Lysis of polyphosphates
Δ	Factor perturbation	b_{PHA}	Rate constant for respiration of X_{PHA}
μ	Mean of the EEs function	K_{PS}	Half saturation parameter for S_{PO_4} uptake
σ	Standard deviation of the EEs function	K_{PP}	Maximum ratio of X_{PP}/X_{PAO}
IF	Interaction among factors	K_{MAX}	Half saturation parameter for X_{PP}/X_{PAO}
μ^*	Mean of the absolute EEs function	K_{IPP}	Half inhibition parameter for X_{PP}/X_{PAO}
r	Sampling repetition for Morris screening method	K_{PHA}	Saturation constant for X_{PHA}/X_{PAO}
n	Model factors number	$K_{O,PAO}$	Half saturation parameter for S_{O_2} for X_{PAO}
$Var(Y)$	Total variance of the model output	$K_{NO_3,PAO}$	Half saturation parameter for S_{NO_3} for X_{PAO}
S_i	First order effect index of the i th factor	$K_{A,PAO}$	Half saturation parameter for S_A for X_{PAO}
S_{Ti}	Total effect index of the i th factor	$K_{NH,PAO}$	Half saturation parameter for S_{NH_4} for X_{PAO}
N_{MC}	Number of Monte Carlo simulations	$K_{P,PAO}$	Half saturation parameter for S_{PO_4} as nutrient (X_{PAO} growth)
S_{Ni}	Normalised interaction index	$K_{ALK,PAO}$	Half saturation parameter for S_{ALK} for X_{PAO}
ρ_s	Spearman's rank correlation index	μ_{AUT}	Maximum growth rate of X_{AUT}
r_p	Pearson correlation index	b_{AUT}	Decay rate for X_{AUT}
PF	Position Factor	$K_{O,A}$	Half saturation parameter for S_{O_2} for X_{AUT}
Rel	Relevance	$K_{NH,A}$	Half saturation parameter for S_{NH_4} for X_{AUT}
NS	Number of simulations	$K_{ALK,A}$	Half saturation parameter for S_{ALK} for X_{AUT}
PAOs	Phosphorus Accumulating Organisms	$K_{P,A}$	Half saturation parameter for S_{PO_4} for X_{PAO}
$Rel_{IMPORTANT}$	Relevance of important factors	$k_{H,BAP}$	Hydrolysis rate coefficient for S_{BAP}
$Rel_{NON-INFLUENTIAL}$	Relevance of non-influential factors	$k_{H,UAP}$	Hydrolysis rate coefficient for S_{UAP}
k_H	Maximum specific hydrolysis rate	$k_{LaT,3}$	Overall oxygen transfer coefficient aerobic tank
$\eta_{NO_3,HYD}$	Correction factor for hydrolysis under anoxic conditions	$k_{LaT,4}$	Overall oxygen transfer coefficient MBR tank
η_{FE}	Correction factor for hydrolysis under anaerobic conditions	Y_H	Yield for X_H growth
K_O	Half saturation parameter for SO_2 for X_H	f_{X_I}	Fraction of X_I generated in biomass decay
S_{O_2}	Dissolved oxygen	Y_{PAO}	Yield for X_{PAO} growth
X_H	Ordinary heterotrophic organisms	Y_{PO_4}	Yield for X_{PP} requirement per X_{PHA} stored
X_S	Particulate biodegradable organics	Y_{PHA}	Yield for X_{PP} storage per X_{PHA} utilised
X_H	Ordinary heterotrophic organisms	Y_A	Yield of X_{AUT} growth per S_{NO_3}
		f_{BAP}	Fraction of S_{BAP} generated in biomass decay
		f_{UAP}	Fraction of S_{UAP} generated in biomass decay

F_{S_F}	Fraction of influent S_F	i_{N,X_I}	Nitrogen content of X_I
F_{S_A}	Fraction of influent S_A	i_{N,X_S}	Nitrogen content of X_S
F_{S_I}	Fraction of influent S_I	$i_{N,BM}$	Nitrogen content of biomass
F_{X_I}	Fraction of influent X_I	i_{P,S_F}	Phosphorus content of S_F
F_{X_H}	Fraction of influent X_H	i_{P,X_I}	Phosphorus content of X_I
β	Erosion rate coefficient of the dynamic sludge	i_{P,X_S}	Phosphorus content of X_S
α	Stickiness of the biomass particles	$i_{P,BM}$	Phosphorus content of biomass
γ	Compressibility of cake	i_{TSS,X_I}	Conversion factor X_I in TSS
f	Substrate fraction below the critical molecular weight	i_{TSS,X_S}	Conversion factor X_S in TSS
λ	Screening parameter	$i_{TSS,BM}$	Conversion factor biomass in TSS
C_E	Efficiency of backwashing	$i_{TSS,X_{PHA}}$	Conversion factor X_{PHA} in TSS
i_{N,S_I}	Nitrogen content of S_I	$i_{TSS,X_{PP}}$	Conversion factor X_{PP} in TSS
i_{N,S_F}	Nitrogen content of S_F		

modeller to identify important input factors (*factors prioritisation*) as well as non-influential input factors (*factors fixing*). The main goal of *factors prioritisation* is to identify factors which determine model variance whereas *factors fixing* identifies factors that may be fixed anywhere within their range of uncertainty without affecting model output variance. Moreover, some GSA methods are also able to quantify the model variance contribution due to the synergistic or co-operative effect among factors called *interaction* or *interaction among factors* (IF) (Saltelli et al., 2004).

In the field of environmental modelling previous studies using GSA have been conducted with different goals (factors prioritisation, factors fixing etc.). Only a limited number of studies focus on wastewater treatment (among others, Brockmann and Morgenroth, 2007; Benedetti et al., 2008; Gernaey et al., 2011; Ruano et al., 2011; Sin et al., 2011; Benedetti et al., 2012; Chen et al., 2012; Flores-Alsina et al., 2012; Ruano et al., 2012).

In the following, five GSA comparison studies, coming from several environmental modelling fields are briefly discussed.

Confalonieri et al. (2010), employing a crop model with 11 parameters, compared the Morris screening method, the regression-based SRC method and two methods based on variance decomposition (Extended-FAST and Sobol). They found almost always similar rankings of important model parameters.

Yang (2011) presented a study in which two methods were proposed to analyse the convergence of sensitivity indices by applying the Central Limit Theorem and the bootstrap technique. The latter was applied for comparing results of five sensitivity analysis methods. Yang found, for a simple model characterised by 5 parameters, a high capability of the Morris screening method in identifying non-influential factors.

Neumann (2012) also presents a comparison among five sensitivity analysis techniques (derivative-based local sensitivity analysis, Morris Screening, Standardised Regression Coefficients, Extended-FAST and an entropy-based method) which were applied to a drinking water model for several objectives including *factors prioritisation*, and *factors fixing*. In general the author found the same parameter ranking results for the different methods. However, for chemicals leading to high non-linearity, the approximation of 1st order effect indices using the local methods or regression-based methods was poor and classification differed among methods.

Finally Sun et al. (2012) compared three sensitivity analysis methods of a water quality hydrology model: the local method, Morris screening method and global sensitivity analysis. They concluded that the three methods were complementary and whenever the number of input factors is too high a more efficient two-step procedure based on a first stage screening process (with a local method) followed by a global sensitivity analysis of the factors identified in the first stage was a feasible approach.

In the wastewater field, Brockmann and Morgenroth (2007) compared Morris screening and FAST methods for a 22 parameter biofilm model for two step nitrification. The authors showed that both methods provide the same set of important parameters despite the fact that information about the variance contribution of each parameter was only provided by the FAST method. They suggest that Morris screening is an excellent method for prior factor fixing while the FAST method is suitable for exploring the variance contribution for the subset of important parameters.

In the wastewater field the Activated Sludge Models (ASM), widely used in modelling of biological treatment processes, are generally characterised by high interaction among factors and important non-linearity. Therefore, the transferability of the knowledge acquired in other modelling fields in terms of GSA application may be limited.

The above review points out that, in the wastewater field, the features of GSA methods have not been investigated much. Indeed wastewater models are mostly complex models (i.e. models characterised by about 100 model factors and easily hundreds of variables and tens of model outputs). For such complex dynamic and stiff models that take a lot of computation time to solve, a modeller is much more interested in limiting the number of simulations than for simple models. The need of limiting the number of simulations in the case of complex models is in contrast with the application of GSA methods that require a higher number of simulations than local methods. Moreover, as far as the authors are aware a comprehensive comparison among the GSA methods for complex biological models, such in the case of ASM used in the wastewater field, has never been performed. In addition, as highlighted by the few studies dealing with convergence of sensitivity index of GSA (e.g. Nossent et al., 2011; Yang, 2011; Nossent and Bauwens, 2012), the high required number of simulations in the case of complex biological models makes it difficult to run a convergence analysis (Benedetti et al., 2011).

