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Micropollutants throughout an integrated urban drainage model: Sensitivity and uncertainty analysis

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ABSTRACT

The paper presents the sensitivity and uncertainty analysis of an integrated urban drainage model which includes micropollutants. Specifically, a bespoke integrated model developed in previous studies has been modified in order to include the micropollutant assessment (namely, sulfamethoxazole – SMX). The model takes into account also the interactions between the three components of the system: sewer system (SS), wastewater treatment plant (WWTP) and receiving water body (RWB).

The analysis has been applied to an experimental catchment nearby Palermo (Italy): the Nocella catchment. Overall, five scenarios, each characterized by different uncertainty combinations of sub-systems (i.e., SS, WWTP and RWB), have been considered applying, for the sensitivity analysis, the Extended-FAST method in order to select the key factors affecting the RWB quality and to design a reliable/useful experimental campaign.

Results have demonstrated that sensitivity analysis is a powerful tool for increasing operator confidence in the modelling results. The approach adopted here can be used for blocking some non-identifiable factors, 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 in the RWB when all model factors (scenario 1) or model factors of SS (scenarios 2 and 3) are varied. If the only factors related to the WWTP are changed (scenarios 4 and 5), the SMX concentration in the RWB is mainly influenced (till to 95% influence of the total variance for $S_{SMX,max}$) by the aerobic sorption coefficient.

A progressive uncertainty reduction from the upstream to downstream was found for the soluble fraction of SMX in the RWB.

1. 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 (carbon, nitrogen, phosphorus). However, the Water protection legislations (e.g. the EU Water Framework Directive (EC, 2000) and the Environmental Quality Standard Directive (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. 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; McCall et al., 2016; Ramin et al., 2016).

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

With this regard, researches have demonstrated the importance of integrated analysis, involving both quantity and quality aspects. The integrated analysis has the advantage of taking into account the interactions between two or more physical systems, i.e. sewer system (SS), WWTP and receiving water body (RWB) (Rauch et al., 2002; Willems and Berlamont, 2002; Freni et al., 2009a,b). An integrated urban drainage model (IUDM) is therefore composed of submodels able to simulate the key processes of each system and the interactions among them. Therefore, IUDMs are often complex and

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involve tens of model parameters and model variables. Thus, the use of such complex models requires a robust database for their calibration and validation before being confidence on the modelled results (Bach et al., 2014).

During the last years, IUDMs have been made further complex by introducing the MP fate and transport (Bach et al., 2014).

Recently, Vezzaro et al. (2012) have introduced an integrated model, combining MP source characterization with dynamic modelling of runoff quality and stormwater treatment. However, authors have calibrated only the hydraulic sub-models due to the MP data lacking. Therefore, modeller cannot completely be confident with the results.

In view of providing results as more reliable as possible, modeller should apply a parsimonious approaches for integrated complex model and/or opportunely collect useful data to be adopted for model calibration/validation.

However, the collection of monitoring data is affected by significant limitations (Freni and Mannina, 2012; Ledin et al., 2013). These limitations can be technical and economical, as the data collection requires huge human and economic resources. Moreover, difficulties of collecting measurements carried out at the watershed outlet are often exhibited in literature (Freni and Mannina, 2012; Vezzaro et al., 2014; Freni and Mannina, 2010). Therefore, the challenge of improving the existing databases is a common practice of dedicated research projects. These difficulties in the data acquiring are amplified for MPs since they are commonly found in low concentrations (in the range of ng/l-mg/l) which are difficult to measure (Vezzaro et al., 2014).

