URBAN DRAINAGE MODELLING 2015

Oral Presentations I

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Global sensitivity analysis for micropollutant modeling by means of an urban integrated approach

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Abstract

The paper presents the sensitivity analysis of an integrated urban water quality system by means of the global sensitivity analysis (GSA). Specifically, an home-made integrated model developed in previous studies has been modified in order to include the micropollutant assessment (namely, sulfamethoxazole - SMX). The model is able to estimate also the interactions between the three components of the system: sewer system (SS), wastewater treatment plant (WWTP) and the receiving water body (RWB).

The analysis has been applied to an experimental catchment nearby Palermo (Italy): the Nocella catchment. Five scenarios each characterized by different combinations of sub-systems (i.e., SS, WWTP and RWB) have been considered applying the Extended-FAST method.

Results demonstrated that GSA is a powerful tool for increasing operator confidence in the modelling results; the approach can be used for blocking some non-identifiable parameters thus wisely modifying the structure of the model and reducing the related uncertainty. The model factors related to the SS have been found to be the most relevant factors affecting the SMX modeling.

Keywords

Contaminants of emerging concerns, mathematical modelling, Monte Carlo simulations, sensitivity analysis, urban water quality.

INTRODUCTION

In the last three decades, scientific research focused on preservation of water environment and on the impact of urban areas pollutants of natural water bodies especially in terms of macropollutants (nitrogen, phosphorus, COD). However, the Water protection legislations (e.g. the EU Water Framework Directive (EC, 2000) and the Environmental Quality Standard Directive (EQS e EC, 2008) also require the reduction of a range of micropollutants (MP), i.e. substances such as drugs, pharmaceuticals, personal care products, biocides, etc.

These substances are characterized of being persistent in the environment, toxic and bioaccumulative (EPA, 2013). Indeed, despite they are not naturally contained in the environment they have been found in some water bodies (Loos et al., 2013). MPs can lead to significant risk on the environment and human health. Indeed, several studies have demonstrated adverse effects of MP on the aquatic life (Coe et al., 2008; Lange et al., 2009). Therefore, the reduction of the discharged load and/or the elimination of these compounds inside the wastewater treatment plant (WWTP) before being discharged in the aquatic environment is an important issue with regard to the quality (Huerta- Fontela et al., 2010).

In this context mathematical modelling can represent an useful tool to assess the MP load discharged in the environment as well as to develop and implement strategies to control MP pollution.

With this regard, researches have demonstrated the importance of integrated analysis, involving both quantity and quality aspects. Thus taking into account the entire integrated system and the interactions between two or more physical systems, i.e. sewer system (SS), WWTP and receiving water body (RWB) (Rauch et al., 2002). With this aim, integrated urban drainage models have been developed introducing the MP fate and transport by putting together single system model. Recently, Vezzaro et al. (2012) introduced an integrated model - combining MP source characterization with dynamic modelling of runoff quality and stormwater treatment. The use of parsimonious approaches can be fundamental to provide useful and reliable modelling results in case of integrated complex model.

In this context, sensitivity analysis (SA) represents a very powerful tool, as it is able to provide information about how the variation in the output of the model can be apportioned to the variation of the input factors. Thus, SA can provide information about the relationships between the different systems of the integrated model (i.e., SS, WWTP and RWB).

This paper presents an integrated water quality urban drainage model that is able to model the sulfamethoxazole (SMX) fate throughout each component of the integrated system (SS, WWTP and RWB). In order to evaluate the role of the processes occurring inside each component of the integrated system on the RWB quality, the global sensitivity analysis has been applied. More precisely, five scenarios have been analyzed and compared by adopting Extended-FAST method, each varying different set of model factors.

