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Combining multimedia models with integrated urban water system models for micropollutants

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ABSTRACT

Integrated urban water system (IUWS) modeling aims at assessing the quality of the surface water receiving the urban emissions through sewage treatment plants, combined sewer overflows (CSOs) and stormwater drainage systems. However, some micropollutants tend to appear in more than one environmental medium (air, water, sediment, soil, groundwater, etc.). In this work, a multimedia fate and transport model (MFTM) is "wrapped around" a dynamic IUWS model for organic micropollutants to enable integrated environmental assessment. The combined model was tested on a hypothetical catchment using two scenarios: on the one hand a reference scenario with a combined sewerage system and on the other hand a stormwater infiltration pond scenario, as an example of a sustainable urban drainage system (SUDS). A case for Bis(2-ethylhexyl) phthalate (DEHP) was simulated and resulted in reduced surface water concentrations for the latter scenario. However, the model also showed that this was at the expense of increased fluxes to air, groundwater and infiltration pond soil. The latter effects are generally not included in IUWS models, whereas MTFMs usually do not consider dynamic surface water concentrations,; hence the combined model approach provides a better basis for integrated environmental assessment of micropollutants' fate in urban environments.

Key words | chemical fate model, dynamic integrated modeling, emerging contaminants, integrated environmental assessment, IUWS, microconstituents

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INTRODUCTION

Integrated modeling of the urban water system has matured substantially over the last decade. In the past, sewers, urban drainage, wastewater treatment and surface waters were modeled separately. However, all these sub-systems are interconnected. Hence, to meet the final aim of water management, being a good ecological status of water bodies, these disciplines have evolved into integrated urban water system (IUWS) modeling (e.g. Schmitt & Huber 2006).

As the presence of some micropollutants in surface water bodies can be of particular concern, the European Commission identified a list of "priority substances" (CEC 2008). Monitoring programmes can be established for surveillance, operational or investigative purposes. However, monitoring is costly, often difficult to perform and, due to the limited sampling frequency, restricted in the amount of collected data necessary to sufficiently reflect temporal variability. Mathematical tools provide a possible solution to complement water quality monitoring. Therefore, in order to model the origin, transport and transfer processes of micropollutants within the urban

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water system in full detail, it is necessary to expand existing urban water quality models with state variables representing these micropollutants (e.g. Lindblom *et al.* 2006). However, micropollutants have the tendency to appear in more than one environmental medium (air, water, sediment, soil, etc.). Harremoës (2002) addresses the point of interrelating the environmental media water, air and soil in "integrated environmental assessment" as a scientific discipline that goes beyond integrated water system modeling.

The behaviour of pollutants in different interconnected environmental media is the subject under study in multimedia fate and transport models (MFTMs) (e.g. Mackay 2001). In comparison to fully dynamic water quality models, the early "unit world" MFTMs show a limited complexity, lack spatial resolution and often assume steady-state or equilibrium distribution between the environmental media. To date, MFTMs have evolved into more realistic and dynamic models: connections with geographical information systems are established, time-variant parameter estimation is included and different sub-models have been coupled in order to represent geographical heterogeneity in the modeled system (e.g. Verdonck 2003; Luo *et al.* 2007). Currently, MFTMs are widely accepted for evaluating the overall fate and transport in the environment of organic chemicals.

This paper introduces a solution for bridging the gap between IUWS models for micropollutants and MFTMs to obtain fully integrated environmental assessment frameworks. This is illustrated through a hypothetical case study and should allow assessment of the impact of source control strategies at the urban scale on surrounding environmental compartments. Moreover, the multimedia model provides the boundary conditions for the urban scale model, such as pollutant (anthropogenic) background concentrations in an upstream river part.

METHODS

Modeling and simulation platform

To illustrate the concept of IUWS and MFTM integration, both models need to be linked. This can be achieved either by interfacing existing stand-alone models (software) or merging both models in a single software.