The objective of this paper is to provide a comprehensive comparison of the most common methods used for assessing model output sensitivity (both in terms of factors prioritisation and factors fixing) for ASM-type models. This comparison highlights the advantages and disadvantages of each method when used in the wastewater field. The methods have been used by employing numerical settings as suggested in literature.

Three sensitivity analysis techniques are compared:

1. the SRC method as proposed by Saltelli et al. (2008);
2. the Morris screening method as modified by Campolongo et al. (2007);
3. the Extended-FAST method proposed by Saltelli et al. (1999).

Common criteria for the comparison have been established below. With regards to the sensitivity threshold for the

identification of the important model parameters a comparable threshold among methods has been identified according to the definition of each sensitivity measure.

An integrated ASM2d-SMP-P model was employed for the method comparison using the water quality data of a University of Cape Town membrane bioreactor (UCT-MBR) pilot plant (Cosenza et al., 2013b).

A detailed analysis of the physical interpretation of sensitivity analysis for the pilot plant under study is provided in Cosenza et al. (2013c).

2. Materials and methods

2.1. The MBR model and case study

The GSA methods are compared for an integrated ASM2d-SMP-P model (Cosenza et al., 2013b). The model couples the biological ASM2d-SMP model (formerly introduced by Jiang et al., 2008) with a physical model derived from Di Bella et al. (2008) and Mannina et al. (2010, 2011b). The model allows simulating the biological nutrient removal processes, the soluble microbial products (SMPs) formation/degradation and the cake layer formation. The biological sub-model simulates the main biological processes that take place and it involves 19 model state variables and 73 factors (kinetic, stoichiometric and fractionation related). The physical sub-model, which is characterised by 2 state variables and 6 factors, simulates the formation of the cake layer on the membrane surface, thus taking into account the membrane fouling. This sub-model also takes into account a further reduction of effluent pollution due to the formation of the cake layer that acts as an additional filter.

Table 1 summarises the identifier, symbol, unit, variation range and literature references of each of the model parameters.

For a detailed description of the parameters the reader is referred to Henze et al. (2000), Di Bella et al. (2008), Jiang et al. (2008), Mannina et al. (2011b) and Cosenza et al. (2013b).

The analysis is conducted for a pilot plant with a UCT-MBR scheme, 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 the following samples were obtained: composite influent wastewater samples (section 0), grab mixed liquor samples in each tank (i.e. anaerobic, anoxic, aerobic and MBR tank, respectively, 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, $\text{NH}_4\text{-N}$, $\text{NO}_2\text{-N}$, $\text{NO}_3\text{-N}$, N_{TOT} , P_{TOT} (APHA, 1998). Further details about the model, pilot plant and sampling campaign can be found in Cosenza et al. (2013a,b) 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 and Viviani, 2009a,b; Mannina et al., 2011a). Four different sections of the UCT-MBR plant were considered, in particular, the anaerobic tank (section 1), anoxic tank (section 2), aerobic tank (section 3) and permeate tank (section 5). Model outputs are defined as the average values of the 165 days of simulated time series. Twenty-one model outputs were taken into account for the GSA: COD_{TOT} , S_{NH_4} , S_{NO_2} , S_{PO} for all 5 sections, MLSS for sections 1–3, COD_{SOL} (COD soluble) for section 3, and CTN (total nitrogen) for section 5. Seventy-nine model factors were considered for the GSA (see Table 1).

2.2. Standardised 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 output and the factors considered (Eq. (1)):

$$y = b_0 + \sum_{i=1}^n b_i \cdot x_i + \varepsilon \quad (1)$$

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 SRCs are the standardised regression slopes:

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

where σ_{x_i} and σ_y represent respectively the factor and the model output standard deviation. A high absolute value of β_i indicates a relevant effect of the related i th factor on the model output. The sign of β_i indicates its positive (sign +) or negative (sign –) effect (Saltelli et al., 2004). For linear models $\sum \beta_i^2 = 1$, otherwise this sum which represents the model coefficient of determination R^2 is lower than 1 (Saltelli et al., 2008).

SRCs are valid measures of sensitivity when, as suggested by Saltelli et al. (2004), the coefficient of determination R^2 , which indicates the portion of total variance explained by the regression model, is greater than 0.7. The SRC method explores only the 1st order effects and does not provide any information about the interaction among factors. Therefore, by means of the SRC method the important (factors prioritisation) and non-influential (factors fixing) factors may be correctly distinguished only in case of linear models. Otherwise the SRC method can be applied only in terms of factors prioritisation.

The required number of simulations found in literature is generally between 500 and 1000 (Neumann, 2012).

2.3. Morris screening method

The Morris screening method provides a measure of sensitivity by computing multiple Elementary Effects (EEs). An EE of the i th factor (EE_i) represents the relative difference between the model output obtained after perturbation of the i th factor by Δ , $y(x_1, \dots, x_{i-1}, x_i + \Delta, x_{i+1}, \dots, x_n)$, and the model output obtained without factor perturbation, $y(x_1, \dots, x_n)$.

$$EE_i(x_1, \dots, x_n, \Delta) = \frac{y(x_1, \dots, x_{i-1}, x_i + \Delta, x_{i+1}, \dots, x_n) - y(x_1, \dots, x_n)}{\Delta} \quad (3)$$

where Δ is a value in $\{1/(p-1), \dots, 1-1/(p-1)\}$ and p is the number of levels. Each of the n factors is partitioned into p levels, and the (x_1, \dots, x_n) vector is sampled from a hyperspace which is a n -dimensional p -level grid. EE is computed, for each factor r times (replicates) at different locations in factor space. In order to facilitate the comparison between Morris Screening and the other methods both model outputs (y) and model factors (x) are centred (to the mean) and scaled (divided by standard deviation) to obtain the sensitivity indices. For each factor, the measure of sensitivity is summarised by the mean (μ) and the standard deviation (σ) of the r EEs. μ is a measure of the importance of the factor in determining model output uncertainty whereas σ indicates if the factor is responsible for introducing non-linearity or interactions. A high value of σ means that the model output variation is influenced by non-linearity or interactions. Thus, the Morris screening method is able to detect the interaction among factors (IF) by means of σ . As proposed by Campolongo et al. (2007), in order to avoid the problem of the effects of opposite signs of the EEs, it is better to refer to the mean (μ^*) of the absolute elementary effects. Factors having μ^* greater than an established threshold value are considered to be important. All factors with μ^* lower than an established threshold value are non-influential. The line $\mu^*_{ij} = +2\sigma_i/\sqrt{r}$, where σ_i/\sqrt{r} represents the standard error of the mean, provides information about the factor effect on model output. Factors which lie below this line have a non-linear effect or are involved in interactions (Morris, 1991).

According to the Morris design (Morris, 1991) the required number of simulations is equal to $r^*(n+1)$ as suggested by Campolongo et al. (2007). Typical numbers are $r = 10\text{--}20$ and $p = 4\text{--}8$ (Campolongo et al., 2007).

2.4. 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 ($\text{Var}(Y)$) can 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 $\text{Var}(Y)$ without taking into account the interactions with other factors. It is expressed as:

$$S_i = \frac{\text{Var}_{x_i}(E_{x_i}(Y|x_i))}{\text{Var}(Y)} \quad (4)$$

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:

$$S_{Ti} = 1 - \frac{\text{Var}_{x_i}(E_{x_i}(Y|x_{-i}))}{\text{Var}(Y)} \quad (5)$$

The higher the S_i is, the higher is the influence of the input factor in terms of factor prioritisation. The difference between S_{Ti} and S_i represents the interaction among factors (IF). It is important to underline that in the context of factors fixing (determining the non-influential factors) the analysis of S_{Ti} has to be performed. If the S_i value is small it doesn't mean that the factor may be fixed anywhere within its range because a high S_{Ti} value would indicate that the factor is involved in interactions. Thus only factors with low S_i and low interaction ($S_{Ti} - S_i$) may be classified as non-influential.

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

Table 1
Number of factor order, symbol, unit of measure, variation range and literature references for each model factor.