MATERIAL AND METHODS

The integrated urban drainage model

The system was modelled employing a bespoke integrated model developed during previous studies (Mannina et al., 2006). The integrated model simulates the main phenomena that take place both in the SS, in the WWTP and in the RWB both during dry and wet weather periods. The model is made up mainly of three sub-models: (i) the rainfall-runoff and flow propagation sub-model, which evaluates the qualitative-quantitative features of the storm water; (ii) the WWTP sub-model, which is representative of the treatment processes; (iii) the RWB sub-model, which simulates the pollution transformations inside the RWB (Figure 1).

The integrated model as proposed by Mannina et al. (2006) has been modified in order to include the sulfamethoxazole (SMX) modelling in each sub-model according to literature (Vezzaro et al., 2010; 2012 and Plósz et al., 2012).

The SS and the RWB models have modified including the mathematical modelling of two components: dissolved (S_{SMX}) and particulate (X_{SMX}). Furthermore, the integrated model applied here has the advantage to consider both SMX sorption and biotransformation in sewer networks mostly omitted in regional model-based assessments (e.g. Ort et al., 2009).

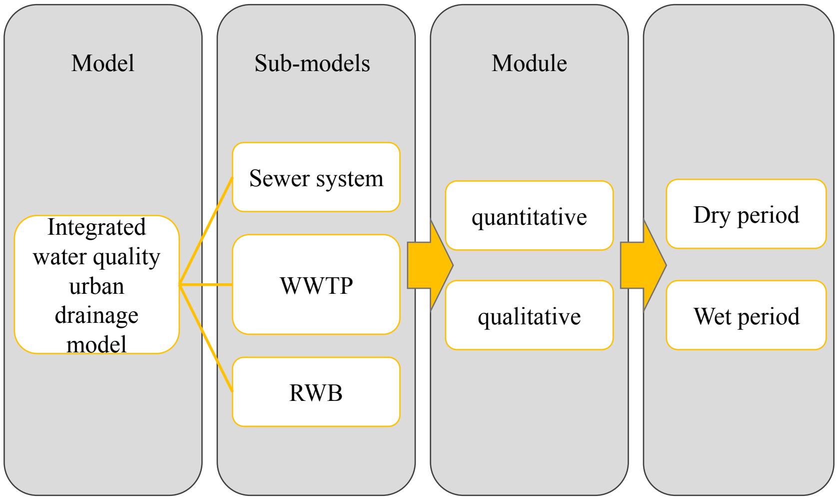

Figure 1. Schematic overview of the integrated model

In Table 1 the processes and the rate are summarized. Such relationships have been considered to describe the SMX fate both in the SS and in the RWB (Vezzaro et al., 2010).

More precisely, the sorption, desorption and the degradation processes have been considered. Important to precise is that anoxic and aerobic degradation processes have only been considered for the RWB, conversely for the SS the only anaerobic degradation process has been considered. The symbol reported in Table 1 has the same meaning as presented in Vezzaro et al. (2010).

Table 1. Process matrix for S_{SMX} and X_{SMX}; adapted from Vezzaro et al. (2010).

Process	Dissolved S_{SMX}	Particulate X_{SMX}	Process rate
Sorption	-1	+1	$k_{sor}\ (X_{TSS}/V)\ S_{SMX}$
Desorption	+1	-1	$(k_{sor}/k_d)\ X_{SMX}$
Aerobic degradation	α_{oxygen}		$k_{aer}\ S_{SMX}$
Anaerobic degradation	$1-\alpha_{oxygen}$		$k_{anaer}\ S_{SMX}$
Anoxic degradation	$1-\alpha_{oxygen}$		$k_{anox}\ S_{SMX}$

The mass balance equations related to the X_{SMX} and S_{SMX} during the wet period are reported in Equations 1 and 2, respectively.

$$X_{SMX} = \left(TSS * f_{SMX} + \frac{L_{SMX}}{Qwet} \right) + k_{sor} TSS * \Delta t * S_{SMX} - \frac{k_{sor}}{k_d} \Delta t * X_{SMX} - k_{anox} (1 - \alpha_{oxygen}) \Delta t * S_{SMX} \qquad (1)$$

$$S_{SMX} = -k_{sor} TSS * \Delta t * S_{SMX} + \frac{k_{sor}}{k_d} \Delta t * X_{SMX} - k_{aer} \alpha_{oxygen} \Delta t * S_{SMX} - k_{anox} (1 - \alpha_{oxygen}) \Delta t * S_{SMX} \qquad (2)$$

where TSS [mg L^{-1}] represents the suspended solids concentration, f_{SMX} [-] is the correlation factor between TSS and SMX, ΔT [sec] represents the time step, L_{SMX} [kg sec^{-1}] is the SMX load and Q_{wet} represents the wet flow rate.