The former avoids time-consuming reimplementation of existing models and allows for preserving the detailed knowledge contained in each dedicated model. However, it requires the creation of interfaces supporting bi-directional data exchange (e.g. Brandmeyer & Karimi 2000), which is a challenging task, due to the discrepancy in level of detail (e.g. different sets of state variables), time scales, spatial resolution, and availability and accuracy of data used in both models. The OpenMI interfacing standard (Gregersen *et al.* 2007) could be a possible solution for a number of problems related to interfacing of models, provided that the model software involved is OpenMI-compliant. However, to our knowledge, no OpenMI-compliant MTFM is currently available.

The latter eliminates the need for interfacing, but requires both models to be available in the same modeling environment. As all components of the IUWS model (see below) in this study were already available in the WEST® modeling and simulation platform (MOSTforWATER, Kortrijk, Belgium), it was decided to illustrate the concept of integrated environmental assessment by implementing a MFTM in WEST®. Both the IUWS model and the MTFM discussed in the next sections are applied to represent a physical system whose hydraulics are modeled in a lumped, simplified way. However, the water quality component of the model is more complex, including most of the physical, chemical and biological processes acting on organic pollution, nutrients and micropollutants. The simplified hydraulics are sufficient to illustrate the concept of IUWS and MTFM coupling.

Dynamic integrated urban wastewater system model for organic micropollutants

The IUWS model consists of different unit process models for each part of the urban water cycle: the simplified KOSIM model (Solvi 2007) is used as hydrological catchment runoff and sewer transport model, ASM2d (Henze *et al.* 2000) for activated sludge processes, the Takacs *et al.* (1991) model for secondary settling, the Universal Stormwater Treatment Model (Wong *et al.* 2006) for stormwater infiltration ponds, and the RWQM1 described in Reichert *et al.* (2001) for river water quality. In the recent EU project ScorePP (www.scorepp.eu), these state-of-the-art water quality models were extended with the fate of micropollutants (Benedetti *et al.* 2009; Vezzaro *et al.* 2010). The relevant removal processes for organic micropollutants in each unit of the urban wastewater system were identified (Table 1) and implemented.

The IUWS model configuration is based on a setup described by Grum *et al.* (2000), which is currently used for simulating IUWS in an e-learning course (Mikkelsen 2009). It consists of a rural catchment, three urban sewer catchments connected to an intercepting combined sewer system, and an activated sludge plant including primary settling, anoxic and aerobic tanks and secondary settling. The treatment plant and the overflow structures at the three urban catchments discharge to a river, which is modeled as five CSTRs in series, each of them in contact with river sediment. The configuration resembles the overall layout of the combined sewerage system of the greater Copenhagen area in Denmark and has been tuned earlier (for educational purposes) to simulate phenomena such as overall nutrient balances, oxygen depletion in rivers, effects of catchment storage on secondary clarification, stormwater source control and treatment, and integrated real time control. A scheme of the model setup is included in the overall IUWS/MFTM scheme shown in Figure 1 and some key properties of the system are listed in Table 2. A five minute temporal resolution rainfall time series is used as dynamic input to the hydrological catchment runoff model.

Multimedia model

Most MFTMs rely on the fugacity concept (Mackay 2001) to quantify the partitioning of a chemical between phases. Fugacity reflects a substance's tendency to flee to a different phase or medium (liquid, solid, or gas). A first possible assumption is that fugacities are equal in all environmental media, which can be used in steady-state models (referred to as level I and II). This allows for equilibrium distribution concentrations to be calculated. Relaxing this assumption and assigning different, yet constant, fugacities to each environmental medium is adopted in level III models. This indicates that the system can be in a non-equilibrium steady-state. As a last option, fugacities can be regarded as fully dynamic by defining them as state variables. This approach is applied in level IV models.