Factor order	Symbol	Description	Unit	MIN	MAX	Reference
1	k_H	Maximum specific hydrolysis rate	$g X_S g X_H^{-1} d^{-1}$	1.5	4.5	Brun et al., 2002
2	$\eta_{NO_3, HYD}$	Correction factor for hydrolysis under anoxic conditions	–	0.402	0.798	Hauduc et al., 2011
3	η_{FE}	Correction factor for hydrolysis under anaerobic conditions	–	0.2	0.6	Hauduc et al., 2011
4	K_O	Half saturation parameter for SO_2 for X_H	$g SO_2 m^{-3}$	0.1	1	Weijers and Vanrolleghem, 1997
5	K_{NO_3}	Half saturation parameter for S_{NO_3} for X_H	$g S_{NO_3} m^{-3}$	0.1	0.625	Weijers and Vanrolleghem, 1997; Brun et al., 2002
6	K_X	Half saturation parameter for X_S/X_H	$g X_S g X_H^{-1}$	0.05	0.15	Brun et al., 2002
7	$K_{O, HYD}$	Half saturation/inhibition parameter for SO_2	$g SO_2 m^{-3}$	0.1	0.3	Brun et al., 2002
8	$K_{NO_3, HYD}$	Half saturation/inhibition parameter for S_{NO_3}	$g N m^{-3}$	0.375	0.625	Brun et al., 2002
9	μ_H	Maximum growth rate of X_H	d^{-1}	0.6	13.2	Jeppsson, 1996
10	q_{FE}	Rate constant for fermentation/Maximum specific fermentation growth rate	$g S_F g X_H^{-1} d^{-1}$	1.5	4.5	Brun et al., 2002
11	$\eta_{NO_3, H}$	Reduction factor for anoxic growth of X_H	–	0.6	1	Brun et al., 2002
12	b_H	Decay rate for X_H	d^{-1}	0.05	1.6	Jeppsson, 1996
13	K_F	Half saturation parameter for S_F	$g S_F m^{-3}$	2	6	Brun et al., 2002
14	K_{FE}	Half saturation parameter for fermentation of S_F	$g S_F m^{-3}$	2	6	Brun et al., 2002
15	K_A	Half saturation parameter for S_A	$g S_A m^{-3}$	2	6	Brun et al., 2002
16	$K_{NH_4, H}$	Half saturation parameter for S_{NH_4} for X_H	$g S_{NH_4} m^{-3}$	0.02	2	Weijers and Vanrolleghem, 1997
17	K_P	Half saturation parameter for S_{PO_4} for X_H	$g S_{PO_4} m^{-3}$	0.005	0.015	Brun et al., 2002
18	$K_{ALK, H}$	Half saturation parameter for S_{ALK} for X_H	$mol HCO_3^- m^{-3}$	0.05	0.15	Brun et al., 2002
19	q_{PHA}	Rate constant for S_A uptake rate	$g X_{PHA} g X_{PAO}^{-1} d^{-1}$	0.3	5.7	Hauduc et al., 2011
20	q_{PP}	Rate constant for storage of polyphosphates	$g X_{PP} g X_{PAO}^{-1} d^{-1}$	0	3.3	Hauduc et al., 2011
21	μ_{PAO}	Maximum growth rate of X_{PAO}	d^{-1}	0.5	1.5	Brun et al., 2002
22	$\eta_{NO_3, PAO}$	Reduction factor for anoxic growth of X_{PAO}	–	0.45	0.75	Brun et al., 2002
23	b_{PAO}	Endogenous respiration rate of X_{PAO}	d^{-1}	0.1	0.25	Henze et al., 2000; Hauduc et al., 2011
24	b_{PP}	Rate constant for lysis of polyphosphates	d^{-1}	0.1	0.25	Henze et al., 2000; Hauduc et al., 2011
25	b_{PHA}	Rate constant for respiration of X_{PHA}	d^{-1}	0.1	0.25	Henze et al., 2000; Hauduc et al., 2011
26	K_{PS}	Half saturation parameter for S_{PO_4} uptake	$g S_{PO_4} m^{-3}$	0.1	0.3	Brun et al., 2002
27	K_{PP}	Maximum ratio of X_{PP}/X_{PAO}	$g X_{PP} g X_{PAO}^{-1}$	0.005	0.015	Brun et al., 2002
28	K_{MAX}	Half saturation parameter for X_{PP}/X_{PAO}	$g X_{PP} g X_{PAO}^{-1}$	0.2	0.51	Rieger et al., 2001
29	K_{IPP}	Half inhibition parameter for X_{PP}/X_{PAO}	$g X_{PP} g X_{PAO}^{-1}$	0.01	0.03	Brun et al., 2002
30	K_{PHA}	Saturation constant for X_{PHA}/X_{PAO}	$g X_{PHA} g X_{PAO}^{-1}$	0.005	0.015	Brun et al., 2002
31	$K_{O, PAO}$	Half saturation parameter for SO_2 for X_{PAO}	$g SO_2 m^{-3}$	0.1	0.3	Brun et al., 2002
32	$k_{NO_3, PAO}$	Half saturation parameter for S_{NO_3} for X_{PAO}	$g S_{NO_3} m^{-3}$	0.375	0.625	Brun et al., 2002
33	$K_{A, PAO}$	Half saturation parameter for S_A for X_{PAO}	$g S_A m^{-3}$	2	6	Brun et al., 2002
34	$K_{NH_4, PAO}$	Half saturation parameter for S_{NH_4} for X_{PAO}	$g S_{NH_4} m^{-3}$	0.025	0.075	Brun et al., 2002
35	$K_{P, PAO}$	Half saturation parameter for S_{PO_4} as nutrient (X_{PAO} growth)	$g S_{PO_4} m^{-3}$	0.005	0.015	Brun et al., 2002
36	$K_{ALK, PAO}$	Half saturation parameter for S_{ALK} for X_{PAO}	$mol HCO_3^- m^{-3}$	0.05	0.15	Brun et al., 2002
37	μ_{AUT}	Maximum growth rate of X_{AUT}	d^{-1}	0.2	1.2	Weijers and Vanrolleghem, 1997
38	b_{AUT}	Decay rate for X_{AUT}	d^{-1}	0.04	0.1605	Hauduc et al., 2011
39	$K_{O, A}$	Half saturation parameter for SO_2 for X_{AUT}	$g SO_2 m^{-3}$	0.1	2	Weijers and Vanrolleghem, 1997; Jeppsson, 1996
40	$K_{NH_4, A}$	Half saturation parameter for S_{NH_4} for X_{AUT}	$g S_{NH_4} m^{-3}$	0.5	1.5	Hauduc et al., 2011
41	$K_{ALK, A}$	Half saturation parameter for S_{ALK} for X_{AUT}	$mol HCO_3^- m^{-3}$	0.25	0.75	Brun et al., 2002
42	$K_{P, A}$	Half saturation parameter for S_{PO_4} for X_{PAO}	$g S_{PO_4} m^{-3}$	0.005	0.015	Brun et al., 2002
43	$k_{H, BAP}$	Hydrolysis rate coefficient for S_{BAP}	d^{-1}	3.705E-07	1.1115E-06	Jiang et al., 2008
44	$k_{H, UAP}$	Hydrolysis rate coefficient for S_{UAP}	d^{-1}	0.0051	0.0153	Jiang et al., 2008
45	$k_{LaT, 3}$	Overall oxygen transfer coefficient aerobic tank	h^{-1}	9.5	10.5	Innocenti, 2005
46	$k_{LaT, 4}$	Overall oxygen transfer coefficient MBR tank	h^{-1}	3.23	3.57	Innocenti, 2005
47	Y_H	Yield for X_H growth	$g X_H g X_S^{-1}$	0.38	0.75	Jeppsson, 1996
48	f_{X_i}	Fraction of X_i generated in biomass decay	$g X_i g X_H^{-1}$	0.05	0.4	Weijers and Vanrolleghem, 1997
49	Y_{PAO}	Yield for X_{PAO} growth	$g X_{PAO} g X_{PHA}^{-1}$	0.42	0.78125	Brun et al., 2002
50	Y_{PO_4}	Yield for X_{PP} requirement per X_{PHA} stored	–	0.38	0.42	Brun et al., 2002
51	Y_{PHA}	Yield for X_{PP} storage per X_{PHA} utilised	$g X_{PP} g X_{PHA}^{-1}$	0.19	0.21	Brun et al., 2002
52	Y_A	Yield of X_{AUT} growth per S_{NO_3}	$g X_{AUT} g S_{NO_3}^{-1}$	0.228	0.252	Brun et al., 2002
53	f_{BAP}	Fraction of S_{BAP} generated in biomass decay	–	0.0069	0.022575	Brun et al., 2002
54	f_{UAP}	Fraction of S_{UAP} generated in biomass decay	–	0.091485	0.101115	Brun et al., 2002
55	F_{S_F}	Fraction of influent S_F	–	0.06	0.18	Brun et al., 2002
56	F_{S_A}	Fraction of influent S_A	–	0.04	0.12	Brun et al., 2002
57	F_{S_i}	Fraction of influent S_i	–	0.114	0.126	Brun et al., 2002
58	F_{X_i}	Fraction of influent X_i	–	0.05	0.15	Brun et al., 2002
59	F_{X_H}	Fraction of influent X_H	–	0.06	0.18	Brun et al., 2002

Table 1 (continued)