The fate of SMX inside the WWTP has been modelled adopting the same principles of ASM-X as proposed by (Plósz et al., 2010; Plósz et al., 2012) without considering the sequestered form of SMX. More precisely, the fate of SMX has been described by using three state variables two in the liquid phase and one in the solid phase. The two state variables of the liquid phase are the chemical concentration (C_{LI}) and the total retransformable chemical concentration (C_{CJ}). The sum between C_{LI} and C_{CJ} represents S_{SMX}. The state variables of the solid is the sorbed concentration (C_{SL}) that represents X_{SMX}. The same processes and rates as proposed by Plósz et al. (2012) have been here considered.

The case study

The analysis was applied to a complex integrated system: the Nocella catchment. The case study is a partially urbanized catchment located nearby Palermo in the north-western part of Sicily (Italy). The entire natural basin has a surface of 99.7 km^2 and has two main branches that flow primarily east to west. The basin closure is located 9 km upstream from the river mouth; the catchment area is 66.6 km^2. The catchment end is equipped with a hydro-meteorological station (Nocella a Zucco). This river reach receives wastewater and stormwater from two urban areas (Montelepre, with a catchment surface equal to 70 ha, and Giardinello, with a surface of 45 ha) drained by combined sewers. Both urban areas are characterized by concrete sewer pipes with steep slopes.

The catchment under study was characterized by two SSs (SS1 – Montelepre and SS2 – Giardinello), two WWTPs (WWTP1 – Montelepre and WWTP2 – Giardinello) and a RWB (Nocella river). Further details concerning the case study and monitoring campaign can be found in Candela et al. (2012).

The global sensitivity analysis – Extended-FAST method

In order to pin down the most influential model parameters of the IUWQ model, the GSA, (namely, Extended-FAST) was applied (Saltelli et al., 2005). The Extended-FAST method belongs to the variance decomposition methods. It is founded on the variance decomposition theorem which states that the total variance of the model output (*Var(Y)*) may be decomposed into conditional variances. This method does not require any assumptions on model structure (linearity, monotonicity etc.). In particular, for each factor *i* two sensitivity indices are defined: the first order effect index (S_i) and the total effect index (S_{Ti}). S_i measures how the *i-th* factor contributes to *Var(Y)* without taking into account the interactions among factors. It is expressed as:

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

(3)

where *E* indicates the expectancy operator and *Var* the variance operator. According to the notation used by Saltelli *et al*. (2004) the subscripts indicate that the operation is either applied ‘‘over the *ith* 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:

$$S_{T\,i} = 1 - \frac{Var_{x_{-i}}\left(E_{x_i}\left(Y|x_{-i}\right)\right)}{Var\left(Y\right)}$$

(4)

The Extended-FAST method requires an $n{\cdot}N_{MC}$ simulations, where n is the number of factors and N_{MC} the number of MC simulations per factor (N_{MC} = 500 – 1000 according to Saltelli *et al*. (2005). It is important to underline that in the context of *factors fixing* the analysis of S_{Ti} has to be performed. If the S_i value is small it doesn't mean that the parameter may be fixed anywhere within its range because a high S_{Ti} value would indicate that the parameter is involved in interactions.

Scenario analysis and numerical setting

Five scenarios have been analysed and compared. For each scenario different set of model factors have been varied during the Extended-FAST application. Details related of each scenario are summarized in Table 2. For each scenario 500 Monte Carlo simulations x number of model factors (N_{MC}) have been performed.

