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Modelling the fate of micropollutants in the water cycle at urban and peri-urban scale – An integrated perspective towards the impacts of water reuse

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Abstract: An integrated model was developed, calibrated and validated to predict the fate of micropollutants (MPs) and the human health risks that these substances pose when wastewater is reused for agricultural purposes. Results showed that pharmaceuticals (e.g., the anti-inflammatory drug paracetamol) can form during in-sewer transit from other metabolites and posing a potential risk (Hazard Quotient for infants = 10^{-2}) if wastewater is not treated before irrigation. The model can represent a relevant decision-support tool to plan barriers for reducing the risk associated to MPs.

Keywords: emerging contaminants; water-energy-food nexus; heat pumps, plant uptake, integrated models

Introduction

Urban areas are major contributors to the discharge of organic micropollutants (MPs) in natural waters. The European Union aimed at reducing the occurrence of MPs by defining environmental quality standards and priority lists, and explicitly requiring integrated approaches. In this context, integrated models can represent valuable tools to predict MP fate across water systems and associated risks. This led to the development of an Integrated Urban Wastewater and Stormwater (IUWS_MP) model library for modelling MP fate in urban wastewater systems (Vezzaro et al., 2014)

Integrated models have mainly been used to evaluate the impacts of discharges from the storm- and wastewater system on the chemical status of different water compartments (e.g. De Keyser et al., 2010). However, there is currently a strong focus on increasing wastewater reuse for irrigation, creating new impact categories related to possible health risk from food crop consumption. Also, the energy sector is moving towards more distributed heat sources across urban areas (e.g., heat pumps using local groundwater reservoirs), introducing a new potential stress factor to the status of the water body. Finally, previously unexplored MP categories (e.g., pharmaceuticals), have been identified as new potential risk factors. Given the properties of these MPs, the existing fate models require to be extended with new processes.

In this study, an integrated model of a urban and peri-urban catchment was developed. The model included drainage system, wastewater treatment plant, receiving water stream, local energy production, and irrigated fields. The objectives of the study were to: (i) extend the IUWS_MP library to simulate new MP categories, (ii) evaluate the model performance against measurements for both conventional pollutants and MPs, and (iii) predict the environmental and human risk associated to MPs in current and future water (re)use practices (irrigation of food crops and heat-pump water use).

Material and Methods

The integrated model utilized an extension of the IUWS_MP model library (Vezzaro et al., 2014), taking into account MP deconjugation as well as the effect of MP ionization on their partitioning. The dynamic model was coupled with a plant-uptake model (Trapp, 2017) to assess health risk linked to consumption of food crops irrigated with reused water. The model was developed to simulate the fate of MP across a urban and peri-urban catchment (Figure 1) located in the north of Italy. The model included MP release sources, transport and transformation across the sewer network, removal in WWTP, and different discharge sources to the downstream canal (e.g. WWTP effluent, heat-pumps discharging contaminated groundwater). Finally, the water of the canal is reused for agricultural purpose, whereby different crops, with respective irrigation and harvesting patterns, were taken into account.

The model performance was evaluated against measurements of conventional pollutants (COD, TSS, N, P) and MPs (e.g. Castiglioni et al., 2018). These were collected at the inlet and outlet of the WWTP, and in the receiving water body. As described in Vezzaro et al. (2014), the IUWS_MP library relies on MP inherent properties, which can be found in public databases and literature. Model uncertainty bounds were estimated by applying a Monte-Carlo approach based on these parameter ranges.

The fate of a range of MPs was simulated (Table 1). Long term (≥ 1 year) management scenarios were considered in order to evaluate exposure concentrations across the integrated system (WWTP inlet and outlet, canal) and in different compartments (edible crop tissues). The estimated exposure was employed to calculate risk indicators for both the ecosystem and humans (expressed as Hazard Quotient–HQ).

