

Can we use a simple modelling tool to validate stormwater biofilters for herbicide removal?

Kefeng ZHANG, Anja RANDELOVIC, Ana DELETIC, Declan PAGE, David McCARTHY

Supplementary material

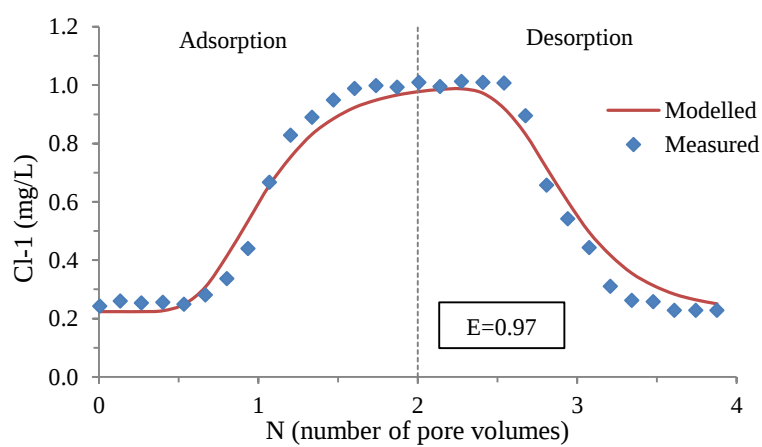


Figure S1 Modelled and measured breakthrough curves for Cl^- from laboratory columns. E: Nash-Sutcliffe coefficient.

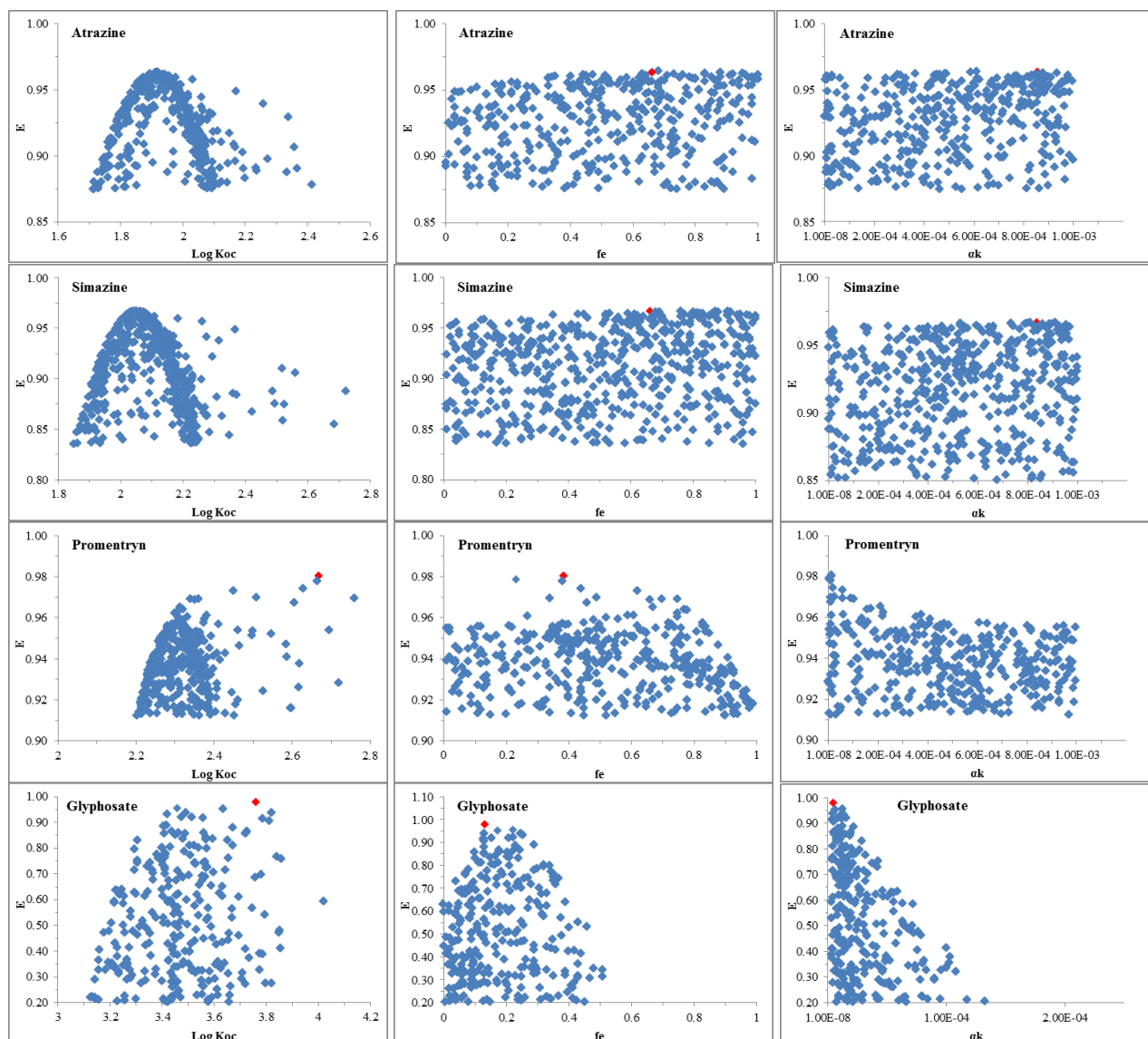


Figure S2 Distribution of adsorption parameters (LogKoc -left, f_e -mid and α_k -right) against Nash-Sutcliffe coefficient (E) for the top k calibrated parameter sets for atrazine, simazine, prometryn and glyphosate. Note: as the intersection (λ) =1 for only 7 simulations for glyphosate, hence $E=0.2$ was adopted here so as to show clear trend of parameters distribution for glyphosate. $K_{oc}=K_d/f_e$

