Pollutant transport modelling in a laboratory setting – what can be learned

Modélisation du transport des polluants en laboratoire : ce que l'on peut en apprendre

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RÉSUMÉ

Le ruissellement des eaux pluviales urbaines est de plus en plus reconnu comme une ressource précieuse dans le contexte de la pénurie d'eau aggravée par le changement climatique. Cependant, la qualité de ce ruissellement est souvent compromise par des micropolluants provenant des matériaux de construction, tels que les pesticides lessivés des membranes bitumineuses de toiture. Cette étude se concentre sur les émissions de l'acide 2-méthyl-4-chlorophénoxyacétique (MCPA), un herbicide couramment associé aux toitures végétalisées et aux matériaux bitumineux. Étant donné la disponibilité limitée des mesures sur le terrain et le coût élevé des campagnes de suivi à grande échelle, nous avons utilisé un dispositif expérimental en laboratoire pour calibrer un modèle de transport de polluants à l'aide du module de qualité de l'eau du logiciel Iber. Cette calibration démontre la faisabilité de reproduire la dynamique de transport du MCPA dans les systèmes de ruissellement urbain, bien qu'un affinage supplémentaire soit nécessaire pour améliorer la précision. Les travaux futurs intégreront des analyses d'incertitude et de sensibilité afin d'évaluer l'influence des facteurs clés sur la performance du modèle, améliorant ainsi la capacité prédictive et soutenant le développement de stratégies robustes pour la gestion de la qualité des eaux de ruissellement urbaines.

ABSTRACT

Urban rainwater runoff is increasingly recognized as a valuable resource in the context of water scarcity exacerbated by climate change. Nevertheless, runoff quality is often compromised by micropollutants originating from building materials, such as pesticides leaching from bituminous roof sheets. This study focuses on emissions of 2-methyl-4-chlorophenoxyacetic acid (MCPA), a herbicide commonly associated with green roofs and bituminous roofing materials. Given the limited availability of field measurements and the high costs of extensive monitoring campaigns, we employed a controlled laboratory setup to calibrate a pollutant transport model using Iber software water quality module. The calibration demonstrates the feasibility of reproducing MCPA transport dynamics within urban runoff systems, although further refinement is required to enhance accuracy. Future work will incorporate uncertainty and sensitivity analyses to evaluate the influence of key factors on model performance, thereby improving predictive capacity and supporting the development of robust management strategies for urban runoff quality.

KEYWORDS

Building materials, Diffuse pollution sources, Micropollutant modelling, Spatio-temporal analysis, Stormwater quality

1 INTRODUCTION

Urban rainwater runoff is increasingly valuable due to water scarcity exacerbated by climate change. However, stormwater can be polluted by micropollutants leached from building materials, including pesticides from bituminous roof sheets. The contribution of pollutants originating from building materials has received increasing research attention over recent decades (Müller et al., 2019). Previous research on pollutant release from building surface materials has focused primarily on metals (e.g., Winters et al., 2015) and pesticides (e.g., Gromaire et al., 2015). In another study, Vialle et al. (2013) found Mecoprop in all runoff samples collected from a suburban catchment, with concentrations reaching up to 4.8 µg/L. The present work is focusing on 2-methyl-4-chlorophenoxyacetic acid (MCPA) emissions, which is commonly used in green roofs and bituminous roofing materials. Studies (e.g., Wicke et al., 2022) show that when used as a root protection agent in bituminous roofing materials, it can leach into stormwater at concentrations that exceed environmental limit values for surface and ground waters. Main problems of pollution by urban water runoff are that the sources are diffuse and the availability of catchment data is low, which hampers the setup of models to describe the pollution. To counter these limitations, present by the low availability of field measurements as well as the expensive measurement campaigns necessary to collect them, this study uses a laboratory setup to calibrate a pollutant transport model for MCPA to showcase the possibilities of such an approach.

