

Treatment of micropollutants in stormwater biofilters: comparing model results with field and lab data

Traitement de micropolluants par une noue filtrante : confrontation d'un modèle aux données expérimentales

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RÉSUMÉ

Les ouvrages de biofiltration traitent les micropolluants transportés par les eaux pluviales urbaines par divers procédés de traitement. Les modèles de transport réactif peuvent être utilisés pour évaluer des hypothèses sur les principaux procédés déterminant la performance du traitement pour un polluant donné et, dans la mesure où ils représentent de façon adéquate les procédés les plus importants, ils peuvent être utilisés pour prévoir la performance et améliorer la conception du système. Dans ce travail, un modèle du traitement des micropolluants est utilisé pour simuler deux études de cas pour lesquelles des données expérimentales de performance de traitement ont été collectées précédemment. Le premier est une noue filtrante, qui a fait l'objet d'une étude de terrain des métaux traces et des micropolluants organiques (hydrocarbures aromatiques polycycliques, alkylphénols, phtalates, bisphénol-A) dans les phases particulaires et dissoutes. La seconde est une étude de biofiltration sur colonne considérant la rétention des métaux traces, en distinguant les fractions particulaires, dissoutes et réellement dissoutes. L'étude sur le terrain montre qu'un modèle représentant l'advection, la dispersion, la sorption et la biodégradation ne décrit pas complètement le traitement des micropolluants dans les biofiltres d'eaux pluviales dans des conditions de terrain complexes. Les résultats du modèle de l'étude en colonne permettront d'évaluer si l'advection, la dispersion et la sorption peuvent représenter avec précision l'élimination des métaux dissous ou réellement dissous dans des conditions contrôlées.

ABSTRACT

Stormwater biofilters treat the micropollutants conveyed by urban stormwater through various treatment processes. Process-based transport models can be used to evaluate hypotheses about the main processes driving treatment performance for a given pollutant and, insofar as they adequately represent the most important processes, can be used to predict performance and improve system design. In this work, a reactive transport model representing micropollutant treatment in stormwater biofilters is used to simulate two case studies for which experimental treatment-performance data has been collected previously. The first is a biofiltration swale, which has been the object of an extensive field study of both trace metals and organic micropollutants (polycyclic aromatic hydrocarbons, alkylphenols, phthalates, bisphenol-A) in both the particulate and dissolved phases. The second is a column study considering trace metal removal, distinguishing the particulate, dissolved and truly-dissolved fractions. Results from the field study show that a model representing advection, dispersion, sorption and biodegradation does not fully describe the processes driving micropollutant treatment in stormwater biofilters under complex field conditions. The results from the model of the column study will allow to evaluate whether advection, dispersion and sorption can accurately represent the removal of dissolved or truly dissolved metals under controlled conditions.

KEYWORDS

Stormwater biofilter, process modelling, micropollutant, metal, reactive transport

1 INTRODUCTION

Urban runoff is contaminated by a wide variety of pollutants, including both trace elements and various organic micropollutants, such as polycyclic aromatic hydrocarbons (PAHs), phthalates and alkylphenols (Zgheib et al., 2011). This pollution can be treated in stormwater biofilters through various processes including sedimentation or physical filtration of particulate pollutants, sorption, volatilisation, biodegradation, photodegradation and accumulation in plants (LeFevre et al., 2014). Confronting modelling and experimental studies is an important approach to gain a more process-based understanding of experimental observations of treatment performance, while identifying the limits of a given theoretical framework and possible improvements to models.

The objective of the present work is to evaluate whether it is relevant to represent the fate of both particulate and dissolved pollutants using a sorption model as surrogate. This is done by comparing confidence intervals (accounting for parameter uncertainty) of model outputs from MPIRe, an existing model representing the reactive transport (advection, dispersion, volatilisation, sorption and biodegradation) of micropollutants through a stormwater biofilter, to two different experimental datasets, a field study of a biofiltration swale in Compans, France (Flanagan et al., 2019) and a column study considering the speciation of metals (Lange et al., 2020).

2 METHODS

2.1 Model description

MPIRe contains both a water flow module and a pollutant transport module; the model used for the present work was simplified from that was developed (and validated for a number of organic micropollutants under controlled conditions) by Randelovic et al. (2016). Flows and compartments irrelevant to the experimental biofilters have been eliminated.