Table 2. Set of model factors varied for each scenario. X represents the variation of a group of model factors of the sub-model

Scenario	SS1	SS2	WWTP1	WWTP2	RWB
1	X	X	X	X	X
2	X				
3		X			
4			X		
5				X	

Table 3 summarises the symbol, unit and the adopted variation range of each of the model factor varied for each sub-model.

Table 3. symbol, unit and the adopted variation range of each of the model factor

	No.	Symbol	Description	Unit	Range
SS1 and SS2	1;18	$t_{channel}$	Channel detention time	min	8-30
	2;19	W_0	Initial hydrological losses	mm	0.1-1
	3;20	Φ	Catchment runoff coefficient	-	0.6-0.98
	4;21	K1	Catchment reservoir constant	min	0.1-55
	5;22	K2	Sewer reservoir constant	min	0.1-65
	6;23	Accu	Build-up coefficient	kg ha^{-1} d^{-1}	0.1-20
	7;24	Disp	Decay coefficient	d^{-1}	0.01-1
	8;25	Arra	Wash-off coefficient	mm^{-Wh} h$^{(Wh-1)}$	0.01-1
	9;26	W_h	Wash-off factor	-	0.1-3.5
	10;27	M	Erosion coefficient	g h^{-1}	0.1-3
	11;28	K_{susp}	Sewer suspension delay	h	0.01-0.8
	12;29	K_{bed}	Sewer bed transport delay	h	0.01-1
	13;30	r_{th}	Theoretical dilution coefficient	-	1.1-2
	14;31	r	Dilution coefficient	-	2-4
	15;32	k_d	Solid-water partition coefficient	1000*m^3 gTSS^{-1}	1.44-1.76
	16;33	k_{sor}	Sorption rate	m^3 gTSS^{-1} d^{-1}	0.144-0.176
	17;34	k_{anaer}	Anaerobic biodegradation rate	1000*d^{-1}	2.17-2.66
WWTP1 and WWTP2	35;39	k_{d_ox}	Aerobic solid-liquid sorption coefficient	L gTSS^{-1}	0.28-0.34
	36;40	k_{dec_ox}	Aerobic biotransformation rate coefficient	L gTSS^{-1} d^{-1}	6.12-7.48
	37;41	k_{bio_ox}	Aerobic biotrasf. rate coefficient for C_{Li}	L gTSS^{-1} d^{-1}	0.4-0.45
	38;42	η_{Dec}	Correc. factor for Ss inhibiition on C_{Li} formation	-	1.8-2.2
RWB	43	kQ	Reservoir flow constant	sec^{-1}	240-297
	44	kC	Reservoir concentration constant	sec^{-1}	193-236
	45	k_{BOD}	BOD removal coefficient rate	1000*sec^{-1}	3.76-4.59
	46	K_{NH}	N-NH$_4$ removal coefficient rate	1000*sec^{-1}	4.93-6.03
	47	k_{sor}	Sorption rate	m^3 gTSS^{-1} d^{-1}	0.099-0.121
	48	k_d	Solid-water partition coefficient	m^3 gTSS^{-1}	0.0099-0.0121
	49	k_{aer}	Anaerobic biodegradation rate	d^{-1}	0.024-0.029
	50	k_{anaer}	Anaerobic biodegradation rate	1000*d^{-1}	2.17-2.66

The Extended-FAST has been applied varying the model factors reported in Table 3 (according the scenarios as reported in Table 2) considering as reference the model outputs summarized in Table 4.
Table 4. Model output taken into account for each sub-model

