Dynamic Transport and Fate Models for Micro-pollutants in Integrated Urban Wastewater Systems

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ABSTRACT

The modelling of urban water quality (i.e. wastewater, stormwater) is a growing issue in water management. New regulations stress the importance of estimating the loads and the fate of micro-pollutants (MPs) in the urban water cycle. The models available to simulate the transport and removal of "traditional" pollutants such as overall organic pollution, nutrients and suspended solids in the different components of the urban water system (i.e. sewer network, stormwater treatment units, wastewater treatment plant, receiving waters) were extended with processes affecting the fate of MPs (i.e. physical, chemical and biological) depending on the compound's inherent properties. This paper describes the modelling approach and some possible applications of these unit process models including their combination to simulate urban water systems by means of three examples, developed within the EU project SCOREPP.

KEYWORDS: Integrated water quality modelling, priority pollutants, environmental quality standards

INTRODUCTION

The overall aim of the SCOREPP project (www.scorepp.eu) is to develop comprehensive and appropriate source control strategies that authorities, cities, water utilities and chemical industry can employ to reduce emissions of micro-pollutants (MPs) from urban areas into the receiving water environment. The SCOREPP project focuses on the 33 priority substances (PSs) and substance groups identified in the Water Framework Directive (WFD), and specifically on those defined as priority hazardous substances (PHSs) (European Commission, 2000, 2008a, which need to be phased out of discharges within a short time range (Mikkelsen et al., 2008; Eriksson et al., 2009).

The scientific objectives of the SCOREPP project are to identify the sources of micro-pollutants (MPs) in urban areas, to identify and assess appropriate strategies for limiting the release of MPs from urban sources and for treating wastewater and stormwater containing MPs on a variety of spatial scales. Furthermore, the aim is to develop GIS-based spatial decision support tools for identification of appropriate emission control measures, to develop integrated dynamic urban scale source-and-flux models that can be used to assess the effect of source control options on MP emissions and to optimise monitoring programmes, and to assess the direct and indirect costs, the cost-effectiveness and the wider societal implications of source control strategies. The developed approaches, models and assessments are used to formulate a set of appropriate MP emission reducing strategies, and a multi-criteria approach is used to compare and evaluate these strategies in relation to their economic, societal and environmental impacts.

In this context, integrated, dynamic urban scale source-and-flux models were developed. The models are used for quantifying the release of MPs from urban sources and the fate of MPs within different treatment systems. These models – which can be linked to simple, river basin scale multimedia models used in ecological risk assessment – enable "what-if" scenarios to assess the effect of emission barriers as well as to evaluate their potential in enabling monitoring systems and sampling programmes to be optimised. An integrated, dynamic model is able to predict the dynamic fate of MPs and therefore it assesses the compliance with Environmental Quality Standards (EQS, annual averages and peak concentrations). Although the integrated, dynamic model is general for application to several types of chemical pollutants, focus is given to fate processes specific for MPs.

In this article, the integrated urban wastewater system (IUWS) and its unit processes are first introduced. Then, the MP fate modelling approach is described and three cases are presented to show possible applications of the developed model library.

METHODOLOGY

The Integrated Urban Wastewater System

The elements and the boundaries of the urban system that are included in the IUWS model are sketched in Figure 1. The fate models used to represent the IUWS components can be subdivided into two families, according to the influence of human activities:

- *"Technosphere" fate models:* include anthropogenic systems, which are built and managed with specific objectives by humans living in the urban area. For example, a sewer network is built and managed to route stormwater and wastewater out of the urban area.
- *"Environmental" fate models:* are used to simulate systems where natural processes are the driving force. Human activities can affect the behaviour of these systems, but cannot have a complete control of all the processes and reactions. An example is the river model.

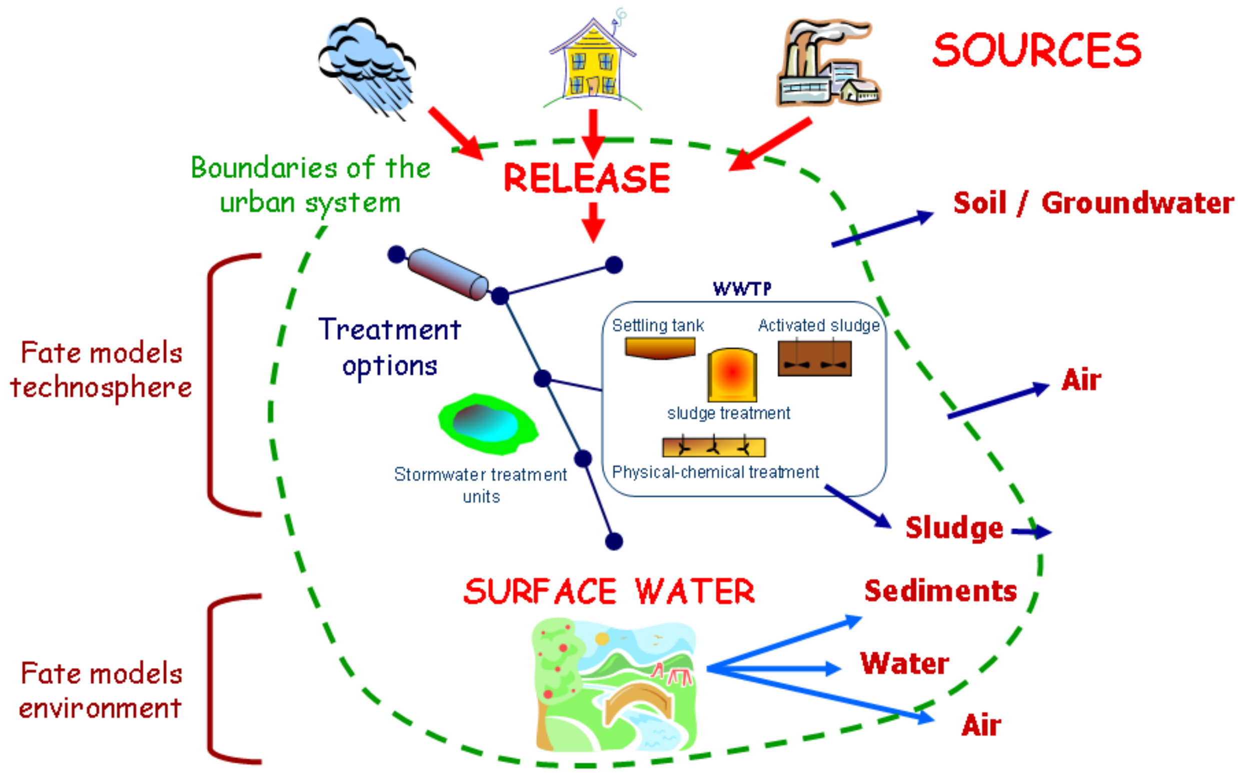

Figure 1. Schematic representation of the IUWS elements and boundaries.