2 METHOD

2.1 Laboratory setup

The experimental study was conducted in the Street Model facility located at CITEEC research centre at the Universidade da Coruña (Spain), using a scaled physical model designed to represent an idealized urban catchment (for example, also used in Pritsis et al., 2023a). The hypothetical city consisted of 25 cubic building blocks arranged in a 5 × 5 layout. Each block measured 30 × 30 cm at the base with a height of 20 cm. The spacing between adjacent blocks was set to 10 cm, representing the road network within the modelled district. The building array was positioned near the outlet of the catchment to reproduce downstream urban conditions. The artificial catchment was constructed from rough concrete and shaped with a major slope of 1% directing flow toward the outlet, complemented by a minor cross slope of 1‰. Each building block was fabricated with a hybrid structure: the roof was made of transparent plexiglass, while the remaining surfaces were constructed from PVC. A general overview of the experimental setup is provided in Figure 1 on the left. The physical model was designed to preserve similarity with a corresponding real-world urban district. The geometrical scaling factor was 1:125, so the model catchment represents a prototype area of 0.23 km², each model building corresponds to a structure with a 24 × 24 m footprint and road prototype width is 8 m. Applying Froude similarity, these scaling ratios ensure geometric, kinematic, and dynamic consistency between the laboratory system and the idealized full-scale urban setting. A rain simulator was installed above the experimental catchment to generate a controlled rainfall cl intensity of 30 mm h^{-1} during the experiments. To ensure uniform rainfall distribution across the catchment, a metal mesh was positioned beneath the nozzles. This mesh homogenized the spray pattern and facilitated the formation of realistic raindrop sizes, thereby reproducing natural rainfall characteristics over the artificial urban surface (Naves et al. 2020).

2.2 Experimental phase

MCPA was introduced into the system at two designated injection points located adjacent to the building blocks. At each point, a 7 mL pulse of MCPA solution (100 µg L^{-1}) was applied, representing pollutant emissions from individual roofs. The positions of the two injection locations (S1 and S2) are shown in Figure 1 on the right. Prior to each injection, the rain simulator was operated at an intensity of 30 mm h^{-1} to establish steady-state hydraulic conditions across the catchment. Immediately after the MCPA pulse was introduced at S1 or S2, water samples were collected at the catchment outlet. For S1, ten samples were taken within the first 120 seconds following injection, while twelve samples were collected over the same period for S2.

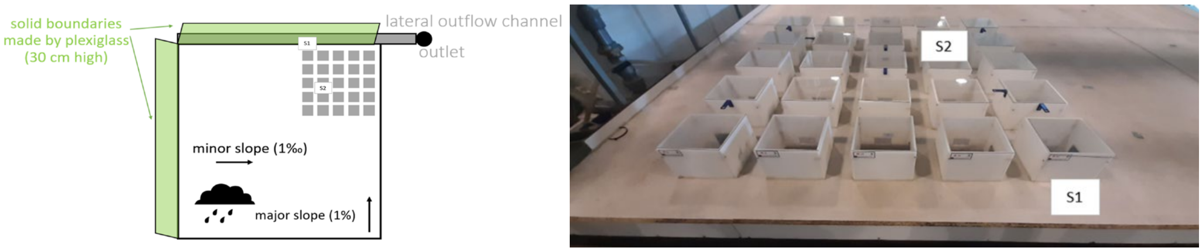


Figure 1: Laboratory setup of the scaled urban catchment model.

(left) Schematic layout showing the 5 × 5 building arrangement, major and minor slopes, and the outlet position.

