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A model library for dynamic transport and fate of micropollutants in integrated urban wastewater and stormwater systems

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ABSTRACT

The increasing efforts in reducing the emission of micropollutants (MP) into the natural aquatic environment require the development of modelling tools to support the decision making process. This article presents a library of dynamic modelling tools for estimating MP fluxes within Integrated Urban Wastewater and Stormwater system (IUWS – including drainage network, stormwater treatment units, wastewater treatment plants, sludge treatment, and the receiving water body). The models are developed by considering the high temporal variability of the processes taking place in the IUWS, providing a basis for the elaboration of pollution control strategies (including both source control and treatment options) at the small spatial scale of urban areas. Existing and well-established water quality models for the different parts of the IUWS (e.g. ASM models) are extended by adding MP fate processes. These are modelled by using substance inherent properties, following an approach commonly used in large-scale MP multimedia fate and transport models. The chosen level of complexity ensures a low data requirement and minimizes the need for field measurements. Next to a synthesis of model applications, a didactic example is presented to illustrate the potential of the use of the developed model library for developing, evaluating and comparing strategies for reduction of MP emissions from urban areas.

Software availability

Name of the software: IUWS_MP model library
Software requirements: WEST 3.7.6 (or higher)
Program Language: Model Specification Language (MSL)
Program Size: approximately 25 MB
Availability: The source code for the IUWS_MP model library can be obtained for free; please contact Prof. Peter Steen Mikkelsen, Technical University of Denmark, Department of Environmental Engineering, Miljøvej, Building 113, 2800 Kgs. Lyngby, Denmark – e-mail: psmi@env.dtu.dk.

1. Introduction

The reduction of emission of micropollutants (MP) from urban areas is an essential step towards the improvement of the environmental status of natural waters, as required by legislation such as the European Water Framework Directive (WFD – European Commission (2000)). This can be achieved through the implementation of emission control strategies dealing with the entire Integrated Urban Wastewater and Stormwater system (IUWS). These emission control strategies include a wide variety of control options (source control, treatment, etc.) whose efficiency needs to be assessed and compared before a final decision on implementation is taken. Urban water managers can thus benefit from the application of mathematical models (see for example Benedetti et al., 2013) to evaluate the effects of the various MP pollution control strategies and to identify the option (or combination thereof) which ensures the most cost-effective solution. Also, models can be used for training and education purposes, enabling

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the understanding of the complex interactions and processes which affect MP fluxes across the urban water systems.

Various modelling tools are available for estimating MP concentrations at the river basin scale (e.g. Feijtel et al., 1997; Keller et al., 2007; Koormann et al., 2006; Schowanek et al., 2001; Williams et al., 2009), but they often assume steady state conditions and focus on wastewater treatment plants (WWTP) and river stretches, neglecting or excessively simplifying the sewer network. Given (i) the complexity of the urban water system, (ii) the highly dynamic processes taking place in it, (iii) the number of possible control options and (iv) the wide variety in characteristics of the considered substances, it is important to apply an approach which includes the entire IUWS. Recent studies (e.g. Gasperi et al., 2012; Launay et al., 2013) highlighted how Combined Sewer Overflows (CSO) can represent an important MP source which can affect the overall quality of the receiving water body. Therefore, limiting the model to river and WWTP strongly reduces the ability to simulate the effect of MP control strategies specifically acting at the relatively small scale of urban areas (e.g. local handling of storm- and wastewater, CSO treatment, WWTP tertiary treatment).

Furthermore, the major driver of the system, rainfall, is characterized by a highly dynamic behaviour. Therefore, steady state or equilibrium multimedia fate models, commonly applied in chemical risk assessment (e.g. Feijtel et al., 1997; Koormann et al., 2006; Struijs, 1996), might not be appropriate to fully describe the highly dynamic processes and the effect of specific pollution control strategies (e.g. CSO treatment). This was already recognized in this discipline because Boeije et al. (1997), for example, presented a stochastic approach to take into account spatial and temporal variability in chemical risk assessment, while employing steady-state models to describe the fate of chemicals.

The development of dynamic IUWS modelling tools was among the main objectives of the ScorePP project (Source Control Options for Reducing Emissions of Priority Pollutants – www.scorepp.eu), which focused on the 33 priority substances (PSs) and substance groups identified in the European legislation, i.e. the EU Environmental Quality Standard (EQS) directive (European Commission, 2008). This directive defines the Maximum Allowable Concentration (MAC-EQS) and Annual Average (AA-EQS) which should not be exceeded in the receiving water. Among these 33 substances, the ScorePP project specifically focused on those defined as priority hazardous substances, whose release into the environment should be eliminated within a short time frame (European Commission, 2000).

Within the ScorePP project, a model library that allows creating integrated dynamic models for the estimation of MP sources and fluxes at the urban scale was developed and it is presented in this contribution. The developed models are aimed to provide results that can be used to evaluate the performance of different MP control strategies, including compliance with legal requirements on the quality of receiving waters, e.g. the EU Environmental Quality Standards (European Commission, 2008). Specifically, these dynamic MP transport and fate models allow the quantification of the MP release from urban sources and their fate within different treatment systems (Plósz et al., 2013) and different environmental compartment (e.g. sediments, groundwater, atmosphere). The outputs of these models can subsequently be used to perform Substance Flow Analysis (SFA) for various MPs at the urban scale (e.g. Bjorklund et al., 2011), allowing for the comparison of different scenarios for MP emission control (e.g. Revitt et al., 2013). The models can be linked to river basin scale Multimedia Fate and Transport Models (MTFMs) commonly used in chemical risk assessment (De Keyser et al., 2010a). This allows the simulation of the interaction between the small-scale urban environment, where the assessment of e.g. short term toxic effects requires a detailed temporal resolution, and the surrounding environmental compartments, which are characterized by processes that can be represented in a less detailed manner (for example, long-range transport of MP and wet deposition, effect of stormwater control strategies on groundwater). An example is presented in De Keyser et al. (2010a).

This article presents the IUWS_MP model library by illustrating the main concepts that were adopted during the model development. The structure of the various units included in the model is subsequently introduced, and examples of application of the IUWS_MP model in the literature are then summarized. The results presented in this study describe a tool which can be used by urban water managers for control of MP releases at the urban scale.

2. Model library development

The development of the various sub-models included in the IUWS_MP system followed the procedure commonly adopted in model development (Carstensen et al., 1997; Dochain and Vanrolleghem, 2001; Jakeman et al., 2006; Refsgaard et al., 2007). These include (Fig. 1): (i) definition of model purpose (Section 2.1) and (ii) model context (Section 2.2); (iii) system conceptualization, including specification of available data, models and other prior knowledge (Section 2.3); and (iv) definition of model structure and