Factor order	Symbol	Description	Unit	MIN	MAX	Reference
60	β	Erosion rate coefficient of the dynamic sludge	–	1.00E-04	2.10E-02	Mannina et al., 2011b
61	α	Stickiness of the biomass particles	–	0	1	Mannina et al., 2011b
62	γ	Compressibility of cake	kg m ⁻³ s	5.56E-04	2.78E-03	Mannina et al., 2011b
63	f	Substrate fraction below the critical molecular weight	–	0.001	0.99	Mannina et al., 2011b
64	λ	Screening parameter	m ⁻¹	1000	2.00E+03	Mannina et al., 2011b
65	C_E	Efficiency of backwashing	–	0.996	0.999	Mannina et al., 2011b
66	i_{N,S_i}	N content of S_i	g N g S_i^{-1}	0.0075	0.0125	Brun et al., 2002
67	i_{N,S_F}	N content of S_F	g N g S_F^{-1}	0.0225	0.0375	Brun et al., 2002
68	i_{N,X_i}	N content of X_i	g N g X_i^{-1}	0.015	0.025	Brun et al., 2002
69	i_{N,X_S}	N content of X_S	g N g X_S^{-1}	0.03	0.05	Brun et al., 2002
70	$i_{N,BM}$	N content of biomass	g N g X_{BM}^{-1}	0.0665	0.0735	Brun et al., 2002
71	i_{P,S_F}	P content of S_F	g P g S_F^{-1}	0.005	0.015	Brun et al., 2002
72	i_{P,X_i}	P content of X_i	g P g X_i^{-1}	0.005	0.015	Brun et al., 2002
73	i_{P,X_S}	P content of X_S	g P g X_S^{-1}	0.005	0.015	Brun et al., 2002
74	$i_{P,BM}$	P content of biomass	g P g X_{BM}^{-1}	0.015	0.025	Brun et al., 2002
75	i_{TSS,X_i}	Conversion factor X_i in TSS	g TSS g X_i^{-1}	0.7125	0.7875	Brun et al., 2002
76	i_{TSS,X_S}	Conversion factor X_S in TSS	g TSS g X_S^{-1}	0.7125	0.7875	Brun et al., 2002
77	$i_{TSS,BM}$	Conversion factor biomass in TSS	g TSS g X_{BM}^{-1}	0.855	0.945	Brun et al., 2002
78	$i_{TSS,X_{PHA}}$	Conversion factor X_{PHA} in TSS	g TSS g X_{PHA}^{-1}	0.57	0.63	Brun et al., 2002
79	$i_{TSS,X_{PP}}$	Conversion factor X_{PP} in TSS	g TSS g X_{PP}^{-1}	3.0685	3.3915	Brun et al., 2002

2.5. Factors classification, simulation conditions and numerical settings for GSA methods

The thresholds for the assessment of the important factors were chosen according to previous studies (Sin et al., 2011). In particular, the threshold value of 0.1 was employed for the absolute value of β_i and for μ^* whereas 0.01 was used for S_i . The choice of the threshold value of 0.01 for S_i is related to the fact that for a linear model $S_i = \beta_i^2$. All factors having μ^* lower than 0.1 have been considered non-influential for the Morris screening application. For each model output, the non-influential factors for Extended-FAST have been classified on the basis of a normalised index (S_{Ni}), introduced in this paper and defined as:

$$S_{Ni} = \frac{S_{Ti} - S_i}{\max(S_{Ti} - S_i)} \quad (6)$$

where $S_{Ti} - S_i$ represents the interaction of the i -th model parameter related to one model output, while $\max(S_{Ti} - S_i)$ represents the maximum value among the interactions for that model output. The main reason for using the normalised index is related to the fact that the several model outputs (21) have different behaviour in terms of total order effect because the interaction is quite different. Thus, for comparing results we need to deal with a normalised index of the interaction with respect to the maximum value of the interaction for each model output. By applying this procedure it is possible to fix the same threshold for all model outputs and at least one factor will be classified as factor with high interaction for each model output (Weijers and Vanrolleghem, 1997). All model factors for which S_{Ni} is lower than 0.6 are classified as non-influential factors.

For the discussion of the results in terms of degree of model linearity the following coefficients were analysed: the linear model determination coefficients (R^2) and the sum of the squares of the standardised regression coefficients $S_{Ni} = S_{Ti} - S_i / \max(S_{Ti} - S_i)$ for the SRC method; the average of the standard deviations on the total number of model factors ($\sum \sigma_i / n$) (which provides an average order of magnitude of the interaction/non-linearity among factors for each model output) for the Morris screening method; the sum of the first order indices ($\sum \beta_i^2$) and the averaged interaction $\sum (S_{Ti} - S_i) / n$ for the Extended-FAST method.

Each of the three GSA methods was applied considering a uniform distribution for all factors. The ranges of the values are listed in Table 1.

For each method the number of simulation runs was established on the basis of literature recommendations (Morris, 1991; Saltelli, 2000; Saltelli et al., 2004; Campolongo et al., 2007).

In order to apply the Extended-FAST method 39,500 model runs were conducted corresponding to 500 simulations for each factor. For the SRC method application 800 model runs were carried out using Latin Hypercube Sampling. The Morris screening application was performed using levels $p = 5$, perturbation factor $\Delta = 2/3$, replicates $r = 10$ and running 800 model simulations.

2.6. Comparison of the sensitivity analysis methods

The sensitivity techniques are based on different philosophies and hypotheses as also pointed out in the literature (Yang, 2011). We make the comparison by considering the most reliable method (Extended-FAST) as the reference method.

The main features of GSA methods we are interested in are:

- a. similarity of sensitivity indices compared to the reference method (factors prioritisation);
- b. similarity of ranking of sensitivity indices compared to the reference method (factors prioritisation);
- c. similarity of classification into important/non-influential factors compared to the reference method (factors prioritisation and factors fixing);
- d. methods' capability to detect interaction among factors;
- e. methods' ability to provide results in a reasonable time.

In order to perform the comparison the following criteria have been considered:

- i) Pearson correlation r_p between sensitivity indices (feature a) varying between -1 (high negative correlation) and 1 (high positive correlation), in case $r_p = 0$ no correlation exists;
- ii) Spearman's ρ_s rank correlation index computed on the sensitivity indices (feature b), providing a measure of statistical dependence between two variables and varying between -1 and $+1$. For ρ_s equal to 1 or -1 the variables are perfectly monotonically related (the sign of ρ_s represents the positive or negative relation of dependence);
- iii) Modified position factor (PF) (Ruano et al., 2012) (feature b). The PF related to the comparison of the position ranking order obtained for the n factors by applying two different methods (i and j) is defined as (Ruano et al., 2012):

$$PF = \sum_{k=1}^n \frac{|P_{k,i} - P_{k,j}|}{\mu_{P_{k,i}, P_{k,j}}} \quad (7)$$

where $P_{k,i}$ and $P_{k,j}$ respectively represent the position of the k -th factor in the ranking obtained by applying method i and j respectively and $\mu_{P_{k,i}, P_{k,j}}$ is the average of $P_{k,i}$ and $P_{k,j}$. PF quantifies the differences among the factors ranking. PF is null in case the ranking of all factors is the same. PF is maximum in case the ranking of all factors is completely different for the two different methods. For example, for $n = 3$ and $P_{1,i} = 1, P_{2,i} = 2, P_{3,i} = 3$ the maximum value of PF occurs when $P_{1,j} = 3, P_{2,j} = 1, P_{3,j} = 2$. For 79 factors the maximum value of PF is 81.84. The minimum, maximum and average values of PF, computed over all model outputs, have been analysed for the comparison.

- iv) relevance (Rel) (feature c) varies between 0 (no model factor is important or non-influential) and 1 (all model factors are important or non-influential) (Beck et al., 1997; Saltelli et al., 2008). Rel represents an integral criterion taking into account all model outputs at the same time. One factor is considered important (or non-influential) if it is important (or non-influential) for at least for one variable.

$$Rel = \frac{\text{number of important/non-influential factors}}{\text{total number of factors}} \quad (8)$$

- v) number of simulations (NS) (feature e);
- vi) visual comparisons of scatter plots of sensitivity indices (feature a);
- vii) Venn Diagrams to visualise classification into important or non-influential (feature c).

In the sequel, details on how these criteria are used to assess the five features are provided.

2.6.1. Similarity of sensitivity indices compared to the reference method (feature a, factors prioritisation)

For the present case study the comparison in terms of similarity of sensitivity indices has been performed by Pearson correlation (i) and visually by means of scatter plots (criterion vi). Specifically, in order to perform the comparison in terms of similarity of sensitivity indices, as suggested in the literature (Campolongo et al., 2007; Saltelli et al., 2008), the comparison between SRC and Extended-FAST results has been carried out by comparing β_i^2 and S_i values as β_i^2 represents a linear approximation of S_i . The comparison between Morris screening and Extended-FAST has been done by comparing μ^* and S_{Ti} values. Moreover Campolongo et al. (2007) have shown that μ^* is a good indicator of S_{Ti} (Saltelli et al., 2008). The Pearson correlation coefficient r_p (i) is therefore evaluated for the comparisons β_i^2 vs S_i and μ^* vs S_{Ti} and the scatter plots (vi) are assessed for β_i^2 vs S_i and μ^* vs S_{Ti} .

2.6.2. Similarity of ranking of sensitivity indices compared to the reference method (feature b, factors prioritisation)

The analysis of the similarity of ranking of sensitivity indices has been performed by means of Spearman's ρ_s rank correlation (ii) and modified position factor (PF) (iii).

Specifically, in order to perform the comparison in terms of ranking between SRC and Extended-FAST, both ρ_s and PF have been computed considering, for each factor, the ranking position associated to the absolute value of β_i and to the S_i value. Conversely, the comparison between Morris Screening and Extended-FAST has been performed by calculating ρ_s and PF on the basis of the ranking position due to μ^* and S_i values.