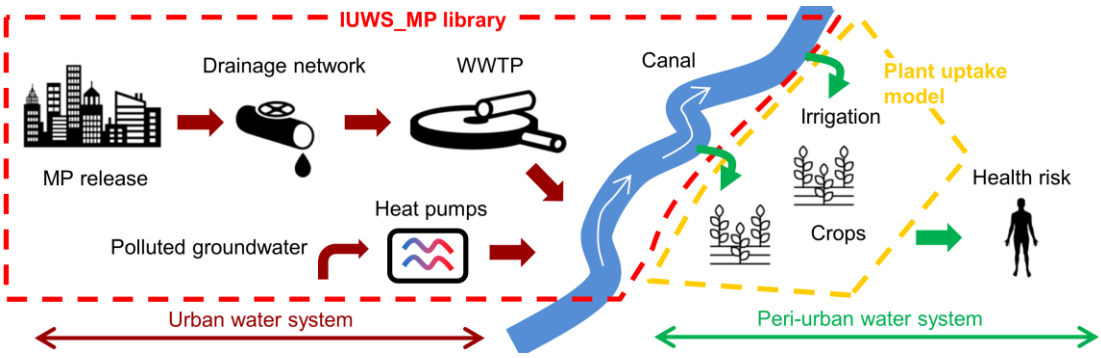

Figure 1 Conceptual scheme of the integrated model of the urban and peri-urban water system.

Table 1 List of simulated substances.

Category	Substances
Antibiotics	Clarithromycin, Sulfamethoxazole
Non-steroideal anti-inflammatory drugs	Diclofenac, Ibuprofen, Paracetamol
Anticonvulsants	Carbamazepine
Diuretics	Furosemide
Estrogens	17α-ethinylestradiol, 17β-estradiol, Estrone
Perfuorinated chemicals	Perfluorooctanoic acid, Peruorooctane sulfonate
Biocides	Triclosan

The management scenarios were defined to assess the effect of the existing infrastructure (e.g., presence of the WWTP), as well as possible future scenarios (e.g., installation of heat-pumps in areas with potential groundwater contamination).

Results and Discussion

The ability of the integrated model to dynamically simulate daily and seasonal variations of MP concentrations (diclofenac, triclosan) in the downstream river is exemplified in Figure 2. It can be seen that available measurements fall within the model uncertainty bounds.

Figure 3a shows the water concentrations of paracetamol predicted at different locations in the catchment. Along the integrated system, a consistent decrease (around three orders of magnitude) in paracetamol concentration was simulated, as a result of the high biodegradability of this pharmaceutical. Formation of paracetamol was predicted to occur during transport in sewers, following the deconjugation of other excreted metabolites.

Figure 3b shows the concentrations in rice (one of the crops considered in the model), and the corresponding health risk for two different water reuse scenarios, where irrigation is performed in the presence and in the absence of the WWTP (i.e., by using untreated wastewater). Following irrigation and uptake in crops, the predicted concentration of paracetamol in rice grains at harvest was 0.01 ng/g_{dw}, resulting in negligible risk for the most vulnerable indicator (infants). If untreated wastewater is used for irrigation, a 10^4-fold increase in the predicted HQ was shown, indicating a substantially higher chance of exceeding the safety threshold of 0.1.