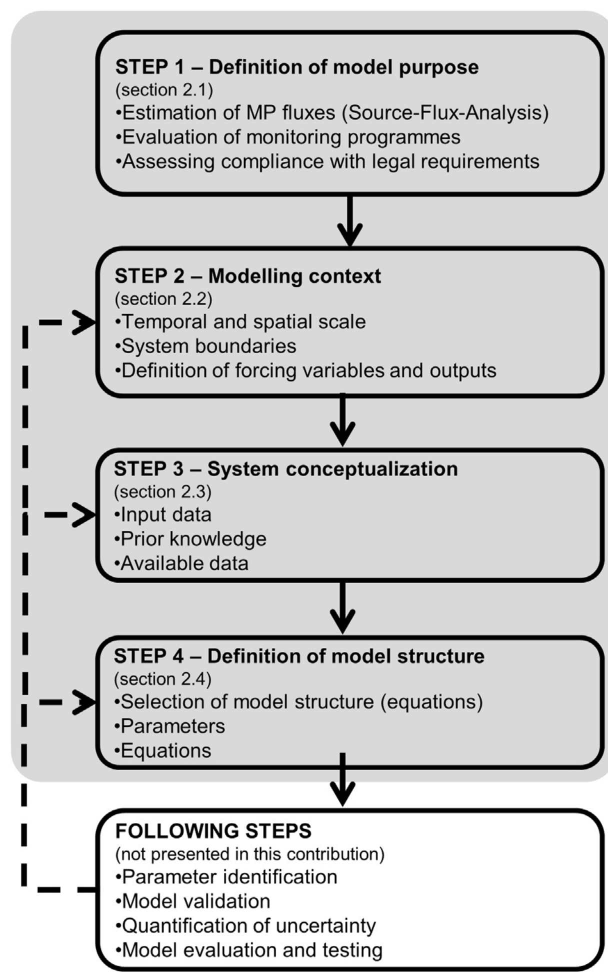

Fig. 1. Steps in the development of the IUWS_MP model that are presented in this article (in grey).
Adapted from Carstensen et al. (1997), Dochain and Vanrolleghem (2001), Jakeman et al. (2006), and Refsgaard et al. (2007).

parameters (Section 2.4). Additional steps, such as model parameter identification, model validation, sensitivity analysis, uncertainty quantification and model testing were performed separately for individual elements of the IUWS_MP (see Section 3.1), but a thorough analysis of the integrated model using these tools is not included in this paper for space reasons. However, it is stressed that these steps are essential when modelling results are used for decision making (see the discussion for MTFM in Buser et al. (2012)) and the integrated model should not be applied without them.

2.1. Definition of modelling purpose

The IUWS_MP model library was developed within the context of the ScorePP project, which aimed at investigating, developing, and assessing different options for reducing MP emissions from urban areas. Therefore, the IUWS_MP model library provides a model platform that allows for the comparison of control strategies by:

1) *Estimating MP fluxes in integrated urban wastewater and stormwater systems* – this objective allows the estimation of the effect of mitigation strategies for control of MP emissions (e.g. "how much does this source control/treatment reduce the emission of this MP?");
2) *Evaluating monitoring programmes* – this objective allows the optimisation of monitoring programmes (e.g. "when and where should one sample?");
3) Assessing compliance with legal requirements, such as concentration limits in the receiving water bodies (expressed both as average and peak concentrations) – this objective allows the assessment of the overall benefit of the proposed strategy on the water environment (e.g. does the strategy achieve a "good environmental status"?).

These points are further referred in the manuscript as "objectives".

2.2. Modelling context

2.2.1. Temporal and spatial scale

To ultimately decide on the type of models that will be used, decisions are required regarding the temporal and spatial aspects that need to be covered by the model. Given the fact that dynamics need to be simulated and that the urban catchment is to be described by the model in some detail, the proposed model library is based on lumped (spatially aggregated) dynamic models. The use of detailed approaches is impracticable in urban areas, where systems are complex and information is scarce. Therefore simplified approaches need to be adopted, where the modeller needs to define the optimal level of simplification given the available information (e.g. the number of pipes and tanks used to simulate a specific subcatchment).

The choice of dynamic models, in contrast with widely applied steady-state approaches, is explained both by the models' purpose and by the characteristics of the modelled system and processes. In fact, estimation of MP fluxes (objective 1) can also be achieved by using annual average fluxes derived from "release strings" (as in the example presented by Eriksson et al., 2011) or by using simple static models (assuming, for example, equilibrium between the environmental compartments, as in multimedia fate models – e.g. Mackay, 2001). However, these approaches are based on assumptions which can fail in representing dynamic processes taking place at the IUWS scale (e.g. rainfall-runoff generation, combined sewer overflows, accidental spills, changes in WWTP operations). Moreover, objectives (2) and (3) require the dynamic estimation of MP concentrations in different parts of the IUWS, and of the impacts on the receiving waters (i.e. acute toxicity), which are caused by short-term events.

The large number of MP sources and of possible control strategies that can be implemented across urban areas requires physically distributed models. Partially lumped approaches (e.g. based on continuously stirred tank reactors – CSTR) provide a compromise between the need to describe the spatial heterogeneity of MP processes and the available resources (information about the model system, time).

2.2.2. Forcing variables and model outputs

Models are structures that provide the model user desired output variables for given inputs (forcing variables). Together with MP release from households, the main forcing function in urban wastewater systems is rainfall, which causes large differences between the behaviour of the system in dry- and wet-weather conditions in a short time scale (minutes-hours). On top of that the concentrations of the MP and traditional pollutants need to be provided as they will affect the model outputs. In Section 2.3.3 the approach taken to obtain the necessary time series is presented. The desired model outputs are time series of MP fluxes (to fulfil objective 1) and MP concentrations (to achieve objectives 2 and 3, which require the estimation of MP concentrations in different environmental compartments.

2.2.3. System boundaries

To clearly identify which aspects of a system need to be considered, the system boundaries need to be defined. The following elements are considered to be included within the borders of the IUWS_MP system (Fig. 2):

- *Sources*: water and pollutant flows are generated by point and diffuse sources across the urban catchment. MP sources are identified after catchment characterization, which links the information on land use and economical activities to potential MP sources. This process is based on MP sources classification, such as the one presented in Lützhøft et al. (2012). When using the IUWS_MP model library it is advisable to generate the MP release time series through the application of the input generator presented by De Keyser et al. (2010b) (see Section 2.3.3). Simulation of MP sources is also relevant for the simulation of source-control pollution control strategies (see the source control example in Section 3.2.2).
- *Sewer network*: water flows from combined and separate systems are collected and routed across the catchment. Also, water can be detained by storage units (e.g. detention basins, etc.) or discharged directly into receiving waters through overflow structures.
- *Stormwater treatment systems*: flows from separated stormwater systems are treated before eventual discharge to the receiving surface water or groundwater.
- *Wastewater treatment systems*: several physical, chemical and biological processes and their combinations are used to treat wastewater.
- *Sludge treatment systems*: the residues from wastewater treatment are treated before final disposal.
- *Receiving water*: natural surface waters (e.g. rivers, lakes) are the final recipients of the water flows from urban areas. These should be connected to the urban wastewater and stormwater system to assess the compliance with water quality criteria (objective 3).

As the interaction between urban areas and the surrounding environmental compartments (atmosphere, groundwater, etc.)