2.6.3. Similarity of classification into important/non-influential factors

The comparison in terms of similarity of classification into important and non-influential factors has been performed numerically by quantifying the *Rel* criterion value for each method (criterion iv) and also by analysing Venn diagrams (criterion vii). *Rel* of important factors for the comparison between SRC and Extended-FAST has been calculated considering the factors that resulted to be important at least for one of the variables taken into account according to the values of $|\beta_i|$ and S_i . The comparison of Morris screening and Extended-FAST in terms of factors fixing has been performed by computing the *Rel* of non-influential factors ($Rel_{NON-INFLUENTIAL}$) considering all factors that were non-influential for at least one variable according to the values of μ^* and S_{Ni} .

2.6.4. Methods' capability to detect interaction among factors

The methods' capability to detect interaction among factors is a feature of the methods. As known by literature SRC and Morris screening do not provide the possibility of quantifying interaction among factors. However, Morris screening method provides qualitative information about factors involved in interactions or inducing non-linearity. Conversely, with the Extended-FAST method it is possible to quantify the interaction among factors by means of the difference between S_{Ti} and S_i .

2.6.5. Methods' ability to provide results in a reasonable time

The comparison in terms of simulation time required has been performed on the basis of the required number of simulations (NS).

3. Results and discussion

3.1. Extended-FAST (reference method)

Fig. 1 summarises the important factors for each subgroup of output variables (on the basis of $S_i > 0.01$ for at least one of the variables in each subgroup) in terms of factor prioritisation, with regard to Extended-FAST (see Table 1 for the detailed results).

In Cosenza et al. (2013c) an in-depth analysis of these results is presented and the knowledge gains as well as the implications for modelling the current system are discussed. In the following section we highlight the main results for $COD_{TOT,1}$, $S_{PO_{4,1}}$, $S_{NO_{3,2}}$, $S_{PO_{4,3}}$ and $COD_{TOT,5}$ (the numbers in the subscript indicate the plant sections where the output is measured). These variables have been selected as representative of the main processes occurring in each reactor. For instance, in the anaerobic tank the most important process is the release of phosphorus by the PAO organisms. Therefore, for the anaerobic tank, the COD and S_{PO} are the model state variables that are expected to vary the most. Similar considerations have been used for the other tanks.

The following factors are important for $COD_{TOT,1}$: $\{\mu_H, f, b_H, K_H, C_E\}$ (see Fig. 1a and Appendix 1). The influence of the factors related to the physical separation process $\{f, C_E\}$ is mainly due to the recycled sludge fluxes from tank to tank. In particular, the influence of the parameter f on $COD_{TOT,1}$ can be attributed to the fact that with increasing f a decrease in $COD_{TOT,5}$ concentration takes place which is propagated throughout the system. The sum of the first order effect indices S_i explains 57% of the total variance indicating that the model is non-linear and/or non-additive. A high degree of interaction occurs for important factors indicated by the sum of S_{Ti} for this variable (11.42). For $COD_{TOT,1}$ the model factors with S_{Ni} greater than 0.6 are also important in terms of S_i value. Such result confirms that for $COD_{TOT,1}$ the degree of interaction among the important factors in terms of S_i is high. It is mainly due to the fact that the biological processes occurring in the section 1 have a slight influence on the $COD_{TOT,1}$ concentration.

The following factors are important for $COD_{TOT,5}$: $\{f, \mu_H, b_H, K_{NH,H}, \mu_{AUT}, k_H, C_E\}$ (see Fig. 1a and Appendix 1). The importance of these factors is consistent with the modeller's experience. Indeed, this factor set shows the impact of the heterotrophic biomass activity and of the membrane separation on the $COD_{TOT,5}$ concentration. Indeed, the fact that factor f was the most important factor for $COD_{TOT,5}$ was attributed to the higher influence of physical separation for permeate than for the other sections. Even though factors α and γ , both related to the physical sub-model, are not classified as being important due to the low value of S_i (0.0079 and 0.0014, respectively), they cannot be fixed anywhere in their variation range due to their high S_{Ti} value (0.25 and 0.24, respectively). Indeed, the S_{Ni} value of factors α and γ is equal to 0.610 and 0.601 respectively. Thus, in terms of factor fixing factors α and γ cannot be considered non-influential.

The following factors were found to have a significant impact on $S_{NO_{3,2}}$ in terms of S_i value: $\{\mu_H, Y_H, b_H, k_H, f_{X_1}, \eta_{NO_{3,HYD}}, F_{SF}\}$ (see Fig. 1c and Appendix 1). Among the important factors, for $S_{NO_{3,2}}$ factors μ_H and Y_H are directly connected to the anoxic growth of heterotrophic organisms on acetate and fermentable substrate. Thus μ_H and Y_H influence the S_{NO_3} concentration inside the anoxic tank. 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 showing some interaction among factors.

For $S_{PO_{4,1}}$ the following factors appear to have a significant impact on the basis of S_i : $\{b_H, q_{PHA}, q_{PP}, Y_H, k_H, f_{X_1}, \eta_{FE}, \mu_H, \mu_{AUT}, F_{SF}, K_O, \mu_{PAO}, F_{X_1}, F_{SA}, i_{N,X,S}, K_{NH,H}\}$ (see Fig. 1d and Appendix 1). Among these factors, q_{PHA} is certainly the most important from a process point of view since it influences the storage of X_{PHA} (poly-hydroxy alkanooates and organic storage polymer) which occurs in the anaerobic tank. The impact of the factors b_H, f_{X_1} and η_{FE} is related to the fact that these three factors influence the lysis of PAO and of slowly biodegradable substrate. Moreover, due to the fact that S_{Ni} is greater than 0.6 and their high interaction contribution (always higher than $IF = 0.14$), the following factors cannot be fixed everywhere in their range: $\{K_{O,A}, K_{NH,A}, K_{P,A}, K_{H,BAB}, K_{H,UAB}, Y_{PAO}\}$ even though they are not important in terms of factors prioritisation (see Appendix 1). The sum of the first order indices for $S_{PO_{4,1}}$ explains 99% of the total variance (see Appendix 1) indicating that the model is almost linear and/or additive.

The following factors were found to have a significant impact on $S_{PO_{4,3}}$: $\{i_{P,X,S}, \mu_H, q_{PP}, b_{PAO}, i_{P,SF}, i_{P,X}, q_{PHA}, f_{X_1}, b_H, F_{SA}, k_H\}$ (see Fig. 1d and Appendix 1). Among them $\{i_{P,X,S}, \mu_H, b_{PAO}\}$ have high affinity with the biological process of phosphorus uptake which occurs in the aerobic tank. The factor $i_{P,X,S}$ influences the aerobic hydrolysis as well as the X_{PAO} lysis, which reduce the S_{PO_4} content in the aerobic tank. The factor b_{PAO} indirectly influences the phosphorus luxury uptake process by means of X_{PAO} lysis. S_{Ni} greater than 0.6 and a high interaction contribution (higher than 0.1) was also found for $\eta_{NO_{3,HYD}}, K_O, K_{NO_3}, K_{PHA}, K_{O,PAO}, K_{NO_3,PAO}, K_{NH,PAO}, \mu_{AUT}$ and $i_{TSS,X,S}$. For $S_{PO_{4,3}}$ the sum of S_i is equal to 0.63 (63% of model variance) and the sum of S_{Ti} is equal to 3.5, showing a poor linearity and/or interaction.