Several components can be identified within the borders of the IUWS model:

- *Sources:* water and pollutants flows are generated by point and diffuse sources across the catchment. This element is not included within the IUWS borders, but it is a *sine qua non* of the IUWS model. In fact, pollutant and water fluxes are estimated by a specifically developed application (De Keyser *et al.*, 2008a, 2009a) and the resulting emission (or release) time series for the different sub-catchments are used as input to the IUWS model.
- *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 by overflow structures.
- *Stormwater treatment systems:* flows from stormwater separated systems are treated before eventual discharge to the receiving surface or ground-waters.
- *Wastewater treatment systems:* several physical, chemical and biological treatments and their combinations are used to treat wastewater (e.g. domestic, from combined systems, industrial, etc).
- *Sludge treatment systems:* the residues from wastewater treatment are treated before the final disposal.
- *Receiving water:* natural waters (e.g. rivers, lakes) are the final recipients of the water flows from urban areas. The objective of the entire MP reduction strategy is the fulfillment of the quality requirements for this component of the IUWS.

Generating Input for the IUWS Model

The need for a structured and quantitative description of emission sources and patterns led to the construction of a database with emission strings (Lützhøft *et al.,* 2009). Each emission string characterises a priority pollutant emission source, together with a default temporal release pattern. A database of typical daily, weekly and yearly release patterns was set up to support the emission string concept.

A stand alone application was built to generate emission time series according to the specified release patterns, based on phenomenological modelling of an unlimited number of emission generating events and allowing the incorporation of stochasticity. This tool is applicable to MPs, traditional pollutants (COD, etc.) and wastewater flow rates, and its inputs can be provided by the emission strings database or by manually entering the information (De Keyser *et al.*, 2008a, 2009a).

The Modelling and Simulation Platform

To illustrate the concepts of IUWS modelling, the models need to be linked. This could either be achieved by interfacing existing stand-alone models (software) or by merging the models within a single software application. As some components of the IUWS model (see below) were already available in the WEST® modelling and simulation platform (MOSTforWATER, Kortrijk, Belgium), it was decided to implement all models in WEST®.

The IUWS models have simplified hydraulics (tanks in series), but a high level of complexity for water quality including most of the physical, chemical and biological processes acting on organic pollution, nutrients and micropollutants.

Modelling of Micro Pollutants Removal Processes in the IUWS

Several models were already available to simulate the removal of compounds in the different components of the urban water system (i.e. sewer network, stormwater treatment units, wastewater treatment plant, receiving waters). However, these models are mainly focusing on the removal of traditional pollutants such as overall organic matter, nutrients and suspended solids. The removal of specific organic compounds requires the consideration of more complex processes (i.e. physical, chemical and biological), depending on the compound's inherent properties. To be able to simultaneously simulate the fate of these pollutants and the traditional pollutants in the different components of the urban water system, existing models need to be extended with a pollutant fate sub-model.

The KOSIM hydrological catchment runoff and sewer transport model (ITWH, 2000), the IWA activated sludge models (Henze *et al.,* 2000), the Universal Stormwater Treatment Model (Wong *et al.,* 2006), and the river water quality model no.1 (RWQM1) by Reichert *et al.* (2001), were chosen as basic water quality models. They are extended with pollutant fate sub-models to predict the behaviour of micropollutants in sewer systems, wastewater treatment plants, stormwater treatment systems and receiving waters, respectively.

The selection of the equations used to model MPs was based on simple principles:

- *Process relevance:* the different MP removal processes are included in the unit models only if the process is relevant, i.e. 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 in the different elements of the IUWS have been preferred, in order to provide a common structure across the integrated model. Different formulations and/or conceptual models have been utilized whenever the characteristics of the unit required peculiar features (e.g. settling in sewer pipes, different components in the river, etc.).
- *Data availability:* the processes are modelled according to the parameters that can be retrieved from the SCOREPP database (Lützhøft *et al.,* 2008). For example, (pseudo) first-order kinetics have been preferred whenever process half-lives are available in the database. Table 2 shows the relevant parameters that are used in the mathematical formulation of the MP removal processes.

Table 1. Relevant MP removal processes in the various units of the IUWS.

Processes \ **Unit**	Sewer	Stormwater treatment (water)	Stormwater treatment (sediment)	Primary settling	Activated sludge tank	Secondary settling	Sludge thickener	Sludge anaerobic digester	Sludge dewatering	River (water)	River (sediment)
Physical processes											
Sedimentation	+	+		+		+	+			+	
Resuspension	+		+								+
Volatilization	+	+		+	+	+	+	+	+	+	
Physico-chemical											
Sorption-desorption	+	+	+	+	+	+	+	+		+	+
Hydrolysis	+	+	+	+	+	+	+			+	
Photolysis		+			+					+	
Biological											
Aerobic biodegradation	+	+	+	+	+	+	+			+	+
Anoxic biodegradation	+	+	+	+	+	+	+	+		+	+

Partition of the simulated MP is included in the model by using two component species: dissolved (S_{MP}) and particulate (X_{MP}). The majority of fate processes are assumed to affect only the dissolved species. Only sorption and desorption processes affect the particulate species. The *pKa* 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 is reported as total concentration, 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.

Table 2. MP removal processes and relevant parameters.

Process	Parameter retrieved from MP database*	Other relevant parameters
Physical processes		
Sedimentation and resuspension	-	Water depth, bottom shear stress, critical shear stress, erodibility constant
Volatilization	Henry's law constant, molecular weight	Water depth, wind speed, water currents and temperature
Physico-chemical		
Adsorption-desorption	Partition coefficient (k_d or k_{OC})	TSS concentration, organic fraction
Hydrolysis	First-order degradation rate	pH, temperature
Photolysis	Half-life	Light intensity, water depth, water pollution
Biological		
Aerobic biodegradation	Half-life	Oxygen concentration, temperature
Anoxic biodegradation	Half-life	Oxygen/nitrate concentration, temperature

** see Lützhøft et al. (2008)*

Multimedia Model

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. 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 heterogeneity 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.