In this context, sensitivity analysis (SA) can represent a very powerful tool to provide useful information required to design an effective (both in economical and usefulness terms) sampling campaign. Indeed, SA provides information about how the model output variation can be apportioned to the input factors variation. Therefore, SA allows the selection of the key factors mostly affecting the model results. Among the SA methods, global sensitivity analysis (GSA) has several advantages. GSA can help modeller to identify important input factors (factors prioritisation) as well as non-influential input factors (factors fixing) (Saltelli et al., 2005). Moreover, some GSA methods are also able to quantify the model variance contribution due to the synergistic or co-operative effect among factors (Saltelli et al., 2005, Cosenza et al., 2013). Therefore, in the IUDM context GSA can provide information about the relationships among the different sub-systems (i.e., SS, WWTP and RWB).

GSA should also provide an answer to the milestone for an effective monitoring campaign designing: i. What are the most significant/important factors contributing to the uncertainty for IUDM? ii. How does the uncertainty related to the data lacking affect the RWB results?

Thus, 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 effect of the uncertain of model parameters on the RWB quality, the GSA has been applied. More precisely, five scenarios have been analysed and compared by adopting Extended-FAST method, each considering a set of model factors as unknown. Furthermore, the he uncertainty propagation from the SS to the RWB has been evaluated.

2. Material and methods

2.1. 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 taking place in the SS, WWTP and RWB during both dry and wet weather period. The model is made up of three sub-models, each divided into a quantity and quality module for the simulations of the hydrographs and pollutographs, respectively (Fig. 1). More precisely, the integrated model is divided into: (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 (Fig. 1).

The integrated model proposed by Mannina et al. (2006) has been modified in order to include the SMX modelling in each sub-model according to previous literature (among others, Vezzaro et al., 2010, 2012; Plósz et al., 2012). A description of each sub-model will be provided below; further details about the model can be found in literature (Mannina et al., 2006; Mannina and Viviani, 2009, 2010a,b,c).

2.1.1. SS sub-model

The SS sub-model simulates the quality–quantity features of rain water during a storm event, which is applied to combined sewer systems receiving both domestic sewage and stormwater. Specifically, the quantity module evaluates the net rainfall from the measured hyetograph by adopting the loss function that takes into account the surface storage and soil infiltration. The net rainfall is then used to simulate the net rainfall–runoff transformation process and the flow propagation. This latter is evaluated by means of a cascade of two linear reservoirs in series and a linear channel. The linear channel allows to split the hydraulic phenomena in the catchment from those in the SS.

Regarding the quality module, the build-up and the wash-off phenomena on the catchment surfaces are modelled coupled with the sediment deposition and erosion processes inside the sewer. The build-up on the catchment surfaces is modelled by using the exponential function as proposed by Alley and Smith (1981). The solid wash-off that occurs during the storm event was modelled according to Jewell and Adrian (1978). The transport equation proposed by Parchure and Mehta (1985) coupled to the bed sediment structures hypothesized by Skipworth et al. (1999) were used to simulate the sediment erosion rate in the SS.

The SMX concentration inside the SS has been modelled by using two state variables: dissolved (S_{SMX}) and particulate (X_{SMX}). In Table 1 the transformation processes and the rates for SMX concentration in the SS are summarized. The SS sub-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) (Table 1). Further-

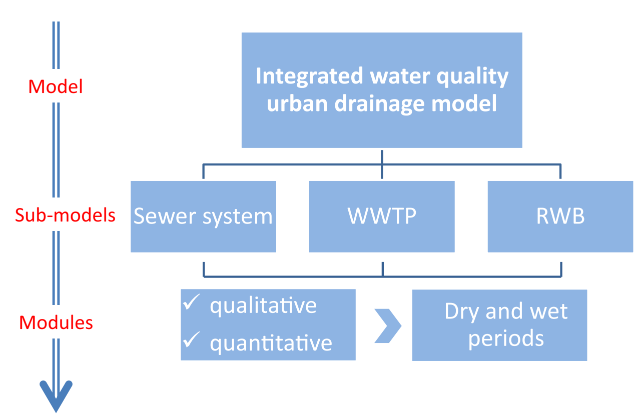

Fig. 1. Schematic overview of the integrated model.