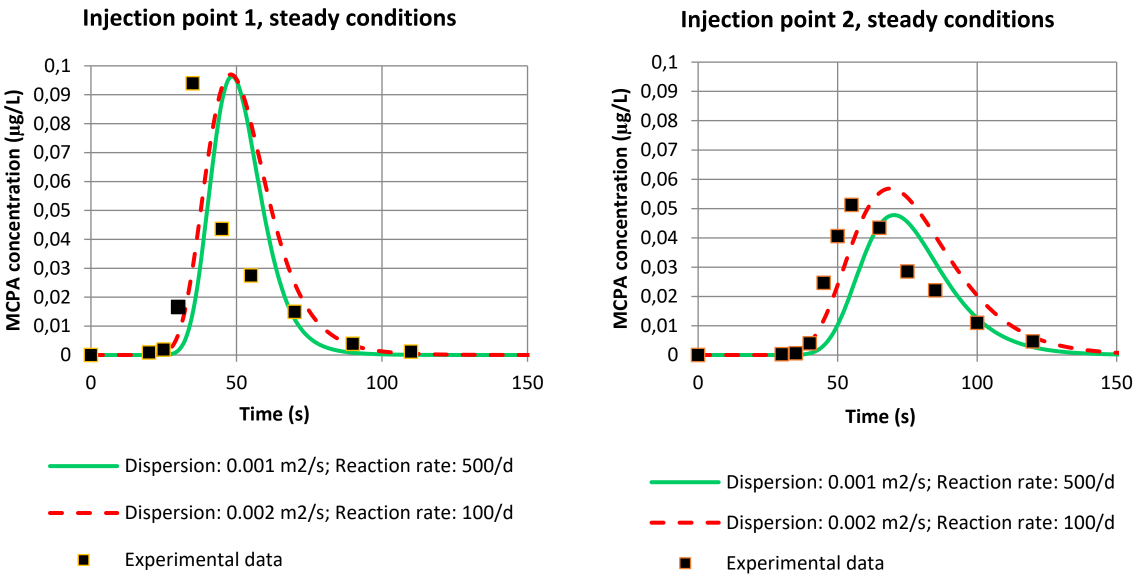
(right) Photograph of the physical model with the 25 building blocks and the two MCPA injection points (S1 and S2).

2.3 Modelling

The purely hydrological model of Pritsis et al. (2023b) was adapted to reproduce the two scenarios numerically using the Iber model (Bladé et al., 2014). Iber is a two-dimensional shallow-water numerical model that also includes capabilities for simulating water-quality processes (García-Feal et al., 2020), like dispersion [m^2/s] and reaction rate [1/d]. Following the methodology introduced in the contribution of Pritsis et al. (2023a), Iber was employed to simulate the spread of an MCPA concentration spot. Physical terrain was captured as a non-uniform rational B-spline (NURBS) surface in GID (GUI software which is coupled with Iber), based on the design characteristics of the laboratory catchment and in that area the mesh was developed. The houses were omitted from that NURBS surface, and their boundaries were set as reflective boundaries in Iber. The computational mesh was unstructured and consisted of a total of 22.358 triangular elements with an average element size of 0.05 m^2. The hydrological module of Iber was activated to convert rainfall into runoff in a fully distributed manner. The Decoupled Hydrological Discretisation (DHD) numerical scheme, which is well suited for hydrological applications, was used in the simulations, and the wet–dry threshold was set to 0.01 mm. The Manning coefficient was set to 0.0225 on the surface domain.

3 RESULTS AND DISCUSSION

The results (see Figure 2) show that although the calibration can still be improved, we can reproduce the transport of the pollutant MCPA using the water quality module of Iber at the catchment outlet.


Injection point 1, steady conditions

Injection point 2, steady conditions

Figure 2: Modelled and measured MCPA concentrations at the outlet of the catchment.

The differences are mainly based on a delay in the model in reaching the peak concentration. This can have several reasons, but the most likely explanation is that the simulation has a certain timelag to the measurement data, which can be caused by measurement and model discrepancies, that need further investigation. Using unsteady conditions, the match at the peak is better, but the increment from zero to a different value is way bigger than the experimental data. At the steady conditions there wasn't any couple of numbers that being compared could give a "perfect match", hinting again at a measurement induced difference. While the dispersion coefficient was being increased, the maximum value was decreasing, at that level, that even with zero reaction rate, the maximum quantity was significantly smaller than the experimental one. A manual trial and error led to improvements; however, a global sensitivity analysis could be beneficial to see what the most influential parameter is and then try to find a calibration scheme for scenarios with greater dispersion number, and smaller reaction rate.

4 CONCLUSION

The study showed the possibility to model pollutant transport within an urban catchment with assumed point pollution sources, as for example from rain downpour spouts. The presented dataset can be a starting point for benchmarking models which would like to model this behaviour, and this study showed the capabilities of Iber in this regard. Future work will include an uncertainty and sensitivity analysis to improve the model and using the data of washoff from all roofs to run a combined model with point input at each of the roofs to look at the mixing behaviour on a catchment scale.

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