Combining multimedia models with integrated urban water system models for micropollutants

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ABSTRACT
Integrated urban water system (IUWS) modelling 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 have the tendency to occur in more than one environmental medium. 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: a reference scenario and 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 a reduced surface water concentration for the latter scenario. However, the model also showed that this was at the expense of increased fluxes to air and groundwater.

KEYWORDS
Dynamic integrated modelling; integrated environmental assessment; IUWS; micropollutants.

INTRODUCTION

Integrated modelling of the urban water system has matured substantially over the last decade. In the past, sewers, urban drainage, wastewater treatment and surface waters were modelled separately. However, since all of these sub-systems are interconnected, and because the final aim of water management is a good ecological status of water bodies, these disciplines have evolved into integrated urban water system (IUWS) modelling (e.g. Schmitt and 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. A possible solution is to use mathematical tools to complement water quality monitoring. Therefore, to model the origin, transport and transfer processes of micropollutants within the urban 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 occur in more than one environmental medium (i.e. air, water, sediment, soil, …). Harremoës (2002) therefore addressed the point of interrelating the environmental media water, air and soil in "integrated environmental assessment" as a scientific discipline going beyond integrated water system modelling.

The behaviour of pollutants in different interconnected environmental media is studied in multimedia fate and transport models (MFTMs) (e.g. Mackay, 2001). Compared 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. Over the years, these MFTM evolved into more realistic and more dynamic models: connections with geographical information systems were established, time-variant parameter estimation was included and different sub-models were coupled together in order to represent geographical heterogenity in the modelled system (e.g. Verdonck, 2003; Luo *et al.*, 2007). Today MFTMs are widely accepted for evaluating the overall fate and transport of organic chemicals.

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

METHODS

Modelling and simulation platform

To illustrate the concept of IUWS and MFTM integration, both models need to be linked. This could either be achieved by interfacing existing stand-alone models (software) or by merging the two models within a single software. As all components of the IUWS model (see below) were already available in the WEST® modelling 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 represent a simple system whose hydraulics are modelled in a simplified way, but at a high complexity level for water quality including most of the physical, chemical and biological processes acting on organic pollution, nutrients and micropollutants.

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) as hydrological catchment runoff and sewer transport model, the 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 a currently running EU project, ScorePP (www.scorepp.eu), these state-of-the-art water quality models were extended with the fate of micropollutants (Vezzaro *et al.*, 2009). The relevant removal processes for organic micropollutants in each unit of the urban wastewater system were identified (Table 1) and implemented.

Table 1. Fate processes important in the various components of the urban water system

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	+	+		+	+	+	+	

The IUWS model configuration was based on a setup described by Grum *et al.* (2000). It consists of a rural catchment, three urban sewer catchments connected to an intercepting combined sewer system, an activated sludge plant including primary settling, two aerated tanks and secondary settling. The treatment plant and the overflow structures at the three urban catchments discharge to a river modelled as a series of five completely mixed tanks, each of them in contact with river sediment. A scheme of the model setup is included in the overall IUWS/MFTM scheme shown in Figure 1.

Multimedia model

Most MFTMs rely on the fugacity concept (Mackay, 2001) to quantify the partitioning of a chemical between phases. For steady-state modelling (called level I and II), equilibrium distribution concentrations can be calculated from the fugacity, which is considered equal in all environmental media. Level III models assign different fugacities to each environmental medium, recognizing that the system can be in a non-equilibrium steady-state. By writing the fugacity equations as differential equations, dynamic conditions can be calculated in a level IV model.

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 using the micropollutant's mass or concentration in each environmental compartment as the main state variable in the differential equations, similar to the mass balances commonly used in IUWS sub-models. This implies that the MTFM implemented in WEST® can be used as a fully dynamic (level IV) model. Moreover, SimpleBox only requires a limited amount of data 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 are: air, soil (natural, agricultural and urban), water (fresh and sea), sediment and above ground vegetation (natural and agricultural). For the purpose of this work, the WEST® implementation of SimpleBox (De Keyser *et al.*, 2008) was modified: the vegetation compartment was omitted and the soil and water compartments were implemented as generic soil and water models, which can be finetuned to different soil and water types by adjusting the parameter values. Next, the model was extended with a 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.