In WEST®, a multimedia fate and transport model (MFTM) is "wrapped around" a dynamic IUWS model for organic micropollutants to enable integrated environmental assessment (Figure 2) (De Keyser *et al.*, 2009b). 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). The WEST® implementation of SimpleBox (De Keyser *et al.*, 2008b) is slightly different from the original SimpleBox: the vegetation compartment was omitted and the soil and water compartments were implemented as generic soil and water models, which can be fine tuned 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.

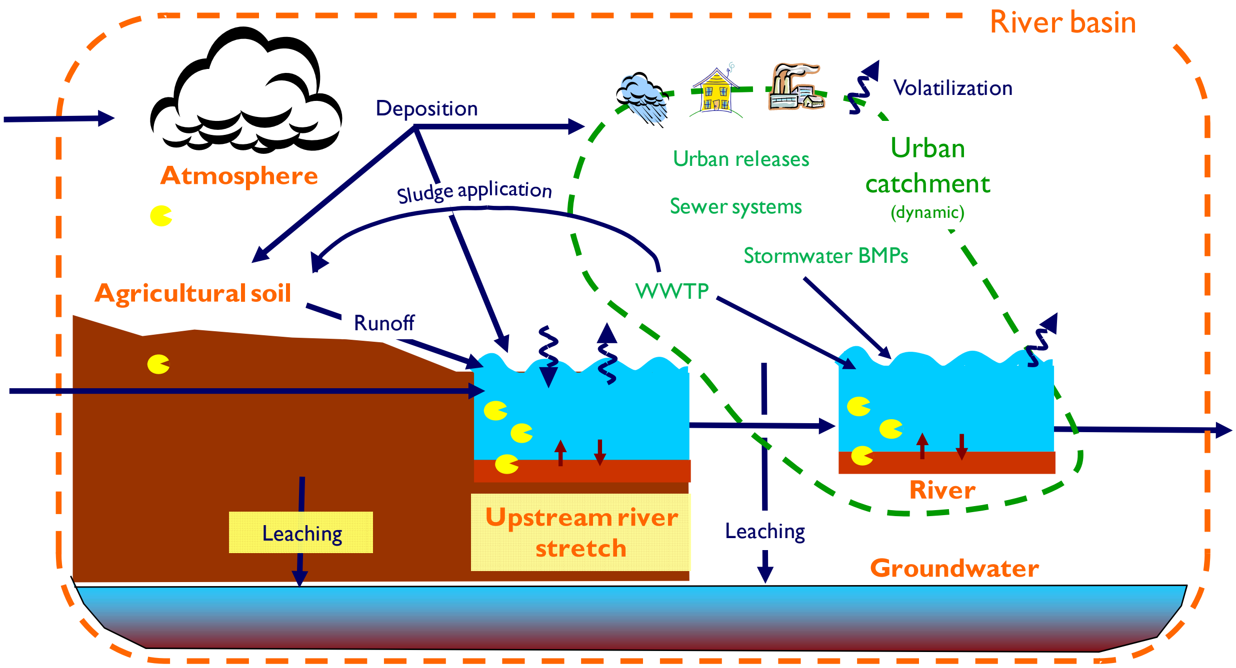

Figure 2. Components of the implemented multimedia model and links with the IUWS model.

EXAMPLES

Modelling Removal of Micropollutants in Stormwater Treatment Systems

The water quality modelling of stormwater treatment facilities is a growing issue in urban water management. An important number of MPs are found in stormwater (e.g. Eriksson et al., 2007; Lützhøft et al., 2008) and the discharge of urban runoff can represent a relevant contamination path for substances with stormwater-related sources (e.g. traffic, roof corrosion, etc.). The need for reducing the impacts of stormwater pollutants on the receiving waters and the removal of MPs stresses the importance of predicting the removal efficiency of stormwater treatment options.

To address these needs, a new model for simulating the MP fate in stormwater treatment options (also called structural Best Management Practices – BMPs) was developed. As part of the IUWS model, the development of this model followed the approach described earlier (i.e. focus on process relevance, data availability and common mathematical formulation). Also, the model structure should be flexible enough to simulate a wide range of BMP facilities.

Given the general lack of data regarding MPs in stormwater systems, the assessment of the BMP removal potential should be based on the inherent properties of the pollutant and the processes potentially occurring in a treatment system: it can be expected that some BMPs are more suitable for removing MPs from the water phase than others (Scholes *et al.*, 2008). Several models are available to simulate the removal of pollutants in BMPs. Various approaches and equations are applied to describe the pollutant removal processes, with different levels of complexity. As for the other elements of the IUWS , present models mainly focus on the removal of "traditional" pollutants such as overall organic matter measured as COD or BOD, total suspended solids (TSS), nutrients, as well as some heavy metals (for a review see e.g. Huber *et al.*, 2006). Also, the removal processes are usually lumped into a generic removal rate and only the most relevant are included (e.g. settling).

The developed model reuses the knowledge from existing models for traditional pollutants and expands them with MPs fate processes. The fate processes equations used in the model are common to other IUWS units: the stormwater unit is usually connected to the sewer units, so the modelled pollutants coincide in those two components of the IUWS model.

The model is characterized by a series of completely stirred tank reactors (CSTRs). Each tank is subdivided into two compartments (water and sediment), which interact as shown in Figure 3. This approach is an expansion of the Universal Stormwater Treatment model presented by Wong *et al.* (2006).

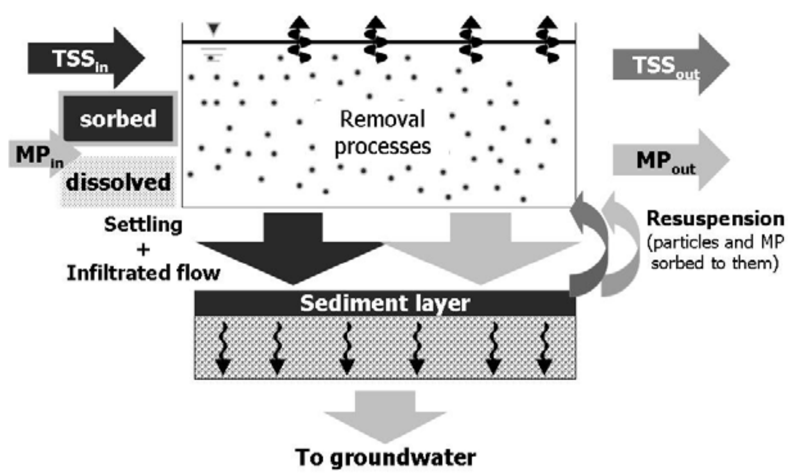

Figure 3. Conceptual scheme of a two-compartment tank.