	Symbol	**Description**	**Unit**
SS1 and SS2	$Q_{SS,max}$	Maximum effluent flow rate	$m^3\ sec^{-1}$
	$TSS_{,max}$	Maximum effluent TSS concentration	$mg\ L^{-1}$
	$BOD_{,max}$	Maximum effluent BOD concentration	$mg\ L^{-1}$
	LTSS	Total TSS effluent load	$kgTSS\ sec^{-1}$
	LBOD	Total BOD effluent load	$kgBOS\ sec^{-1}$
	$X_{SMX,max}$	Maximum effluent X_{SMX} concentration	$ng\ L^{-1}$
	$S_{SMX,max}$	Maximum effluent S_{SMX} concentration	$ng\ L^{-1}$
WWTP1 and WWTP2	$BOD_{,max}$	Maximum effluent BOD concentration	$mg\ L^{-1}$
	$S_{NH,max}$	Maximum effluent ammonia concentration	$mg\ L^{-1}$
	$X_{SMX,max}$	Maximum effluent X_{SMX} concentration	$ng\ L^{-1}$
	$S_{SMX,max}$	Maximum effluent S_{SMX} concentration	$ng\ L^{-1}$
RWB	$Q_{RWB,max}$	Maximum effluent flow rate	$m^3\ sec^{-1}$
	$BOD_{,max}$	Maximum effluent BOD concentration	$mg\ L^{-1}$
	$X_{SMX,max}$	Maximum effluent X_{SMX} concentration	$ng\ L^{-1}$
	$S_{SMX,max}$	Maximum effluent S_{SMX} concentration	$ng\ L^{-1}$

RESULTS AND DISCUSSION

Scenario analysis results

For sake of shortness only the relevant results related to the model outputs of the RWB (with particular reference to SMX) will be discussed (Scenario 1). Thus, attention will be focused on the role of model factors related to the upstream sub-model on the RWB quality in terms of MPs pollution. Furthermore, the comparison among the results of the 5 scenarios will be discussed in terms of maximum values of Si for each sub-model.

In Figure 2 the results related to $X_{SMX,max}$ (Fig. 2a) and $S_{SMX,max}$ (Fig. 2b) for the scenario 1 are shown.