The MFTM implemented in WEST® is based on the 'regional' scale of the SimpleBox model (den Hollander *et al.* 2003). It is a level III/level IV Mackay-type model, but uses the micropollutant's mass or concentration (instead of its fugacity) in each environmental compartment as the main state variable in the differential equations, which is similar to the mass balances commonly used in IUWS sub-models for traditional pollutants. This implies that the MTFM implemented in WEST® can be used as a fully dynamic (level IV) model, in contrast to the original Excel-implemented SimpleBox. Moreover, only a limited amount of data needs to be provided by the user, as a large number of parameter values can be estimated by the model based on the micropollutant's physical-chemical properties. The environmental compartments considered in SimpleBox

Table 1 | Fate processes included in the various components of the IUWS model

Processes	Sewer	Stormwater unit (water)	Stormwater unit (sed.)	Primary settling	Aeration tank	Secondary settling	River water	River sediment
Adsorption-desorption	+	+	+	+	+	+	+	+
Aerobic biodegradation	+	+	+		+		+	+
Anoxic biodegradation	+	+	+		+		+	+
Hydrolysis	+	+	+		+		+	
Photolysis		+			+		+	
Sedimentation	+	+		+		+	+	
Resuspension	+		+					+
Sediment-water exchange							+	+
Volatilization	+	+		+	+	+	+	

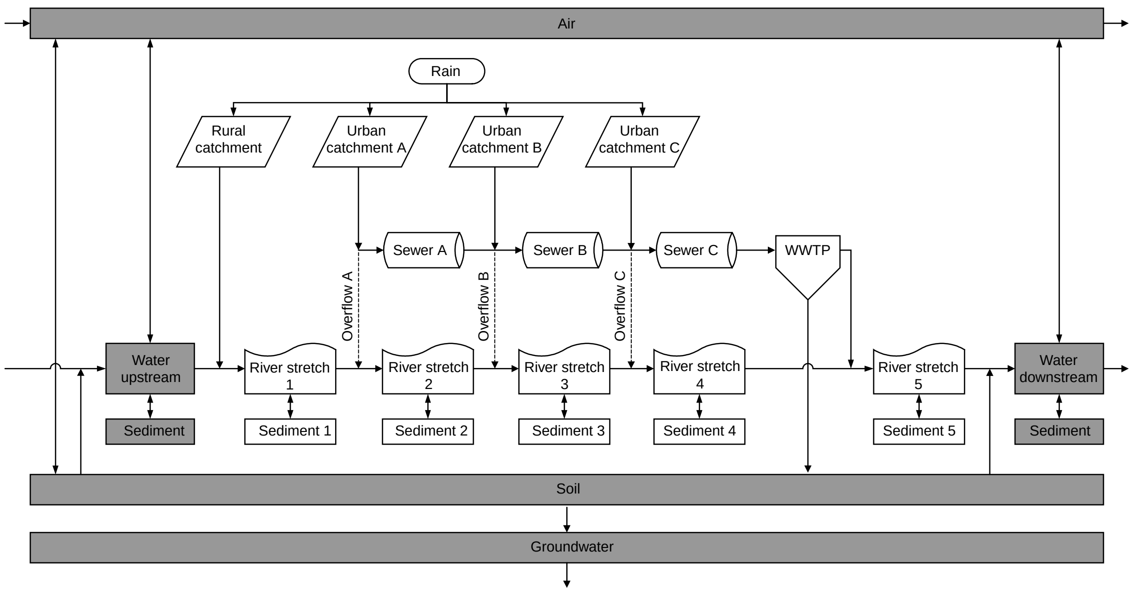

Figure 1 | Schematic representation of the integrated environmental model (IUWS model (white blocks) and MFTM (grey blocks)).

are: air, soil (natural, agricultural and urban), water (fresh and sea), and sediment and above ground vegetation (natural and agricultural). For the purpose of this work, the WEST® implementation of SimpleBox (De Keyser *et al.* 2008) is modified: the vegetation compartment is omitted and the soil and water compartments are implemented as generic soil and water models. The latter can be fine-tuned to different soil and water types by adjusting the parameter values. Next, the model is extended with a basic groundwater compartment, acting as a fixed volume completely stirred tank reactor (CSTR) where no biological degradation of the micropollutant occurs. A schematic overview of the model setup is part of the overall scheme in Figure 1 (grey blocks) and some key properties of the system are listed in Table 2.