Table 1
Process matrix for S_{SMX} and X_{SMX} modelling related to the SS sub-model. Where: k_{sor} = Sorption rate; X_{TSS} = suspended solids concentration; α_{oxygen} = Aerobic (1)/anaerobic (0) switch parameter; k_d = Solid-water partition coefficient; k_{anaer} = Anaerobic biodegradation rate.

Process	S_{SMX}	X_{SMX}	Process rate
Sorption	−1	+1	k_{sor} (X_{TSS}) S_{SMX}
Desorption	+1	−1	(k_{sor}/k_d) X_{SMX}
Anaerobic degradation	−1		$(1-\alpha_{oxygen})k_{anaer}$ S_{SMX}

more, the anaerobic degradation of SMX inside the SS has been considered (Table 1).

For example, the mass balance of S_{SMX} and X_{SMX} during the wet period are reported in Eqs. (1) and (2), respectively.

$$X_{SMX} = \left(X_{TSS} * f_{SMX} + \frac{L_{SMX}}{Q_{wet}}\right) + k_{sor}X_{TSS} * \Delta t * S_{SMX} - \frac{k_{sor}}{k_d}\Delta t * X_{SMX} \tag{1}$$

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

where f_{SMX} [–] is the correlation factor between X_{TSS} and SMX; ΔT [sec] is the time step resolution; L_{SMX} [kg sec^{-1}] = SMX load; Q_{wet} = wet flow rate.

2.1.2. WWTP sub-model

The WWTP has been modelled by adopting the Activated Sludge Model no 1 (ASM1) (Henze et al., 2000). The ASM1 model takes into account the main biological processes inside a WWTP involving both autotrophic and heterotrophic biomass. Specifically, the ASM1 model takes into account the following processes: aerobic and anoxic growth of heterotrophic bacteria; aerobic growth of autotrophic bacteria; decay of both autotrophic and heterotrophic bacteria; hydrolysis of both organic nitrogen and entrapped organic material; ammonification. These processes are included in the WWTP sub-model integrating with the overall urban drainage model.

The ASM1 model has been modified in order to include the SMX modelling. In particular, the fate of SMX inside the WWTP has been modelled by adopting the same principles of ASM-X as proposed by Plósz et al. (2010) and 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 $S_{SMX.}$ While, C_{SL} is the state variable related of the solid phase concentration that represents X_{SMX}. The same processes and rates as proposed by Plósz et al. (2012) have been here considered. Table 2 summarizes the stoichiometric matrix of the modified ASM1 related only to the SMX modelling.

2.1.3. RWB sub-model

The RWB has been modelled as proposed by literature (Mannina and Viviani, 2010a,b,c). More precisely, the RWB sub-model describes both the flow propagation along the river (quantity module) and the concentration of the biodegradable oxygen demand (BOD), dissolved oxygen (DO), ammonia (NH_4) and nitrate-nitrate (NO). During the flow propagation process, the hydrograph is characterized by two main relevant phenomena: a hydrograph flow delay and a hydrograph flow reduction. Further details about the model equations and parameters can be found in literature (Mannina and Viviani, 2010a,b,c).

RWB sub-model has been modified including the mathematical modelling of both S_{SMX} and X_{SMX}. Table 3 summarizes the processes and the rates considered. More precisely, the sorption, desorption and the degradation processes have been considered. Important to precise is that aerobic and anoxic degradation processes have been considered for the RWB. The symbol reported in Table 3 has the same meaning of that reported in Table 1.