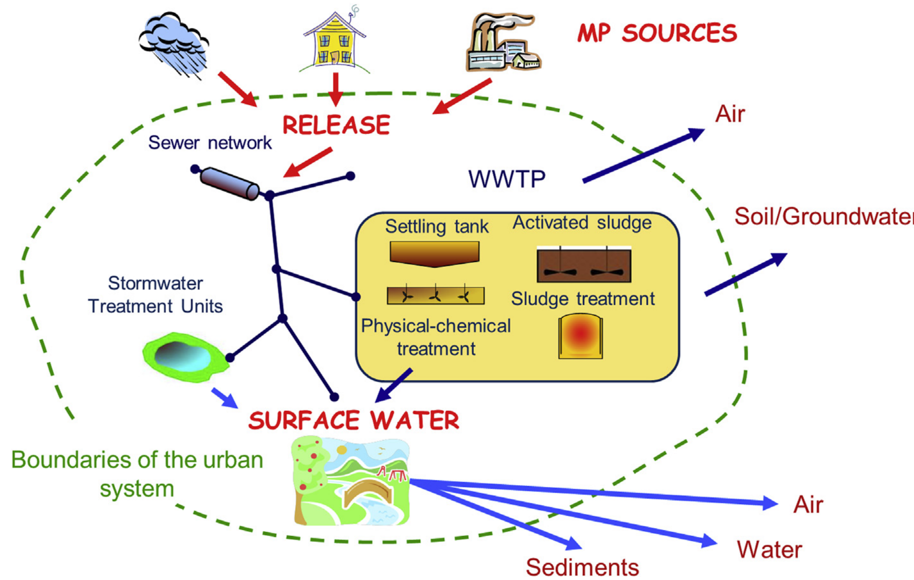

Fig. 2. Schematic representation of the IUWS_MP elements and boundaries of the modelled system.

cannot be neglected, the IUWS_MP model can be connected to river-basin catchment scale multimedia transport and fate models (see the example presented by De Keyser et al., 2010a). This allows for the consideration of processes such as long-range MP atmospheric transport, MP accumulation in soil and sediments, and MP contamination of groundwater.

2.3. System conceptualisation

2.3.1. Prior knowledge

Several dynamic models were already available in literature to simulate fluxes of pollutants in the different components of the IUWS. However, these models are mainly focussing on traditional pollutants such as overall organic matter, nutrients and suspended solids, as in the example presented in Bauwens et al. (1996), Meirlaen et al. (2001), Erbe and Schuetze (2005). While some MP fate processes can be modelled by linking MP fate to already modelled components (e.g. sorption links MP fate to Total Suspended Solids (TSS), but this is valid only for MP with strong tendency to sorb), other MP processes (e.g. volatilization) require the inclusion of additional fate processes.

Similarly, several models have been developed over the past decades to simulate MP transport fate in different elements of the IUWS (e.g. Bjorklund et al., 2011; Feijtel et al., 1997; Keller et al., 2007; Koormann et al., 2006; Lindblom et al., 2011; Schowanek et al., 2001; Williams et al., 2009). However, either they are characterized by a large scale (river basin), or they focus only on a single element of the IUWS, commonly the WWTP (Plosz et al., 2012; Seth et al., 2008; Struijs, 1996). It is thus necessary to find a compromise between the different available levels of complexity and the modelling context presented in Section 2.2. For example, the number of parameters and degradation pathways which are well representing the MP fate in a WWTP might be excessive when trying to simulate MP fate in the sewer network.

The IUWS_MP model library merges the major strengths of these two model groups (integrated dynamic water quality models and MP fate and transport models) into a tool which allows for the simultaneous simulation of both MP and traditional pollutants in the different components of the urban water system. This is relevant to simulate MP fate processes that are affected by “traditional” pollutants (e.g. biodegradation in activated sludge tanks, sorption to sludge in clarifiers).

2.3.2. Available data for chemical properties

The ScorePP project underlined how information about MP sources and behaviour in the environment is limited (Lützhøft et al., 2012). Therefore, the models included in the IUWS_MP library utilize parameters (substance physical–chemical properties, such as solid/water partition coefficient, degradation half-lives, Henry’s Law constant, etc.) which can be easily retrieved from existing chemical databases, such as the one compiled by Lützhøft et al. (2009), focussing on the substances listed in the WFD, and publically available websites (e.g. the Hazardous Substances Data Bank (HSDB), the European chemical Substances Information System (ESIS)). This approach, common to the one applied in MTFM models (e.g. Mackay, 2001), limits the model data requirements while ensuring the application to a wide range of MPs (i.e. all the non-polar substances for which the equations listed in Section 2.4 are valid can be simulated). Additional information obtained from field measurements and laboratory experiments can improve the accuracy of model predictions and reduce the uncertainty linked to the representativeness of the information retrieved from existing databases for the specific study area.

2.3.3. Model input generation

The need for a structured and quantitative description of emission sources and patterns led to the construction of a database classifying MP sources (e.g. Lützhøft et al., 2012). In this classification MP sources are categorized based on different classification codes listing chemicals, production processes, and economical activities involved in the MP emission (defined as “release strings”). For each priority pollutant emission source a default temporal release pattern is defined. Model inputs for each MP can thus be generated by (i) identifying the MP sources in the catchment by GIS-based information (e.g. the number of activities X in the study areas), and (ii) by combining this information with the estimated MP release (e.g. each activity X releases on average Y mass of MP per year). An example of this model input generation method is presented in Lützhøft et al., 2009).

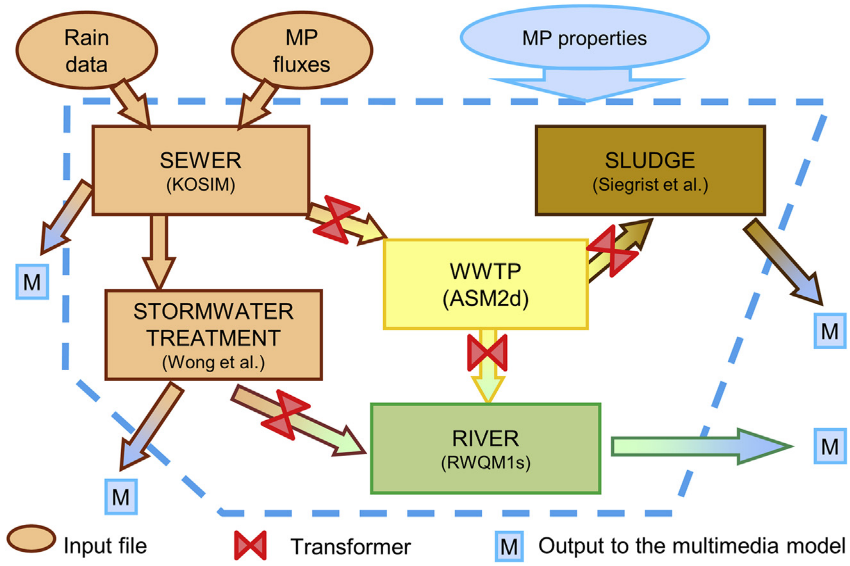

Fig. 3. Connections between the different water quality components used in the IUWS_MP model library.

A stand-alone application was built within the ScorePP project (De Keyser et al., 2010b) to generate emission time series according to the specified release patterns, based on phenomenological modelling of a large number of emission generating events and allowing the incorporation of stochasticity of MP emissions. This tool is applicable to MPs, traditional pollutants (COD, etc.) and wastewater flow rates, and its inputs can be provided by the release strings database or by manually entering the information (for further information the reader is referred to De Keyser et al., 2010b).

2.4. *Definition of IUWS_MP model structure*

2.4.1. *Existing models*

Among the various models that are available in literature to model the elements of the IUWS system, the following were chosen as starting point: the KOSIM hydrological catchment runoff and sewer transport model (ITWH, 2000), the Activated Sludge Model no. 2d (ASM2d; Henze et al., 2000; Gernaey et al., 2004), the Universal Stormwater Treatment Model (Wong et al., 2006), the simplified version of the River Water Quality Model no. 1 (Reichert et al., 2001) introduced in Benedetti et al. (2010) (RWQM1s), and the anaerobic digestion model by Siegrist et al. (1993). These are well-known state-of-the-art models, widely applied in literature and already available in various software packages.