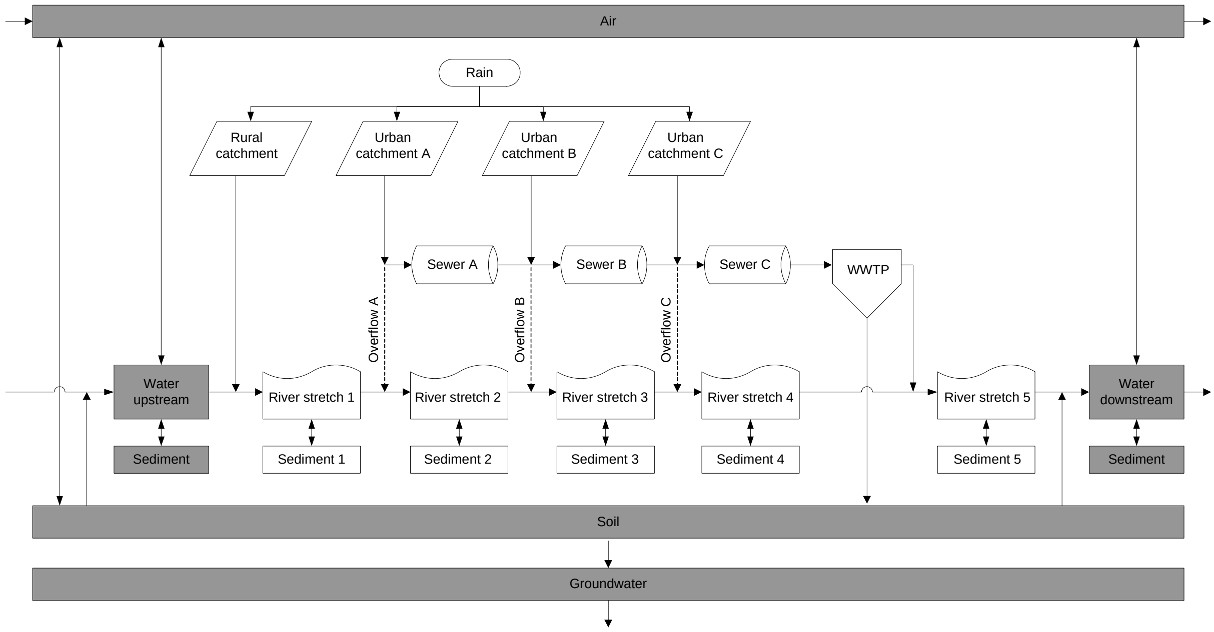

Figure 1. Schematic representation of the integrated environmental model (IUWS model (white blocks) and MFTM (grey blocks))

Integrated environmental model

Using the two submodels discussed above, an integrated IUWS/MFTM model was set up. The characteristics of the two models can be found in De Keyser *et al.* (2008). In the reference scenario, the following links between both models were 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 was 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) was simulated, with volatilization and infiltration processes occuring (Figure 2). Wet and dry deposition as well as diffusion are considered as exchange processes between the compartments air and soil in the multimedia model, but similar links between the air and the urban catchments were neglected because the surface area of the urban catchments causes the fluxes to be a factor 1000 smaller than the assumed emissions onto the urban surface.

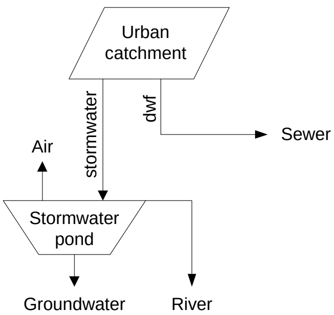

Figure 2. Addition of storm water infiltration ponds to the previously modelled setup

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

The parameter values were 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, the chemical's presence in the environment is of growing concern. Cousins and Mackay (2003) assume EU production and consumption tonnages of 595,000 and 476,000 tons of DEHP per year respectively. They use emission factors of 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, based on Parkerton and Konkel (2001). Emission estimates were converted to a *per capita* basis and scaled to the size of the case study. Urban emissions to water were assumed to go to wastewater, whereas emissions to soil were supposed to accumulate on the urban surface and to be washed off with runoff.

Table 2. Key parameters of the micropollutant DEHP used in the case study (European Commission, 2008; Lützhøft *et al.*, 2008)

Parameter	Unit	Value
Molecular weight	$g \cdot mole^{-1}$	390.54
Vapor pressure	Pa	3.4E-5
Henry constant	$Pa \cdot m^3 \cdot mole^{-1}$	4.43
Water solubility	$\mu g \cdot l^{-1}$	3.0
K_{OC}	$l \cdot kg^{-1}$	1E5
K_d	$l \cdot kg^{-1}$	1.5E4
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	3000
Adsorption rate constant	$m^3 \cdot d^{-1} \cdot g_{solids}^{-1}$	0.1
Background concentration in air entering the system	$ng \cdot m^{-3}$	10
Background concentration in water entering the system	$\mu g \cdot l^{-3}$	0.10

RESULTS AND DISCUSSION

Initialization

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

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. On the other hand, the figure also shows that the stormwater infiltration ponds reallocate the DEHP flows to groundwater and air. The increased air concentrations are transient due to photochemical breakdown and advective transport out of the modelled 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 with measured concentrations reported in the literature, which are for urban areas usually below or around one $\mu g \cdot l^{-1}$ (European Commission, 2008). Further research will reveal to what extent such simplified model setup can be tuned to yield more realistic environmental concentrations.

