

# SIMPLIFIED MODEL TO EVALUATE THE FATE OF MICROPOLLUTANTS IN AN INTEGRATED URBAN DRAINAGE SYSTEM: SENSITIVITY ANALYSIS

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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 takes into account 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 in order to select the key factors affecting the RWB quality and to design a reliable/useful experimental campaign. 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.

# 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 (nitrogen, phosphorus, COD). However, the Water protection legislations (e.g. the EU Water Framework Directive (EC, 2000) and the Environmental Quality Standard Directive (EQS, 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. 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). An integrated urban drainage model is therefore composed of sub-models able to simulate the key processes of each system and the interactions among them. Therefore, integrated urban drainage models are often complex and 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. During the last years integrated urban drainage models have been made further complex by introducing the MP fate and transport by putting together single system models or modifying the existing one. Recently, Vezzaro et al. (2012) 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 to provide results as more reliable as possible modeller should apply a parsimonious approaches in case of integrated complex model and/or opportunely collect data useful to calibrate/validate model. However, the collection of monitoring data is affected by significant limitations (Freni and Mannina, 2012). 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, representative of the combined effects of all processes throughout the overall system, are often exhibited in literature (Freni and Mannina, 2012; Vezzaro et al., 2015). Therefore, the improving of the existing databases is only a common practice of dedicated research projects. These difficulties in the data acquiring are amplified in case of MPs as commonly found in low concentrations (in the range of ng/lmg/l), which are difficult to measure (Vezzaro et al., 2015). 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 provide information about how the variation in the output of the model can be apportioned to the variation of the input factors thus allowing the selection of the key factors affecting the model results. Among the SA methods, global approach (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 (Cosenza et al., 2013). Therefore, in the IUDM context GSA can provide information about the relationships between the different systems of the integrated model (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 of the integrated system on the RWB quality, the GSA has been applied. More precisely, five scenarios have been analyzed and compared by adopting Extended-FAST method, each considering a set of model factors as unknown. Furthermore, the he uncertainty propagation form the SS to the RWB has been evaluated.

# 2. Materials 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 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 submodels each divided into a quantity and quality module for the simulations of the hydrographs and pollutographs (Figure 1). More precisely, the integrated model is divided into:(i) the rainfall-runoff and flow propagation submodel, 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).

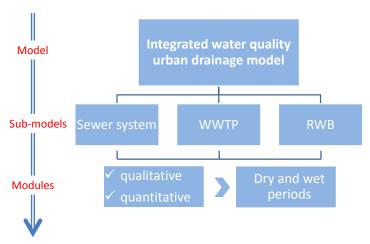


Figure 1. Schematic overview of the integrated model

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., 2012; Plósz et al., 2012). A brief description for each sub-model will be provided below; furthers details about the model equations and parameters can be found in Mannina et al. (2006) and Mannina and Viviani (2010). A detailed description will be instead provided for the model modification that include the SMX modelling.

### 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 that receive both domestic sewage and stormwater. Specifically, the quantity module evaluates the net rainfall from the measured hyetograph by adopting 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 that allows to split the hydraulic phenomena in the catchment from those in the SS. Regarding to 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 inside the SS. SMX inside the SS has been modelled by using two state variables: dissolved ( $S_{SMX}$ ) and particulate ( $X_{SMX}$ ). In Table 1 the processes and the rates considered 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). Furthermore, the anaerobic degradation of SMX inside the SS has been considered (Table 1).

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

Process	S <sub>SMX</sub>	X <sub>SMX</sub>	Process rate		
Sorption	-1	+1	$k_{sor} (X_{TSS}) S_{SMX}$		
Desorption	+1	-1	$(k_{sor}/k_d) X_{SMX}$		
Anaerobic degradation	$1\!-\alpha_{\text{oxygen}}$		k <sub>anaer</sub> S <sub>SMX</sub>		

### 2.1.2. WWTP sub-model

The WWTP has been modelled by adopting the ASM1 (Henze et al., 2000) model. 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 modelled . 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; 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 ( $C_{SJ}$ ). 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  $C_{SMX}$ . The same processes and rates as proposed by Plósz et al. (2012) have been here considered.