For example, the mass balance of S_{SMX} and X_{SMX} during the wet period is reported in Eqs. (3) and (4), respectively.

$$X_{SMX} = \left(X_{TSS} * f_{SMX} + \frac{L_{SMX}}{Qwet}\right) + k_{sor}X_{TSS} * \Delta t * S_{SMX} - \frac{k_{sor}}{k_d}\Delta t * X_{SMX} - k_{anox}(1-\alpha_{oxygen})\Delta t * S_{SMX} \tag{3}$$

$$S_{SMX} = -k_{sor}X_{TSS} * \Delta t * S_{SMX} + \frac{k_{sor}}{k_d}\Delta t * X_{SMX} - k_{aer}\alpha_{oxygen}\Delta t * S_{SMX} - k_{anox}(1-\alpha_{oxygen})\Delta t * S_{SMX} \tag{4}$$

Symbols reported in Eqs. (3) and (4) have the same meaning as in Eqs. (1) and (2).

2.2. 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 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 (i.e., >10%).

The catchment under study was characterized by two SSs (SS1 – Montelepre and SS2 – Giardinello), two WWTPs (WWTP1 – Montelepre and WWTP2 – Giardinello) and as RWB a river stretch (Nocella river). Further details concerning the case study and monitoring campaign can be found in literature (Candela et al., 2012; Freni et al., 2012, 2011).

2.3. The global sensitivity analysis – Extended-FAST method

In order to pin down the most influential model parameters of the integrated urban drainage model, the GSA (namely, the Extended-FAST method) 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:

$$S_i = \frac{Var_{xi}(E_{x_{-i}}(Y|x_i))}{Var(Y)} \tag{5}$$

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}.

Table 2
Gujer matrix of the SMX modelling; symbol and meaning of the parameters are reported in Table 3.

Component i → Process j ↓	1 C_{Li}	2 C_{Cj}	3 C_{SL}	Process rate
De-sorption	1		−1	$k_{des} \cdot C_{SL}$
Aerobic sorption	−1		1	$k_{des} \cdot K_{d\_ox} \cdot C_{Li} \cdot \frac{S_O}{K_O+S_O} \cdot X_{TSS}$
Aerobic parent compound retransformation	1	−1		$k_{dec\_ox} \cdot C_{CJ} \cdot \frac{K_S \cdot \eta_{Dec}}{K_S \cdot \eta_{Dec}+S_S} \cdot \frac{S_O}{K_O+S_O} \cdot X_{TSS}$
Aerobic biotransformation	−1			$k_{dec\_ox} \cdot C_{CJ} \cdot \frac{K_S \cdot \eta_{Dec}}{K_S \cdot \eta_{Dec}+S_S} \cdot \frac{S_O}{K_O+S_O} \cdot X_{TSS}$
Anoxic sorption	−1		1	$k_{des} \cdot K_{d\_ax} \cdot C_{Li} \cdot \frac{S_O}{K_O+S_O} \cdot X_{TSS}$
Anoxic parent compound retransformation	1		−1	$k_{dec\_ax} \cdot C_{Cj} \cdot \frac{K_S \cdot \eta_{Dec}}{K_S \cdot \eta_{Dec}+S_S} \cdot \frac{K_O}{K_O+S_O} \cdot X_{TSS}$
Anoxic biotrasformation	−1			$k_{Bio\_ax} \cdot C_{Li} \cdot \frac{K_S \cdot \eta_{Bio}}{K_S \cdot \eta_{Bio}+S_S} \cdot \frac{K_O}{K_O+S_O} \cdot X_{TSS}$

Table 3
Process matrix for S_{SMX} and X_{SMX} modelling related to the RWB sub-model. k_{aer} = Aerobic biodegradation rate; k_{anox} = Anoxic biodegradation rate.

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

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

$$S_{T_i} = 1 - \frac{Var_{x_{-i}}(E_{x_i}(Y|x_{-i}))}{Var(Y)} \quad (6)$$

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 Vanrolleghem et al. (2015).

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 does not 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.

2.4. Scenario analysis and numerical setting

Five scenarios have been analysed and compared. For each scenario different set of model factors have been considered as unknown in order to quantify the effect of their uncertainty on the RWB quality. The set of unknown model factors has been varied during the Extended-FAST application for each scenario.