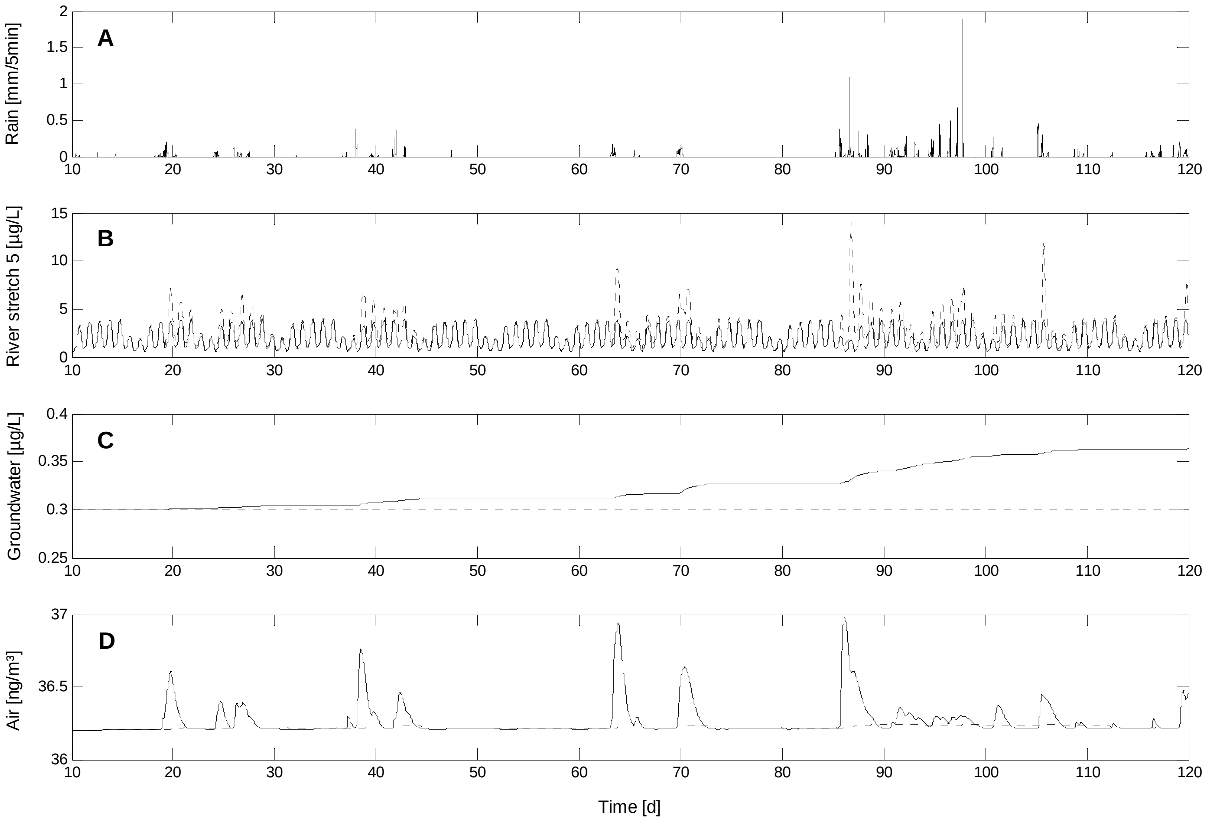

Figure 3. Input rainfall series (A) and simulated DEHP concentration in the two modelled scenarios (basic scenario in dotted line, scenario with the stormwater infiltration ponds in solid line) in the last river stretch of the IUWS model (B), in the groundwater compartment of the MFTM (C) and in the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

Figure 4 shows an overview of all mean DEHP mass fluxes, removal rates and concentrations in the modelled system, but with the IUWS represented as one compartment. The averages are calculated with data obtained from 120 days of dynamic simulation with a 15 minute output interval. Note that 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 that mass fluxes towards downstream water and soil have decreased, while DEHP fluxes to the groundwater and the air compartment have increased. The latter may in this example not have a vast impact, but without the MFTM shell around the IUWS model, this effect could not have been assessed at all.