### 2.1.3. RWB sub-model

The RWB has been modelled as proposed by Mannina and Viviani (2010). More precisely, the RWB submodel describes both the flow propagation along the river (quantity module) and the pollution concentration of the biodegradable oxygen demand (BOD), dissolved oxygen (DO), ammonia (NH<sub>4</sub>), and nitrate-nitrate (NO). During the flow propagation process, the hydrograph is characterised by two main relevant phenomena: a

hydrograph flow delay and a hydrograph flow reduction. Furthers details about the model equations and parameters can be found in Mannina and Viviani (2010).

WB sub-model has been modified including the mathematical modelling of both  $S_{SMX}$  and  $X_{SMX}$ . In Table 2 summarizes the processes and the rates considered. More precisely, the sorption, desorption and the degradation processes have been considered. Important to precise is that anoxic and aerobic aerobic and anoxic degradation processes have been considered for the RWB. The symbol reported in Table 2 has the same meaning as reported in Table 1.

**Table 2**. 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 <sub>SMX</sub>	X <sub>SMX</sub>	Process rate	
Sorption	-1	+1	$k_{sor}\left(X_{TSS}\right)S_{SMX}$	
Desorption	+1	-1	$(k_{sor}/k_d) X_{SMX}$	
Aerobic degradation	$lpha_{oxygen}$		$k_{aer}  S_{SMX}$	
Anoxic degradation	$1-lpha_{\text{oxygen}}$		$k_{anox}  S_{SMX}$	

# 2.1.4. 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 km² 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 km². 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).

# 2.1.5. 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. On the other hand,  $S_{Ti}$  allows evaluating the interactions among factors. 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.

# 2.1.6. 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 thus allowing to quantify the effect of their uncertainty on the RWB quality. The set of unknown model factors have varied during the Extended-FAST application for each scenario.

Details related of each scenario are summarized in Table 3.

Scenario
SS1
SS2
WWTP1
WWTP2
RWB

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**Table 3**. Set of un-known model factors ( ) varied for each scenario.

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 only of one sub-system at time. Such scenarios allow to assess the weight of the uncertainty of each sub-system and allow to gain insight about the uncertainty propagation throughout the sub-systems.

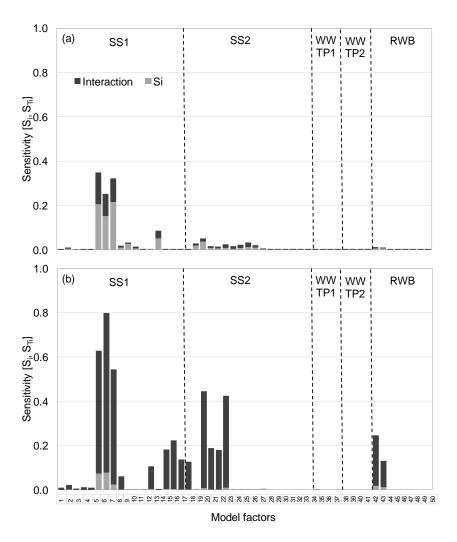
For each scenario 500 Monte Carlo simulations x number of model factors ( $N_{MC}$ ) have been performed. Furthermore, the uncertainty propagation form the SS to the RWB has been evaluated in terms of ratio between standard deviation ( $\sigma$ ) and average ( $\mu$ ) value of the model output taken into account. The smaller this ratio value, the more the modelled output is condensed around the average value.

### 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 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. Finally, the uncertainty propagation for each scenario will be also discussed.

# 3.1. Scenario analysis results

In Figure 2 the results related to X<sub>SMX,max</sub> (Fig. 2a) and S<sub>SMX,max</sub> (Fig. 2b) for the scenario 1 are shown.



