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Variance-based sensitivity analysis for wastewater treatment plant modelling

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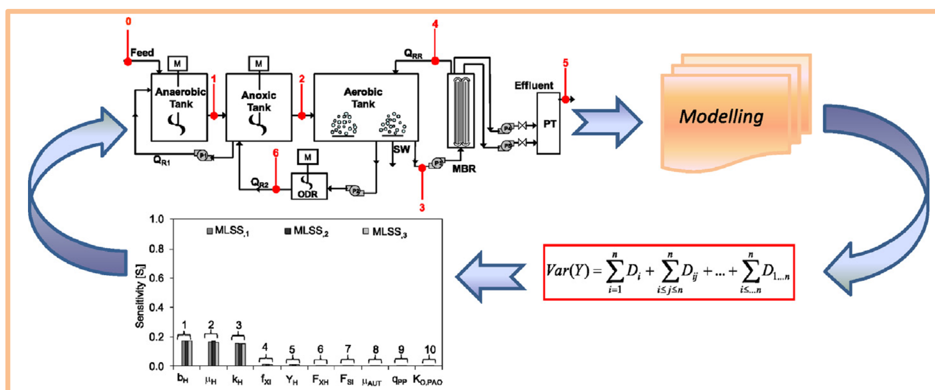
HIGHLIGHTS

- The Extended-FAST method was applied to an integrated membrane bioreactor model.
- The explored factor space was wider than in other studies.
- The relationship between variables and factors was non-linear and non-additive.
- Significant interactions among the model factors were found.

GRAPHICAL ABSTRACT



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ABSTRACT

Global sensitivity analysis (GSA) is a valuable tool to support the use of mathematical models that characterise technical or natural systems. In the field of wastewater modelling, most of the recent applications of GSA use either regression-based methods, which require close to linear relationships between the model outputs and model factors, or screening methods, which only yield qualitative results. However, due to the characteristics of membrane bioreactors (MBR) (non-linear kinetics, complexity, etc.) there is an interest to adequately quantify the effects of non-linearity and interactions. This can be achieved with variance-based sensitivity analysis methods. In this paper, the Extended Fourier Amplitude Sensitivity Testing (Extended-FAST) method is applied to an integrated activated sludge model (ASM2d) for an MBR system including microbial product formation and physical separation processes. Twenty-one model outputs located throughout the different sections of the bioreactor and 79 model factors are considered. Significant interactions among the model factors are found. Contrary to previous GSA studies for ASM models, we find the relationship between variables and factors to be non-linear and non-additive. By analysing the pattern of the variance decomposition along the plant, the model factors having the highest variance contributions were identified. This study demonstrates the usefulness of variance-based methods in membrane bioreactor modelling where, due to the presence of membranes and different operating conditions than those typically found in conventional activated sludge systems, several highly non-linear effects are present. Further, the obtained results

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highlight the relevant role played by the modelling approach for MBR taking into account simultaneously biological and physical processes.

1. Introduction

Activated sludge models (ASMs) (Henze et al., 2000) are widely applied (for design, control or optimization) in their original form or modified in order to simulate adapted systems such as membrane bioreactors (MBR) (Fenu et al., 2010; Mannina and Cosenza, 2013). However, these models are complex and generally over-parameterized. On account of this, wastewater treatment plant (WWTP) modelling requires a considerable number of assumptions on model structure, model parameter values and model input variables. In the following we use the term factors for both model parameters and model inputs adopting the terminology often applied in the sensitivity analysis (SA) literature. SA provides useful support in determining which input factors are important (*factor prioritization*) and which factors are non-influential (*factor fixing*). Especially global sensitivity analysis (GSA) techniques can provide valuable support for the application of mathematical models. According to Saltelli et al. (2008), the GSA techniques can be divided into: (i) screening methods, e.g. Morris screening method (Morris, 1991; Campolongo et al., 2007); (ii) regression/correlation-based methods such as the Standardised Regression Coefficients (SRCs) method; (iii) variance decomposition methods such as Extended Fourier Amplitude Sensitivity Testing (Extended-FAST) (Cukier et al., 1973; Schaibly and Shuler, 1973; Sobol, 1993; Saltelli et al., 1999).

Recently, GSA applications have started to emerge in the wastewater modelling field (among others, Ruano et al., 2011; Sin et al., 2011; Benedetti et al., 2012; Chen et al., 2012; Flores-Alsina et al., 2012). In most cases, regression-based methods have been applied (Benedetti et al., 2012; Flores-Alsina et al., 2012; Sin et al., 2011). For instance, Flores-Alsina et al. (2012) have applied the SRC method in order to assess how the range of values in design assumptions influences the final design of a plant. Sin et al. (2011) applied the SRC method to an ASM model, in which 26 parameters were taken into account. They found a high ability of the SRC method in identifying the sources of uncertainty and quantifying their impact on performance criteria. Benedetti et al. (2012) applied the SRC method to a complex wastewater model (65 model factors) for selecting the most important factors and assessing the relative importance of factors in view of output uncertainty. Other applications of GSA in the wastewater field refer to screening methods. In particular, Ruano et al. (2011) applied the Morris screening method to a fuzzy logic-based control system for an ASM model, in which 17 model parameters were involved.

Variance-based sensitivity analysis methods have recently been applied in the drinking water modelling field by Neumann et al. (2007) and Neumann et al. (2009) to improve the understanding of oxidation and disinfection processes. In the wastewater modelling field two applications of variance-based sensitivity analysis have been conducted. Brockmann and Morgenroth (2007) applied the quantitative variance-based FAST method to a biofilm model for two step nitrification in order to compare with the results obtained by applying the qualitative screening method of Morris. Recently, Chen et al. (2012) found that complex ASM-MBR models can be highly nonlinear and that variance-based sensitivity analysis methods can be of use in helping the modeller to find which factors are involved in interactions.

In order to extend the knowledge on the application of variance-based sensitivity analysis in the wastewater modelling field, the paper presents the application of the Extended-FAST method to an integrated ASM no.2d – soluble microbial product – (ASM2d–SMP) model applied to a University Cape Town (UCT) MBR pilot plant. The study presented here contains several differences compared to Chen et al. (2012):

- In this study the mathematical model is an integrated MBR model that takes into account both physical (fouling prediction) and biological processes (including nutrient removal), coupled with the SMP formation/degradation processes;
- The integrated MBR model used here is able to simulate the phosphorus removal process, often neglected in the modelling literature (Zuthi et al., 2013)
- Real wastewater has been considered for the pilot plant feeding;
- The Extended-FAST method is applied by using an approach based on plant sections: different model outputs for different plant sections are considered.

Specifically, the principal objectives of this study are: (i) to identify important factors (factor prioritization); (ii) to identify non-influential factors (factor fixing); (iii) to identify interacting factors and (iv) to quantify the variance contribution of the factors to various model variables across the plant.

2. Materials and methods

2.1. Extended-FAST

Let us consider the simplified model:

$$Y = g(x) \tag{1}$$

where x is a vector of n factors and Y the model output; whenever g can be decomposed as a sum of n functions g_i, each of which is a function only of the relative factor x_i, model (1) is defined additive (Saltelli et al., 2004).

According to the variance decomposition theorem, the total variance of the model output ($Var(Y)$) may be decomposed into conditional variances.

The total variance $Var(Y)$ is decomposed as follows:

$$Var(Y) = \sum_{i=1}^{n} D_i + \sum_{i \le j \le n}^{n} D_{ij} + \ldots + \sum_{i \le \ldots n}^{n} D_{1\ldots n} \tag{2}$$

where D_i represents the first order effect for each factor x_i and $D_{ij}\ldots D_{1\ldots n}$ the interaction effects. Specifically, the first order effects represent the variance of the conditional expectation $Var_{xi}\left(E_{x_{-i}}(Y|x_i)\right)$. According to the notation used by Saltelli et al. (2004), the subscripts indicate that the operation is either applied "over the *ith* factor" X_i, or "over all factors except the i-th factor" X_{-i}.

The Extended-FAST method allows calculating two different sensitivity indices in order to evaluate the contribution of each factor to the total variance: the first-order effect index (S_i) and the total effect index (S_{Ti}). S_i is evaluated according to Eq. (3):

$$S_i = \frac{Var_{xi}\left(E_{x_{-i}}\left(Y\middle|x_i\right)\right)}{Var(Y)}. \tag{3}$$

S_i measures how the i-th factor contributes to $Var(Y)$ without taking into account the interactions among factors.

Assuming non-correlated input factors and an additive model (no interactions present) Eq. (4) is valid:

$$\sum_{i=1}^{n} S_i = 1 \tag{4}$$

where n is the total number of input factors.