Integrated environmental model

Using the two submodels discussed above, an integrated IUWS/MFTM model is set up. The characteristics of the two models can be found in De Keyser *et al.* (2008) and Benedetti *et al.* (2009). In the reference scenario, the following links between both models are considered (Figure 1): an upstream MFTM water compartment provides the input to the IUWS river model, a downstream MFTM water compartment receives the IUWS river water, and primary and secondary waste sewage sludge is conveyed to the MFTM soil compartment after treatment in a thickener. Furthermore, a combined sewer system is implemented with treatment in the WWTP before discharge into the surface water. In a second scenario, with separate sewer system, the installation of stormwater infiltration ponds as best management practice (BMP) is simulated, with volatilization and infiltration processes occurring (Figure 2). Wet and dry deposition as well as diffusion are considered as exchange processes between the air and soil compartments in the multimedia model, but similar links between the air and the urban catchments are not included as they are negligible compared to fluxes due to direct emissions onto the urban surface.

Bis(2-ethylhexyl) phthalate (DEHP) as a case study

The substance-inherent physical-chemical parameter values are adapted to simulate the fate of bis(2-ethylhexyl) phthalate (DEHP) in the integrated system (Table 2). Because of the high production volume and widespread use of DEHP, this chemical's presence in the environment is of growing concern. Cousins & Mackay (2003) assume EU production and consumption tonnages of 595,000 and 476,000 tons of DEHP per year respectively. Based on Parkerton & Konkel (2001), they use emission factors of

Table 2 | Key parameters used in the case study

	Parameter	Unit	Value
IUWS model*	Sewer catchment size (incl. industry, in population equivalent)	PE	127,500
	Impervious area (catchment surface for runoff)	km^2	3.36
	Total length of the intercepting combined sewer system	km	8.0
	Volume of activated sludge tanks in WWTP	m^3	53,000
	Organic carbon content of WWTP sludge	–	0.37
	Total length of the river upstream of WWTP discharge point	km	9.0
	Length of the river segment downstream of WWTP discharge point	km	11.0
	Base river flowrate	$m^3\,s^{-1}$	15
	Mean DEHP emission to urban surface, susceptible to runoff	$g\,PE^{-1}\,d^{-1}$	2.63×10^{-4}
	Mean DEHP emission to sewer system, via dry weather flow	$g\,PE^{-1}\,d^{-1}$	1.5×10^{-2}
	Total volume of storm ponds	m^3	11,250
Multimedia model†	Air-soil interface area	km^2	5,000
	Air-water interface = water-sediment interface area	km^2	150
	Air height	m	1,000
	Sediment depth	m	0.03
	Water depth	m	3.0
	Fraction air in soil	–	0.2
	Fraction water in soil	–	0.2
	Fraction water in sediment	–	0.8
	Organic carbon content of soil and sediment	–	0.1
	Annual precipitation	$mm\,year^{-1}$	700
	Fraction of rainfall infiltrating to soil	–	0.25
	Wind speed 10 m above earth surface	$m\,s^{-1}$	3.0
	Air residence time	d	0.245
	Water residence time	d	174
	Settling velocity of solids	$m\,d^{-1}$	2.5
	DEHP emission to air	$kg\,d^{-1}$	618.6
	DEHP background concentration in air entering the system	$ng\,m^{-3}$	10
	DEHP background concentration in water entering the system	$\mu g\,l^{-3}$	0.10
Micropollutant DEHP‡	Molecular weight	$g\,mole^{-1}$	390.54
	Vapor pressure	Pa	3.4×10^{-5}
	Henry constant	$Pa\,m^3\,mole^{-1}$	4.43
	Water solubility	$\mu g\,l^{-1}$	3.0
	K_{OC}	$l\,kg^{-1}$	1×10^{-5}
	K_d	$l\,kg^{-1}$	1.5×10^{4}
	Half-life in air	d	1
	Half-life in soil and sediment	d	300
	Photolysis half-life in nearsurface water	d	0.5
	Biodegradation half-life in aerobic water	d	25
	Biodegradation half-life in anoxic water	d	3,000
	Adsorption rate constant	$m^3\,d^{-1}\,g_{solids}^{-1}$	0.1

*Grum *et al.* (2000).
†De Keyser *et al.* (2008).
‡Staples *et al.* (1997), European Commission (2008) and Lützhøft *et al.* (2008).

