# Transfer of S-Metachlor and its metabolites in the vadoze zone : experiments and modelling

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# EXPERIMENTAL AND MODELLING APPROACHES OF TRANSFER OF S-METOLACHLOR AND ITS METABOLITES IN THE VADOZE ZONE

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To improve transfer modelling of pesticides into groundwater, it is necessary to characterize the role of the vadoze zone. This study aims to characterize flow processes and geochemical interactions for an herbicide, S-metolachlor, and its two main metabolites, ESA-metolachlor and OXA-metolachlor, in the vadoze zone of a fluvio-glacial aquifer (South-East of France). Sandy lithofacies, Sx, and sand-gravel bimodal lithofacies, Gcm, were collected and studied for size fraction [0-2mm] and [0-10mm] respectively. Non-saturated columns (dia. 10 cm x H 30 cm) were performed under steady-state water flow in darkness at 15°C. The breakthrough curves were analyzed using the method of moments (Hanna et al., 2012). Inverse modelling with Hydrus 1D code (Simunek et al., 2013) were conducted in a two steps approach: determination of the hydrodynamic parameters based on the tracer (bromide) experiment and fitting of the reactive transport of the studied parent molecule and its metabolites. The second step was realized by using 2 modeling options: chemical non-equilibrium (i.e. chemical kinetics) and non-physical non-equilibrium (i.e. adsorption surface sites in the immobile water fraction).

Tracer columns experiments showed a fractionation of flow into mobile and immobile compartments in both materials. However, immobile water content is estimated as 3 times higher for Gcm columns than for Sx. Compared to bromide, S-metolachlor breakthrough curve is delayed with deficit mass balance because of retention in columns. ESA-metolachlor and OXA-metolachlor breakthrough curve are almost bromide similar because of very less retentions estimated. Consequently, both metabolites leaching behavior seems to be mostly governed by water flow pattern. Higher sorption parameter of S-metolachlor than those of its metabolites is in agreement with batch sorption experiments. Nevertheless, retention parameters obtained from column tests are lower than those calculated from the batch experiments because of time dependence of retention. The contact time between solutes and the matrix is shorter in column experiments than contact time used in equilibrium batch adsorption. These results emphasize retention processes are solute dependent and chemical composition matrix dependent. Moreover, interactions are impacted by contact time which has important implications for the fate and transport of pesticides and metabolites as demonstrated here for S-metolachlor and its metabolites in vadoze zone. Reactive transport of both pesticides and metabolites was rarely discussed in literature, and this study takes part in first investigations in vadoze zone.

Hanna K., Lassabatère L. & Bechet B. (2012) Transport of two naphtoic acids and salicylic acid in soil : Experimental study and empirical modeling. Water Research, Vol. 46, Issue 14, 4457-4467.

Šimůnek J., van Genuchten M.T. & Sejna M. (2013) The Hydrus-1D software package for simulating the one-dimensional movement of water, heat, and multiple solutes in variably-saturated media. Version 4.16, *HYDRUS Software Series 3,* Department of Environmental Sciences, University of California Riverside, Riverside, California, 330p.