The computation of all higher order terms leads to the estimation of the total effect index (S_{Ti}) defined as follows:

$$S_{Ti} = 1 - \frac{Var_{x_{-i}}\left(E_{x_i}\left(Y \middle| x_{-i}\right)\right)}{Var(Y)}. \tag{5}$$

S_{Ti} allows evaluating the interactions (S_{Si}) among factors as in the following:

$$S_{Si} = S_{Ti} - S_i. \tag{6}$$

Moreover, a comparison between S_i and S_{Ti} may help modellers to evaluate whether the model under study is additive or not. Indeed, for additive models $S_i = S_{Ti}$, while for non-additive models $S_{Ti} > S_i$.

It is important to underline that in the context of *factor fixing* the analysis of S_{Ti} has to be performed. If the S_i value is small, it does not necessarily 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.

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

We compute Extended-FAST indices using the package for sensitivity analysis developed by Pujol (2007) within the R programming environment (R Development Core Team, 2007).

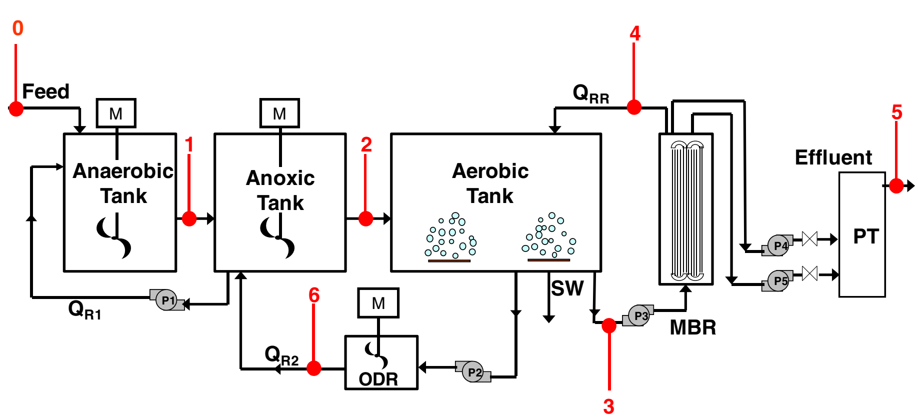
2.2. The case study

The case study is developed around a pilot plant according to the UCT-MBR scheme (Fig. 1). More specifically, the plant consists of five reactor sections: anaerobic (mean volume 72 L) (Section 1), anoxic (mean volume 165 L) (Section 2) and aerobic (mean volume 327 L) (Section 3), respectively, followed by an aerobic tank (mean volume 52 L) (Section 4), in which two submerged hollow fibre membrane modules (Zenon Zeeweed, ZW 10) are installed, and a tank, in which permeate is collected (Section 5). The pilot plant was feed with 40 L/h (Q_{FEED}) of municipal wastewater. Biomass is recycled from the membrane tank to the aerobic tank ($Q_{RR} = 5$–$6\ Q_{FEED}$), from the aerobic to the anoxic tank ($Q_{R2} = 6\ Q_{FEED}$), from the anoxic to the anaerobic tank ($Q_{R1} = 3\ Q_{FEED}$) in order to maintain the biomass concentration required for biological activity. Within the recycle from the aerobic to the anoxic tank, an oxygen depletion reactor (ODR) is interposed in order to ensure anoxic conditions. The permeate extraction is operated by means of an ad hoc permeate extraction pump which is able to impose a maximum depression of −50 kPa providing an average flux of 21 L m^{-2} h^{-1}. The pilot plant was operated for 165 days under non-controlled climatic conditions with constant permeate flux. The membranes were periodically subjected to physical (manual cleaning) and chemical cleaning (using a solution of 2 g L^{-1} of citric acid). The pilot plant was operated until the 76th day under complete sludge retention. Subsequently the sludge retention time was set to approximately 36 days. During the pilot plant operation, composite samples of influent wastewater (Section 0) and grab samples of mixed liquor in Sections 1–4, the mixed liquor in ODR (Section 6) and the permeate (Section 5) were taken three times per week and 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). Daily measurements in each section were also conducted for dissolved oxygen (DO), pH and temperature (T) using a handheld Multi-metre 340i (WTW). Further details about the sampling campaign, the influent characteristics and the membrane cleanings can be found in Cosenza et al. (2013b,d) and Di Trapani et al. (2011).

2.3. The ASM-MBR model

The pilot plant described above was modelled by means of an integrated ASM2d–SMP model developed in a previous study (Cosenza et al., 2013a). The model is divided into two sub-models (biological and physical), globally involving 19 biological state variables, 2 physical state variables and 79 factors (kinetics, stoichiometry, physical factors and fractionation coefficients).

The biological sub-model is able to simulate the biological nutrient removal processes occurring in a UCT–MBR system (where the biomass separation process occurs by means of a membrane) and the soluble microbial products' (SMPs) formation/degradation. The need to introduce the SMP modelling arises from the fact that SMPs have a relevant influence on the effluent concentration in terms of COD and on membrane permeability (Meng et al., 2009). The biological sub-model is a modified version of ASM2d and takes into account two new state variables, S_{UAP} (soluble utilization associated product) and S_{BAP} (soluble biomass associated product), and six new processes (anaerobic, aerobic and anoxic hydrolysis of both UAP and BAP) (Jiang et al., 2008). The sum of S_{UAP} and S_{BAP} is equal to the modelled SMP. Moreover, four new parameters are introduced: f_{BAP} (fraction of BAP generated per biomass decayed), f_{UAP} (fraction of UAP generated in biomass decay), $k_{H,BAP}$ and $k_{H,UAP}$ (hydrolysis rate coefficient respectively for S_{BAP} and S_{UAP}).



LEGEND			
M	Mixer	Q_{R1}-Q_{R2}	Mixed Liquor Recycle
PT	Permeate tank	RR	Retained Recycle
P1-P2- P3	Pump of the mixed liquor recycle	SW	Sludge wasting
P4- P5	Permeate extraction pump		Bidirectional valve
ODR	Oxygen Depletion Reactor		Sampling section point

Fig. 1. Schematic overview of the UCT–MBR pilot plant.

Table 1
Symbol, description, unit of measure, variation range and literature references for each model factor; symbols reported in Table 1 are in agreement with the nomenclature used by Henze et al. (2000), Jiang et al. (2008), Mannina et al. (2011b) and Cosenza et al. (2013a). The reference temperature is 20 °C.