As the selected models use different water quality components, connections between the elements of the IUWS_MP library were ensured by ad hoc transformer models (Fig. 3). These were developed based on the following principles:

- when components in the two models to be connected are equivalent (e.g. NH_4 from the sewer system entering the WWTP), no transformations are performed. As shown in Fig. 3, sewer and stormwater treatment units used the same water components, so no transformation was needed;
- components are fractionated or lumped when the upstream/downstream submodel employs a different description of the component (e.g. KOSIM simulates organic matter as dissolved and particulate COD, while the ASM2d model simulates six different organic pollution components);
- when a component is absent in the upstream model (e.g. biomass is not simulated by the KOSIM model, but is needed as input by the ASM2d model), typical values from literature are used as input to the downstream model. Specific dynamic input generators, which are capable of creating input time series (e.g. the WWTP inflow generator presented by Bechmann et al., 1999; or the input generator presented in De Keyser et al., 2010b) are not part of the model library. Rather their outputs are used as inputs to the simulation models through input files.

The chosen traditional pollutant models were extended with micropollutant fate sub-models to predict the behaviour of micropollutants (Section 2.4.2). In all models, the mixing and transport in the different units (sewer pipes, detention basins, activated sludge tanks, river stretches, etc.) are simulated by means of CSTR tanks (in series).

2.4.2. *Variables and equations*

Micropollutants are affected by a wide range of fate processes, which define their distribution and fate between environmental compartments. As the inclusion of all these processes in all the elements of IUWS would significantly increase model complexity, MP fate processes (and the respective mathematical formulations) included in an IUWS element were selected according to simple principles:

- *Flexibility*: MP removal processes have been defined to ensure the simulation of a wide range of MP without requiring structural modification of the model, i.e. different substances can be simulated by simply modifying the model parameters.
- *Process relevance*: the different MP removal processes are included in the unit models only if the process is relevant, i.e. if it is likely to have a significant influence on the MP fate. Table 1 shows the processes that are included in the various model units.
- *Common mathematical formulation*: common equations that can be applied to the different elements of the IUWS_MP have been preferred, in order to provide a common structure across the integrated model. The Gujer matrix, summarizing the stoichiometry of the MP fate processes included in IUWS_MP and their process rates, is presented in Table 2.
- *Data availability*: the processes are modelled according to the parameters that can be retrieved from available literature (including the ScorePP database – Lützhøft et al., 2009). For

Table 1
MP removal processes included in the various unit models of the IUWS_MP.

Unit	Sewer		Stormwater treatment (water)	Stormwater treatment (sediment)	WWTP				Sludge			River	
	Sewer (water)	Sewer (sediment)			Primary settling	Activated sludge tank	Secondary settling	Filter	Sludge thickener	Sludge anaerobic digester	Sludge dewatering	River (water)	River (sediment)
Physical processes													
Settling	+		+		+		+		+			+	
Resuspension		+		+									+
Volatilization	+		+		+	+	+		+	+	+	+	
Filtration/separation				+				+					
Physico-chemical													
Sorption-desorption	+	+	+	+	+	+	+		+	+		+	+
Hydrolysis	+		+	+	+	+	+		+			+	
Photolysis			+			+						+	
Biological													
Aerobic biodegradation	+		+	+	+	+	+		+			+	+
Anoxic/Anaerobic biodegradation	+	+	+	+	+	+	+		+	+		+	+

example, (pseudo) first-order kinetics is preferred whenever process half-lives were available in the database. The relevant parameters that are used in the mathematical formulation of the MP removal processes are shown in Table 3. Following the *data availability* principle, parent compounds and transformation products are not included in the model. It is relevant to note that for some processes (e.g. settling, resuspension) the majority of the relevant parameters are related to "traditional" pollutants (e.g. settling velocity is related to TSS). Therefore, the estimation of these parameters can benefit from measurements of these "traditional" water quality parameters, which are easier to measure and are more abundant in literature than MP data.

Table 1 lists the MP fate processes which were selected and implemented in the IUWS_MP model library. As shown in the stoichiometric matrix (Table 2), partitioning of the simulated MP is included in the model by using two components: dissolved (S_{MP}) and particulate (X_{MP}). The majority of MP fate processes is assumed to only affect the dissolved species. Only sorption, desorption and TSS-related processes (filtration, settling and resuspension) affect the particulate species in the water column (while in sediments also biodegradation is included). The *p*Ka value is used to calculate the ionized fraction. All processes only affect the non-ionized fraction of MPs. The influence of temperature on the process rates is calculated by using the Arrhenius equation. Whenever the pollutant inflow (defined – for example – by the input generator described in Section 2.3.3) is reported as total concentration, equilibrium is assumed and the pollutant is split into the dissolved and particulate species according to the solid/water partition coefficient (K_d) and the TSS concentration in the inflow. The interaction with other water quality components can be directly expressed in the stoichiometry (for example, sorption and desorption process rates are linked to TSS concentrations, anoxic/anaerobic biodegradation in some units can be regulated by the nitrate and oxygen

Table 2
Gujer matrix of the proposed model IUWS_MP library for the components related to MP fate processes (parameters and state variables are listed in Table 3 – further details are provided in the additional information).

	S_{MP}	X_{MP}	Process rate [g_{MP}. l^{-1} d^{-1}]
Physical processes			
Settling[a,b]		-1[c]	$\frac{v_{sed}}{h_w}\cdot\left(1-\frac{\tau_b}{\tau_{crit,set}}\right)\cdot\left(\frac{C_{TSS}}{C^*_{TSS}}-1\right)\cdot X_{MP}$
Resuspension[d]		$+1$[c]	$E_0\left(\frac{\tau_b}{\tau_{crit,res}}-1\right)^n\frac{A_b}{M_s}X_{MP}$
Volatilization[e]	-1		$k_{l,O_2}\sqrt{\frac{MW_{MP}}{MW_{O_2}}}\cdot S_{MP}$
Filtration/separation		-1	$K_{TSS,filter}\cdot F_{X_{MP},in}$
Physico-chemical			
Sorption[f]	-1	$+1$	$k_{sor}C_{TSS}S_{MP}$
Desorption[f]	$+1$	-1	$\frac{k_{sor}}{K_d}X_{MP}$
Hydrolysis	-1		$k_{hyd}S_{MP}$
Photolysis	-1		$k_{pho,0}\frac{I}{I_0}\frac{D}{D_0}\frac{1-e^{-h_w\alpha_D(\lambda^*)}}{h_w\alpha_D(\lambda^*)}\cdot S_{MP}$
Biological			
Aerobic biodegradation	-1		$\alpha_{oxygen}k_{aerb}S_{MP}$
Anoxic/Anaerobic biodegradation[g]	-1	-1[h]	$(1-\alpha_{oxygen})\cdot k_{anoxb}S_{MP}$

[a] Settling in clarifiers is simulated by using the model by Takacs et al. (1991).
[b] In the river model $C^*_{TSS} = C_{TSS}/2$.
[c] Value for the water compartment (in sediment compartments the sign is opposite to withheld the mass balance).
[d] In the river model $n = 1$.
[e] Valid for adimensional Henry's constant >0.04 (Trapp and Harland, 1995).
[f] In the river model instantaneous sorption/desorption is assumed, so these processes are neglected.
[g] In model units where oxygen and nitrates are included among the water components, dependency to these two water components is included in the process rate (e.g. in the form $S_{O_2}/(S_{O_2}+K_{O_2})$ for oxygen).
[h] Only in sediment compartments.

Table 3
MP removal processes along with their relevant parameters, state variables, inputs and outputs listed in Table 2.