The present water flow module is one-dimensional and contains two compartments: a ponding zone and a filter zone. The ponding zone has two inflows (direct rainfall, Q_{rain} , and runoff, Q_{in}) and two outflows (flow into the filter media, Q_{pf} , and overflow, Q_{over}). Q_{pf} is determined according to modified Darcy's law; when ponding water depth exceeds a fixed value, the exceeding volume is transformed into Q_{over} . Q_{pf} is the only inflow to the filter zone; outflows include flow in the drain and evapotranspiration.

The pollutant transport model represents all pollutants as existing in the dissolved phase (i.e. sedimentation, filtration and colloidal transport are not represented). The ponding zone is represented as a continuously stirred tank reactor (CSTR) with only volatilisation as a reactive process. The transport through the filter zone is represented by a one-dimensional advection-dispersion scheme for unsaturated soil. In this zone, three reactive processes are represented: instantaneous sorption, kinetic sorption and biodegradation. Parameters for this model are the filter media's dispersivity (α_L), as well as the pollutant's intrinsic properties: Henry's constant (H_c), organic carbon-water partition coefficient (K_{oc}), the fraction of sites with instantaneous sorption (f_e), half-life of biodegradation ($T_{1/2}$), rate constant of kinetic sorption (α_k). These parameters have been collected from the scientific literature (e.g. Mackay, 2006). As reported values vary greatly between studies, their estimation is subject to substantial uncertainty, which is accounted for in the following applications using a stochastic approach.

2.2 Application to Compans biofiltration swale

The first application of the model is to a biofiltration swale located in Compans, France. The biofiltration swale, which was both drained and lined, with 0.5 m of filter media containing 0.9% organic carbon and no submerged zone, was the object of an in-depth monitoring campaign involving rainfall and flow measurements, as well as analysis of a wide range of micropollutants in untreated runoff, drained water and the system's filter media. Inlet and outlet masses of several micropollutants, including Cu, Zn, pyrene (Pyr), phenanthrene (Phen), octylphenol (OP), nonylphenol (NP) and bis(2-ethylhexyl) phthalate (DEHP), have been estimated for the first 13 months of the facility's operation, according to a stochastic approach, allowing for uncertainty quantification (Flanagan et al., 2019). The objective of the present study is to simulate outlet masses for the same period using MPIRe in order to compare predicted long-term load reductions (i.e. difference between the mass of pollutants entering the facility and leaving the facility through the drain and overflow over the 13-month period) and identify deviations in real versus theoretical behaviour. Uncertainties due to parameters estimation were quantified by varying parameters within distributions of possible values (Table 1) and repeating simulations 1500x per pollutant.

After adaptation to the site's geometry, hydraulic conductivity and ponding depth (parameters difficult to estimate reliably in the field for this site) were calibrated simultaneously, ultimately leading to a Nash-Sutcliffe of 0.61 for the first period and 0.7 for the second period.

Table 1. Parameter distributions. Besides α_L , uniform distributions of possible values (Mackay, 2006) were used.

Pollutant	H_c (Pa.m ³ /mol)	K_{oc} (L/kg)	$T_{1/2}$ (days)	f_e	α_K (s ⁻¹)	α_L (m)
Cu	-	$5.9 \cdot 10^5 - 1.8 \cdot 10^6$	-	0-1	$1 \cdot 10^{-7} - 5 \cdot 10^{-5}$	Log-normal distribution, $\mu_{ln}=-2.44$, $\sigma_{ln}=1.30$
Zn	-	$1.4 \cdot 10^5 - 4.3 \cdot 10^5$	-			
Pyr	0.92 – 2.0	$2.6 \cdot 10^4 - 6.3 \cdot 10^6$	200 – 1900			
Phen	2.4 – 5.6	$2.6 \cdot 10^2 - 1.0 \cdot 10^6$	11 – 200			
OP	0.18 – 0.70	$2.5 \cdot 10^3 - 7.4 \cdot 10^3$	0.26 – 69			
NP	0.11 – 3.4	$1.3 \cdot 10^4 - 4.0 \cdot 10^4$	0.29 – 99			
DEHP	0.013 – 3.6	$1.3 \cdot 10^4 - 2.0 \cdot 10^6$	1.4 – 57			

2.3 Application to Luleå column tests

The model will also be applied to a data set of bioretention columns treating semi-synthetic stormwater (Lange et al., 2020). In these experiments, trace metals were analysed in total, dissolved (<0.45 μ m) and truly dissolved (filtration with a 3 kDa ultrafilter) fractions at both the inlet and the outlet of the columns, which were operated under different drying and wetting regimens. Confidence intervals of model predictions will be compared with measured outlet concentrations for different fractions to test whether the model can represent behaviour of total concentrations of metals or whether it is more adapted for representing the dissolved or truly dissolved fraction.