The water compartment is assumed to be aerobic, while the bottom unit is assumed to be in anaerobic conditions. Additionally to other components of the IUWS model, photolysis is implemented in the water phase (see Table 1). Annual and diurnal variations of photolysis rate are modelled by using a sinusoidal function. The model can also simulate the fate of other "traditional" water quality components (TSS, COD, nitrogen, phosphorus) by using the *k-C** approach presented in Wong *et al.* (2006). The *k-C** approach is also implemented in the extension of the sewer components (based on the KOSIM model).

The model was tested by simulating a stormwater treatment pond in Lilla Essingen, Stockholm (Sweden). The pond is part of a treatment train used to treat highway runoff before filtering and discharge to a receiving water body. Flow and quality measurement used here were taken in the period between March and September 2004. The pond has a permanent volume of ca. 150 m^3, a maximum volume of 200 m^3, with an emptying time needed to restore dry-period conditions of about 69 h (for a more detailed description see Stockholm Vatten, 2006). The pond model was set to obtain a hydraulic efficiency value similar to the value estimated by Jansons et al. (2005) for a similar pond layout. This was obtained by using a model configuration with eight serial tanks.

The model was used to simulate the fate of a heavy metal (Cu) in the pond. Settling was assumed to be the only relevant removal process affecting heavy metals in the system, thus the main parameters used to predict their fate were the settling velocity v_{sed} and the solid-water partition coefficient k_d. Various ranges were found in literature for the fate process parameters (see Table 3). To assess the influence of these variations, both for the single parameters and for combinations thereof, the model was run by sampling several parameter sets from the ranges listed in Table 3. The remaining parameters were optimized by sampling from default parameter distributions.

Table 3. Parameter ranges used to simulate micropollutants fate.

Parameter	Unit	Parameter range	Source
$k_{d,Cu}$	l/kg	$5 \cdot 10^3 - 1 \cdot 10^5$	Shafer *et al.* (2004)
v_{sed}	m/d	17 – 2600	Bentzen *et al.* (2005)

Selected examples from the simulation results for heavy metals are shown in Figure 4. The graph shows that prediction of particulate metal fluxes was mostly affected by the settling process, while sorption/desorption was the major driver for the prediction of dissolved metals fluxes. A peak in particulate Cu may be due to poor settling conditions or resuspension of sediments. Despite the selected parameters ranged by several orders of magnitude, the predicted mass fluxes and concentrations ranged in only a ±50% interval. Similarly, the estimated removal efficiency for heavy metals varied by ±10% for Cu when varying k_d, while minor variations (around 5%) were obtained by varying v_{sed}. The variability in the estimated removal of heavy metals decreased with the increase of the k_d value and it stabilized for a k_d value higher than 10^4. These results confirm that settling is the major removal process for compounds with high sorbent properties and sorption/desorption processes play a minor role.

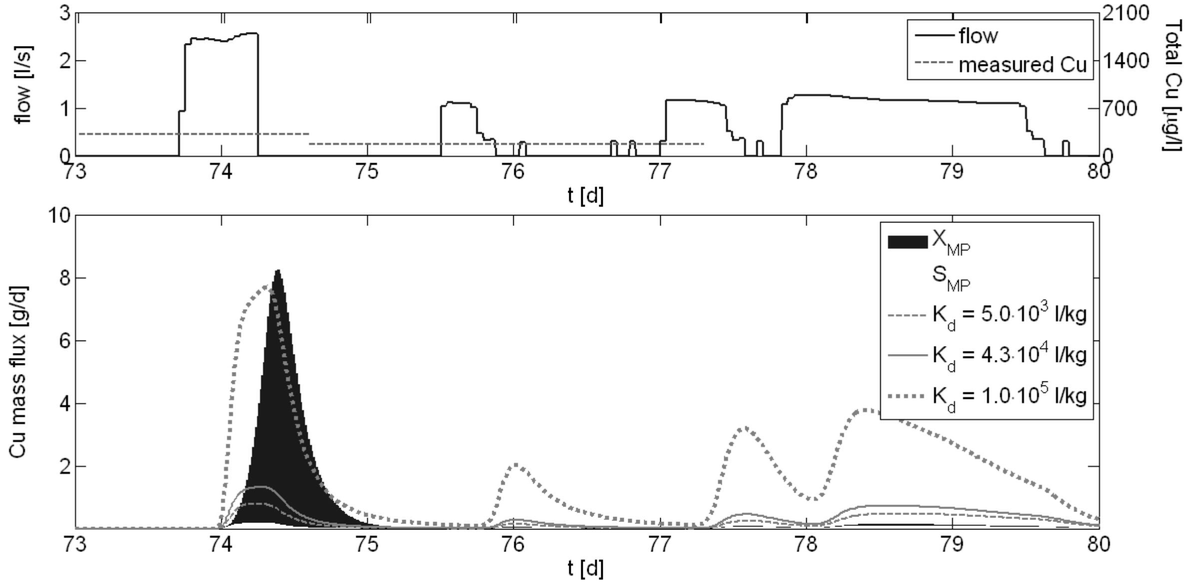

Figure 4. Variation in dissolved Cu fluxes for different solid/water partition coefficients (k_d) and corresponding prediction intervals for particulate Cu (black area).

The material presented here represents the initial experiences with the model. Further investigations will lead to insight into the significance of the modelled processes to the fate of a wide range of micropollutants with highly differing properties, which are potentially found in stormwater runoff (e.g. Eriksson *et al.,* 2007; Lützhøft *et al.,* 2008). More details on this study can be found in Vezzaro *et al.* (2009).

Evaluating Compliance with Environmental Quality Standards in Rivers

The objective of this example is to evaluate the added value of dynamic pollutant fate models for implementing the WFD. The selected model is a simplified version of the River Water Quality Model No. 1 (RWQM1), incorporating the environmental fate of organic pollutants. Two realistic scenarios are designed and described in the following section. They comprise a combination of two rivers, representative for Western Europe, and one chemical. For each scenario, the model predictions and the compiled monitoring data are compared with the Maximum Allowed Concentration (MAC) and Annual Average (AA) Environmental Quality Standards (EQS) values.

For the design of two scenarios, one chemical and two Belgian rivers were selected. Hereby, attention was paid to select rivers that are representative for Western Europe in order to support conclusions relevant for all rivers in this part of Europe. The studied chemical is nonylphenol (NP), which is solely used in the industry, and it is in the WFD priority list.