Symbol	Description	Unit	Min	Max	Reference
k_H	Maximum specific hydrolysis rate	$g\ X_s g\ X_H^{-1} d^{-1}$	1.5	4.5	Brun et al. (2002)
$\eta_{NO3,HYD}$	Correction factor for hydrolysis under anoxic conditions	–	0.402	0.798	Hauduc et al. (2011)
η_{FE}	Correction factor for hydrolysis under anaerobic conditions	–	0.2	0.6	Hauduc et al. (2011)
K_O	Half saturation parameter for SO_2 for X_H	$g\ S_{O2}.m^{-3}$	0.1	1	Weijers and Vanrolleghem (1997)
K_{NO3}	Half saturation parameter for S_{NO3} for X_H	$g\ S_{NO3}.m^{-3}$	0.1	0.625	Weijers and Vanrolleghem (1997), Brun et al. (2002)
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)
$K_{O,HYD}$	Half saturation/inhibition parameter for SO_2	$g\ S_{O2}.m^{-3}$	0.1	0.3	Brun et al. (2002)
$K_{NO3,HYD}$	Half saturation/inhibition parameter for S_{NO3}	$g\ N.m^{-3}$	0.375	0.625	Brun et al. (2002)
μ_H	Maximum growth rate of X_H	d^{-1}	0.6	13.2	Jeppsson (1996)
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)
$\eta_{NO3,H}$	Reduction factor for anoxic growth of X_H	–	0.6	1	Brun et al. (2002)
b_H	Decay rate for X_H	d^{-1}	0.05	1.6	Jeppsson (1996)
K_F	Half saturation parameter for S_F	$g\ S_F.m^{-3}$	2	6	Brun et al. (2002)
K_{FE}	Half saturation parameter for fermentation of S_F	$g\ S_F.m^{-3}$	2	6	Brun et al. (2002)
K_A	Half saturation parameter for S_A	$g\ S_A.m^{-3}$	2	6	Brun et al. (2002)
$K_{NH,H}$	Half saturation parameter for S_{NH4} for X_H	$g\ S_{NH4}.m^{-3}$	0.02	2	Weijers and Vanrolleghem (1997)
K_P	Half saturation parameter for S_{PO4} for X_H	$g\ S_{PO4}.m^{-3}$	0.005	0.015	Brun et al. (2002)
$K_{ALK,H}$	Half saturation parameter for S_{ALK} for X_H	$mol\ HCO_3^-.m^{-3}$	0.05	0.15	Brun et al. (2002)
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)
q_{PP}	Rate constant for storage of polyphosphates	$g\ X_{PP}.g\ X_{PAO}^{-1}.d^{-1}$	0	3.3	Hauduc et al. (2011)
μ_{PAO}	Maximum growth rate of X_{PAO}	d^{-1}	0.5	1.5	Brun et al. (2002)
$\eta_{NO3,PAO}$	Reduction factor for anoxic growth of X_{PAO}	–	0.45	0.75	Brun et al. (2002)
b_{PAO}	Endogenous respiration rate of X_{PAO}	d^{-1}	0.1	0.25	Henze et al. (2000), Hauduc et al. (2011)
b_{PP}	Rate constant for lysis of polyphosphates	d^{-1}	0.1	0.25	Henze et al. (2000), Hauduc et al. (2011)
b_{PHA}	Rate constant for respiration of X_{PHA}	d^{-1}	0.1	0.25	Henze et al. (2000), Hauduc et al. (2011)
K_{PS}	Half saturation parameter for S_{PO4} uptake	$g\ S_{PO4}.m^{-3}$	0.1	0.3	Brun et al. (2002)
K_{PP}	Maximum ratio of X_{PP}/X_{PAO}	$g\ X_{PP}.g\ X_{PAO}^{-1}$	0.005	0.015	Brun et al. (2002)
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)
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)
K_{PHA}	Saturation constant for X_{PHA}/X_{PAO}	$g\ X_{PHA}.g\ X_{PAO}^{-1}$	0.005	0.015	Brun et al. (2002)
$K_{O,PAO}$	Half saturation parameter for SO_2 for X_{PAO}	$g\ S_{O2}.m^{-3}$	0.1	0.3	Brun et al. (2002)
$K_{NO3,PAO}$	Half saturation parameter for S_{NO3} for X_{PAO}	$g\ S_{NO3}.m^{-3}$	0.375	0.625	Brun et al. (2002)
$K_{A,PAO}$	Half saturation parameter for S_A for X_{PAO}	$g\ S_A.m^{-3}$	2	6	Brun et al. (2002)
$K_{NH,PAO}$	Half saturation parameter for S_{NH4} for X_{PAO}	$g\ S_{NH4}.m^{-3}$	0.025	0.075	Brun et al. (2002)
$K_{P,PAO}$	Half saturation parameter for S_{PO4} as nutrient (X_{PAO} growth)	$g\ S_{PO4}.m^{-3}$	0.005	0.015	Brun et al. (2002)
$K_{ALK,PAO}$	Half saturation parameter for S_{ALK} for X_{PAO}	$mol\ HCO_3^-.m^{-3}$	0.05	0.15	Brun et al. (2002)
μ_{AUT}	Maximum growth rate of X_{AUT}	d^{-1}	0.2	1.2	Weijers and Vanrolleghem (1997)
b_{AUT}	Decay rate for X_{AUT}	d^{-1}	0.04	0.1605	Hauduc et al. (2011)
$K_{O,A}$	Half saturation parameter for SO_2 for X_{AUT}	$g\ S_{O2}.m^{-3}$	0.1	2	Weijers and Vanrolleghem (1997), Jeppsson (1996)
$K_{NH,A}$	Half saturation parameter for S_{NH4} for X_{AUT}	$g\ S_{NH4}.m^{-3}$	0.5	1.5	Hauduc et al. (2011)
$K_{ALK,A}$	Half saturation parameter for S_{ALK} for X_{AUT}	$mol\ HCO_3^-.m^{-3}$	0.25	0.75	Brun et al. (2002)
$K_{P,A}$	Half saturation parameter for S_{PO4} for X_{PAO}	$g\ S_{PO4}.m^{-3}$	0.005	0.015	Brun et al. (2002)
$k_{H,BAP}$	Hydrolysis rate coefficient for S_{BAP}	d^{-1}	3.705E−07	1.1115E−06	Jiang et al. (2008)
$k_{H,UAP}$	Hydrolysis rate coefficient for S_{UAP}	d^{-1}	0.0051	0.0153	Jiang et al. (2008)
$k_{LaT,3}$	Overall oxygen transfer coefficient aerobic tank	h^{-1}	9.5	10.5	Innocenti (2005)
$k_{LaT,4}$	Overall oxygen transfer coefficient MBR tank	h^{-1}	3.23	3.57	Innocenti (2005)
Y_H	Yield for X_H growth	$g\ X_H.g\ X_S^{-1}$	0.38	0.75	Jeppsson (1996)
f_{XI}	Fraction of X_I generated in biomass decay	$g\ X_I.g\ X_H^{-1}$	0.05	0.4	Weijers and Vanrolleghem (1997)
Y_{PAO}	Yield for X_{PAO} growth	$g\ X_{PAO}.g\ X_{PHA}^{-1}$	0.42	0.78125	Brun et al. (2002)
Y_{PO4}	Yield for X_{PP} requirement per X_{PHA} stored		0.38	0.42	Brun et al. (2002)
Y_{PHA}	Yield for X_{PP} storage per X_{PHA} utilized	$g\ X_{PP}.g\ X_{PHA}^{-1}$	0.19	0.21	Brun et al. (2002)
Y_A	Yield of X_{AUT} growth per S_{NO3}	$g\ X_{AUT}.g\ S_{NO3}^{-1}$	0.228	0.252	Brun et al. (2002)
f_{BAP}	Fraction of S_{BAP} generated in biomass decay	–	0.0069	0.022575	Brun et al. (2002)
f_{UAP}	Fraction of S_{UAP} generated in biomass decay	–	0.091485	0.101115	Brun et al. (2002)
F_{SF}	Fraction of influent S_F	–	0.06	0.18	Mannina et al. (2011a)
F_{SA}	Fraction of influent S_A	–	0.04	0.12	Mannina et al. (2011a)
F_{SI}	Fraction of influent S_I	–	0.114	0.126	Mannina et al. (2011a)
F_{XI}	Fraction of influent X_I	–	0.05	0.15	Mannina et al. (2011a)
F_{XH}	Fraction of influent X_H	–	0.06	0.18	Mannina et al. (2011a)
β	Erosion rate coefficient of the dynamic sludge	–	1.00E−04	2.10E−02	Mannina et al. (2011b)
α	Stickiness of the biomass particles	–	0	1	Mannina et al. (2011b)
γ	Compressibility of cake	$Kg\ m^{-3}\ s$	5.56E−04	2.78E−03	Mannina et al. (2011b)
f	Substrate fraction below the critical molecular weight	–	0.001	0.99	Mannina et al. (2011b)
λ	Screening parameter	m^{-1}	1000	2.00E + 03	Mannina et al. (2011b)
C_E	Efficiency of backwashing	–	0.996	0.999	Mannina et al. (2011b)
$i_{N,SI}$	N content of S_I	$g\ N.g\ S_I^{-1}$	0.0075	0.0125	Brun et al. (2002)
$i_{N,SF}$	N content of S_F	$g\ N.g\ S_F^{-1}$	0.0225	0.0375	Brun et al. (2002)
$i_{N,XI}$	N content of X_I	$g\ N.g\ X_I^{-1}$	0.015	0.025	Brun et al. (2002)
$i_{N,XS}$	N content of X_S	$g\ N.g\ X_S^{-1}$	0.03	0.05	Brun et al. (2002)
$i_{N,BM}$	N content of biomass	$g\ N.g\ X_{BM}^{-1}$	0.0665	0.0735	Brun et al. (2002)
$i_{P,SF}$	P content of S_F	$g\ P.g\ S_F^{-1}$	0.005	0.015	Brun et al. (2002)
$i_{P,XI}$	P content of X_I	$g\ P.g\ X_I^{-1}$	0.005	0.015	Brun et al. (2002)

Table 1 (*continued*)