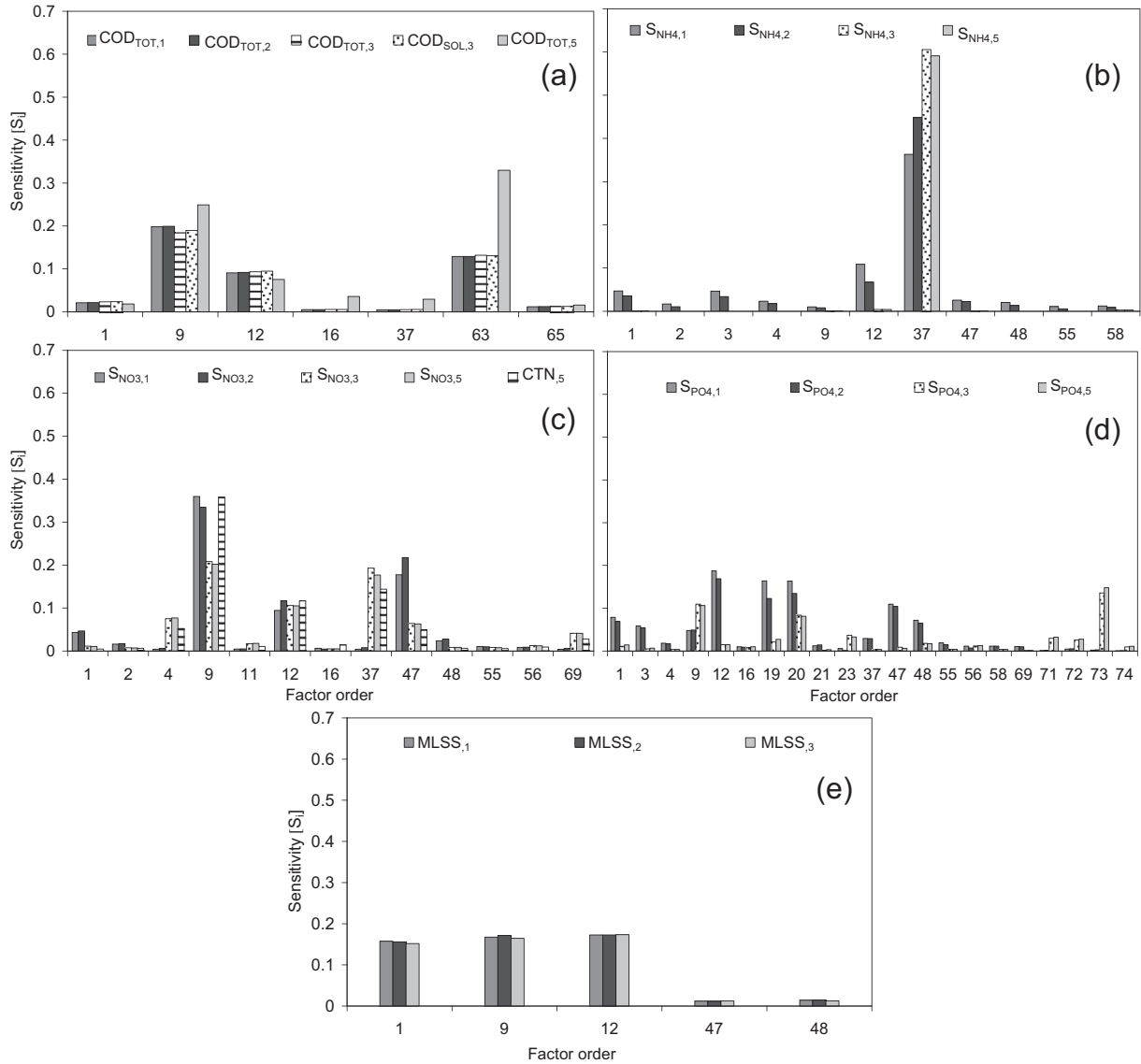


Fig. 1. Important model factors classified on the basis of S_i value according to the Extended-FAST method at least for one of the variables: COD_{TOT,1}, COD_{TOT,2}, COD_{TOT,3}, COD_{SOL,3} and COD_{TOT,5} (a); S_{NH4,1}, S_{NH4,2}, S_{NH4,3} and S_{NH4,5} (b); S_{NO3,1}, S_{NO3,2}, S_{NO3,3}, S_{NO3,5} and CTN₅ (c); S_{PO4,1}, S_{PO4,2}, S_{PO4,3} and S_{PO4,5} (d); MLSS₁, MLSS₂ and MLSS₃ (e).

In the next section we discuss how the two other methods, SRC and Morris Screening, are able to approximate these results obtained with Extended-FAST.

3.2. Comparison among methods

3.2.1. General results

Important model characteristics appear when analysing the summary Table 2 (and Appendix 1, 2 and 3):

- i) regarding the Extended-FAST results, model factors are almost always involved in interactions as shown above $\sum(S_{Ti}-S_i)$ ranges between 2.37 and 21.33. Compared to the $\sum S_i$ such values show that, despite $\sum S_i$ in some cases to be close to 1, the S_{Ti} is much greater than S_i (Table 2).
- ii) regarding the SRC results the R^2 values (0.23–0.49) for all model variables were found to be <0.7, which means that the SRC technique is applied outside its application range. The lower values of the R^2 compared to other applications of ASM

models (see for example Sin et al., 2011) could be due to the fact that in this work the investigated factor region is wider and/or a more complex model was studied (e.g. membrane processes, SMP, etc.).

- iii) for the Morris screening the important factors have a high positive value of σ (see Appendix 3) which is always greater than the value corresponding to the line $\mu^*_i = +2\sigma_i/\sqrt{r}$ (where r represents the repetition number). This indicates the presence of non-linearity or interactions for these factors. The total interaction among the factors calculated as the ratio between the sum of standard deviations and the total number of factors (n) ranges between 0.08 and 0.16. These values correspond to a sum of standard deviations respectively equal to 6.32 and 12.64 with highest contributions found for S_{PO} variables (Table 2).

3.2.2. Similarity of sensitivity indices compared to reference method (factors prioritisation)

Although the SRC method is found to be outside its range of applicability (R^2 is always <0.7) the high correlation between β_i^2 and

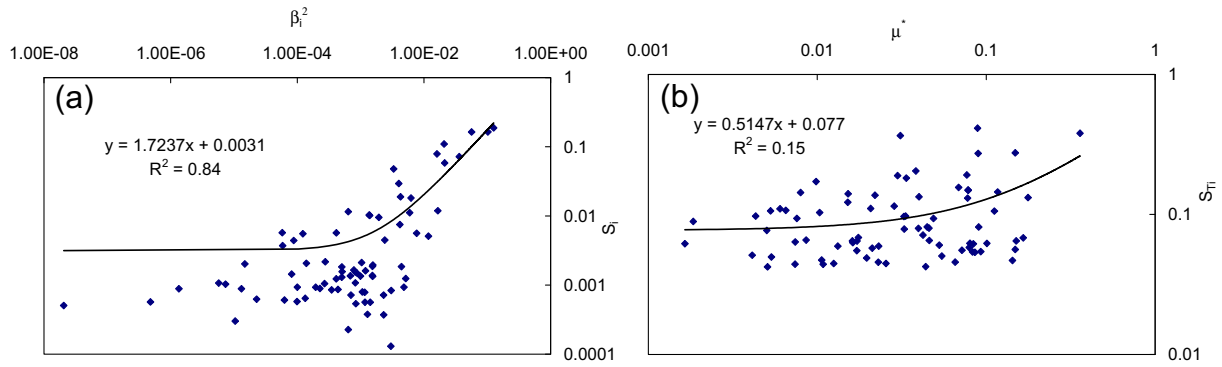


Fig. 2. Scatter plots, interpolating curves and equations of regressions obtained comparing S_i and β_i^2 and S_{Ti} and μ_i^* for $S_{PO_{4,1}}$ (a and b) (the axes are logarithmic).

ranking order is negative for a considerable number of variables (Table 3). Again, we thus find a poor ability of the Morris screening method to reproduce the results of Extended-FAST.

The comparison of the ranking of sensitivity indices with the reference method has also been done in terms of position factor PF (Table 4). The minimum, maximum and mean values of the position factor PF confirm the better correspondence between Extended-FAST and SRC than between Extended-FAST and Morris Screening. For comparing the similarity between Extended-FAST and SRC or Morris screening it seems better to use the Pearson correlation instead of the rank correlation as the modeller is generally not really interested in a good correspondence of the ranking of non-influential factors. Indeed, non-influential factors have too much influence in determining rank correlation. Moreover, the minimum maximum and average values of PF obtained by applying two different methods provide general information about the correspondence among ranking positions.

3.2.4. Similarity of classification into important/non-influential factors

Analysing the relevance values Rel for the case of important factors ($Rel_{IMPORTANT}$) reported in Table 4 one may observe that both SRC and Extended-FAST provide a similar number of globally important factors. Moreover, it is also evident that the Morris screening approach overestimates the number of important factors as demonstrated by the higher value of $Rel_{IMPORTANT} = 0.45$. $Rel_{NON-INFLUENTIAL}$ values related to the Morris screening (0.55) and Extended-FAST (0.24) methods show that the Morris screening method also overestimates the number of non-influential factors.

Fig. 3 shows the Venn diagrams for the comparison of the factor classification of the SRC (Fig. 3a) and Morris screening methods (Fig. 3b and c) with the results of Extended-FAST, for

$S_{PO_{4,1}}$ (in terms of important and non-influential factors). Very similar patterns are found for the other variables. In Fig. 3a one may observe that except for the factor no. 49 all model factors found to be important for SRC are also important for Extended-FAST. However, Extended-FAST detects a larger number of factors as being important which are not detected by SRC. This is probably due to the fact that the β_i^2 underestimate S_i and thereby, by using the same cut-off level, SRC will underestimate the number of important factors (Neumann, 2012). When comparing the results of Extended-FAST and Morris screening for $S_{PO_{4,1}}$ a poor consistency among the results was obtained in terms of factor prioritisation (Fig. 3b).

In terms of factors fixing Fig. 3c shows that for $S_{PO_{4,1}}$ a large fraction of non-influential factors are obtained by Extended-FAST and Morris screening methods. However, also in this case, the Morris screening method overestimates the number of non-influential factors. Such a result may have important consequences in case the Morris screening method is used for selecting factors to be calibrated in an ASM model as the case study presented here. Indeed, for $S_{PO_{4,1}}$ a subset of factors (17) that are non-influential according to Morris screening is important according to Extended-FAST. The disagreement between Morris screening and Extended-FAST results, as discussed above, is probably due to convergence issues. It is important to state that the presented results in terms of similarity of classification into important/non-influential factors depend on the threshold of the sensitivity measures selected for identifying the important/non-influential factors.