Process	Parameter retrieved from MP database[a]			Other relevant parameters			State variables, inputs and outputs		
	Name	Unit	Description	Name	Unit	Description	Name	Unit	Description
Physical processes									
Settling				C^*_{TSS}	gTSS/l	Background TSS concentration[b]	C_{TSS}	gTSS/l	TSS concentration
				v_{sed}	m/d	Average settling velocity for particles	h_w	m	Water level
				$\tau_{crit,sed}$	Pa	Critical shear stress for settling	τ_b	Pa	Bottom shear stress
Resuspension				E_0	g/m^2/d	Erodability constant	M_s	g	Mass of settled solids
				A_b	m^2	Surface of sediments	$F_{X_{MP},in}$	gMP/s	Flux of particulate MP entering the unit
				$\tau_{crit,res}$	Pa	Critical shear stress for resuspension			
				n	–	Power of erosion term			
Volatilization	MW_{MP}	g/mol	MP molecular weight	k_{l,O_2}	1/d	Reaeration coefficient			
				MW_{O_2}	g/mol	Oxygen molecular weight			
Filtration/separation				$K_{TSS,filter}$	–	Fraction of particles retained by the filter/infiltration system			
Physico-chemical									
Sorption-desorption	k_{sor}	m^3/g$_{TSS}$/d	MP sorption rate						
	K_d	m^3/g$_{TSS}$	MP solid-water partition coefficient						
Hydrolysis	k_{hyd}	1/d	First order hydrolysis rate						
Photolysis	$k_{pho,0}$	1/d	Near-surface degradation rate for photodegradation	$\frac{I}{I_0}$	–	Ratio of the total solar radiation and the radiation when $k_{pho,0}$ was measured	h_w	m	Water level
				$\frac{D}{D_0}$	–	Ratio of radiance distribution function and its value at the surface			
				$\alpha_D(\lambda^*)$	1/m	Apparent attenuation coefficient at the maximum light adsorption wavelength			
Biological									
Aerobic biodegradation	k_{aer}	1/d	Aerobic biodegradation rate	α_{oxygen}	–	Aerobic (1)/anoxic (0) switch parameter[c]			
Anoxic/Anaerobic biodegradation	k_{anorb}	1/d	Anoxic biodegradation rate						

[a] see Lützhøft et al. (2009).
[b] The so-called background concentration (Wong et al., 2006) represents the unsetteable fraction of TSS, following the concept implemented in the Universal Stormwater Treatment Model (Wong et al., 2006).
[c] In units where oxygen and nitrates are included among the water components, dependency to these two water components is included in the process rate (e.g. in the form $S_{O_2}/(S_{O_2}+K_{O_2})$). In the remaining units (e.g. sewer network) α_{oxygen} is fixed throughout the simulation.

concentrations) or it can be indirect (e.g. resuspension of TSS in sewer units also affect resuspension of X_{MP}).

2.4.3. Software selection

To implement an IUWS_MP model of a system, the models of the various IUWS elements need to be combined into a single model. This could either be achieved by interfacing software that each allows simulating existing stand-alone models or by implementing the models of the different IUWS elements within a single software application. The latter was selected as the most appropriate solution, and the prototype of the IUWS_MP model library was implemented in the WEST® modelling and simulation platform (www.mikebydhi.com), as most of the elements of the IUWS system (sewer, WWTP, river, sludge) were already available for modelling the traditional pollutants (Solvi, 2006). Nevertheless, the IUWS_MP model library can also be implemented in other software platforms, such as SIMBA® (used for example in Erbe and Schuetze, 2005) or CITYDRAIN© (Achleitner et al., 2007). As mentioned before, model inputs can, for instance, be generated by using the stand-alone application presented by De Keyser et al. (2010b) and supplied as input files to the simulation.

3. Model applications

3.1. Examples of application of the IUWS_MP model

The various elements composing the IUWS_MP model library have already been applied in different case studies, which illustrate how the presented models can be applied to achieve the objectives listed in Section 2.1.

- MP fluxes were estimated both in single elements of the IUWS system (e.g. stormwater treatment units, WWTP) and at the catchment scale. Vezzaro et al. (2011a) simulated the fate of four organic MPs (iodopropynyl butylcarbamate – IPBC, benzene, glyphosate, and pyrene) in a stormwater detention pond. Cloutier et al. (2012) estimated the fate of various MP (17α-estradiol, trichloroethylene and bis(2-ethylhexyl)phtalate (DEHP)) in different wastewater treatment trains. At catchment scale, the IUWS_MP library was applied to calculate the fluxes of three MPs (zinc, copper, fluoranthene) discharged from separate stormwater systems (Vezzaro et al., 2011b, 2012).
- Optimal experimental design for parameter estimation and monitoring of an MP emission control strategy was investigated by Pettersson et al. (2010).
- Compliance of receiving waters with Environmental Quality Standard values for two organic MPs (naphthalene and nonylphenol) was evaluated by Gevaert et al. (2009) for a small Belgian river.

Some characteristics of the above applications are summarized: The model library was applied both to real systems (Gevaert et al., 2009; Vezzaro et al., 2012) and to hypothetical systems (the benchmark WWTP in Cloutier et al. (2012), and the semi-hypothetical catchment firstly introduced by De Keyser et al. (2010a)). The scarcity of available MP measurements limited the evaluation of the model performance to a few examples (mainly focussing on the stormwater treatment unit presented in Vezzaro et al. (2010)).

The ability of the proposed modelling approach to provide support for the evaluation of MP pollution control strategies was illustrated by Gevaert et al. (2012). This study, based on a preliminary version of the model library (Benedetti et al., 2009 – which included a smaller number of unit models compared to those listed in Table 1), compared different control strategies in the hypothetical case study introduced by De Keyser et al. (2010a). Vezzaro et al. (2013) evaluated strategies for reducing stormwater MP emissions in a real system (presented in Vezzaro et al. (2012)). The importance of uncertainty quantification was illustrated in this study by performing the comparison while taking into account result uncertainty. Furthermore, De Keyser et al. (2010a,b) connected the IUWS_MP model library to a MTFM to simulate concentrations of an organic MP (DEHP) in different environmental compartments (groundwater, atmosphere, sediments) under two pollution control scenarios. The latter example shows that it is possible to evaluate the impact of MP reduction strategies at a larger scale than the urban catchment.

Despite the chronic scarcity of measured MP concentrations, the examples listed here showed how the IUWS_MP model library can provide useful information to the development of MP control strategies. By applying uncertainty identification and quantification approaches (as in Vezzaro et al., 2011a,b) it is also possible to obtain robust results which allow the comparison of different strategies despite the high result uncertainty (see the examples in Vezzaro and Mikkelsen (2012) for evaluation of discharge limits, and in Vezzaro et al. (2013) for EQS).

The reader is referred to the aforementioned publications for a detailed overview of the performance of the model library in real case studies and in-depth discussion of the obtained results.

3.2. Use of the IUWS_MP model for educational purposes

3.2.1. Hypothetical case study

The IUWS_MP model library has also been used for educational purposes in e.g. PhD courses on xenobiotics in the urban environment (held at the Technical University of Denmark – DTU) and in workshops involving both students and young water professionals (at Université Laval). In these courses the model library was applied to illustrate the importance of quantifying MP fluxes within the urban wastewater and stormwater systems to develop strategies for reducing MP emissions. Moreover, this example illustrates the ability of the integrated model to fulfil the objectives listed in Section 2.1.1 and to operate in a data-scarce situation (Section 2.4.2), as the only available input data consists of rainfall data and additional inputs (MP emission rates, MP properties, etc.) are retrieved from public databases.