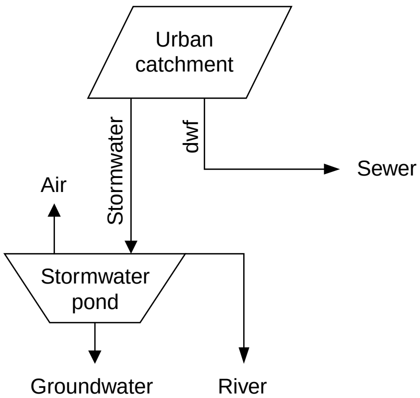

Figure 2 | Addition of storm water infiltration ponds to the reference scenario of Figure 1.

0.0025, 0.00025 and 0.00005 to air, water and soil respectively, due to industrial production, industrial use and transport, and of 0.01, 0.00031 and 0.00065 due to product end use and disposal. Emission estimates are converted to a *per capita* basis and scaled to the size of the case study. Urban emissions to water are assumed to go to wastewater, whereas emissions to soil are supposed to accumulate on the urban surface and to be washed off with runoff.

Initialization of the model

The IUWS model is first initialized using a 120 days steady-state simulation to obtain realistic initial conditions in all components of the IUWS (sewers, treatment plant, river). Then, the average DEHP mass fluxes from the IUWS to the multimedia compartments are calculated and used as steady-state input to initialize the stand-alone MFTM. When a steady-state is reached, both models are coupled and run with the obtained steady-state quantities as initial values, which are in the range of environmental DEHP concentrations reported in literature.

RESULTS AND DISCUSSION

Environmental concentrations and fluxes in the different scenarios

The dynamic simulation results shown in Figure 3 indicate that the installation of stormwater infiltration ponds helps to avoid DEHP peak discharges into the surface water originating from the stormwater after treatment in the WWTP (B). On the other hand, the figure also shows that the stormwater infiltration ponds reallocate the DEHP flows to groundwater (C), air (D) and infiltration pond soil (E). The elevated air concentrations are transient due to photochemical breakdown and advective transport out of the modeled system, whereas the accumulation of DEHP in the groundwater compartment could potentially cause problems in the long term. The simulated river concentrations are relatively high compared to the environmental quality standard defined in the EQS directive (1.3 $\mu g\,l^{-1}$, cf. CEC 2008) and measured concentrations reported in literature. The latter are, for urban areas, usually below or around one $\mu g\,l^{-1}$, although concentrations up to 21 $\mu g\,l^{-1}$ have been observed in industrialized urban areas (European Commission 2008). Further research will reveal to what extent such simplified model setup can be tuned to yield more realistic environmental concentrations.

Figure 4 shows an overview of all mean DEHP mass fluxes, removal rates and concentrations in the modeled system (with and without the infiltration pond). Note that the IUWS is represented as one compartment. The averages are calculated with data obtained from 120 days of dynamic simulation with a 15-minute output interval. By summarizing the data as mean values, the dynamics are not apparent, but without a dynamic model (rainfall input time series) these results could not have been obtained. The main effect of the stormwater infiltration ponds on the outer-urban environment is a decrease of mass fluxes towards downstream water and soil, whereas DEHP fluxes to the groundwater and the air compartment increase. In this example, the latter may not have a vast impact, but without the MFTM shell around the IUWS model, this effect could not have been assessed at all.