Symbol	Description	Unit	Min	Max	Reference
$i_{P,XS}$	P content of X_S	g P.g X_S^{-1}	0.005	0.015	Brun et al. (2002)
$i_{P,BM}$	N content of biomass	g P.g X_{BM}^{-1}	0.015	0.025	Brun et al. (2002)
$i_{TSS,XI}$	Conversion factor X_I in TSS	g TSS.g X_I^{-1}	0.7125	0.7875	Brun et al. (2002)
$i_{TSS,XS}$	Conversion factor X_S in TSS	g TSS.g X_S^{-1}	0.7125	0.7875	Brun et al. (2002)
$i_{TSS,BM}$	Conversion factor biomass in TSS	g TSS.g X_{BM}^{-1}	0.855	0.945	Brun et al. (2002)
$i_{TSS,XPHA}$	Conversion factor X_{PHA} in TSS	g TSS.g X_{PHA}^{-1}	0.57	0.63	Brun et al. (2002)
$i_{TSS,XPP}$	Conversion factor X_{PP} in TSS	g TSS.g X_{PP}^{-1}	3.0685	3.3915	Brun et al. (2002)

The physical sub-model takes into account the cake layer formation (on the membrane surface) during the suction and backwashing phases and the partial COD removal throughout the cake layer. More specifically, by modelling the rate of sludge attachment to and detachment from the membrane surface throughout the suction and backwashing phase, the solid mass deposited on the membrane surface and the cake layer thickness are evaluated. Moreover, according to the deep-bed theory, the COD profile across the cake layer is described (Mannina et al., 2011b). Particles are retained inside the cake layer which, coupled with the fraction of particles retained by the physical membrane, contribute to the reduction of the total COD concentration in the effluent (Di Bella et al., 2008; Mannina et al., 2011b).

As recently demonstrated by Corominas et al. (2012), due to non-linearity, it is possible to obtain a large difference between values obtained with steady-state solutions and averaged values from dynamic solutions for these type of models. Therefore, time-averaged dynamic simulation outputs (over 165 days) for Sections 1–3 and 5 have been used in the analysis. Twenty-one model outputs have been subjected to the SA: namely, COD_{TOT}, S_{NH4}, S_{NO3}, S_{PO}, MLSS, for each section, soluble COD (COD_{SOL}) for Sections 1, 2 and 3, and total nitrogen (C_{TN}) for Section 5.

Table 1 summarizes information on the model factors with symbols according to nomenclature used in previous studies (Henze et al., 2000; Jiang et al., 2008; Mannina et al., 2011b; Cosenza et al., 2013a). For the variance decomposition to be useful, meaningful variation ranges for the factors are required. In Table 1, the variation ranges of factors obtained from an extensive literature search are reported. Due to the lack of knowledge on the model factors' distribution, a uniform prior distribution was considered for each of them. Indeed, Freni and Mannina (2010) have recently demonstrated that in case of a lack of relevant information on model factors, a uniform prior distribution should be preferred.

2.4. Dynamic simulation

The entire plant model was coded in Fortran. Further details about the integrated ASM2d–SMP model (factors and processes involved) can be found in Cosenza et al. (2013a). For dynamic simulation, continuous input time series were used, which were obtained by employing a truncated Fourier series calibrated on discrete measured input data collected during pilot plant monitoring (Mannina and Viviani, 2009a,b).

2.5. Extended-FAST application

In order to apply Extended-FAST, 39,500 model runs were conducted corresponding to 500 Monte Carlo simulations for each model factor. The required number of model runs was confirmed by testing the convergence of the results by increasing the number of Monte Carlo simulations in a stepwise approach and verifying that the difference between two subsequent steps was negligible (Benedetti et al., 2011).

According to the Extended-FAST method, the identification of important and non-influential model factors has been carried out by employing two criteria: S_i (*factor prioritization*) and S_{Ti} (*factor fixing*). More specifically, for each model output, the most important factors have been selected by imposing a threshold for S_i. In particular, factors having a S_i value higher than 0.01 for a model output have been considered important (*factor prioritization*). This threshold value has been selected in line with previous GSA applications on ASM models (Neumann, 2012; Sin et al., 2011). The value of S_{Ti} has been considered in order to define the set of non-influential model factors. Specifically, factors with $S_i < 0.01$ and $S_{Ti} < 0.1$ are defined as being non-influential.

3. Results

Table 2 shows the mean (μ), the standard deviation (σ) and the coefficient of variation (c.v. = σ / μ) of the 21 model outputs. The c.v. values range between 0.2 and 2.21, these values ensure that conducting variance decomposition for the model outputs is a meaningful endeavour: in the case of very small c.v. such as 0.01 understanding how different model factors contribute to model output variance would be little value. Five sub-groups have been formed by clustering all model variables. Clusters are defined for MLSS, COD, NO_3^- (which also includes total nitrogen model output), NH_4^+ and P. Tables 1A–5A (Supplementary material) report the full results for all of the 79 model factors. Fig. 2a–l summarizes the results for the five sub-groups: They report the ten most important factors, in order to be sure that for every variable, the most critical factors are considered. For this, the factors are ranked on the basis of the S_i value of the model output. The sequence of factors in Fig. 2a–l is determined by the model variable exhibiting the highest value of S_i for the top ranked factor. In particular, in Fig. 2a–l, for each model output and for the considered model factors, the values of S_i and S_{Ti} and ranking are reported. Fig. 2a–l shows how the variance contribution changes along the plant sections. The results for each of the subgroups are discussed in the following sections.

3.1. MLSS sub-group

With the exception of f_{Xi} and to some extent k_H the most important model factors are mainly related to the X_H activity with, in all sections, 34% of the variance being explained by b_H and μ_H (see Table 1A, Fig. 2a). The results related to the influence of f_{Xi} are of particular interest within the MBR context: a progressive accumulation of X_i occurs when an MBR operates with complete sludge retention. For this study, this is the case for the first 76 days, where the plant was operated with complete sludge retention. A significant influence of f_{Xi} on the MLSS concentration is expected and has been demonstrated previously by Chen et al. (2012) and Sin et al. (2011). Chen et al. (2012) have demonstrated that the influence of f_{Xi} on the MLSS concentration inside the MBR system increases with increasing sludge retention time (SRT) as shown by an increasing S_i. Non-linearity is important as the first-order effects (sum(S_i)) only explain 60% of variance in the MLSS model outputs.

A substantial reduction of the number of factors can be obtained in the factor fixing setting with 56 factors are classified as non-influential (see Table 1A).

No relevant variation on the S_i and S_{Ti} has been detected along the plant sections (Fig. 2a and b, Table 1A) which corresponds to the fact that the MLSS concentrations are homogeneous throughout the different sections. The MLSS variation is a slow process driven by SRT and not by the local biological processes.

Table 2
Mean (μ), standard deviation (σ) and coefficient of variation (c.v.) for each of the 21 time averaged model outputs used for the Extended-FAST application.

Model output	μ [mg/L]	σ [mg/L]	c.v. [–]
$MLSS_{,1}$	671.12	574.73	0.86
$MLSS_{,2}$	820.61	748.4	0.91
$MLSS_{,3}$	1494.46	1423.2	0.95
$COD_{TOT,1}$	259.23	289.79	1.12
$COD_{TOT,2}$	292.86	377.68	1.29
$COD_{TOT,3}$	532.69	713.52	1.34
$COD_{SOL,3}$	473.42	718.04	1.52
$COD_{TOT,5}$	64.54	30.59	0.47
$S_{NH4,1}$	11.64	1.72	0.15
$S_{NH4,2}$	9.82	1.96	0.2
$S_{NH4,3}$	1.57	2.9	1.85
$S_{NH4,5}$	1.35	2.97	2.21
$S_{NO3,1}$	0.59	1.06	1.81
$S_{NO3,2}$	1.02	1.45	1.42
$S_{NO3,3}$	11.59	2.42	0.21
$S_{NO3,5}$	12.31	2.55	0.21
$CTN_{,5}$	14.38	3.02	0.21
$S_{PO,1}$	7.04	3.32	0.47
$S_{PO,2}$	7.22	3.53	0.49
$S_{PO,3}$	5.09	1.52	0.3
$S_{PO,5}$	5.24	1.54	0.29

3.2. COD sub-group

Concerning factor prioritization, for each variable of the COD sub-group, except for $COD_{TOT,5}$, about 20% of the variance has been attributed to μ_H, which was the most important factor for most COD-related variables (see Fig. 2c and Table 2A). Factor f (substrate fraction able to be retained by the membrane) was the second most important factor for all variables, contributing to 13% of the variance, except for $COD_{TOT,5}$, where f was the most important one (see Fig. 2c and Table 2A). The influence of the factor f for Sections 1, 2 and 3 can be attributed to the recycled fluxes from tank to tank. The fact that factor f was the most important factor only for $COD_{TOT,5}$ can be attributed to the higher influence of physical separation for the permeate in this section compared to the other sections. For $COD_{TOT,5}$ the factors b_H, k_H and C_E (efficiency of backwashing) were also important although a different ranking was found. However, for $COD_{TOT,5}$ also factors $K_{NH,H}$ (half saturation coefficient for ammonia) and μ_{AUT} (maximum growth rate of autotrophic biomass) were important. For the COD sub-group, the contribution of the total variance of COD due to the first order effect was about 60% for Sections 1, 2 and 3 and 90% in Section 5 (see last row on Table 2A) indicating differences in linearity.