Details related of each scenario are summarized in Table 4. The first scenario is characterized by the highest uncertainty; indeed, the variation of the model factors of each sub-system is considered. On the other hand, scenarios 2–5 are those characterized by the variation of the model factors of one sub-system at time. Such scenarios allow to evaluate the weight of the uncertainty of each sub-system and to gain insight on the uncertainty propagation throughout the sub-systems.

For each scenario 500 Monte Carlo simulations x number of model factors (N_{MC}) have been performed (Vanrolleghem et al., 2015). For each scenario, the N_{MC} value has been established by testing the convergence of the sensitivity measure after increasing the number (Vanrolleghem et al., 2015).

Table 5 summarises the symbol, unit and the adopted variation range of each of the model factors varied for each sub-model; the widest variation range found in literature has been adopted for each model factor. The different values of the solid-water partition coefficient (k_d) depends on the different solids properties (Besha et al., 2017).

For each scenario, the Extended-FAST has been applied by varying the model factors reported in Table 5. During the Extended-FAST application the model outputs summarized in Table 6 have been considered as reference.

Furthermore, the uncertainty propagation from the SS to the RWB has been evaluated in terms of coefficient of variation (CV). CV is defined as the ratio between the standard deviation (α) and the average (μ) value of the model output of reference taken into account. Low CV values suggest that the modelled output is close to its average value.

For model running, the temporal resolution of 60 s has been adopted.

3. Results and discussion

For sake of shortness only the relevant results related to the model outputs of the RWB (with particular reference to SMX) will be here discussed (Scenario 1). Thus, attention will be focused on the role that model factors of the upstream sub-models have on the RWB quality in terms of MPs concentration. Furthermore, the comparison among the results of the 5 scenarios will be discussed in terms of maximum values of S_i for each sub-model. Finally, the uncertainty propagation for each scenario will be also discussed.

The fraction of mass for both X_{SMX} and S_{SMX} in each sub-system was: 1) SS1 and SS2, 6% and 94% for S_{SMX} and X_{SMX}, respectively; 2) WWTP1 and WWTP2, 92% and 8% for S_{SMX} and X_{SMX}, respectively; 3) RWB, 22% and 78% for S_{SMX} and X_{SMX}, respectively.

3.1. Scenario analysis results

In Fig. 2 the results related to $X_{SMX,max}$ (Fig. 2a) and $S_{SMX,max}$ (Fig. 2b) for the scenario 1 are shown. Specifically, for each group of model factors (related to SS1, SS2, WWTP1, WWTP2 and RWB) the values of S_i and interactions are reported. The results reported

Table 4
Set of un-known model factors (●) varied for each scenario.

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

Table 5
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 inhibition 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

Table 6
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	kgBOD 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}

in Fig. 2 show that the model factors related to WWTPs have a negligible effect on the variation of the SMX ($X_{SMX,max}$ and $S_{SMX,max}$) concentration in the RWB. This result is mainly due to the partial inhibition of the enzymatic mechanism that allows the SMX degradation within the WWTPs. Indeed, the aforementioned enzymatic mechanism leads to the adoption of the SMX as carbon and ammonium nitrogen source if no other sources are available. However, the real wastewater is rich of readily biodegradable carbon and ammonium. Thus, the SMX degradation enzymatic mechanism is often inhibited and its concentration remains almost intact (Drillia et al., 2005).

By analysing Fig. 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. Factors Accu and Arra influence the sediments build-up inside the SS, while factor Disp influences the wash-off process; thus influencing the TSS content inside the integrated model and consequently inside the RWB (Freni et al., 2009a,b; Vanrolleghem et al., 2015). As suggested by Vezzaro et al. (2011), TSS content is directly connected to the particulate SMX process. However, as shown by the dark grey bars on Fig. 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. Therefore, in order to better model the $X_{SMX,max}$ inside the RWB the improvement of the quantification of the amount of solids inside the sewer system is required.