As river stretches, parts of the Zenne and the Demer, with discharge points situated in the Belgian cities Eppegem and Kermt, respectively, were chosen. In the scenario set-up, it was decided to disregard the presence of wastewater treatment plants (WWTPs), sewer overflows, etc. downstream from the discharge point. Only direct discharge of the chemicals is considered. If dynamic models prove to be useful in this set-up, they will be even more useful when including the aforementioned components, since each of them will add more dynamics on top of the direct discharge pattern. Thus, our set-up can be considered as a worst-case for evaluating the added value of dynamic models.

NP is classified as a PHS, which means that emissions of this substance in the aquatic environment should be phased out by the year 2015. The studied industrial site produces NP 287 days per year by continuous methods, the rest of the year there is no production. In Figure 5, the predicted NP concentrations at the edge of the mixing zone (assumed to be five times the mean river width) in the small and medium-size river stretches are shown for 1 year. Furthermore, the monthly measured concentrations and the MAC–EQS, set at 2μg/L (European Commission, 2008a), are plotted.

Figure 5 shows that the maximum simulated NP concentrations in the small river (scenario 1) and medium-size river stretches (scenario 2) do not exceed the MAC–EQS. The same conclusion is drawn when comparing the highest measured concentrations with the MAC–EQS. However, there are sufficient degrees of freedom in the scenario design to find borderline cases where monitoring would give a different outcome. First, assume that the MAC–EQS for a more toxic priority substance would be set at 0.8μg/L (scenarios 1,2a).

As can be seen from Figure 5, all twelve measured concentrations in the small river stretch are lower than this critical value, although simulation illustrates the exceedance of this value at some days. Secondly, assume that an NP-producing industry releases over 287 d three times more of this substance to wastewater than the selected industrial site during the same period (scenarios 1,2b). This wastewater is also directly discharged into the two river stretches at the same discharge points.

The simulation results and the monitoring data are represented in Figure 6 for 1 year. This figure shows that the predicted NP concentration in the small river stretch exceeds the MAC–EQS on several days, in contrast to the monitoring data. Other degrees of freedom include effluent discharge rate, production method, number of working days, etc.

These two cases clearly illustrate the added value of dynamic tools. Currently, the WFD requires that Member States classify their water bodies using monitoring data. As shown in the above examples, measurements can lead to misclassification of water bodies. If a water body is erroneously qualified to have a “good” chemical quality status, no measures would be taken although aquatic organisms experience acute effects. Beyond and at the edge of the mixing zone, the substance should also comply with the AA–EQS on the average of 1 year. The NP concentration which is expected to protect the aquatic organisms against long-term chronic effects is set by the European Commission (2008a) at 0.3μg/L.

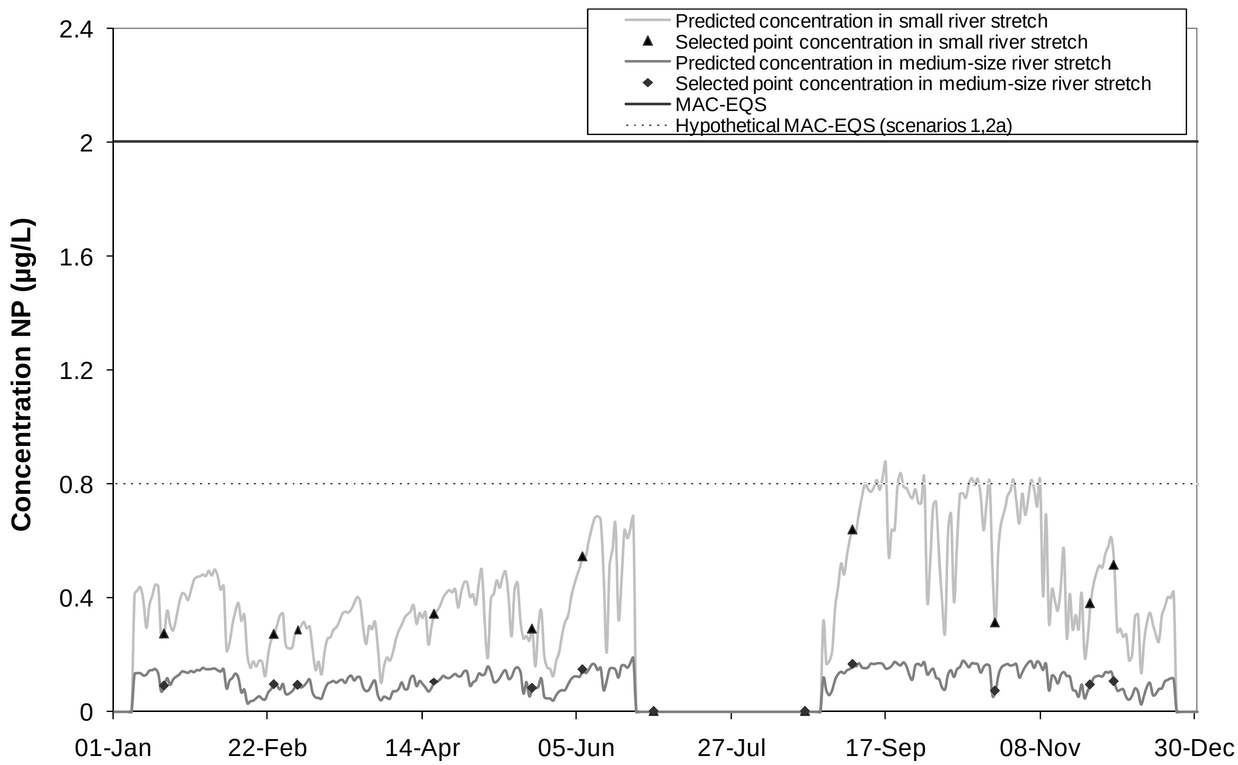

Figure 5. Predicted and selected point concentrations of nonylphenol at the edge of the mixing zone in the small and medium-size river stretches, together with the MAC–EQS and the hypothetical MAC–EQS assumed in scenarios 1,2a (for 1 year).

In Figure 7, the yearly predicted concentrations in both river stretches, together with the annual average measured concentrations and the AA–EQS are represented. As can be seen from Figure 7, the annual average measured NP concentration in the small river stretch 0.32µg/L exceeds the AA–EQS, while for the medium-size river stretch the average value is below the critical limit. It can also be observed from this figure that the predicted NP concentration profile for the small river stretch often exceeds the AA–EQS. Short-term exceedances of the AA–EQS do not result in adverse acute effects since these exceedances remain below the MAC–EQS. However, there are also long-term exceedances that could result in adverse chronic effects. For example, in September–early October, the AA–EQS value is exceeded for a period of 37 d, which is larger than the exposure period used in invertebrate ecotoxicity testing, e.g. 21-days off-spring surviving for Daphnia magna (Comber *et al.,* 1993).