In terms of factor fixing, as reported in Table 2A, one may observe that only 2 factors (among 79) were found to be non-influential (for all variables of the sub-group), thus demonstrating a high interaction among factors for the COD sub-group. Moreover, the factors α (stickiness of the biomass particles) and γ (compressibility of cake layer), both related to the physical sub-model, were found to be of interest in terms of factor fixing. Indeed α and γ had a high interaction value (0.24) for the simulated average concentration of $COD_{TOT,5}$ and cannot be considered non-influential for the COD sub-group (see Table 2A). For $COD_{TOT,5}$ the factors related to heterotrophic metabolism (μ_H, b_H), wastewater fractionation (F_{SI}, F_{XH} and F_{SA}), physical separation (α, γ and λ) and growth of autotrophic biomass (μ_{AUT}) had the highest interaction contribution. For the COD sub-group (see Fig. 2c and d) the variance contribution is more or less stable in every plant section, except for Section 5. This result is not surprising as the physical separation process by means of the membrane (which also involves the cake layer formation) has a greater contribution on $COD_{TOT,5}$ than in the other sections. Indeed in Section 5, the value of S_i related to the factor f (rank order 1) for COD_{TOT} is almost three times higher than in the other sections (see Fig. 2c and d). In terms of S_{Ti} (see Fig. 2d), k_H, μ_{AUT} and γ show also some peculiarities for Section 5. In particular, the contribution of k_H to the total variance of $COD_{TOT,5}$ (S_{Ti} equal to 0.17) is lower than in the other sections.

3.3. NH_4^+ sub-group

Regarding factor prioritization, for the ammonia sub-group and for each plant section, the most important factor was μ_{AUT}. The highest influence of μ_{AUT} was on $S_{NH4,3}$ with the first order effect equal to 0.61 (see Fig. 2e and Table 3A). This is consistent with process understanding as the nitrification process occurs in Section 3. Factors Y_H and f_{XI} were also important in Sections 1 and 2 (see Table 3A). The influence of the latter two factors, related to sludge production, confirms the relationship between sludge production and nitrifying organism activity for MBR systems, as discussed by Sin et al. (2011). More specifically, when increasing the sludge production (obtained by withdrawing sludge) a negative effect on the nitrification process occurs due to a reduction of autotrophic bacteria. The influence of the factors b_H and k_H for the S_{NH4} in Sections 1 and 2 is attributable to the metabolic use of ammonia by the heterotrophic biomass.

In terms of factor fixing, as reported in Table 3A, no factor was found to be non-influential for all variables. Thus, no factor could be fixed for this sub-group (in case all variables are considered). This result is due to the high interaction among factors. Indeed, for the sum of first order effects, which range between 0.64 and 0.99 (see last row in Table 3A) one might expect an unimportant effect related to interactions, especially in Sections 1 and 2, where the sum of S_i is equal to 0.99 and 0.86, respectively. However, when assessing S_{Ti}, strong interactions were found. More specifically, in Sections 1 and 2, interactions are present and only very few factors can be fixed (Table 3A). However, in Sections 2 and 4, the contribution of the interaction is low and 68 factors are non-influential for $S_{NH4,3}$ and $S_{NH4,5}$ (Table 3A). For $S_{NH4,1}$, five factors had the highest interaction contribution: the oxygen switch coefficients for heterotrophic and PAO biomass (K_O and $K_{O,PAO}$), the correction factor for hydrolysis under anoxic conditions ($\eta_{NO3,HYD}$), the half saturation coefficient for acetate (K_A) and the maximum growth rate of autotrophic biomass (μ_{AUT}). Such a result is consistent with the process knowledge. Indeed, by increasing K_O and $\eta_{NO3,HYD,}$ the denitrification rate increases. Moreover, μ_{AUT} influences the nitrification process and consequently the recycled ammonia load from the aerobic to the anoxic tank is influenced. One also observes strong interaction of nitrification/denitrification factors coupled with the PAO metabolism (e.g. $K_{NH,PAO}$ and $K_{NO3,PAO}$). The interaction of PAO activity is probably due to the influence of the denitrifying phosphorous accumulating organisms on the nitrification/denitrification processes. Almost the same set of factors is identified in Section 2, although with a weaker interaction. Such results are likely due to the fact that $S_{NH4,1}$ and $S_{NH4,2}$ are influenced by the nitrification processes occurring in the aerobic tank (Section 3), which cause the variation of the recycled ammonia load.

For the ammonia sub-group, a high variability for S_i and S_{Ti} is shown along the plant sections (see Fig. 2e and f). More specifically, in terms of S_i, the variability is more evident for the factor μ_{AUT} (see Fig. 2e). On the contrary, in terms of S_{Ti} value, except for μ_{AUT}, all factors show a high variability along the system (Fig. 2f). For $S_{NH4,3}$ and $S_{NH4,5}$ (except for μ_{AUT}, $K_{A,}$ and F_{Xi}), factors reported in Fig. 2f always have S_{Ti} close to 0.1 or lower than 0.1, showing a low total variance contribution.

The higher values of S_i in Sections 3 and 5 than in Sections 1 and 2 are most likely due to the fact that the main process (nitrification) that influences the ammonia in the system occurs in the aerobic tank (Section 3). Moreover, the $S_{NH4,5}$ is also influenced only by the nitrification process. On the other hand, the higher values of S_{Ti} in Sections 1 and 2 than in Sections 3 and 5 may be attributed to the influence of recycled fluxes and to the high interaction of factors.