Sensitivity to boundary conditions and model layout

The discussed simulation outputs serve as an illustration of the modeling concept and its behavior. As is the case for any model, results heavily depend on assumptions made and fixing of inputs during the modeling process. The latter should be borne in mind. E.g. the simulated effect in the air compartment is transient due to the short residence time of air in the modeled system

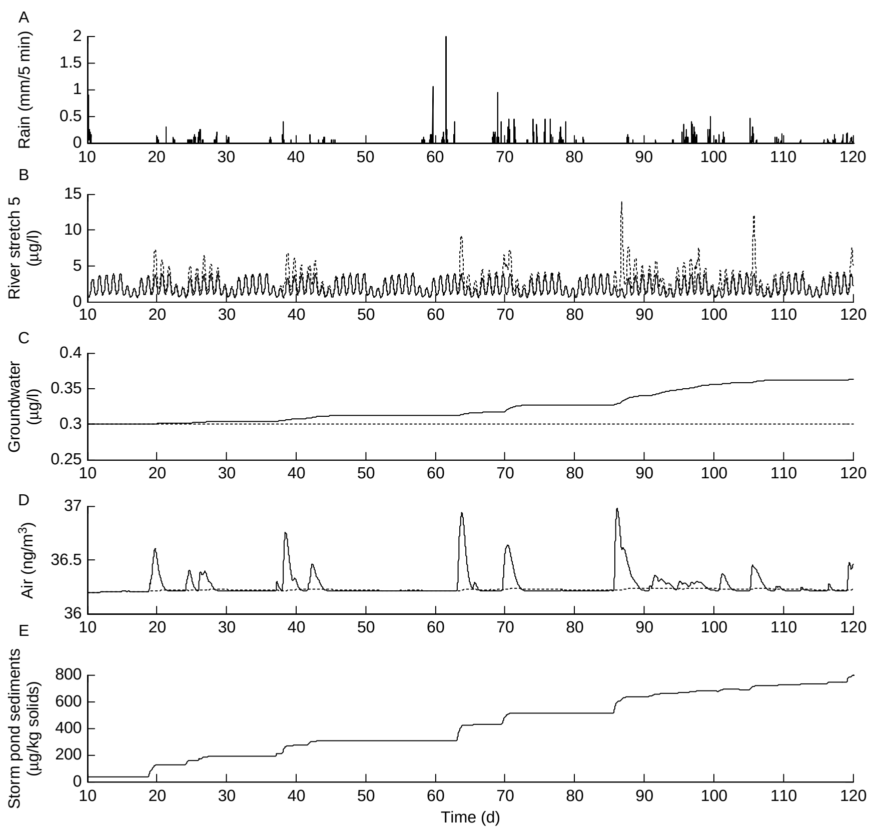

Figure 3 | Input rainfall series (A) and simulated DEHP concentration in the two modeled scenarios (basic scenario in dotted line, scenario with the stormwater infiltration ponds in solid line) in the last river stretch of the IUWS model (B), in the groundwater compartment of the MFTM (C), in the air compartment of the MFTM (D) and in the soil of the infiltration ponds (E).

(less than 6 hours). Increase of the MFTM compartments' dimensions further reduces the impact of such advective transport processes. On the other hand, if the multimedia model is so extensive that it contains multiple cities, and yet simplified assuming no spatial heterogenity, then it is needed to assume that the same measures are applied in all cities within the region to observe an effect in the MFTM compartments. Besides model layout properties, also the estimated emissions to the modeled system influence the results. Moreover, detailed emission data is in many cases not available as micropollutant emissions are often diffuse, complex and expensive to register. Hence, the emissions need to be estimated based on rough emission factors, which causes large uncertainties on the output magnitudes. A more rigorous sensitivity and uncertainty analysis could be performed to investigate this. This was, however, outside the scope of this work.

Outlook for further research

Two potential aspects for future studies with the aim to further increase the confidence in the interpretation of simulation results are uncertainty and time scales.

The former can be as high as several orders of magnitude in multimedia models (Hennes & Rapaport 1989). For the more complex urban water models, the prediction performance is known to be better in terms of traditional pollutant concentrations (Mannina *et al.* 2006), although this is not known yet for micropollutants since, to our knowledge, no uncertainty evaluations have been conducted so far for micropollutants in the whole IUWS. This topic deserves further attention in order to make integrated environmental assessment based on coupled IUWS/MFTM models more reliable.