For $S_{SMX,max}$ (Fig. 2b) a great number of model factors showed to have an high contribution in terms of interaction both for SS1 and SS2. Specifically, the following factors resulted to strongly influence the $S_{SMX,max}$ inside the RWB; factors affecting the sediments build-up (Accu, No. 6, Arra, No. 8) and wash-off (Disp, No. 7) inside the SS1; the sorption of SMX inside the SS1 ($K_{sor,}$ No. 16); the hydrological loos (ϕ – No. 20) and the sediments build-up (Arra, No. 23) inside the SS2; the nitrification inside the RWB (K_{NH}, No. 16). Such a fact means that the soluble fraction of SMX, which has a maximum value of one order of magnitude higher than the particulate fraction, is strongly related to the TSS compound. Therefore, the sorption/desorption process play a key role on the maximum concentration of S_{SMX} in the RWB. Further, the above result confirms that the reduction of the solid compounds released inside the RWB can have an important role in reducing the MP concentration in the acquatic system (Vezzaro et al., 2010). Similarly, the results reported in Fig. 2b suggest that in order to improve the $S_{SMX,max}$ modelling inside the RWB, modeller has to enhance the

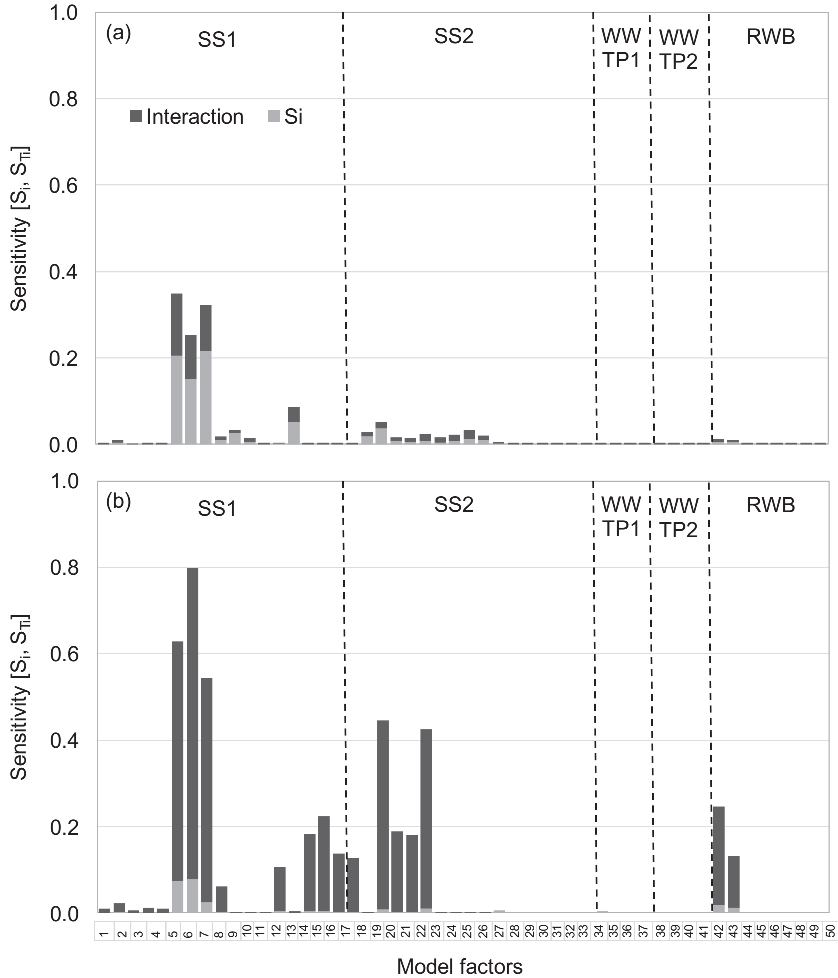

Fig. 2. Results of S_i and interaction related to $X_{SMX,max}$ (a) and $S_{SMX,max}$ (b) for RWB.

quantification of the amount of solids inside the SS. Furthermore, K_{NH} should be measured by using respirometric techniques.