In the example from the PhD course held at DTU, the IUWS_MP model was applied to a semi-hypothetical urban catchment, which is a simplified representation of a catchment located in the western suburbs of Copenhagen (Denmark). This semi-hypothetical catchment has been used for educational purposes at DTU during the last decade, with main focus on the integrated modelling of traditional pollutants (TSS, COD and nutrients). The characteristics of the system are defined to exacerbate some phenomena (e.g. the modelled pipe capacity is limited to cause CSO, the design of the secondary clarifier is such that sludge losses occurs during hydraulic overloading of the WWTP, etc), thus providing the students a better understanding of the interactions within an integrated system. The catchment provided the basis for the integration between MTFM models and the IUWS_MP system illustrated in De Keyser et al. (2010a). The model area is composed of three subcatchments connected to a WWTP (Fig. 4), which performs nitrification-denitrification treatment through activated sludge. The catchment is connected to a natural stream by discharge from the WWTP and by overflow structures located along the sewer network. MP concentrations and fluxes in the river are monitored at three stations (located upstream the catchment, after the WWTP discharge, and at the river mouth, 11 km downstream the WWTP). The main characteristics of the system are listed in Table 4. Rainfall data collected by a rain gauge managed by the Danish

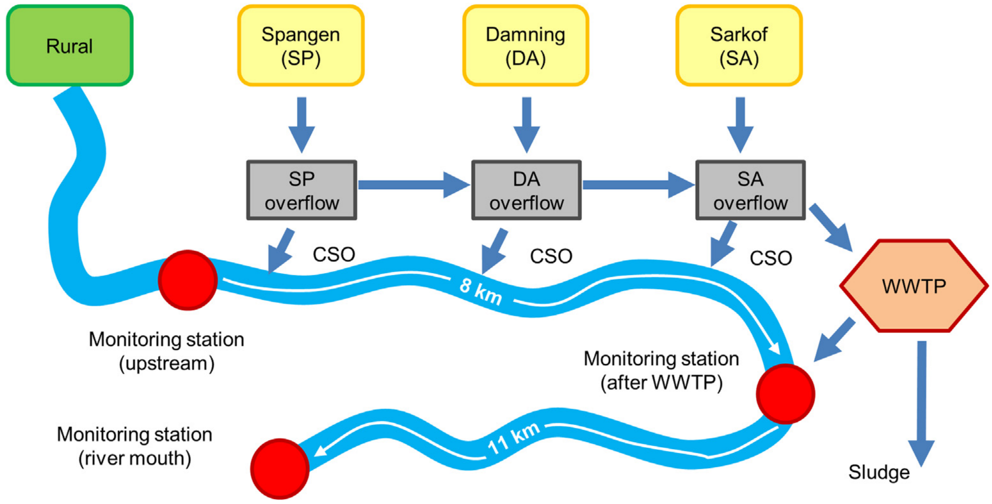

Fig. 4. Scheme of the simulated theoretical catchment.

Table 4
Main characteristics of the simulated theoretical catchments.

Catchment	Rural	Spangen	Damning	Sarkof
Total area [ha][a]	600	120	450	120
Length of downstream connection [m]	–	4000	3250	750
WWTP				
Volume of anoxic tank [m^3]	25,000			
Volume of aerobic tank [m^3]	28,000			
River				
Length of river upstream WWTP discharge [m]	8000			
Length of river downstream WWTP discharge [m]	11,000			

[a] a hydrological reduction factor of 0.8 was assumed, with a population density of 16,000 inhabitants/km^2 and an average wastewater production of 150 L/day.

Meteorological Institute (Jørgensen et al., 1998) were used as input to the integrated model to estimate yearly MP fluxes. Information regarding traditional pollutants (e.g. TSS concentration in wastewater) were defined according to typical literature values (Henze et al., 2002).

3.2.2. Simulated substances and scenarios

The model was applied to simulate three different organic MP: Bisphenol A (CAS 80-05-7), Glyphosate (CAS 71-83-6) and Pyrene (CAS 129-00-0). These substances were selected to show the flexibility of the proposed modelling approach when modelling MP with a range of different properties. In fact, Pyrene shows a high tendency to sorb to particles (high K_{OC} and K_{OW}), while Bisphenol and Glyphosate have different biotic and abiotic degradability (Bisphenol A has a shorter aerobic half-life, while it does not undergo photo- and anaerobic degradation – see the properties listed in Table 5). Also, these three MP have different sources in urban areas: Bisphenol A is mainly present in wastewater, while Glyphosate and Pyrene are mostly found in stormwater (see Table 6).

Constant concentrations were assumed for stormwater (thus disregarding accumulation and wash-off processes), while diurnal and weekly variations in wastewater (based on typical observed patterns) were simulated (with average concentrations listed in Table 6 and same diurnal and weekly variation as for the traditional pollutants). As the simulated substances are not included in the European legislation (EQS directive – European Commission, 2008), EQS values from national legislation (Bisphenol A, Pyrene – Danish Ministry of Environment, 2010) or proposed EQS (Glyphosate – UKTAG, 2012) were used (Table 7). An exceedance event for Maximum Allowed Concentrations (MAC-EQS) was arbitrarily defined as a concentration exceeding the EQS after more than 3 h from the last exceedance.

The model was used to simulate different scenarios, which involved estimation of MP fluxes, simulation of monitoring stations along the receiving water body, and evaluation of compliance with water quality registration. This enabled (i) the assessment of contributions of the different sources in the urban catchment, (ii) the evaluation of MP fate in the urban water system, and (iii) the effect of different pollution control options on the loads discharged to the receiving waters and on the compliance with EQS. The simulation period covered a 1-year period with a 15 min output resolution. A variable time-step Runge–Kutta solver was used to more efficiently (in terms of computation time) simulate the dynamic processes with a time scale faster than 15 min – e.g. CSO events). Three arbitrary scenarios, created to cover a range of different MP control strategies, were simulated:

Table 5
Main physico-chemical properties of the simulated MP (HSDB, 2006, 2008, 2010).

	Bisphenol A (CAS 80-05-7)	Glyphosate (CAS 71-83-6)	Pyrene (CAS 129-00-0)
Molar mass [g/mol]	228.29	169.07	202.26
Koc [l/kg]	796	3400	76,000
Log Kow [–]	3.32	−4.00	4.88
Water solubility [mg/l]	120	12,000	0.135
Vapour pressure [mmHg]	$3.9 \cdot 10^{-7}$	$2.89 \cdot 10^{-10}$	$4.5 \cdot 10^{-6}$
Henry's constant [atm m^3/mol]	$1 \cdot 10^{-11}$	$4.08 \cdot 10^{-19}$	$1.19 \cdot 10^{-5}$
Aerobic degradation half-life [d]	3	66	400
Anaerobic degradation half-life [d]	Not degraded	8.1	~Years
Photodegration half-life [d]	Potential	28	0.04

Table 6
Average wastewater concentration values of the three simulated MP (HSDB, 2006, 2008, 2010).

	Bisphenol A (CAS 80-05-7)	Glyphosate (CAS 71-83-6)	Pyrene (CAS 129-00-0)
Average concentrations			
Wastewater[a] [μg/l]	2.5	Not detected[b]	0.96
Stormwater [μg/l]	0.003	2.69	30.0

[a] Average value.
[b] To avoid numerical problems, a value of 1 ng/l was used in the simulations.