The second important factor in studies conducted with coupled IUWS/MFTM systems is the huge range of time constants to be considered. Processes in the IUWS

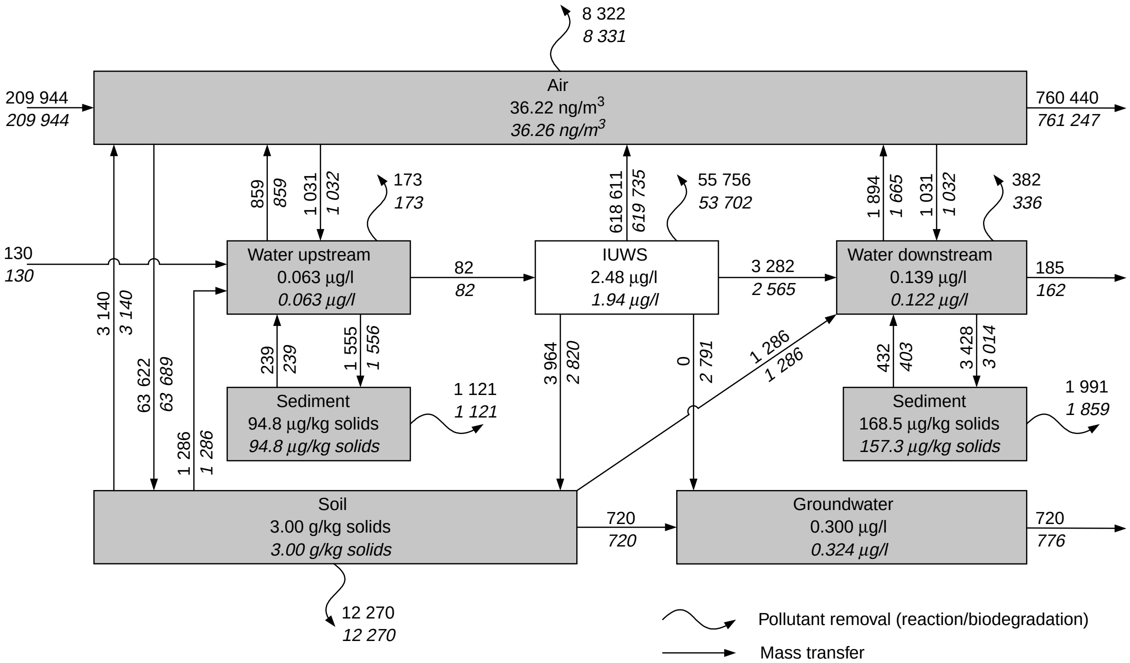

Figure 4 | Mean DEHP mass fluxes (in $g\,d^{-1}$) and concentrations in the modeled system: reference scenario (normal typeface) and after the implementation of stormwater infiltration ponds (italic typeface); values in the IUWS block are concentrations in the receiving water after mixing, i.e. at the outflow of river stretch 5.

model like adsorption, desorption, biodegradation, etc. can have small time constants and therefore make the system respond quite fast to dynamics acting on the system, like rainfall and time-varying emissions. In multimedia models, however, large time constants in the order of years are inherent to the system. It should be investigated whether the choice of the initial conditions for the dynamic simulations influences the conclusions and, moreover, whether better alternatives than the use of a calculated steady-state exist.

CONCLUSIONS

The added value of wrapping a multimedia fate and transport model (MTFM) around an integrated urban water system (IUWS) model is twofold: (1) the multimedia model provides boundary conditions to the IUWS, and (2) it allows a holistic assessment of the overall environmental status of the modeled system beyond urban surface water quality. A combined MFTM/IUWS model is presented and used to simulate the fate of the micropollutant DEHP in two scenarios: a reference and a scenario with stormwater infiltration ponds. The main effect of the stormwater infiltration ponds on the outer-urban environment is shown to be that mass fluxes towards downstream water and soil decrease, whereas fluxes to the groundwater and the air compartment increase. The creation of a combined MFTM/IUWS model can either be achieved by establishing an interface between two existing models or by merging them into one ‘supermodel’. Both approaches can be challenging, depending on the flexibility of the simulation platform. Nevertheless, once these models are implemented, a simple change of parameters allows for studying the fate of a huge range of micropollutants in the urban environment under dynamic conditions.

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