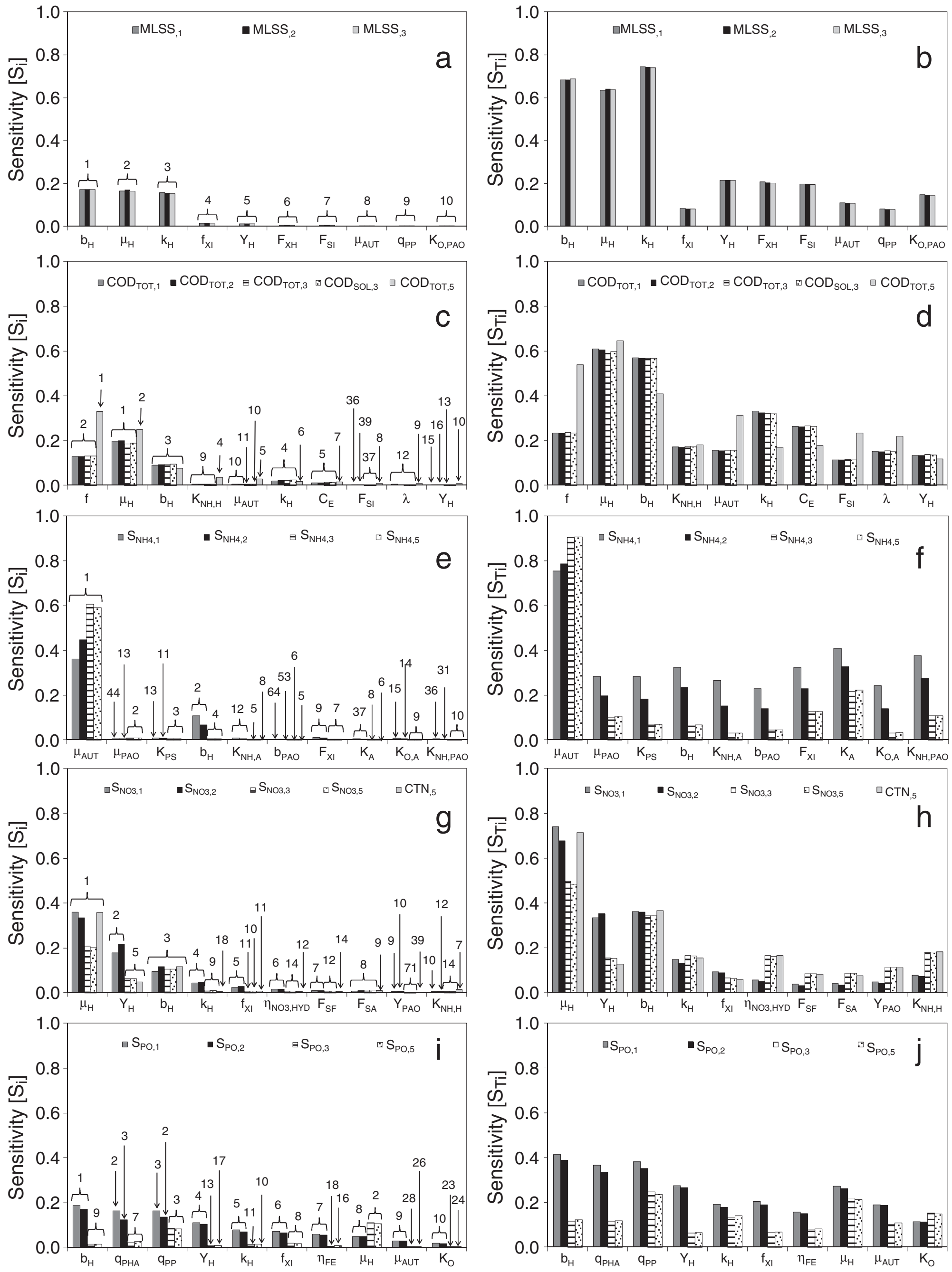


Fig. 2. S_i and S_{Ti} for the important factors for MLSS sub-group (a and b), COD sub-group (c and d), ammonia sub-group (e and f), nitrate and total nitrogen sub-group (g and h) and P sub-group (i and l). The 10 most important factors for the model variable exhibiting the highest value of S_i for the top ranked factor are displayed: $MLSS_{,3}$ (a and b), $COD_{TOT,5}$ (c and d), $S_{NH4,3}$ (e and f), $S_{NO3,1}$ (g and h), $S_{PO,1}$ (i and l); number indicates the rank order established on the basis of S_i values.

3.4. NO_3^- sub-group

In terms of factor prioritization, for the nitrate sub-group, the most important factor was μ_H, contributing on average to 29% of the variance (see Fig. 2g and Table 4A). This indicates the strong influence of the denitrification process for the entire nitrate sub-group.

The influence of factor μ_H (see Table 4A) is in agreement with the results obtained by Chen et al. (2012). Such a result reflects, for the employed integrated ASM2d–SMP model, the magnitude of the denitrification process under anoxic conditions (Chen et al., 2012). The heterotrophic decay factor (b_H) was the third most important model factor, indicating the importance of the decay of heterotrophic biomass (see Fig. 2g). Indeed, factors μ_H, b_H and Y_H are important for S_{NO3} in Sections 1 and 2 and are connected to the anoxic growth of heterotrophic organisms (denitrification) on S_A (acetate) and S_F (fermentable substrate). However, b_H has an indirect influence, as confirmed by the high value S_{Ti} for this factor (see Fig. 2h and Table 4A).

In terms of factor fixing, one may observe that 72 factors (among the 79) could be fixed for Sections 1 and 2 (Table 4A). However, for Sections 3 and 5, different results have been obtained due to the high interaction among factors.

Regarding $S_{NO3,1}$ and $S_{NO3,2}$ it is important to note that the highest degree of interaction contribution is provided by those factors that are also important in terms of S_i. Such factors are related to the activity of the heterotrophic biomass (among them μ_H, b_H, Y_H, k_H) involved in different processes. For $S_{NO3,3}$ and $S_{NO3,5}$, the same set of non-influential (14) factors (except for K_P) was found (Table 4A). For $C_{TN,5}$ 33 factors were found to be non-influential (Table 4A). For the nitrate sub-group, factors μ_H (Fig. 2g) and μ_{AUT} (Table 4A) have a relevant variation in terms of S_i along the plant sections. As expected, μ_{AUT} has the highest value of S_i (0.45) for $S_{NO3,2}$. Concerning S_{Ti}, the factors have a non-uniform behaviour along the system (see Fig. 2h and Table 4A).

3.5. Phosphorus sub-group

Regarding factor prioritization, factors b_H, q_{PP} and q_{PHA} were important and contributed on average to 17% and 14% of the variance for Sections 1 and 2, respectively (see Fig. 2i and Table 5A). 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 alkanoates and organic storage polymer), which occurs in the anaerobic tank and is fundamental for the aerobic phosphate uptake. Indeed, the magnitude of the first order effect for q_{PHA} was higher in the first two plant sections (0.16 and 0.12, respectively) than in the others (see Table 5A). On the contrary, factor q_{PP} mainly influences the aerobic and anoxic phosphorus uptake kinetics of phosphorus accumulating organisms (PAOs), which may indirectly influence the S_{PO} concentration in the other plant sections (by means of the recycled sludge). However, the results demonstrated a high magnitude of the first order effect for q_{PP} (rate constant for PHA storage by PAO) in the first two plant sections too (0.16 and 0.13), showing that for the case study, the recycled fluxes had a strong influence. The factors b_H and f_{XI} were the first and sixth most influential factors for S_{PO} respectively in Sections 1 and 2. This result was related (similarly to η_{FE}) to the fact that these two factors influence the lysis of PAO and the hydrolysis of the slowly biodegradable substrate. Factor μ_H was important for S_{PO} in every plant section, with a greater influence for Sections 3 and 5 (S_i equal to 0.11) (Fig. 2i, Table 5A). Indeed μ_H influences S_{PO} in Sections 3 and 5 through competitive heterotrophic aerobic growth on fermentable organic matter and acetate. The influence of μ_H for $S_{PO,1}$ and $S_{PO,2}$ was mainly an indirect influence, as represented by the high magnitude of the S_{Ti} value compared to S_i.

In terms of factor fixing, very similar results were obtained for Sections 1 and 2, and Sections 3 and 5. It is mainly related to the similarity of biological processes occurring in these sections affecting S_{PO}. The influence of μ_{AUT} for $S_{PO,1}$ and $S_{PO,2}$ (see Table 5A) was mainly indirect, because it regulates the presence of nitrate in the recycled sludge flux from the aerobic to the anoxic tank and consequently, from the anoxic to the anaerobic tank.

The variance contribution of factors b_H, q_{PHA} and Y_H varies along the system both in terms of S_i and S_{Ti} (see Fig. 2i and l).

4. Discussion

4.1. Significance of interactions

The analysis of the sums of S_i and S_{Ti} (Tables 1A–5A (last row)) shows that the model is not additive and strong interactions among model factors occur. Indeed, despite the fact that in some cases the sum of S_i was close to 1 (see for example variables $S_{NH4,1}$ or $C_{TN,5}$), S_{Ti} values were always greater than the corresponding S_i values (see last row in Tables 1A–5A). This result is more pronounced for the variables $COD_{TOT,5}$, $S_{NH4,1}$, $S_{NH4,2}$, $S_{NO3,2}$, $S_{NO3,3}$, $S_{NO3,5}$ and $C_{TN,5}$, where the sum of S_i and the sum of all S_{Ti} varied in the range 0.86–0.99 and 10.51–22.23, respectively (see last row of Tables 1A–5A). This may be attributed to the influence of recycled fluxes and to the high interaction of factors for nitrogen removal processes. The high interaction among factors is also attributed to the wider factor variation range explored in this study compared to other studies (Sin et al., 2009, 2011; Chen et al., 2012). By broadening the variation range of each model factor, the interaction among factors and the non-linear behaviour of the model become more apparent. Fig. 3 summarizes the first ten factors having the highest interaction value for $COD_{TOT,5}$, $S_{NH4,1}$, $S_{NH4,2}$, $S_{NO3,2}$, $S_{NO3,3}$, $S_{NO3,5}$ and $C_{TN,5}$. The factors involved in interactions (Fig. 3) are almost all related to the biological transformation processes of nitrogen inside the system. This shows how the nitrogen removal process is strongly influenced by all other processes (and their corresponding factors). Consequently, for the case study, both S_i and S_{Ti} need to be assessed in order to quantify the degree of interaction among processes and factors. Thus, it is highlighted here that it is not sufficient to perform a simpler GSA method, such as SRC.

4.2. Comparison among sub-groups

4.2.1. Factor fixing

In terms of factor fixing, very different results were obtained among the sub-groups. For the NH_4^+ sub-group, no factor was found to be non-influential for all variables (Table 3A). This result is also due to the thresholds chosen for determining non-influential factors. Thus, it is suggested to modellers of observing the influence of the choice of threshold when the GSA is aimed at reducing the number of factors to be calibrated. For the MLSS and P sub-groups, a high percentage of factors (71% and 49% respectively) could be fixed (considering all variables of each sub-group), thus significantly reducing the number of model factors to be taken into account in case, for example, of model calibration. Conversely, for the COD and NO_3^- sub-groups, due to the high interaction among factors, only 4% and 14% of the factors, respectively, could be considered non-influential.