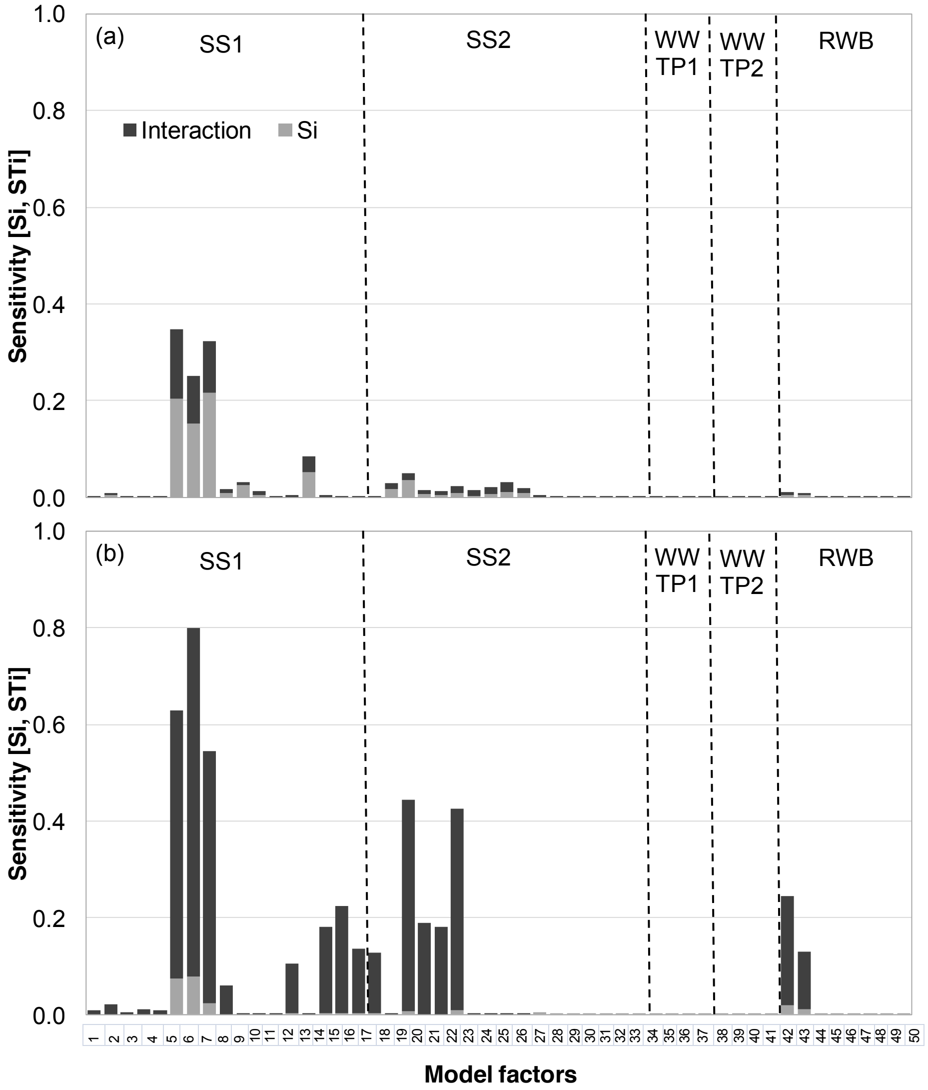

Figure 2. Results of Si and interaction related to $X_{SMX,max}$ (a) and $S_{SMX,max}$ for RWB (b)

Specifically, for each group of model factors (related to SS1, SS2, WWTP1, WWTP2 and RWB) the values of Si and interactions are reported. By analysing Figure 2a one can observe that the most important model factors for $X_{SMX,max}$ in the RWB are Accu (no. 6), Disp (no. 7) and Arra (no. 8) related to the SS1 which account for 20% , 15% and 21% of the variance, respectively. This result is mainly debit to the role of these three factors in influencing the TSS content inside the integrated model and consequently inside the RWB (Vanrolleghem et al., 2015). Indeed, the TSS content is directly connected to the particulate SMX process (Vezzaro et al., 2011). However, as shown by the dark grey bars on Figure 2a these three model factors contribute for 14%, 9% and 10% to the total variance in terms of interaction. This result is mainly due to the role of these factors in influencing other model output.

For $S_{SMX,max}$ (Figure 2b) a great number of model factors showed to have an high contribution in terms of interaction both for SS1 and SS2. This means that the soluble compound of SMX is strongly related to the TSS compound. Thus, underlying the key role of sorption/desorption process on the maximum concentration of S_{SMX} in th RWB. Thus confirming that the reduction of the solid compounds released inside the RWB can have an important role in reducing the MP pollution in the acquatic system (Vezzaro et al., 2010).

Comparison among the scenarios. Table 5 summarizes the results for each scenario and model output of the maximum value of Si. By analysing the results reported in Table 5 one can observe that in scenarios 1, 2 and 3 model factors connected with the SS modelling has the highest contribution to the total variance for all model outputs. Regarding the SMX model outputs, the same results as discussed before can be observed from Table 5. Indeed, from scenario 1 to scenario 3 both $X_{SMX,max}$ and $S_{SMX,max}$ are strongly influenced by the model factors related to SS. Thus emphasizing the role of the upstream processes on the MP concentration inside the RWB.

