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# Predicting the fate of pharmaceuticals in integrated urban wastewater systems

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**Summary:** A new category of substances, Pharmaceutical Active Compounds (PhACs), has been detected in different parts of integrated urban wastewater and stormwater (IUWS) systems. PhACs are characterized by different fate processes compared to those included in existing MP (MicroPollutants) fate modelling libraries. Thus, existing modelling tools cannot predict the fate of PhACs, and it is not possible to estimate the human and environmental risk due to their discharge in natural water. In this work a dynamic model library was developed to enable the simulation of PhACs across different IUWS elements (sewers, wastewater treatment plants, receiving water bodies). The model performance was assessed by simulating the fate of four PhACs in two different IUWS systems, where measurements were available. Model prediction capability was good, highlighting how the model can be a valuable support tool for a sustainable management of water in urban areas.

**Keywords**: Integrated water quality modelling; control strategies; risk assessment.

## 1. Introduction

Pharmaceutical active compounds (PhACs) can pose an environmental and human health risk when discharged in surface waters (Letsinger and Kay, 2019). Thus strategies to ensure a sustainable management of water in urban areas require knowledge of PhACs fate, but data related to their presence in environmental compartments are often lacking. Integrated models can be used to fill the information gap that water managers are facing. However, existing MP (MicroPollutants) modelling tools cannot predict the fate of PhACs since these compounds are characterized by different fate processes. In this work we presented a modelling library allowing simulating a wide range of PhACs in integrated urban wastewater and stormwater (IUWS) systems by utilizing information which is available in scientific literature and open-access available databases. Model validation was performed comparing model prediction bounds against available measurements in two IUWS systems. The library can then be used to assess PhACs environmental risk and identify risk minimization strategies.

## 2. Materials and methods

Based on the most recent developments in scientific knowledge, significant extensions were introduced to the IUWS_MP model library (Vezzaro et al., 2014). Specifically, modifications included a consumption-excretion model to link sales data with soluble (*S*) and particulate (*X*) model state variables ($S_{MP}$, $X_{MP}$, $X_{MP,seq}$ and $S_{conj,gluc}$) to input to the sewer model, minimizing the effort of pharmacokinetic data collection (i.e. using only excretion rate). Additional fate processes such as deconjugation, sequestration and sorption equilibrium to account for ionisable and re-transformable fractions of PhACs (also known as conjugates) were also added. The model performance was assessed by simulating the fate of four PhACs (ibuprofen, furosemide, paracetamol and diclofenac) in two different IUWS systems, located in two countries (Denmark and Italy) where measurements were available. Model input-parameters (e.g. sales data, excretion rates, first-order biodegradation rates, etc.) were retrieved from available database and literature, and associated uncertainties propagated to model output by applying a forward Monte-Carlo approach (1,000 runs).

## 3. Results and conclusions

The dynamic concentrations from the 1,000 Monte Carlo simulations were aggregated in box-plots (Figure 1) to enable the comparison against measurements (which are mostly based on 24-h composite samples). The prediction bounds (i.e. width of the whiskers) shows the ranges of predicted concentrations over the week when samples were taken, while measured concentrations are shown as maximum, median and minimum values. Model prediction bounds were in good agreement with available measurements across the simulated systems, confirming the robustness of the modelling approach across different systems. Possible applications include: i) assessment the environmental risk by evaluating compliance with Environmental Quality Standards (EQS) for the receiving water body and ii) evaluation of the effect of PhACs emission reduction strategies in reducing the risk for both aquatic environment and human health (as in water-reuse scenarios). In conclusion, the proposed modelling approach allows simulating a wide range of PhACs, minimizing the need of expensive data collection campaigns, enabling a wide application of the library.

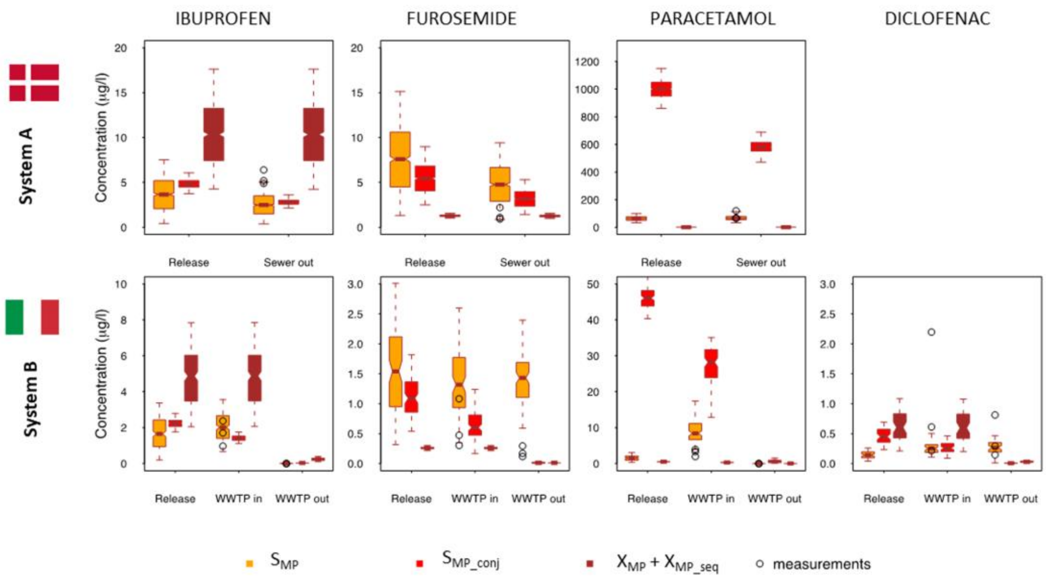


**Figure 1** Comparison between measurements (circle) and model predictions (box-plot) for different fractions of PhACs at different comparison points.

## REFERENCES

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