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### Conceptual Modeling of Micropollutant Fate in Sewer Systems – A GIS-Based Approach to Define Model Structure

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**Abstract:** A new approach to automate the challenging task of defining the complexity level for conceptual modelling of micropollutant (MP) fate in sewer system is here presented. The approach combines GIS information and advanced statistical techniques (e.g., cluster analysis) and provides for a realistic description of in-sewer hydraulic residence time (HRT), which is fundamental for simulating MP removal processes occurring during in-sewer transport. The conceptual model was first tested in a full-scale catchment, where HRT distribution was determined based on spatial distribution of discharge sources and following calibration against high-frequency flow rate data. The model was then used to predict the dynamics of an ideal MP (biodegradation half-life = 2.5 h) at the outlet of the sewer system, revealing higher removal during in-sewer transport when considering an average HRT compared to a discrete HRT distribution. These results demonstrate that an intermediate complexity level, between highly detailed hydrodynamic models and simplified models, could be adopted for MP fate predictions while keeping computational demands reasonable. This latter aspect can be also of particular interest when an integrated modelling perspective (e.g., sewer and WWTP) is considered.

Keywords: GIS; cluster analysis; sewer system modelling.

#### **1. INTRODUCTION**

The development of models that properly describe transport and biochemical processes within a sewer is a challenging task due to the complex nature of the sewer itself and the lack of available information such as sewer network geometry. When dealing with the fate of reactive organic micropollutants (MP), further challenges arise due to the uncertainties linked to measurements and the poor mechanistic knowledge of the processes involved. Where available, detailed hydrodynamic models have been used to simulate pollutants fate (Shahvi et al., 2016) or to extract information that is relevant for MP fate estimation, such as hydraulic residence time (HRT) and MP discharge profiles (McCall at al., 2017). However, when such information is not available and computational demands are limited, conceptual modes can provide a valid alternative to simulate the transport and transformation of MPs. In large catchments, conceptual approaches have been proposed to simulate water quality at the inlet of wastewater treatment plants (WWTP) and their main focus has been on traditional water quality indicators (e.g., Flores-Alsina et al., 2014). The model library described in Vezzaro et al. (2014) provided a conceptual approach to simulate the fate of various MPs across the whole integrated urban wastewater system. When focusing on MP fate description, relevant parameters (especially the in-sewer hydraulic residence time, HRT)



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need to be considered in the model construction. HRT is in fact linked to the main MP fate processes (biodegradation, sorption) (Ramin et al., 2016), and its correct description is a key point for predicting MP occurrence in sewer outlets. However, hydrodynamic models of sewer catchments are rarely available, especially for large urban areas, and alternative data on water supply (e.g., water consumption, consumer locations) and sewer networks (pipeline) stored in Geographical Information Systems (GIS) may represent a valid option. In this study, we aimed at testing a new approach, which relies on available GIS information and advanced statistical techniques (cluster analysis), for defining the level of optimum complexity for conceptual sewer models where MP fate prediction is the primary objective.

#### 2. MATERIALS AND METHODS

#### 2.1 Case Study

The conceptual model approach was developed for a large sewer catchment with negligible industrial contribution. No detailed hydrodynamic model of the catchment is currently available. Water network data were provided by the local water utility, including shape files of the sewer pipeline network, the catchment area, the geographical location of points for potable water consumption along the drinking water distribution system (around 28.000), and the water consumption for each point over a reference period (1 year). WWTP inlet flow data (at 5-minute resolution) were available for the study period (January 2016-December 2016).

#### 2.2 Overview of the approach

The developed approach comprised three steps, which are detailed below with respect to the procedures and the algorithms used.

#### Step 1: Sewer Network Analysis and Daily Wastewater Profile Generation.

The distance d (m) between each wastewater generation point (equal to drinking water consumption point) and the WWTP inlet was calculated through the "networkx" python module using the Dijkstras algorithm. This provided a probability density distribution (*pdd*), where the mean represents the average household distance from the WWTP. The diurnal wastewater profile generation was estimated based on the pattern for diurnal drinking water (*ddw*) consumption reported by Candelieri and Archetti (2014). Finally, the wastewater profile was obtained by scaling the *ddw* profile by the annual water consumption. Water losses (e.g. water gardening) were also taken into account and assumed equal to 2% of the annual consumption (Butler et al., 2004).

#### Step 2: Gaussian Mixture Model for Cluster Analysis.

The *pdd* of the network distance was divided by an average flow velocity v (0.8 m<sup>3</sup>/s, value after calibration against high-resolution influent flow rate measurements), to obtain a *pdd* for in-sewer HRT. Also, an automatic model calibration was performed to estimate groundwater infiltration. The HRT *pdd* was then used as input to the iterative Expectation-Maximation (EM) algorithm to optimise the Gaussian mixture model likelihood. The EM algorithm was used to determine the mean and variance of a number n of Gaussian sub-distributions (also known as components), the combination of which fits the HRT *pdd*. The components denote the different sub-catchments, in which the main catchment was subdivided.



Step 3: Construction of the conceptual model.

The model was built by using the elements in the IUWS-MP library (Vezzaro et al., 2014), where the sewer network was simulated as a series of non-linear reservoirs (Saagi et al., 2016) in WEST® 2014 (DHI, Hørsholm, Denmark). For each sub-catchment the number of non-linear tanks was optimised to match the estimated HRT mean of step 2.

#### **3. RESULTS AND DISCUSSION**

#### 3.1 Sewer Network Analysis and cluster analysis

The results of the cluster analysis and the conceptual model are shown in Figure 1a and b, respectively. The algorithm selected six components, indicating that six mean HRT values were sufficient for a proper representation of the HRT distribution in the catchment. Accordingly, six separate sub-catchments were identified and used for the definition of the conceptual model (Figure 1b).



**Figure 1.** a) Result of the cluster analysis with identification of the sub-catchments and their corresponding HRT values (mean of each Gaussian distribution); b) conceptual model in WEST environment.

#### 3.2 Model results

The conceptual model allowed to properly simulate flow dynamics (Figure 2a), being within the 10<sup>th</sup> and 90<sup>th</sup> percentile of measured data (180 days). Figure 2b presents the concentration profiles at the sewer outlet of an ideal non-sorptive MP with biodegradation half-life = 2.5 h when a six-catchment model (red curve) and a single-catchment model (green area) is considered. For the single-catchment model, an average HRT value of approximately 2.5 hours (the mean of the HRT distribution) was assumed. The simulated MP profile differed for the two cases, with approximately 10% lower removal efficiency from excretion point to WWTP inlet for the six-catchment model. This observation highlights the influence of HRT description on the estimation of MP removal via biodegradation within the sewer system.



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Figure 2. a) Comparison between measured data (red lines, median of 180 days) and the model (blue line) when six sub-catchments are considered; b) Comparison of profiles for an ideal non-sorptive and biodegradable MP when two different conceptual sewer models are considered (6 subcatchments in red, 1 subcatchment in green).

#### CONCLUSIONS

Through the combination of GIS-based information and statistical analysis, we were able to identify the optimal structure of a conceptual model aiming at simulating in-sewer HRT in a large urban catchment, while keeping model complexity as simple as possible. This approach allowed for successful simulation of flow dynamics and implications for MP fate predictions were evaluated. Preliminary simulation results revealed that multi-catchment models should be preferred, especially for degradable MPs, to avoid overestimation of their removal during in-sewer transport. Further investigation is currently ongoing to assess the effect of complexity level on in-sewer removal of MPs of different characteristics (e.g., higher or lower degradability).

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