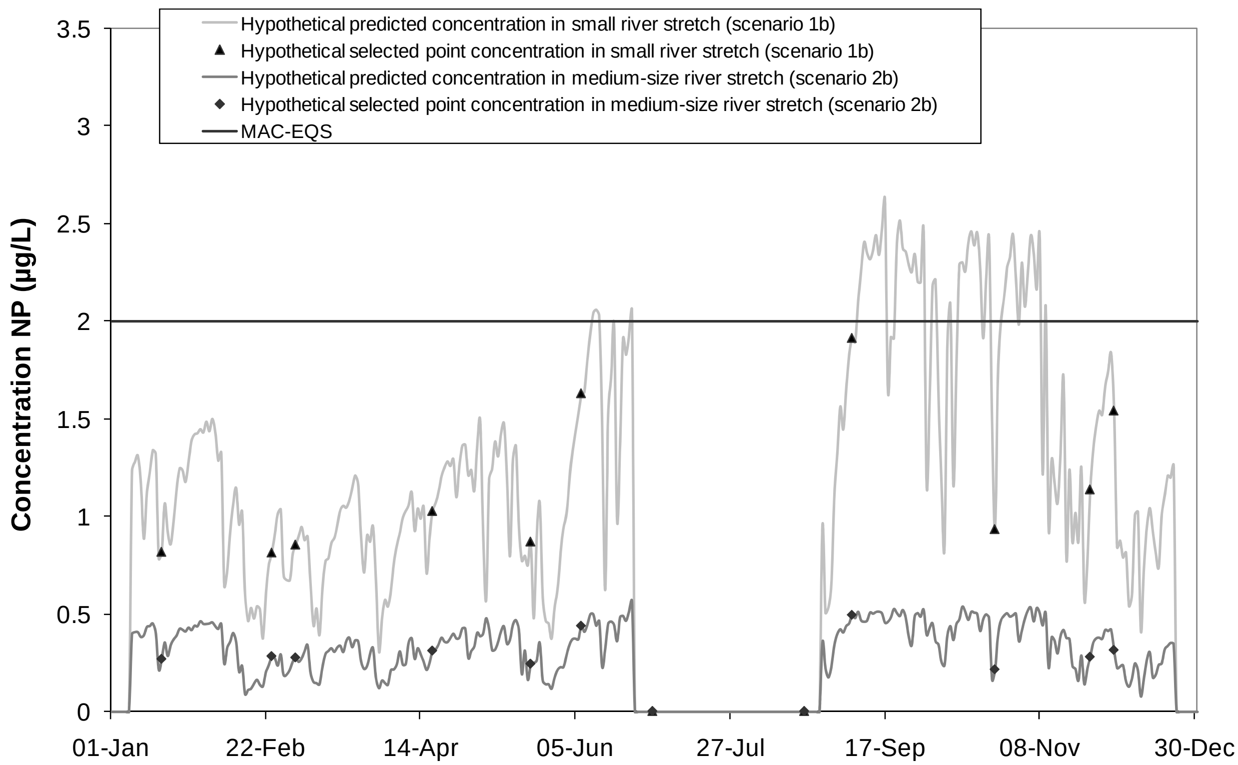

Figure 6. Hypothetical predicted and selected point concentrations of nonylphenol at the edge of the mixing zone in the small (scenario 1b) and medium-size river stretches (scenario 2b), together with the MAC–EQS (for 1year).

For the medium-size river stretch, the model predictions do not exceed the critical value of 0.3µg/L. In conclusion, both procedures, i.e. monitoring and dynamic modelling, result in the same conclusion for both river stretches. One should note that the same discharge load can cause chronic effects to the aquatic organisms in small rivers and not in larger rivers, which have a higher dilution factor. This assessment could lead to situations in which the discharger could fully utilize the assimilative capacity of the water body up to the concentration values provided by the EQSs. However, one should also comply with the emission limit values, as imposed by the combined approach in the WFD. These have not been agreed on a European level, so it is up to the member states to define ELVs nationally. There are again sufficient degrees of freedom to find situations where monitoring and modelling would give opposite conclusions. Suppose that the AA–EQS for a less toxic substance is set at 0.4µg/L (scenarios 1,2c). The annual average measured concentration in the small river stretch would, in that case, be lower than the critical value, meaning that no chronic effects of aquatic organisms would be observed based on monthly monitoring. The model predictions, on the other hand, exceed the AA–EQS during a whole month, which could result in adverse chronic effects.