Table 5. Maximum Si value for each scenario and model output

		Maximum S_i				
		Scenario 1	**Scenario 2**	**Scenario 3**	**Scenario 4**	**Scenario 5**
SS1	$Q_{SS,max}$	0.5 (K1)	0.5 (K1)	-	-	-
	$TSS_{,max}$	0.3 (Accu)	0.3 (Accu)	-	-	-
	$BOD_{,max}$	0.22 (Arra)	0.22 (Arra)	-	-	-
	LTSS	0.52 (Accu)	0.52 (Accu)	-	-	-
	LBOD	0.5 (Accu)	0.5 (Accu)	-	-	-
	$X_{SMX,max}$	0.29 (Accu)	0.29 (Accu)	-	-	-
	$S_{SMX,max}$	0.37 (Accu)	0.37 (Accu)	-	-	-
SS2	$Q_{SS,max}$	0.25 (K1)	-	0.36 (K1)	-	-
	$TSS_{,max}$	0.51 (K_{susp})	-	0.47 (K_{susp})	-	-
	$BOD_{,max}$	0.55 (K_{susp})	-	0.51 (K_{susp})	-	-
	LTSS	0.36 (Accu)	-	0.3 (Accu)	-	-
	LBOD	0.28 (Accu)	-	0.25 (Accu)	-	-
	$X_{SMX,max}$	0.45 (K_{susp})	-	0.41 (K_{susp})	-	-
	$S_{SMX,max}$	0.35 (K_{susp})	-	0.33 (K_{susp})	-	-
WWTP1	$BOD_{,max}$	0.38 (Accu)	0.38 (Accu)	-	-	-
	$S_{NH,max}$	0.4 (Accu)	0.4 (Accu)	-	-	-
	$X_{SMX,max}$	0.52 (Accu)	0.59 (Accu)	-	0.94 (k_{d_ox})	-
	$S_{SMX,max}$	0.42 (Accu)	0.53 (Accu)	-	0.9 (k_{d_ox})	-
WWTP2	$BOD_{,max}$	0.18 (W_h)	-	0.18 (W_h)	-	-
	$S_{NH,max}$	0.23 (W_h)	-	0.24 (W_h)	-	-
	$X_{SMX,max}$	0.24 (Accu)	-	0.24 (Accu)	-	0.75 (k_{d_ox})
	$S_{SMX,max}$	0.27 (Accu)	-	0.23 (W_h)	-	0.8 (k_{d_ox})
RWB	$Q_{RWB,max}$	0.15 (Φ)	0.6 (Φ)	0.26 (Φ)	-	-
	$BOD_{,max}$	0.2 (Arra)	0.3 (Arra)	0.34 (Φ)	-	-
	$X_{SMX,max}$	0.2 (Arra)	0.55 (Accu)	0.27 (Φ)	0.85 (k_{d_ox})	0.65 (k_{d_ox})
	$S_{SMX,max}$	0.08 (Disp)	0.28 (Arra)	-	0.95 (k_{d_ox})	0.65 (k_{d_ox})

Regarding the last two scenarios (4 and 5), the results reported in Table 1 show that the most relevant factor affecting the SMX modelling is represented by the aerobic solid-liquid sorption coefficient

(k_{d_ox}). Indeed, this factor affect till to 95% of the total variance of $S_{SMX,max}$ (scenario 4). Thus demontrating that the predominat processes inside the WWTP are the desorption/sorption. Such a result is in line with previous findings which demonstrate that MP fate throughout wastewater treatment systems strongly depends on their sorption behaviour (e.g. Song et al., 2006; Plósz et al., 2013).

CONCLUSIONS

A home-made integrated model able to model the SMX (both as particulate and soluble compounds) has been used in this study. The Extended-FAST model has been employed to evaluate the role of the key factors affecting the quality of several model outputs of the catchment under study. Five scenarios have been analyzed by varying different combinations of model factors.
The key findings of this study can be summarized as in the following:

- For the scenario 1 (i.e, all the model factors selected for SS1, SS2, WWTP1, WWTP2 and RWB are varied) both $X_{SMX,max}$ and $S_{SMX,max}$ in the RWB are strongly influenced by the model factors that control the TSS load from the SS. Thus, the role of solids contents both for the desorption and sorption processes of SMX is relevant.
- The comparison among the scenarios have underlined that the SMX concentration inside the RWB is mainly influenced by the SS model factors (scenarios 1, 2 and 3). Whenever, the only factors related to the WWTP are changed (scenarios 4 and 5) the factor mainly affecting the SMX concentration inside the RWB is represented by the aerobic sorption coefficient (till to 95% influence of the total variance for $S_{SMX,max}$).

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