3.2.5. Capability of detecting interaction

By applying the three methods the knowledge acquired in literature concerning the ability of each method to detect interaction among factors has been confirmed. Despite, as known, the fact that the SRC method is unable to quantify interaction among factors, the non-linearity of the used ASM model is revealed by the low R^2 values (always lower than 0.7). For the Morris screening method the degree of interaction and/or non-linearity among factors has been provided by σ values that have always been greater than the value corresponding to the line $\mu_i^* = +2\sigma_i/\sqrt{r}$. The quantification of the interaction among factors has been performed by applying the Extended-FAST method which shows that the highest interaction among factors occurs for $S_{NH_4,1}$ as reported in Table 2 (last row).

3.2.6. Methods' ability to provide results in a reasonable time

When applying literature recommendations the highest number of simulations is required for the Extended-FAST method (39500) and thus SRC (800) is computationally more efficient than Extended-FAST (in the current case study by 1–2 orders of magnitude) ensuring a good agreement of the results in terms of factor prioritisation. The Morris screening method (with 800

Table 4
Criteria indices of the comparison among the sensitivity methods.

	Method		
	SRC	Morris screening	Extended-FAST
Methods' property			
CE	Medium	Medium	Low
IF	No	No	Yes
Criteria			
NS	800	800	39,500
$Rel_{IMPORTANT}^*$	0.3	0.45	0.32
$Rel_{NON-INFLUENTIAL}$	—	0.55	0.24
PF**	(44.02–58.73) 51.15	(49.64–63.60) 57.30	—

NS: number of simulation; CE: computational efficiency; R: relevance; IF: ability of the sensitivity analysis method to take into account the interaction among factors; PF: position factor among the factors respect to Extended-FAST results. (*) Computed on the basis of $|\beta_i|$, S_i or μ_i^* value; (**) (a–b) c for each factor means: (a–b) is the minimum and the maximum and c is the average value.

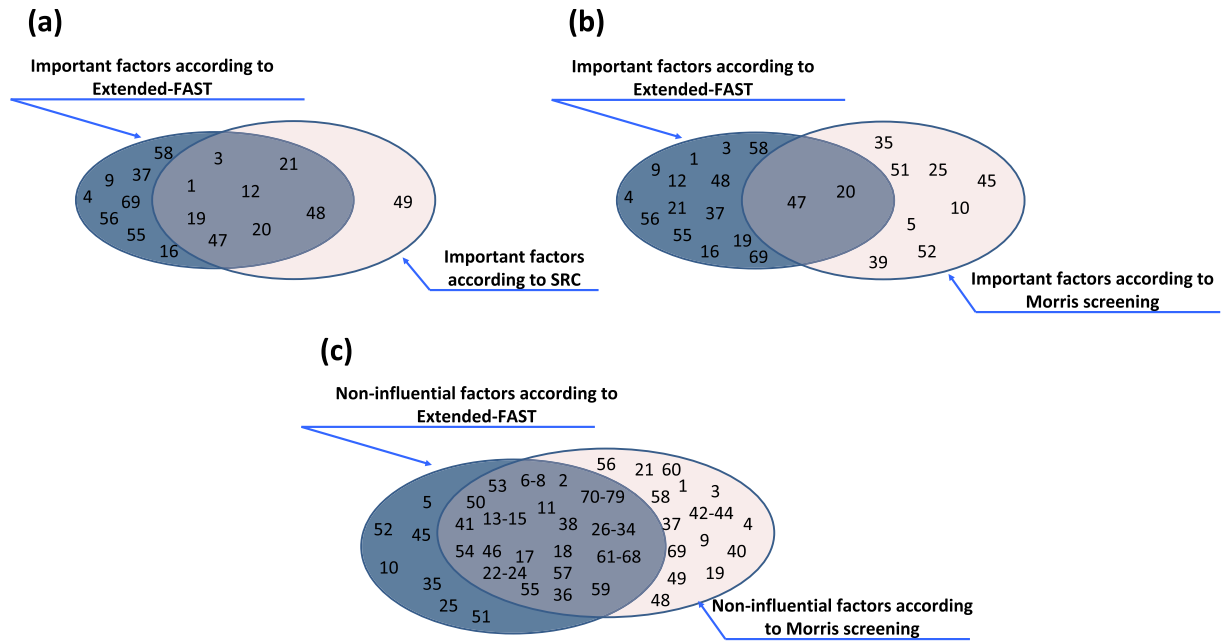


Fig. 3. Venn diagram related to the comparison of important and non-influential factors obtained by applying SRC and Morris screening with that of Extended-FAST for the model output $S_{PO_{4.1}}$; numbers refer to the factor order (according to Table 1). The important model factors reported in the Venn diagram have been classified on the basis of $|\beta_i|$ (for SRC), S_i (for Extended-FAST) and μ^* (for Morris screening).

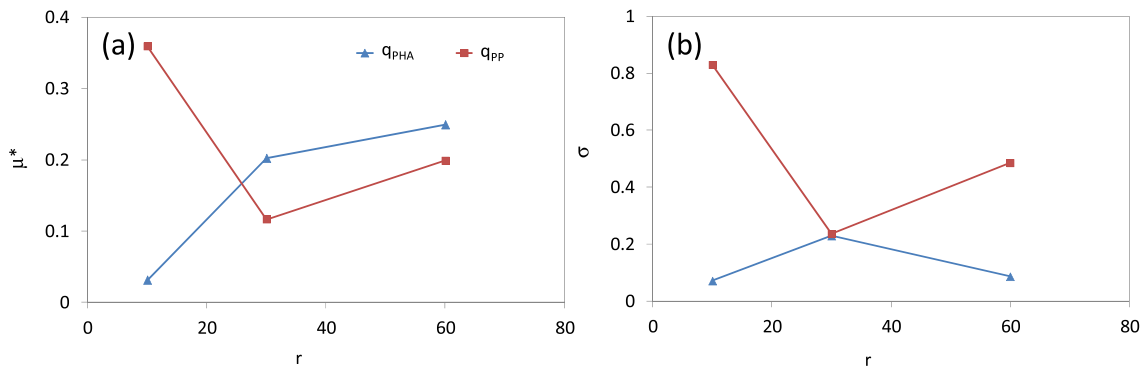


Fig. 4. Variability of μ^* (a) and σ (b) with the increase of the replication, r , in the Morris GSA method as applied to the factors q_{PHA} and q_{PP} for the variable $S_{PO_{4.1}}$.

simulations) seems to be efficient in terms of computational demand but doesn't provide reasonable results if applied using literature recommendations for the required number of replicates.

3.2.7. Convergence of Morris screening

As previously discussed the application of the Morris screening method, employing a number of replicates as suggested in the literature, leads to different results compared to SRC and Extended-FAST. This finding has been hypothesised to be due to the fact that convergence for the Morris method has not been achieved with the literature suggestion for the number of replicates. Even though a full analysis of this convergence issue is beyond the scope of this work, a further analysis has been performed in order to evaluate the effect of the number of replicates. In particular, three scenarios were analysed by changing the number of replicates r , equal to 10, 30 and 60. For all scenarios the number of levels was $p = 5$ and $\Delta = 2/3$. The results of each test in terms of sensitivity analysis index, μ^* (and σ), were compared in order to verify the stability of the sensitivity of each factor with increasing number of replicates. For sake of conciseness in Fig. 4 only the results (μ^* and σ) obtained for the sensitivity of $S_{PO_{4.1}}$ towards q_{PHA} and q_{PP} are shown. Fig. 4 shows a high variability of the sensitivity indices even for a

number of r much higher than the recommended one in literature. Thus, the modeller cannot be confident with these results obtained with the Morris screening method as convergence is not reached for this model when using numerical settings found in the sensitivity analysis literature. For a deeper investigation into the convergence issue, the readers are referred to Mannina et al. (2013).

4. Conclusions

- It was found that, even though the SRC method was applied outside its range of applicability ($R^2 < 0.7$), the ranking of important model factors (*factors prioritisation*) was very similar to the results obtained with Extended-FAST, except for the MLSS variables.
- The Pearson correlation r_P values calculated to compare Morris screening and Extended-FAST in terms of μ^* and S_{Ti} are lower than those calculated to compare SRC and Extended-FAST in terms of β_i^2 and S_i .
- The low similarity between Morris screening and Extended-FAST results is expressed both in the number and type of influential/non-influential factors.

- It is hypothesised that the discrepancy between the results of Morris screening (with default settings for the number of simulation) and Extended-FAST is attributed, for this case study, to convergence problems.
- 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. This is due to the fact that when non-linearity increases β_i^2 underestimate S_i .
- The MBR model for the presented application showed a non-linear behaviour and interacting factors.
- In case the modeller is only interested in factor prioritisation then the use of the less computationally demanding SRC is suggested because it identifies the same factors as the Extended-FAST method.
- The use of multiple sensitivity analysis methods in a GSA study allows increasing the robustness of the conclusions made. Here, using the three methods simultaneously allowed identifying problems with Morris Screening as the two other methods provided consistent results.