3 RESULTS AND DISCUSSION

3.1 Modeled biofiltration swale load reductions

Median pollutant load reductions (E_{50}) predicted by the model were between 73-80% except for NP (52%); the level of uncertainty in this prediction varied greatly between pollutants, depending on the variability of pollutant parameters found in the literature (Figure 1a). 95% confidence intervals covered spans of 13-94% load reduction, with the highest levels of uncertainty observed for Phen, due to very K_{oc} . Modelled E_{50} were higher than experimental E_{50} for all pollutants compared with experimental results, with no overlap observed between 95% confidence intervals of load reduction for Cu, OP and DEHP.

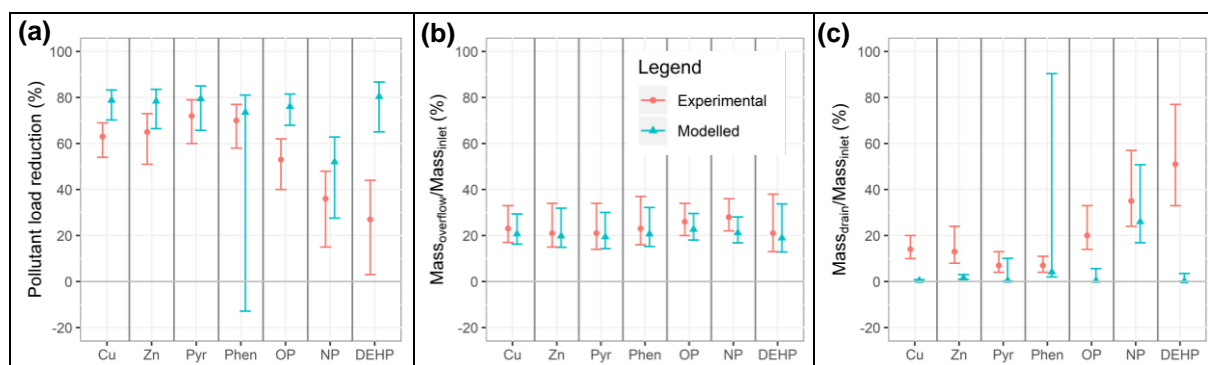


Figure 1. Median and 95% confidence interval of experimental and modelled (a) pollutant load reduction, (b) proportion of inlet mass overflowing from the system and (c) proportion of inlet mass drained from the system.

Drained masses rather than overflowed masses appear to be mainly responsible for the model's overestimation of load reduction (Figure 1b and 1c). Indeed, modelled median drained masses ($M_{drain,50}$) were always lower than experimental values, with no overlap in 95% confidence intervals for Cu, Zn, OP and DEHP. The underestimation is not due to the model's water balance, which actually overestimates outflow through the drain. This indicates that the pollutant transport and reaction processes represented in the filter zone (advection, dispersion, equilibrium and kinetic sorption, biodegradation) provide "overly optimistic" results and do not sufficiently represent the retention of pollutants in the filter zone. In the cases of OP and DEHP, this is likely due to emissions from pollutant construction materials, which lead to higher outlet concentrations than would otherwise have

occurred (Flanagan et al., 2019). For metals, it is likely that other processes besides sorption (e.g. particle and colloidal transport) are also driving performance.

4 CONCLUSIONS AND FUTURE WORK

Applying a pollutant transport model to experimental biofiltration data can be an important tool for better understanding treatment processes. However, both experimental and modelling data entail uncertainties, which must be quantified when making comparisons. Such a comparison revealed that a model representing the advection, dispersion, sorption (kinetic and instantaneous) and biodegradation of micropollutants overestimates load reductions. Therefore, other factors must also drive pollutant removal performance. These may include pollutant speciation, transport of particulate and colloidal phases, preferential flows and emissions of micropollutants from materials used in the biofilter's construction. Modelling the Luleå column experiments will provide an opportunity to test hypotheses about the model's ability to predict the behaviour of species of metals under controlled conditions.

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