- *Baseline scenario*: fluxes in the actual system were evaluated, distinguishing between the contribution of wastewater and stormwater.
- *Source control scenario*: the simulated MP is banned from households, i.e. the concentration in wastewater is below the detection limit. In this scenario concentrations are assumed not to vary in stormwater (thus neglecting the effect that banning would have on stormwater pollution sources). This is simulated by reducing the MP concentration in wastewater (a value of 1 ng/l was used to avoid numerical problems which might arise with zero concentrations).
- *CSO control scenario*: direct discharge of untreated wastewater through CSOs is reduced by construction of detention basins at the overflow structures. The size of the basins is defined to avoid overflows by increasing the storage capacity. The sizes are the following: Spangen 6000 m^3, Damning 8000 m^3, and Sarkof 3750 m^3.
- *End-of-pipe treatment scenario*: Tertiary treatment of the WWTP outlet by using a filter (Cloutier et al., 2012) with a particle removal efficiency of 99%.

3.2.3. Simulation results

The simulated MP fluxes for the baseline scenario are shown in Fig. 5. From these results, the main conclusions that can be drawn about the system are:

- The major MP fluxes are discharged from the WWTP (over 99% for Bisphenol and Glyphosate).
- The WWTP shows different MP removal efficiencies (calculated as the ratio between the inlet and outlet load from the WWTP) according to the properties and the sources of the simulated MP: 20% for Bisphenol A (which, according to the model, is mainly removed by aerobic biodegradation), 5% for Glyphosate (which has low degradability and tendency to sorb) and 90% for Pyrene (mainly removed through sorption to TSS and their consequent removal).
- Similarly, the MP load removed with the WWTP waste sludge depends on the MP properties, with 37% of the Pyrene (strongly bound to particles) entering the plant removed with the sludge (while this is 5.5% for Bisphenol and 2% for Glyphosate)

Table 7
Environmental Quality Standard values used for the hypothetical case study.

	Bisphenol A (CAS 80-05-7)	Glyphosate (CAS 71-83-6)	Pyrene (CAS 129-00-0)
Annual Average (AA) [μg/l]	0.1[a]	196[b]	0.0046[a]
Maximum Allowed Concentration (MAC) [μg/l]	10[a]	398[b]	0.023[a]

[a] Value from Danish water regulation (Danish Ministry of Environment, 2010).
[b] Value proposed by UKTAG (2012).

- The MP loads caused by overflows represent an important pollution source only for Pyrene, as about 15% of the total load transported by the river originates from the CSO structures, whereas for Bisphenol A and Glyphosate the CSO contribution to the river load was less than 0.02% and 0.23%, respectively.
- Annual Average EQS are fulfilled for all the simulated MP. The MAC-EQS for Pyrene is exceeded both after the WWTP (29 times/year) and at the river mouth (16 times/year) as a consequence of CSO events (23 events/year at SP and 3 events/year events at SA: one of these major CSO events is shown in the detailed illustration of Fig. 6). MAC-EQS for the two remaining substances was fulfilled.

A more detailed analysis of the continuous results (Fig. 6) allows evaluating compliance with EQS and stressed the importance of CSO events for the quality status of the river. The average concentrations in the river for the simulated year (approximately 12 ng/l for Bisphenol A, 1 ng/l for Glyphosate, and 6 ng/l for pyrene) were in the same order of magnitude of the values listed in literature (HSDB, 2006, 2008, 2010). The comparison of the simulated COD and MP concentrations in the river (Fig. 6c,d) shows the clear correlation between those water quality parameters (CSO events generate peaks in both COD and MP). Dispersion, along with fate processes, is responsible for the decreasing number of MAC-EQS exceedances along the river. This is relevant information for selection of potential locations for the installation of monitoring stations along the river stretch. Concentration peaks at the river mouth occurred about 2–3 h after overflow events took place at the SP overflow structure. This information is useful to plan dedicated sampling and/or interpret the results from monitoring campaigns regarding river quality. For example, if MP monitoring is performed only at the river mouth station, the increase of MP concentrations (Fig. 6d) caused by a small rain event (which does not cause CSO events but hampers the removal performance of the WWTP) would be overlooked.

The reductions of MP fluxes by the different scenarios are listed in Table 8. Depending on the main source and the physical characteristics of the simulated MP, different reductions in MP emissions to the natural environment were obtained:

- Bisphenol A is mainly found in wastewater, therefore banning of this substance from households results in a complete eradication of MP emission (the remaining 0.2% at the WWTP outlet is due to the 1 ng/l value used to avoid numerical problems). On the other hand, this scenario achieves limited reductions for Glyphosate and Pyrene, because the stormwater contribution is also relevant for these MP.
- The decrease of overflow volumes (from about 28700 m^3 to 2350 m^3) leads to an increase of the load of stormwater-related MP (Glyphosate and Pyrene) to the WWTP, and the increased hydraulic overloading of the plant also results in slightly larger loads discharged into the river. CSO control contributed to improve the peak quality in the river for Pyrene (the occurrence of MAC-EQS exceedance is almost halved at the river mouth, decreasing from 16 times/year to 9 times/year).
- The installation of a filter at the WWTP outlet achieves different reductions depending on the characteristics of the simulated MP, with better removal for MP with high tendency to sorb (up to 45% for Pyrene). Not surprisingly, this End-of-Pipe scenario increases the MP removal of the WWTP (from 20% to 35% for Bisphenol A, from 5% to 23% for Glyphosate, and from 90% to 94% for Pyrene), while the remaining scenarios do not affect the plant removal performance.
- Overall, none of the simulated scenarios manages to achieve the desired water quality in the river (i.e. non-exceedance of EQS for

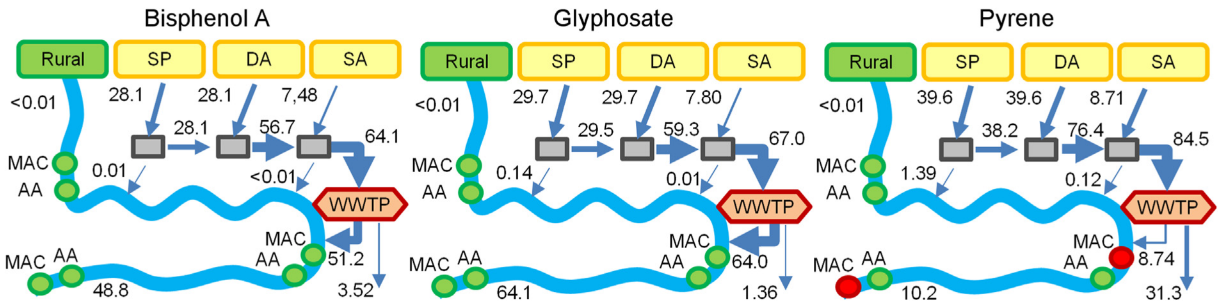

Fig. 5. Substance Flow Analysis for the baseline scenario for Bisphenol A (a), Glyphosate (b) and Pyrene (c). MP fluxes are expressed as average daily loads [g/d]. Green and red circles indicate compliance with EQS criteria (MAC = Maximum Allowable Concentration, AA = Annual average) at the different monitoring stations along the river. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