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

Specifically, for each group of model factors (related to SS1, SS2, WWTP1, WWTP2 and RWB) the values of  $S_i$  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. 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 (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 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. Therefore, results reported in Figure 2a suggest that 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  $S_{SMX,max}$  (Figure 2b) a great number of model factors showed to have an high contribution in terms of interaction both for SS1 and SS2. Specifically 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 ( $K_{SOf}$ , no. 16), the hydrological loos ( $\Phi$  – no. 20) and the sediments

build-up (Arra, no. 23) inside the SS2 and the nitrification inside the RWB ( $K_{NH}$ , no. 16) resulted to strongly influence the  $S_{SMX,max}$  inside the RWB. 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., 2012). Similarly for the  $X_{SMX,max}$ , form the results reported in Figure 2b one can conclude that in order to improve the  $S_{SMX,max}$  modelling inside the RWB modeller has to enhance the quantification of the amount of solids inside the SS. Furthermore,  $K_{NH}$  should be measured by using respirometric techniques.

# 3.1.1. Comparison among the scenarios

Table 4 summarizes the results for each scenario and model output of the maximum value of  $S_i$ . By analysing the results reported in Table 4 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 4. 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.

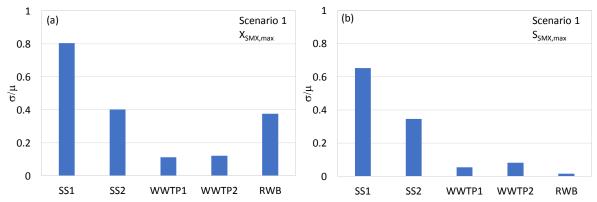
Regarding the last two scenarios (4 and 5), the results reported in Table 4 show that the most relevant factor affecting the SMX modelling is represented by the aerobic solid-liquid sorption coefficient ( $k_{d_ox}$ ). Indeed, this factor affect till to 95% of the total variance of  $S_{SMX,max}$  (scenario 4). Thus demonstrating that the predominant 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. Plósz et al., 2013). Therefore, in order to improve the model performances modeller should better identify factor related with solids modelling and quantify the  $k_{d_ox}$  by using batch tests.

### 3.2. Uncertainty propagation

Results related to the uncertainty propagation from the SS1 to the RWB are reported in Figure 3 with the specific reference to the scenario 1 and SMX model outputs. From Figure 3a one may observe that the peaks in the  $X_{SMX,max}$  concentration decreases from SS1 to WWTP2 as revealed by the low  $\sigma/\mu$  value. This result reveals that from upstream to the downstream the uncertainty due to the unknown model factors progressively reduce. However, as shown in Figure 3a the  $\sigma/\mu$  value inside the RWB increases. This results is likely due to the combination effect on the  $X_{SMX,max}$  concentration of the poor knowledge of the model factors related to the RWB with all the other factors. By analyzing Figure 3b one may observe that the peaks in the  $S_{SMX,max}$  concentration profile are much smaller in the RWB, as represented by the low  $\sigma/\mu$  value. Thus revealing that in case of soluble form of SMX, the uncertainty definitely decrease from upstream to downstream.