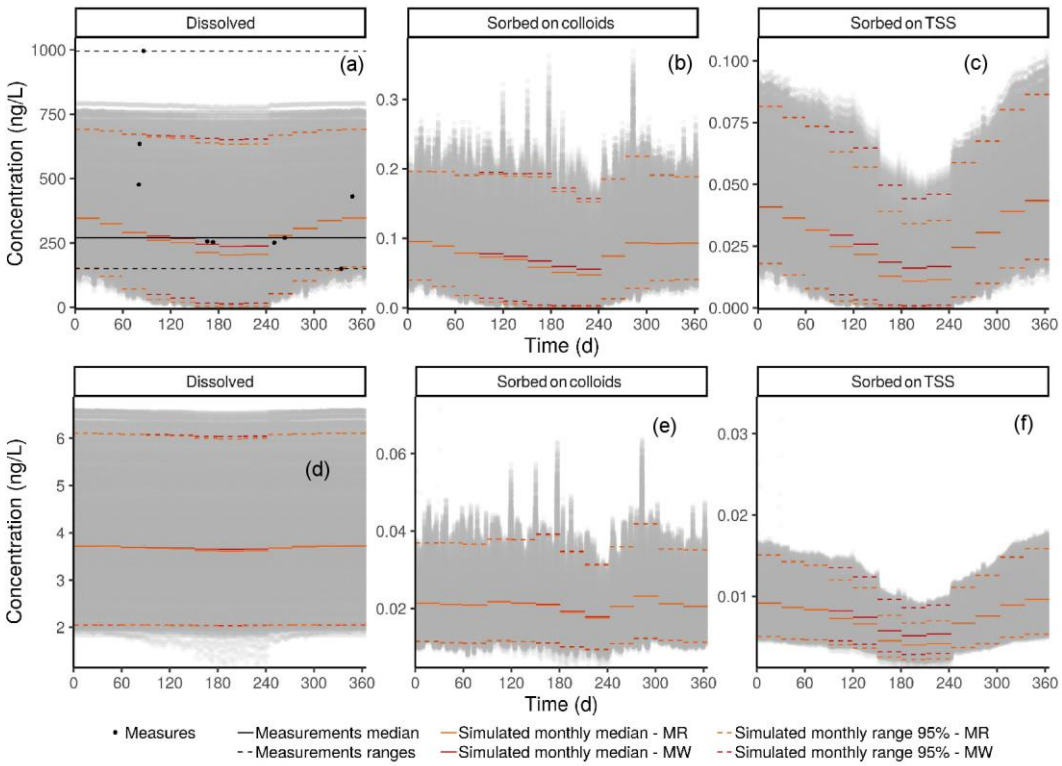

Figure 2 Predicted concentration (12:00 ranges of (a) diclofenac and (b) triclosan at the outlet of the simulated canal stretch. Measured values were only available for dissolved diclofenac. The simulation started on 1st January (day 0) and ended on 31st December (day 365).

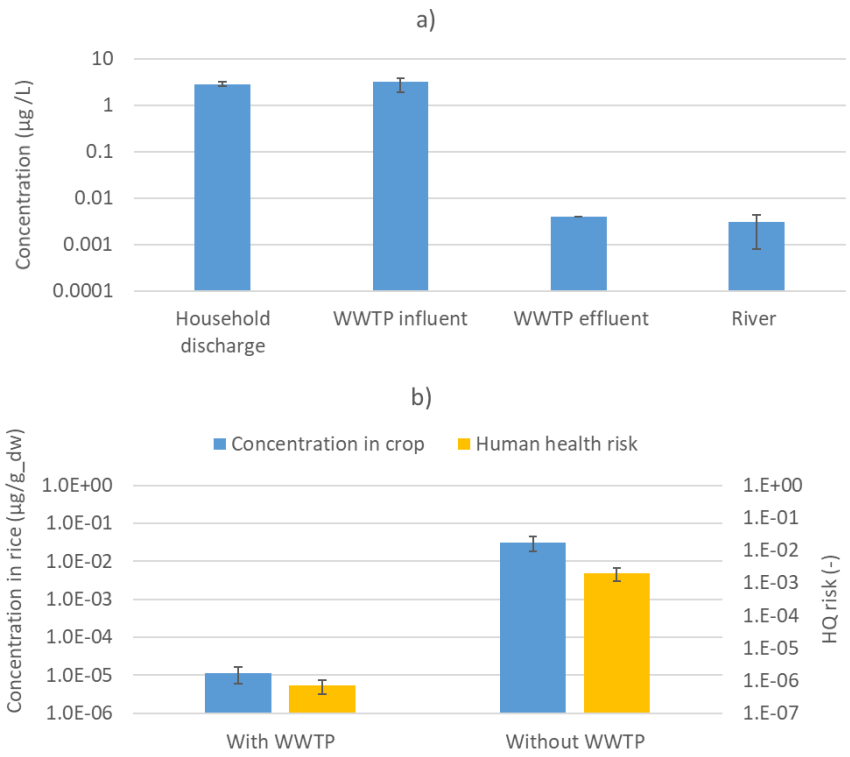

Figure 3 (a) paracetamol water concentration in different elements of the integrated urban water system, b) paracetamol concentration in rice grains and associated risk (HQ) when irrigation is done with treated and untreated wastewater. Results are expressed as annual means and 5th–95th percentile ranges.

Conclusions

The integrated model developed in this study was capable of predicting the fate and occurrence of MPs at different locations in a (peri-)urban water system, allowing to estimate the risk associated to existing water reuse practices. The model can represent a relevant decision-support tool to evaluate alternative scenarios and identify possible mitigation strategies and barriers for reducing the risk associated to MPs.

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