$\text{Log}K_{oc}$, f_e α_k are sensitive parameters for prometryn and glyphosate, while for Simazine and Atrazine, Log Koc is the only sensitive parameter. The different patterns of sensitivity are mainly attributed to the different adsorption properties of the studied herbicides. Glyphosate was the most different one from others, as it has the highest adsorption potential (evident by its highest calibrated logKoc value – 3.8; Table 1 of the manuscript) and it not only attaches to organic matter in the media but also can form phosphonate anions that can be retained through many processes (e.g. ligand exchange, electrostatic ion-exchange reactions, etc)

(Strange - Hansen et al., 2004; Zhang et al., 2015). As for triazines (simazine, atrazine and prometryn), adsorption onto media is relatively lower mainly through weak physical mechanisms (e.g. proton-transfer and hydrogen bonding) (Zhang *et al.*, 2015), with relatively lower logKoc values of 2.0 for atrazine, 2.1 for simazine, and 2.7 for prometryn (Table 1).

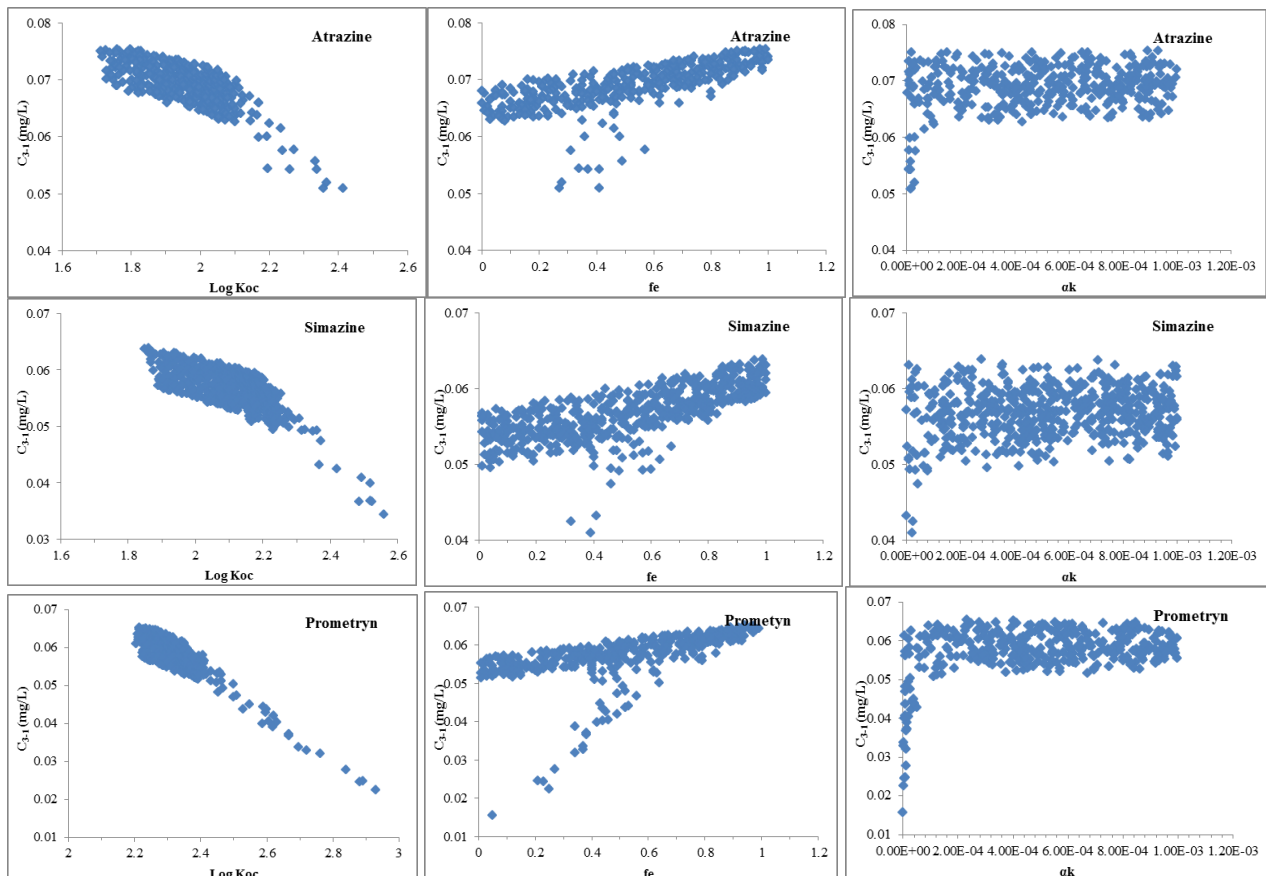


Figure S3 Plots displaying the relationship between three adsorption parameters (LogKoc - left, fe-mid and αk -right) and the first outflow concentration of the 3rd challenge test (C3-1) for the top k calibrated parameter sets for atrazine, simazine and prometryn.

Reference:

- Strange - Hansen, R., Holm, P.E., Jacobsen, O.S. and Jacobsen, C.S., 2004. Sorption, mineralization and mobility of N - (phosphonomethyl) glycine (glyphosate) in five different types of gravel. *Pest Management Science* 60(6), 570-578.
- Zhang, K., Deletic, A., Page, D. and McCarthy, D.T., 2015. Surrogates for herbicide removal in stormwater biofilters. *Water Research* 81(0), 64-71.