Acknowledgements

Peter Vanrolleghem holds the Canada Research Chair in Water Quality Modelling. The authors wish to acknowledge the support provided by the IWA Task Group on Design and Operations Uncertainty (DOU). This work was partly funded by the Natural Sciences and Engineering Research Council of Canada (NSERC) and Primodal Inc.

Appendix A. Supplementary data

Supplementary data related to this article can be found at <http://dx.doi.org/10.1016/j.envsoft.2013.07.009>.

References

- Beck, M.B., Ravetz, J.R., Mulkey, L.A., Barnwell, T.O., 1997. On the problem of model validation for predictive exposure assessments. *Stochastic Hydrology and Hydraulics* 11 (3), 229–254.
- Benedetti, L., Batstone, D.J., De Baets, B., Nopens, I., Vanrolleghem, P.A., 2008. Global sensitivity analysis of biochemical, design and operational parameters of the Benchmark Simulation Model no. 2. In: *Proceedings of: International Congress on Environmental Modelling and Software (iEMSs2008)*. Barcelona, Spain, July 7–10 2008, vol. 2, pp. 1322–1330.
- Benedetti, L., Batstone, D.J., De Baets, B., Nopens, I., Vanrolleghem, P.A., 2012. Uncertainty analysis of WWTP control strategies made feasible. *Water Quality Research Journal of Canada* 47 (1), 14–29.
- Benedetti, L., Claeys, F., Nopens, I., Vanrolleghem, P.A., 2011. Assessing the convergence of LHS Monte Carlo simulations of wastewater treatment models. *Water Science and Technology* 63 (10), 2219–2224.
- Brockmann, D., 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.
- Brun, R., Kühni, M., Siegrist, H., Gujer, W., Reichert, P., 2002. Practical identifiability of ASM2d parameters: systematic selection and tuning of parameter subsets. *Water Research* 36, 4113–4127.
- Campolongo, F., Cariboni, J., Saltelli, A., 2007. An effective screening design for sensitivity analysis of large models. *Environmental Modelling & Software* 22 (10), 1509–1518.
- Chen, L., Tian, Y., Cao, C., Zhang, S., Zhang, S., 2012. Sensitivity and uncertainty analyses of an extended ASM3-SMP model describing membrane bioreactor operation. *Journal of Membrane Science* 389, 99–109.
- Confalonieri, R., Bellocchi, G., Bregaglio, S., Donatelli, M., Acutis, M., 2010. Comparison of sensitivity analysis techniques: a case study with the rice model WARM. *Ecological Modelling* 221, 1897–1906.
- Cosenza, A., Di Bella, G., Mannina, G., Torregrossa, M., Viviani, G., 2013a. Biological nutrient removal and fouling phenomena in a UCT-MBR treating high nitrogen loads. *Journal of Environmental Engineering* 139 (6), 773–780.
- Cosenza, A., Mannina, G., Neumann, M.B., Viviani, G., Vanrolleghem, P.A., 2013b. Biological nitrogen and phosphorus removal in membrane bioreactors: model development and parameter estimation. *Bioprocess and Biosystems Engineering* 36 (4), 499–514.
- Cosenza, A., Mannina, G., Vanrolleghem, P.A., Neumann, M.B., 2013c. Variance-based Sensitivity Analysis in Wastewater Applications (submitted for publication).
- Cukier, R.I., Fortuin, C.M., Shuler, K.E., Petschek, A.G., 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., 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., 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., Neumann, M.B., Vanrolleghem, P.A., 2012. Assessing the use of activated sludge process design guidelines in wastewater treatment plant projects: a methodology based on global sensitivity analysis. *Environmental Modelling & Software* 38 (12), 50–58.
- Gernaey, K.V., Flores-Alsina, X., Rosen, C., Benedetti, L., Jeppsson, U., 2011. Dynamic influent pollutant disturbance scenario generation using a phenomenological modelling approach. *Environmental Modelling & Software* 26 (11), 1255–1267.
- Hauduc, H., Rieger, L., Ohtsuki, T., Shaw, A., Takács, I., Winkler, S., Héduit, A., Vanrolleghem, P.A., Gillot, S., 2011. Activated sludge modelling: development and potential use of a practical applications database. *Water Science and Technology* 63 (10), 2164–2182.
- Henze, M., Gujer, W., Mino, T., 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., Saltelli, A., 1996. Importance measures in global sensitivity analysis of nonlinear models. *Reliability Engineering and System Safety* 52, 1–17.
- Innocenti, V., 2005. *Modello di depurazione biologica secondo lo standard ASM3 con doppio step di nitrificazione* (Degree thesis). Università degli Studi di Firenze, Italy (in Italian).
- Jiang, T., Myngheer, S., De Pauw, D.J.W., Spanjers, H., Nopens, I., Kennedy, M.D., Amy, G., Vanrolleghem, P.A., 2008. Modelling the production and degradation of soluble microbial products (SMP) in membrane bioreactors (MBR). *Water Research* 42 (20), 4955–4964.
- Mannina, G., Cosenza, A., Neumann, M.B., Vanrolleghem, P.A., 2013. *Global Sensitivity Analysis for Urban Water Quality Modelling: Convergence Analysis and Comparison of Different Methods* (submitted for publication).
- Mannina, G., Cosenza, A., Vanrolleghem, P., Viviani, G., 2011a. A practical protocol for calibration of nutrient removal wastewater treatment models. *Journal of Hydroinformatics* 13 (4), 575–595.
- 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., Di Bella, G., Viviani, G., 2011b. An integrated model for biological and physical process simulation in membrane bioreactors (MBR). *Journal of Membrane Science* 376 (1–2), 56–69.
- Mannina, G., Viviani, G., 2009a. Separate and combined sewer systems: a long-term modelling approach. *Water Science and Technology* 60 (3), 555–565.
- Mannina, G., Viviani, G., 2009b. Hybrid moving bed biofilm reactors: an effective solution for upgrading a large wastewater treatment plant. *Water Science and Technology* 60 (5), 1103–1116.
- Morris, M.D., 1991. Factorial sampling plans for preliminary computational experiments. *Technometrics* 33 (2), 161–174.
- Neumann, M.B., 2012. Comparison of sensitivity analysis techniques for modelling micropollutant oxidation in water treatment. *Science of the Total Environment* 433 (1), 530–537.
- Nossent, J., Bauwens, W., 2012. Multi-variable sensitivity and identifiability analysis for a complex environmental model in view of integrated water quantity and water quality modeling. *Water Science & Technology* 65 (3), 539–549.
- Nossent, J., Elsen, P., Bauwens, W., 2011. Sobol' sensitivity analysis of a complex environmental model. *Environmental Modelling & Software* 26, 1515–1525.
- Ruano, M.V., Ribes, J., Ferrer, J., Sin, G., 2011. Application of the Morris method for screening the influential parameters of fuzzy controllers applied to wastewater treatment plants. *Water Science and Technology* 63 (10), 2199–2206.
- Ruano, M.V., Ribes, J., Seco, A., Ferrer, J., 2012. An improved sampling strategy based on trajectory design for application of the Morris method to systems with many input factors. *Environmental Modelling & Software* 37 (11), 103–109.
- Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M., 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., Chan, K.P.S., 1999. A quantitative model-independent method for global sensitivity analysis of model output. *Technometrics* 41 (1), 39–56.
- Saltelli, A., Ratto, M., Tarantola, S., Campolongo, F., 2005. Sensitivity analysis for chemical models. *Chemical Reviews* 105, 2811–2827.
- Saltelli, A., Tarantola, S., Campolongo, F., Ratto, M., 2004. *Sensitivity Analysis in Practice. A Guide to Assessing Scientific Models*. In: *Probability and Statistics Series*. John Wiley & Sons Publishers.

- Schaibly, J.H., 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., Gernaey, K.V., Neumann, M.B., van Loosdrecht, M., Gujer, W., 2011. Global sensitivity analysis in wastewater treatment plant model applications: prioritizing sources of uncertainty. *Water Research* 45, 639–651.
- Sobol, I.M., 2001. Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. *Mathematics and Computers in Simulation* 55 (1–3), 271–280.
- Sun, X.Y., Newham, L.T.H., Croke, B.F.W., Norton, J.P., 2012. Three complementary methods for sensitivity analysis of a water quality model. *Environmental Modelling & Software* 37, 19–29.
- Weijers, S.R., Vanrolleghem, P.A., 1997. A procedure for selecting best identifiable parameters in calibrating activated sludge model No.1 to full-scale plant data. *Water Science and Technology* 36 (5), 69–79.
- Yang, J., 2011. Convergence and uncertainty analyses in Monte-Carlo based sensitivity analysis. *Environmental Modelling & Software* 26 (4), 444–457.