4.2.2. Factor prioritization

In terms of factor prioritization, no particular differences among sub-groups were extracted from the results. In general, for each sub-group the important factors, selected on the basis of S_i, were strongly related to the main biological or physical processes occurring inside the system.

4.2.3. Spatial variability of variance contributions

As shown in Fig. 2, for some of the model outputs analysed, significant variability of the variance contribution along the plant sections occurs. This variability is mainly present for variables related to the nitrogen removal processes and physical processes. Thus, NH_4^+, NO_3^- and COD sub-groups show quite a high variability of S_i and S_{Ti} for some of the factors. For example, μ_{AUT} has the highest S_i value for S_{NH} in Section 3, where the nitrification process takes place, whereas factor f has the highest value of S_i for $COD_{TOT,5}$, because the physical separation mostly influences the COD_{TOT} concentration in Section 5. In terms of S_{Ti}, a high variability for the P sub-group is obtained (see Fig. 2l). The results in terms of spatial variability of the variance contribution obtained in this study can support experimental design.

4.3. Comparison with previous studies

The Extended-FAST analysis has several distinct characteristics compared to a previous analysis by Chen et al. (2012). The model structure of our study is much more complex due to the configuration and the processes taken into account (nutrient removal processes and physical separation processes are considered in the ASM2d–SMP). Moreover, a wider factors space than Chen's has been explored. As reported in Table 1, the adopted factor range was based on the range of values found in the literature, in view of studying the effect on model behaviour (variance, linearity etc.). Indeed, in Cosenza et al. (2013c), it has been demonstrated that using a broader factors variation range compared to Sin et al. (2011) the model non-linearity is exposed. Here, by using a wider variation range than Chen et al. (2012) the contribution on the model variance due to the interaction among factors is increased. Indeed, contrary to Chen et al. (2012), where the contribution of factors due to higher-order interactions was unimportant for ammonia and nitrate, in this study, a high interaction contribution to the model variance

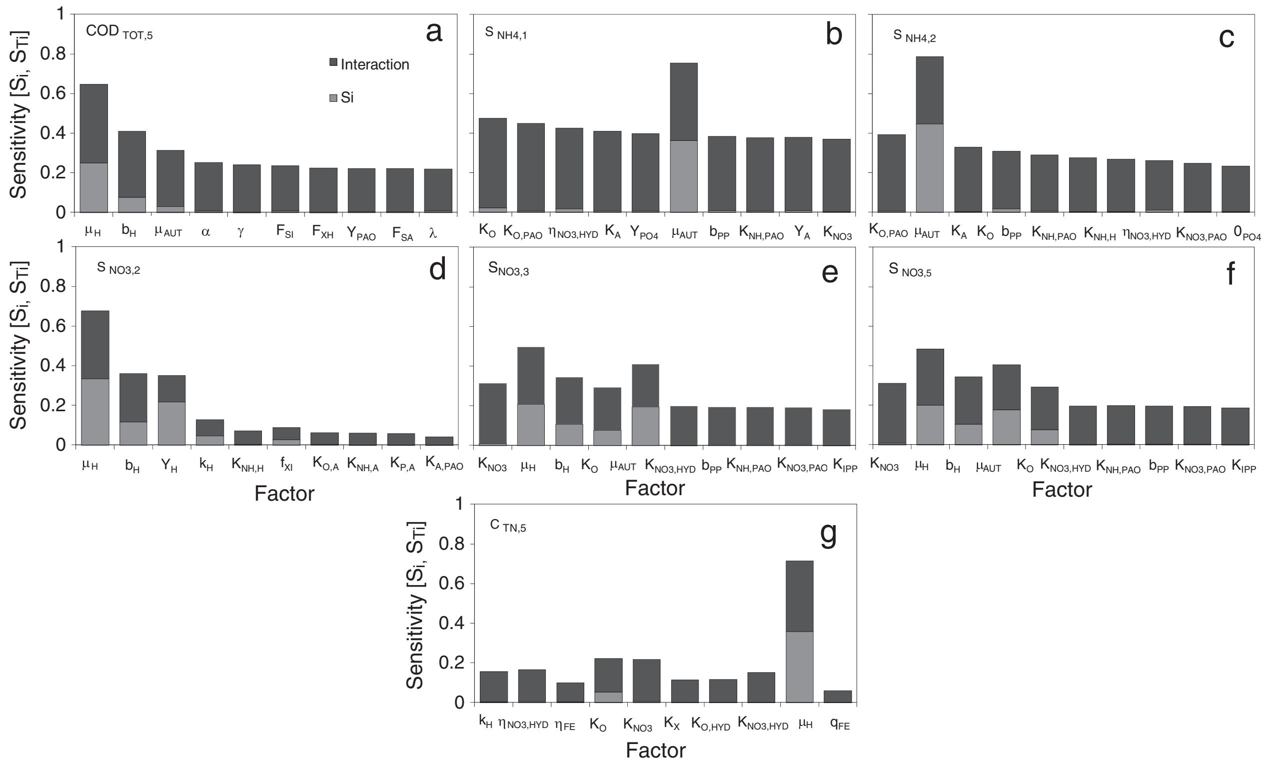


Fig. 3. First ten factors having high interaction value for $COD_{TOT,5}$ (a), $S_{NH4,1}$ (b), $S_{NH4,2}$ (c), $S_{NO3,2}$ (d), $S_{NO3,3}$ (e), $S_{NO3,5}$ (f) and $C_{TN,5}$ (g). Dark-grey bar represents the interaction value, light-grey bar represents S_i while the sum of dark-grey and light-grey bars represents S_{Ti}.

has been obtained. The present case study identifies the presence of non-linearity and interactions for ammonia and nitrate sub-groups.

4.4. Implications for modellers

In case a modeller wants to optimise processes, the results discussed in this paper show how important it is to analyse, according to the specificity of the case under study, whether factors are important or non-influential for each of the plant's sections. Only by analysing the values of S_i and S_{Ti} section by section for all of the relevant variables, the modeller will be able to acquire sufficient information related to the biological processes, which occur in the system under study, going beyond her/his a priori knowledge about the processes. Moreover, an improvement of the experimental design could be obtained by reducing the number of unnecessary measurements. All results have underlined the characteristics of the behaviour of the system under study due to both the presence of the physical sub-model and the plant scheme (the latter entails the presence of several recycled sludge fluxes). Due to these characteristics and the complexity of the involved biological processes, some of the obtained results are specific for the analysed case study and differ from previous studies (Sin et al., 2011; Chen et al., 2012). Specifically, the system exhibits significant interactions, which necessitate the use of more advanced GSA techniques than typically used. Although it is important to underline that the results obtained are case-study dependent the authors believe that both the approach and results presented here are of general value to the systems analysis of MBR models.

5. Conclusions

- GSA was applied to different subgroups of variables to identify differences in importance of factors between compounds:
  - Variation in MLSS was mainly explained by factors related to heterotrophs and was stable across the plant sections. For the MLSS sub-group, a substantial reduction of the number of uncertain factors to be considered was obtained (56 out of 79 factors are non-influential).
  - For the COD sub-group, only 2 out of 79 model factors were classified as being non-influential. Factors α and γ related to the physical model were found to be involved in interactions.
  - For the ammonia, nitrate and P sub-groups, the application of the variance based sensitivity analysis method provided significantly different results in terms of factor sensitivity compared to methods, which do not take into account interaction among factors (e.g. regression-based methods).
- The GSA results depended highly on the choice of compound and the sampling location within the treatment plant. This could be taken advantage of to design experiments in a more efficient way.
- The employed ASM model behaved in a strongly non-linear and non-additive way, contrary to previous GSA applications on simplified ASMs.
- The results underlined the importance of interactions due to both the presence of the physical sub-model and the plant scheme with the presence of several recycled sludge fluxes. The fact that these interactions surfaced in this study may be explained by the complexity of the model on the one hand and the large variation range adopted for each factor. Most importantly, however, the fact that such significant interactions were present, points to the necessity to use the more advanced GSA techniques than typically used. Furthermore, from the modelling point of view, the use of integrated models, which take into account both biological and physical processes simultaneously, is recommended.

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References

APHA WEF. Standard methods for the examination of water and wastewater. 20th ed. Washington, DC, USA: American Public Health Association/American Water Works Association/Water Environment Federation; 1998.

Benedetti L, Claeys F, Nopens I, Vanrolleghem PA. Assessing the convergence of LHS Monte Carlo simulations of wastewater treatment models. Water Sci Technol 2011;63(10):2219–24.