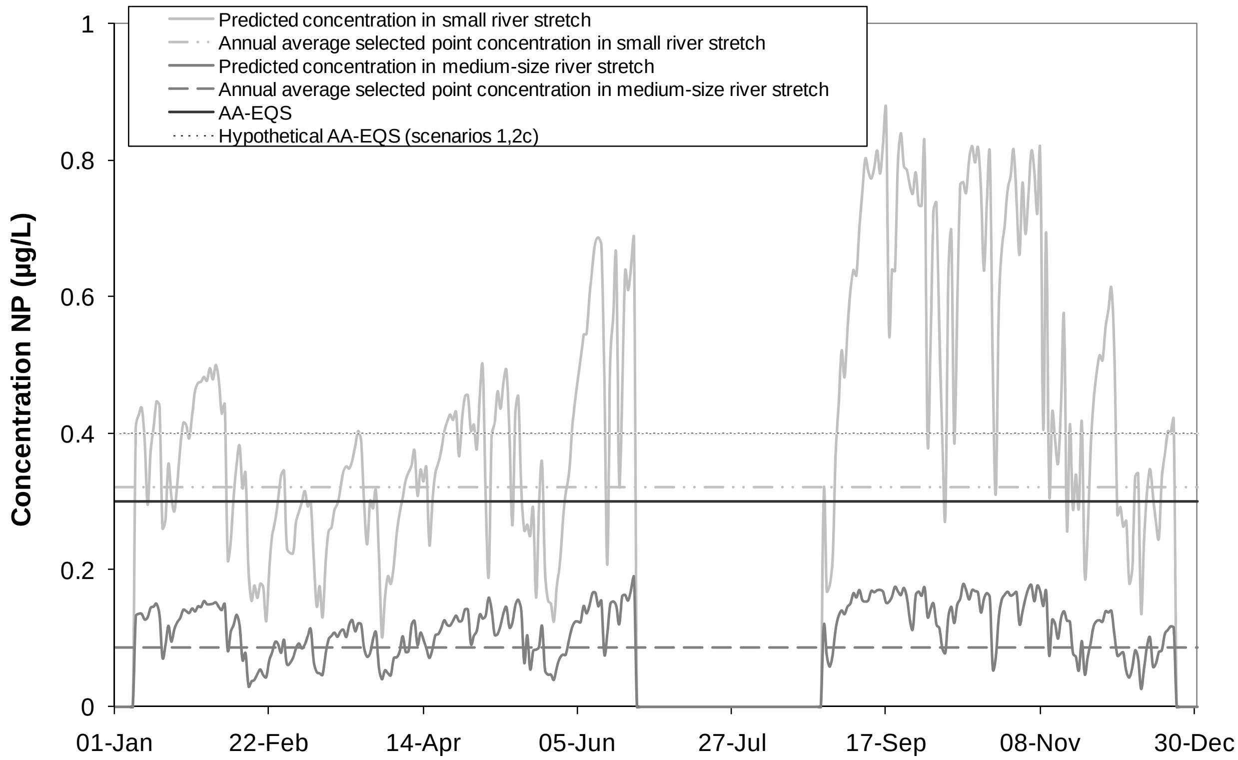

Figure 7. Predicted nonylphenol concentrations and the annual average selected point concentrations of nonylphenol at the edge of the mixing zone in the small and medium-size river stretches, together with the AA–EQS and the hypothetical AA–EQS assumed in scenarios 1,2c (for 1 year).

Integration of IUWS and MFTM Models

A schematic overview of the model setup for this example is given in Figure 8. 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.

The parameter values were adapted to simulate the fate of bis(2-ethylhexyl) phthalate (DEHP) in the integrated system (Table 4). Because of the high production volume and widespread use of DEHP, the chemical's presence in the environment is of growing concern.

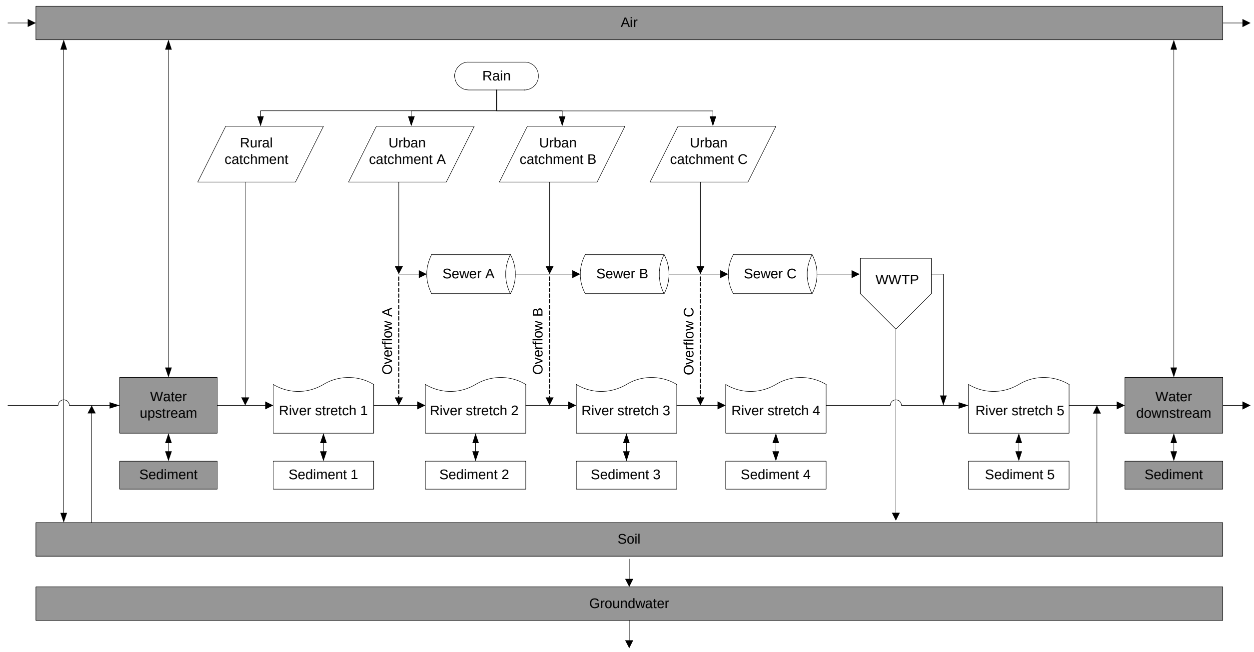

Figure 8. Schematic representation of the integrated environmental model (IUWS model (white blocks) and MFTM (grey blocks))

Table 4. Key parameters of the micropollutant DEHP used in the case study (European Commission, 2008b; 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

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.

In the reference scenario (Figure 8), 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. A combined sewer system was implemented with treatment in the WWTP before discharge into the surface water.

In the second scenario, with separate sewer system, the installation of stormwater infiltration ponds as best management practice (BMP) was simulated, with volatilization and infiltration processes occurring. Wet and dry deposition, as well as diffusion, is 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.