**Table 4**. Maximum S<sub>i</sub> value for each scenario and model output

		Maximum S <sub>i</sub>					
		Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5	
SS1	$Q_{\text{SS},\text{max}}$	0.5 (K1)	0.5 (K1)	-	-	-	
	TSS, <sub>max</sub>	0.3 (Accu)	0.3 (Accu)	-	-	-	
	BOD, <sub>max</sub>	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 <sub>SMX,max</sub>	0.37 (Accu)	0.37 (Accu)	-	-	-	
SS2	$Q_{\text{SS},\text{max}}$	0.25 (K1)	-	0.36 (K1)	-	-	
	TSS, <sub>max</sub>	0.51 (K <sub>susp</sub> )	-	0.47 (K <sub>susp</sub> )	-	-	
	BOD, <sub>max</sub>	0.55 (K <sub>susp</sub> )	-	0.51 (K <sub>susp</sub> )	-	-	
	LTSS	0.36 (Accu)	-	0.3 (Accu)	-	-	
	LBOD	0.28 (Accu)	-	0.25 (Accu)	-	-	
	$X_{\text{SMX,max}}$	0.45 (K <sub>susp</sub> )	-	0.41 (K <sub>susp</sub> )	-	-	
	$S_{\text{SMX},\text{max}}$	0.35 (K <sub>susp</sub> )	-	0.33 (K <sub>susp</sub> )	-	-	
	BOD, <sub>max</sub>	0.38 (Accu)	0.38 (Accu)	-	-	-	
WWTP1	$S_{\text{NH,max}}$	0.4 (Accu)	0.4 (Accu)	-	-	-	
	$X_{\text{SMX,max}}$	0.52 (Accu)	0.59 (Accu)	-	0.94 (k <sub>d_ox</sub> )	-	
	$S_{\text{SMX,max}}$	0.42 (Accu)	0.53 (Accu)	-	0.9 (k <sub>d_ox</sub> )	-	
WWTP2	BOD, <sub>max</sub>	0.18 (W <sub>h</sub> )	-	0.18 (W <sub>h</sub> )	-	-	
	$S_{\text{NH},\text{max}}$	0.23 (W <sub>h</sub> )	-	0.24 (W <sub>h</sub> )	-	-	
	$X_{\text{SMX,max}}$	0.24 (Accu)	-	0.24 (Accu)	-	0.75 (k <sub>d_o</sub>	
	$S_{\text{SMX},\text{max}}$	0.27 (Accu)	-	0.23 (W <sub>h</sub> )	-	0.8 (k <sub>d_ox</sub>	
RWB	Q <sub>RWB,max</sub>	0.15 (Φ)	0.6 (Ф)	0.26 (Ф)	-	-	
	BOD, <sub>max</sub>	0.2 (Arra)	0.3 (Arra)	0.34 (Ф)	-	-	
	$X_{SMX,max}$	0.2 (Arra)	0.55 (Accu)	0.27 (Φ)	0.85 (k <sub>d_ox</sub> )	0.65 (k <sub>d_o</sub>	
	$S_{SMX,max}$	0.08 (Disp)	0.28 (Arra)	0.0013 (Arra)	0.95 (k <sub>d_ox</sub> )	0.65 (k <sub>d_o</sub>	



**Figure 3.** Results of the uncertainty propagation in terms of  $\sigma/\mu$  ratio from the SS1 to the RWB related to the scenario 1 for the  $X_{SMX,max}$  (a) and  $S_{SMX,max}$  (b) model outputs.

Figure 4 reports the comparison among scenarios in terms of uncertainty propagation for each analyzed scenario related to the X<sub>SMX,max</sub> inside the RWB.

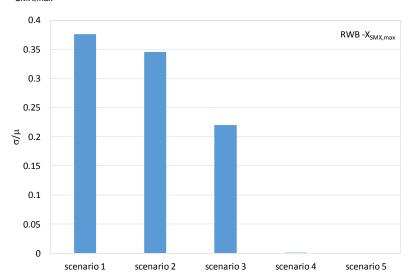


Figure 4. Results of the uncertainty propagation in terms of  $\sigma/\mu$  ratio for each scenario related to the model output  $X_{SMX,max}$  inside the RWB

Results reported in Figure 4 shows that with the increase of the knowledge of the model factors (from scenario 1 to scenario 5) the peaks in the  $X_{SMX,max}$  concentration profile reduces as demonstrated by the decreasing value of  $\sigma/\mu$ .

# 4. Conclusions

The key findings of this study to design an effective sampling campaign are summarized in the following:

✓ In case all model factors are unknown (scenario 1) X<sub>SMX,max</sub> and S<sub>SMX,max</sub> 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.

- 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<sub>SMX,max</sub> concentration inside the rivers; the K<sub>NH</sub> 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<sub>SMX,max)</sub>.
- ✓ The uncertainty propagation from the upstream to downstream shows a progressive reduction for S<sub>SMX,max</sub>.

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