Benedetti L, Batstone DJ, De Baets B, Nopens I, Vanrolleghem PA. Uncertainty analysis of WWTP control strategies made feasible. Water Qual Res J Can 2012;47(1):14–29.

Brockmann D, Morgenroth E. 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 Sci Technol 2007;56(8):85–93.

Brun R, Kühni M, Siegrist H, Gujer W, Reichert P. Practical identifiability of ASM2d parameters: systematic selection and tuning of parameter subsets. Water Res 2002;36:4113–27.

Campolongo F, Cariboni J, Saltelli A. An effective screening design for sensitivity analysis of large models. Environ Model Software 2007;22(10):1509–18.

Chen L, Tian Y, Cao C, Zhang S, Zhang S. Sensitivity and uncertainty analyses of an extended ASM3–SMP model describing membrane bioreactor operation. J Membr Sci 2012;389:99–109.

Corominas L, Flores-Alsina X, Snip L, Vanrolleghem PA. Comparison of different modeling approaches to better evaluate greenhouse gas emissions from whole wastewater treatment plants. Biotechnol Bioeng 2012;109(11):2854–63.

Cosenza A, Mannina G, Neumann MB, Viviani G, Vanrolleghem PA. Biological nitrogen and phosphorus removal in membrane bioreactors: model development and parameter estimation. Bioprocess Biosyst Eng 2013a;36(4):499–514.

Cosenza A, Di Bella G, Mannina G, Torregrossa M, Viviani G. Biological nutrient removal and fouling phenomena in a University Cape Town Membrane Bioreactor treating high nitrogen loads. J Environ Eng ASCE 2013b;139(6):773–80.

Cosenza A, Mannina G, Vanrolleghem PA, Neumann MB. Global sensitivity analysis in wastewater applications: a comprehensive comparison of different methods. Environ Model Software 2013c;49:50–2.

Cosenza A, Di Bella G, Mannina G, Torregrossa M. The role of EPS in fouling and foaming phenomena for a membrane bioreactor. Bioresour Technol 2013d;147:184–92.

Cukier RI, Fortuin CM, Shuler KE, Petschek AG, Schaibly JH. Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients. I Theory. J Chem Phys 1973;59(8):3873–8.

Di Bella G, Mannina G, Viviani G. An integrated model for physical–biological wastewater organic removal in a submerged membrane bioreactor: model development and parameter estimation. J Membr Sci 2008;322(1):1–12.

Di Trapani D, Capodici M, Cosenza A, Di Bella G, Mannina G, Torregrossa M, et al. Evaluation of biomass activity and wastewater characterization in a UCT-MBR pilot plant by means of respirometric techniques. Desalination 2011;269:190–7.

Fenu A, Guglielmi G, Jimenez J, Spèrandio M, Saroj D, Lesjean B, et al. Activated sludge model (ASM) based modelling of membrane bioreactor (MBR) processes: a critical review with special regard to MBR specificities. Water Res 2010;44(15):4272–94.

Flores-Alsina X, Corominas Ll, Neumann MB, Vanrolleghem PA. Assessing the use of activated sludge process design guidelines in wastewater treatment plant projects: a methodology based on global sensitivity analysis. Environ Model Software 2012;38:50–8.

Freni G, Mannina G. Bayesian approach for uncertainty quantification in water quality modelling: the influence of prior distribution. J Hydrol 2010;392:31–9.

Hauduc H, Rieger L, Ohtsuki T, Shaw A, Takàcs I, Winkler S, et al. Activated sludge modelling: development and potential use of a practical applications database. Water Sci Technol 2011;63(10):2164–82.

Henze M, Gujer W, Mino T, van Loosdrecht M. Activated sludge models ASM1, ASM2, ASM2d and ASM3. IWA Task Group on Mathematical Modelling for Design and Operation of Biological Wastewater Treatment. London, UK: IWA Publishing; 2000.

Innocenti V. Modello di depurazione biologica secondo lo standard ASM3 con doppio step di nitrificazione. (Degree thesis)Italy: Universita' degli Studi di Firenze; 2005 [in Italian].

Jeppsson U. Modelling aspect of wastewater treatment process. [PhD thesis]Sweden: Department of Industrial Electrical Engineering and Automation (IEA), Lund Institute of Technology (LTH); 1996.

Jiang T, Myngheer S, De Pauw DJW, Spanjers H, Nopens I, Kennedy MD, et al. Modelling the production and degradation of soluble microbial products (SMP) in membrane bioreactors (MBR). Water Res 2008;42(20):4955–64.

Mannina G, Cosenza A. The fouling phenomenon in membrane bioreactors: assessment of different strategies for energy saving. J Membr Sci 2013;444:332–44.

Mannina G, Viviani G. Separate and combined sewer systems: a long-term modelling approach. Water Sci Technol 2009a;60(3):555–65.

Mannina G, Viviani G. Hybrid moving bed biofilm reactors: an effective solution for upgrading a large wastewater treatment plant. Water Sci Technol 2009b;60(5): 1103–16.

Mannina G, Cosenza A, Vanrolleghem PA, Viviani G. A practical protocol for calibration of nutrient removal wastewater treatment models. J Hydroinformatics 2011a;13(4): 575–95.

Mannina G, Di Bella G, Viviani G. An integrated model for biological and physical process simulation in membrane bioreactors (MBRs). J Membr Sci 2011b;376:56–69.

Meng F, Chae SR, Drews A, Kraume M, Shin HS, Yang F. Recent advances in membrane bioreactors (MBRs): membrane fouling and membrane material. Water Res 2009;43:1489–512.

Morris MD. Factorial sampling plans for preliminary computational experiments. Technometrics 1991;33(2):161–74.

Neumann MB. Comparison of sensitivity analysis techniques for modelling micropollutant oxidation in water treatment. Sci Total Environ 2012;433(1):530–7.

Neumann MB, von Gunten U, Gujer W. Uncertainty in prediction of disinfection performance. Water Res 2007;41:2371–8.

Neumann MB, Gujer W, von Gunten U. Global sensitivity analysis for model-based prediction of oxidative micropollutant transformation during drinking water treatment. Water Res 2009;43:997–1004.

Pujol G. Sensitivity: sensitivity analysis. R package version 1.3-0; 2007.

R Development Core Team. R: a language and environment for statistical computing; 2007.

Rieger L, Koch G, Kühni M, Gujer W, Siegrist H. The EAWAG Bio-P module for activated sludge model No. 3. Water Res 2001;35(16):3887–903.

Ruano MV, Ribes J, Ferrer J, Sin G. Application of the Morris method for screening the influential parameters of fuzzy controllers applied to wastewater treatment plants. Water Sci Technol 2011;63(10):2199–206.

Saltelli A, Tarantola S, Chan KPS. A quantitative model-independent method for global sensitivity analysis of model output. Technometrics 1999;41(1):39–56. [426].

Saltelli A, Tarantola S, Campolongo F, Ratto M. Sensitivity analysis in practice. A guide to assessing scientific models. Probability and Statistics SeriesJohn Wiley & Sons Publishers; 2004.

Saltelli A, Ratto M, Tarantola S, Campolongo F. Sensitivity analysis for chemical models. Chem Rev 2005;105:2811–27.

Saltelli A, Ratto M, Andres T, Campolongo F, Cariboni J, Gatelli D, et al. Global sensitivity analysis. The primer. The Atrium, Southern Gate, Chichester: John Wiley & Sons Ltd.; 2008.

Schaibly JH, Shuler KE. Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients. II applications. J Chem Phys 1973;59(8):3879–88.

Sin G, Gernaey KV, Neumann MB, van Loosdrecht MCM, Gujer W. Uncertainty analysis in WWTP model applications: a critical discussion using an example from design. Water Res 2009;43(11):2894–906.

Sin G, Gernaey KV, Neumann MB, van Loosdrecht M, Gujer W. Global sensitivity analysis in wastewater treatment plant model applications: prioritizing sources of uncertainty. Water Res 2011;45:639–51.

Sobol IM. Sensitivity analysis for non-linear mathematical models. Math Model Comput Exp 1993;1:407–14.

Weijers SR, Vanrolleghem PA. A procedure for selecting best identifiable parameters in calibrating activated sludge model No. 1 to full-scale plant data. Water Sci Technol 1997;36(5):69–79.

Zuthi MFR, Guo WS, Ngo HH, Nghiem L, Hai FI. Enhanced biological phosphorus removal and its modelling for the activated sludge and membrane bioreactor processes. Bioresour Technol 2013;139:363–74.