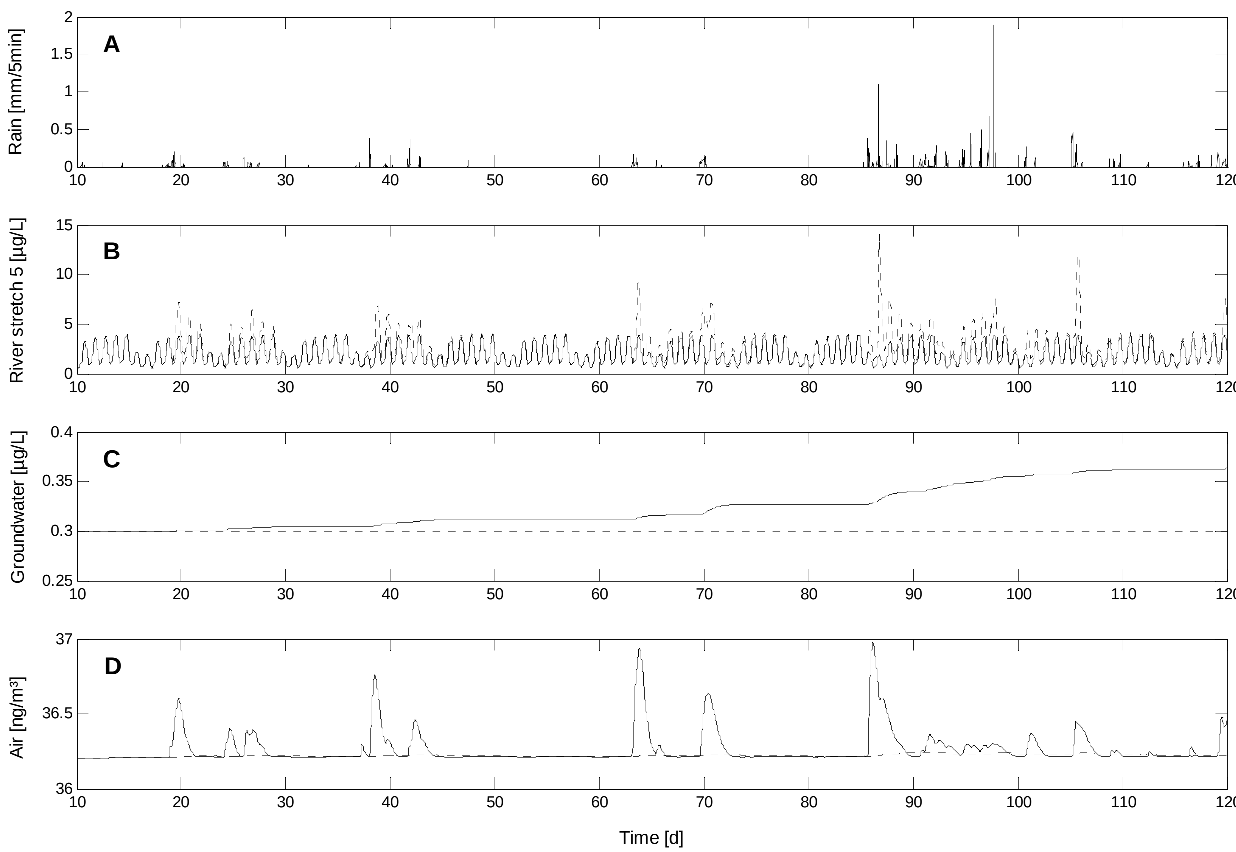

Figure 9. Input rainfall series (A) and simulated DEHP concentration in the two modelled scenarios (basic scenario in dotted line, scenario with the stormwater infiltration ponds in solid line) in the last river stretch of the IUWS model (B), in the groundwater compartment of the MFTM (C) and in the air compartment of the MFTM (D).

The dynamic simulation results shown in Figure 9 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 long term problems.

Figure 10 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. More details on this study can be found in De Keyser *et al.* (2009b).

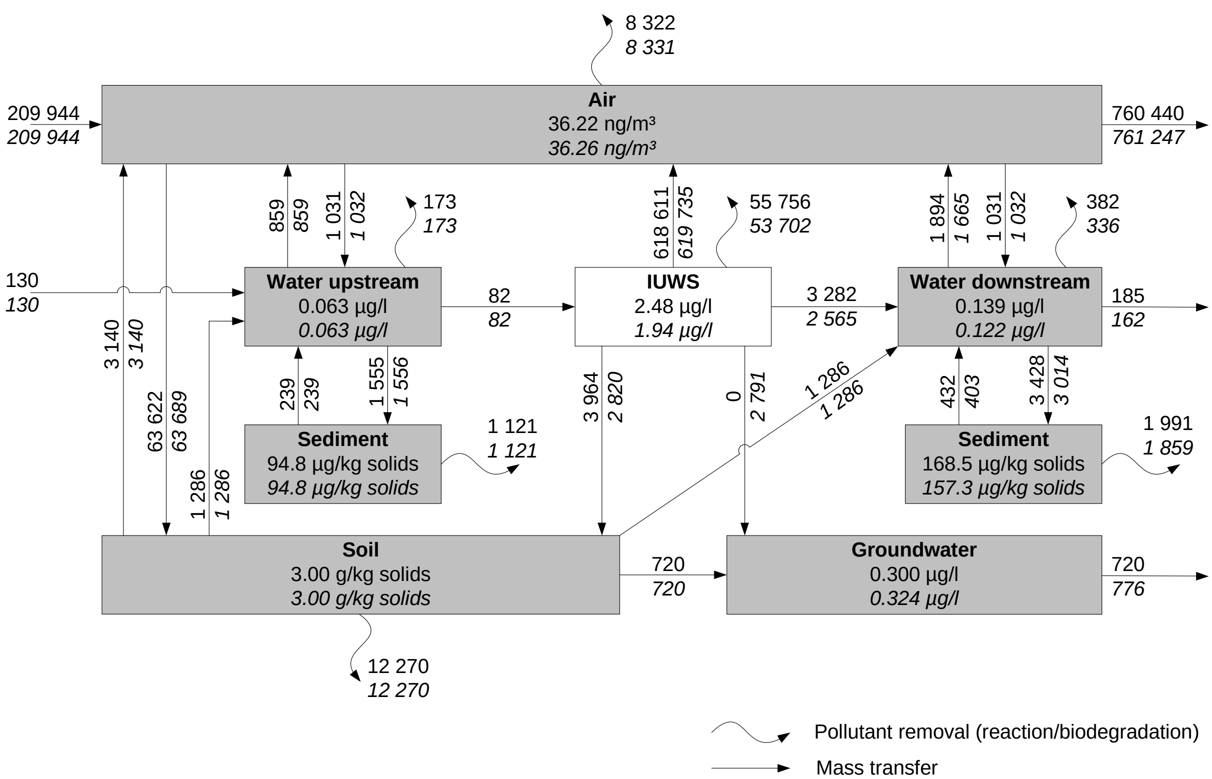

Figure 10. Mean DEHP mass fluxes (in g·d^{-1}) and concentrations in the modelled system: reference scenario (normal typeface) and after the implementation of stormwater infiltration ponds (italic typeface); values in the IUWS block are concentrations in the receiving water after mixing, i.e. at the outflow of river stretch 5.

CONCLUSIONS

Each of the models representing the different components of the urban wastewater system was extended with a pollutant fate sub-model to predict the behaviour of micro-pollutants next to “traditional” pollutants. These extended models are implemented in one simulation platform, WEST®, which is suitable for the modelling of complex dynamic systems and facilitates the connection of the different sub-models. This integrated model can be used to estimate the MP fluxes in the urban area, to assess EQS compliance in the receiving water and to predict the efficiency of different MP removal strategies. In this way, authorities, cities, water utilities and chemical industry can efficiently investigate and employ measures to reduce emissions of micro-pollutants (MPs) from urban areas into the receiving water environment. This was demonstrated by three different examples.

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