Two aspects to take into account in future studies to increase the confidence in the interpretation of simulation results are uncertainty and time scales. The uncertainty of the simulated environmental micropollutant concentrations in multimedia models can be several orders of magnitude (Hennes and 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 studies have been conducted so far on the whole IUWS. This topic deserves further attention in order to make integrated environmental assessment based on IUWS/MFTM coupled models more reliable.

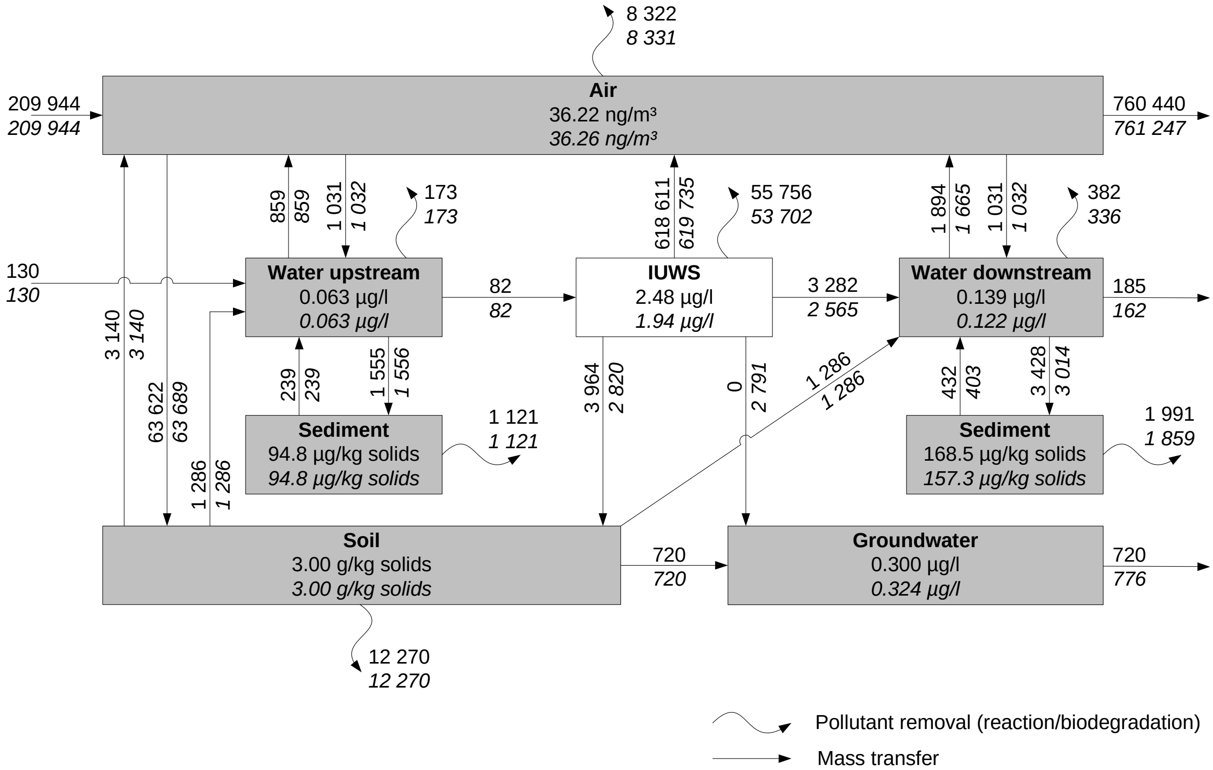

Figure 4. Mean DEHP mass fluxes (in g·d^{-1}) and concentrations in the modelled system: reference scenario (normal typeface) and after the implementation of stormwater infiltration ponds (italic typeface); values in the IUWS block are concentrations in the receiving water after mixing, i.e. at the outflow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

The second important factor in studies conducted with coupled IUWS/MFTM systems is the huge range of time constants. Processes in the IUWS 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 has an influence on the conclusions and, in case, whether there are better alternatives then a calculated steady-state.

CONCLUSIONS

The combination of integrated urban water system (IUWS) models with multimedia fate and transport models (MFTM) can either be done by creating 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. The added value of wrapping a MTFM around an IUWS model is twofold: (1) the multimedia model provides boundary conditions to the IUWS, and (2) it allows to make a holistic assessment of the overall environmental status of the modelled system, beyond urban surface water quality. A combined MFTM/IUWS model was 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 was shown to be that mass fluxes towards downstream water and soil have decreased, while fluxes to the groundwater and the air compartment have increased.

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