Comparison among the scenarios. Table 7 summarizes the results for each scenario and model output of the maximum value of S_i. By analysing the results reported in Table 7 one can observe that for scenarios 1, 2 and 3, the model factors related to the SS modelling have 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 7. 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. Such a result emphasizes the role of the upstream processes on the MP concentration inside the RWB.

Regarding the last two scenarios (4 and 5), the results reported in Table 7 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 affects till to 95% of the total variance of $S_{SMX,max}$ (scenario 4). This result demonstrates that the predominant processes inside the WWTP are the desorption/sorption. Such a result is in line with previous findings which have demonstrated that the MPs fate throughout wastewater treatment systems strongly depends on their sorption behaviour (e.g. Song et al., 2006; Plósz et al., 2013). Therefore, in order to improve the model performances the modeller should better identify factors related with solids modelling and quantify the k_{d_ox} by using batch tests.

3.2. Uncertainty propagation

In Fig. 3, the results related to the uncertainty propagation (from SS1 to the RWB, throughout WWTP1 and from SS2 to the RWB, throughout WWTP2) are reported. Results of Fig. 3 refer to scenario 1 and SMX model outputs.

From Fig. 3a one may observe that the peak in the $X_{SMX,max}$ concentration decreases from SS1 to WWTP1 and from SS2 to WWTP2, as revealed by the low CV value. This result reveals that from upstream to the downstream (from SS1 to WWTP1 or from SS2 to WWTP2) the uncertainty, due to the unknown model factors, progressively reduces. However, as shown in Fig. 3a the CV value inside the RWB increases. This results is likely due to the combined effect of the poor knowledge of the model factors related to the RWB with all the other factors which influences the $X_{SMX,max}$ concentration.

By analyzing Fig. 3b one may observe that the peak in the $S_{SMX,max}$ concentration profile is much smaller in the RWB, as represented by the low CV value. This result reveals that in case of soluble form of SMX, the uncertainty definitely decreases from upstream to downstream.

The different uncertainty due to SS1 and SS2, both for $X_{SMX,max}$ and $S_{SMX,max}$, could be likely due to the different order of magnitude of the total SMX concentration (on average 1 order higher for SS2) (Fig. 3). Conversely, the difference of the uncertainty due to WWTP1 and WWTP2 is quite negligible. Despite the low

Table 7
Maximum S_i 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)	0.0013 (Arra)	0.95 (k_{d_ox})	0.65 (k_{d_ox})