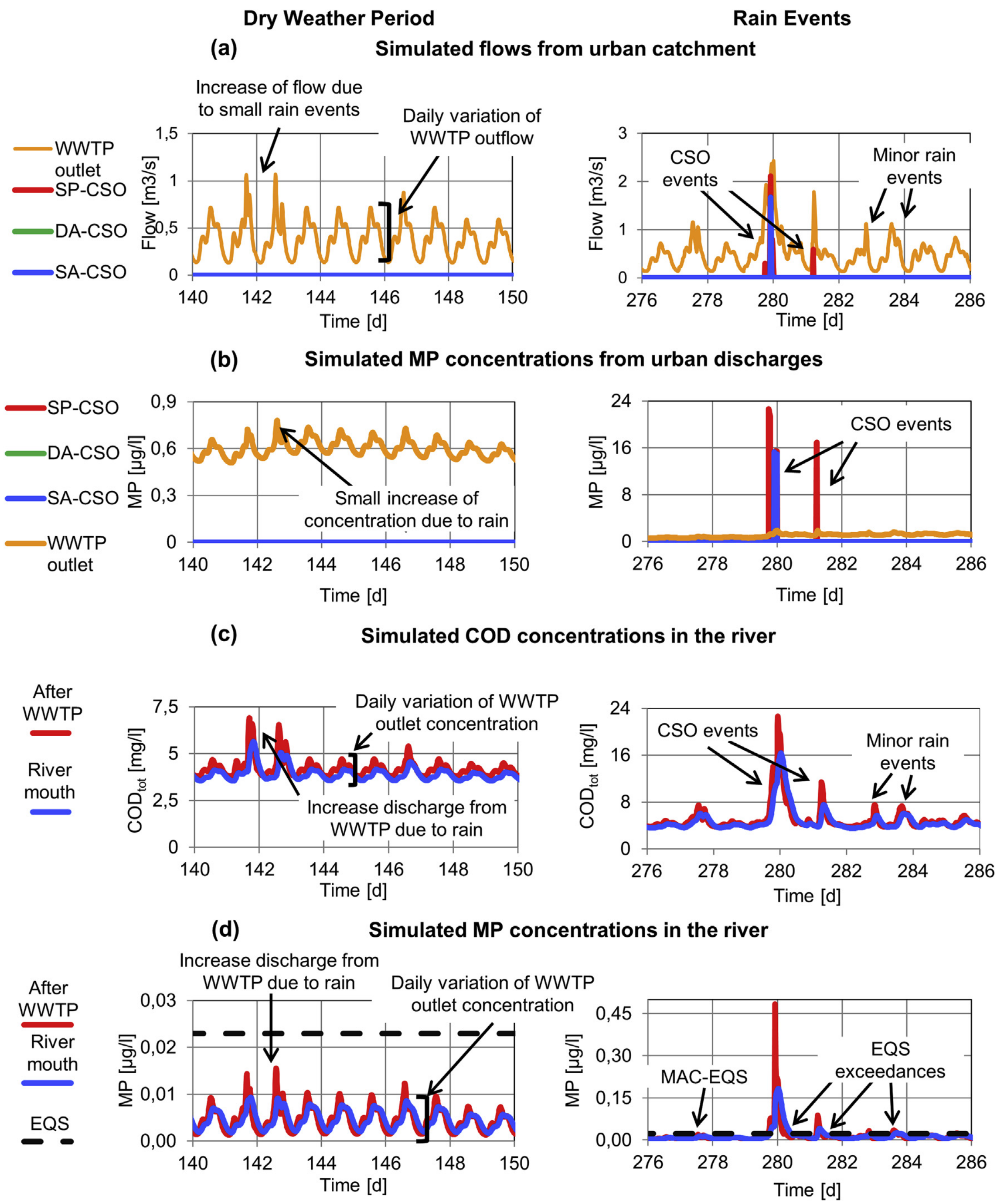

Fig. 6. Examples of simulated results for the baseline scenario for Pyrene and COD: (a) overflows and WWTP outflow; (b) Pyrene concentrations at overflow structures and WWTP outlet; (c) COD and (d) Pyrene concentrations in the river at the monitoring stations downstream the WWTP.

Table 8
Scenario comparison for the three simulated micropollutants. Variations from the baseline scenario are expressed as percentages.

	Scenario		
	Source control	CSO control	End-of-pipe
Bisphenol A			
Total CSO load	−98.6	0	0
MP inlet load to the plant	−99.8	0	0
MP outlet load from the plant	−99.8	0	−19.9
MP load at the river mouth	−99.8	<0.1[a]	−19.9
Glyphosate			
CSO load	<0.01	−94.9	0
MP inlet load to the plant	<0.01	+0.14	0
MP outlet load from the plant	−16.0	+0.11	−19.5
MP load at the river mouth	−16.0	−0.12	−19.5
Pyrene			
CSO load	−1.19	−94.5	0
MP inlet load to the plant	−36.2	+0.91	0
MP outlet load from the plant	−33.4	+1.35	−45.5
MP load at the river mouth	−28.5	−12.9	−36.2
Exceedance of MAC-EQS after WWTP	−24.1	−3.45	0
Exceedance of MAC-EQS at river mouth	−25.0	−43.8	−6.25

all the MP) when considered alone. The simulation results thus suggest that a combination of different control options might be necessary to meet the desired quality objectives.

This didactical example illustrates students how (i) MP behaviour and removal is affected by their sources and inherent properties, (ii) these factors also affect the performance of different control strategies, and (iii) strategies obtaining good performance for one MP might not be sufficient to achieve the goal defined for another MP (suggesting a combination of strategies). Given the increased interest in uncertainty aspects of environmental models (Refsgaard et al., 2007; Belia et al., 2009), the authors want to strongly recommend that, when the model library is to be used in real applications, the uncertainty of these results should be quantified (e.g. by assessing the influence of variations in inputs and parameters on the final model outputs – as shown in the example provided by Vezzaro and Mikkelsen, 2012). In this way the user can considerably increase the robustness of the conclusions drawn (see, for example, the scenario comparison performed in Vezzaro et al., 2013).

4. Conclusions

This article presents an integrated dynamic model and model library for the estimation of MP fluxes across the different elements of urban water systems. This model library can be used to estimate MP fluxes across the different elements of the integrated urban wastewater and stormwater system. As shown through the example applications summarized in this contribution, this allows to

(i) evaluate the effect of pollution control strategies (e.g. "the source control/treatment B reduces the emission of this MP from the city by XX%");
(ii) optimize monitoring programmes (e.g. "to measure this MP, it is better to sample XX hours after a rain event and YY km downstream the overflow structure"); and
(iii) check compliance with Environmental Quality Standards of a proposed control strategy (e.g. "with the strategy A the river is able to fulfil all the Environmental Quality Standards all across the year").

The proposed modelling approach:

- extends state-of-the-art models for the various elements of the urban wastewater and stormwater system with MP-fate models inspired by those that are commonly applied in chemical risk assessment. The integrated model thus benefits from all available information about MPs that can be found in literature and public databases;
- extends state-of-the-art MP fate models by including dynamic descriptions that are especially relevant in urban contexts (e.g. CSOs) and by extending the set of units that are described in some detail;
- provides a dynamic representation of the complex processes taking place in urban areas, providing useful information for planning/implementation of monitoring programs which are difficult to obtain from steady-state approaches;
- allows focussing both on the single elements of the urban water systems (e.g. a single stormwater unit) and on the whole urban area (as in the educational example presented in this study).

The presented model library for traditional and micropollutants in the integrated urban wastewater and stormwater system thus represents an important tool for urban water managers in their effort to reduce city-born MP emissions to the water environment. The use of these models will provide a more solid background for the development and the implementation of pollution control strategies, leading to the desired improvement of the quality of the natural environment downstream urban areas.

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