



Modeling the effect of flow homogeneity on the fate of Cd, Pb and Zn in a calcareous soil

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The fate of pollutants in the vadose zone depends on flow pathways. It is generally assumed that homogeneous flow will allow pollutants to reach most of the sorption sites, whereas preferential flow will transport pollutants through restricted zones and prohibit pollutants to reach sorption sites in more stagnant water (e.g. Lassabatere et al., 2004). However, this hypothesis has so far not been validated nor experimentally nor numerically. Experimental validation would require, in a unique soil, to establish heterogeneous and homogeneous flow conditions for the similar hydric (water content) and hydraulic (flow rate) conditions, which is almost impossible to achieve. Eventually, variations in flow heterogeneity may be obtained by varying hydric and hydraulic conditions. But straightforward conclusions on flow heterogeneity cannot be expected from such multi-variable experimental assets. This study investigates numerically the effect of flow heterogeneity on the fate of three heavy metals in calcareous environments. The solute transport code considers MIM model (mobile-immobile model) for describing flow heterogeneity. Water is divided into mobile water and immobile water fractions. Solutes are transported by convection and dispersion in mobile water and diffuse at the interfaces between mobile and immobile water fractions. The speciation code considers metal dissolution/precipitation of carbonates, and complexation on calcite surfaces and cationic exchange on Fe-oxyhydroxides particles (clay). The numerical code is applied to the experimental results obtained for a calcareous soil in contact with three trace elemental cations (Cd(II), Pb(II), and Zn(II)) under both static (batch experiments) and dynamic conditions (column experiments) (Lassabatere et al., 2007). The model reconstructs accurately the experimental results and then simulates varying contact times (in batches), injection flow rates (in columns), and concentration conditions. Then, the model is used to predict Cd, Pb and Zn elution and retention for several scenarios regarding flow homogeneity. The numerical sensitivity analysis quantifies the effect of the fraction of mobile water and the solute exchange rate between mobile and immobile water fractions. The modeling clearly shows that the degree of flow homogeneity should impact both heavy metal modeled elution and retention in the soil profile. However, the impacts depend on both the hydrodynamics of flow (mobile water fraction and solute exchange rate between mobile and immobile fractions) and the type of geochemical mechanism involved in heavy metal retention and elution (cationic exchange, versus precipitation).

Lassabatere L, Spadini L, Delolme C, et al (2007) Concomitant Zn-Cd and Pb retention in a carbonated fluvio-glacial deposit under both static and dynamic conditions. *Chemosphere* 69:1499–1508.

Lassabatere L, Winiarski T, Galvez Cloutier R (2004) Retention of three heavy metals (Zn, Pb, and Cd) in a calcareous soil controlled by the modification of flow with geotextiles. *Environ Sci Technol* 38:4215–4221.