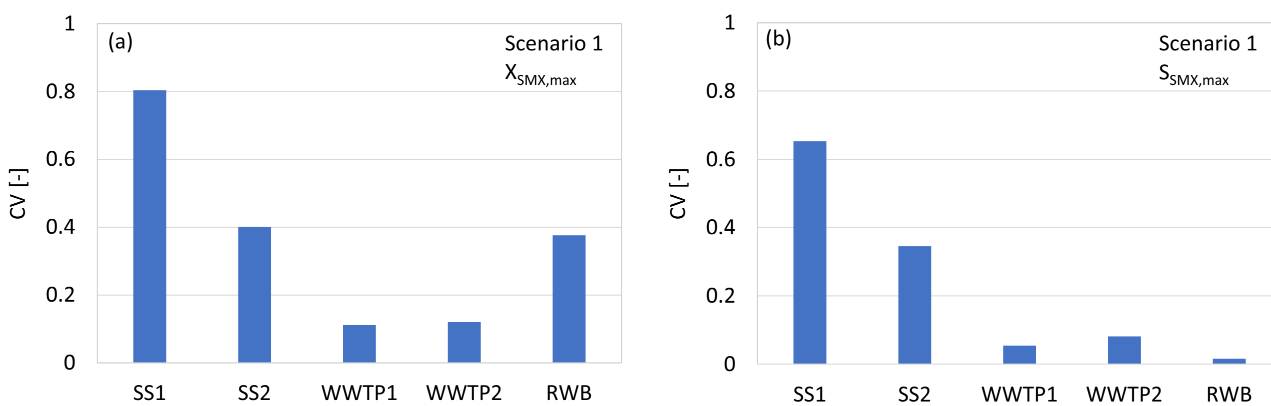

Fig. 3. Results of the uncertainty propagation in terms of CV = σ/μ from the SS1 to the RWB, throughout WWTP1 and from the SS2 to the RWB, throughout WWTP2 related to the scenario 1 for the $X_{SMX,max}$ (a) and $S_{SMX,max}$ (b) model outputs.

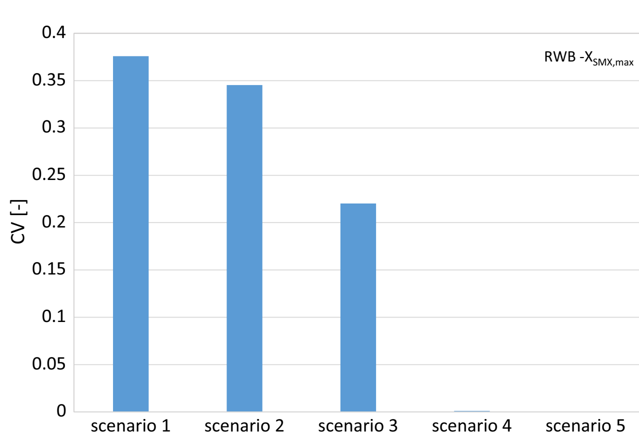

Fig. 4. Results of the uncertainty propagation in terms of CV = σ/μ for each scenario related to the model output $X_{SMX,max}$ concentration in the RWB.

influence of the processes occurring inside the WWTPs on the SMX variation, their complexity lead to CV values different from zero.

Fig. 4 reports the comparison among scenarios in terms of uncertainty propagation for each analyzed scenario related to the $X_{SMX,max}$ concentration in the RWB. Results reported in Fig. 4 shows that with the increase of the knowledge of the model factors (from scenario 1 to scenario 5) the peak in the $X_{SMX,max}$ concentration profile reduces as demonstrated by the decreasing value of CV.

4. Conclusions

A global sensitivity analysis was carried out for micropollutant assessment throughout an integrated urban drainage model. The main findings of this study follow:

- In case all model factors are unknown (scenario 1) $X_{SMX,max}$ 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 solid contents both for the desorption and sorption processes of SMX is relevant.

- Even in case set of model factors related to WWTP and RWB are known (scenarios 2 and 3) both $X_{SMX,max}$ and $S_{SMX,max}$ in the RWB are strongly influenced by the model factors related to TSS load in the SS. The role of key factors related to the TSS load inside the SS is crucial for a good SXM modeling in a IUDM approach, thus suggesting that these factors need to be measured as much as possible.
- The aerobic sorption factor (k_{d_ox}) is the most important for $X_{SMX,max}$ and $S_{SMX,max}$ modelling in RWB (scenarios 4 and 5), therefore this factor has to be measured by using batch tests.
- Nitrification process inside the RWB may have a great influence on the $S_{SMX,max}$ concentration inside the rivers; the K_{NH} factors should be quantified to improve the SMX modeling.
- 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 $S_{SMX,max}$.
- The uncertainty propagation from the upstream to downstream shows a progressive reduction for $S_{SMX,max}$.

Overall, this study allowed us to gain insights into the key model factors which influence the most the SMX in an integrated urban drainage system. Results obtained here could be adopted to design an effective sampling campaign.

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