



Use of advanced geochemical models in vadose zone reactive transport modeling

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Transport of compounds in soils depends on hydrology and the partitioning of the elements between the soil solid phase and soil solution. In the last decade, the development of advanced speciation and surface complexation models to calculate partitioning of inorganic compounds has made much progression. This is especially true for models used to predict complexation of metals by Solid Organic Matter (SOM) and Dissolved Organic Matter (DOM), such as the Non Ideal Competitive Adsorption Donnan (NICA-Donnan) model. These models are important to calculate sorption in the vadose zone as organic matter is often the most important reactive surface here. In principle, such advanced geochemical models can be used for reactive transport calculations. At current, however, mainly simple empirical relations are used for such practical applications. The major advantages of using advanced geochemical models are, first, that they give insight in the processes determining the behavior of metals in soil. Now also speciation of metals in solution can be calculated, especially metal activity, which often determines uptake of metals by plants and metal toxicity for biota. Secondly, such models can be used with generic parameter sets, while more empirical models often require site specific calibration of equilibrium parameters, like exchange constants and sorption constants.

We evaluated the use and practical applicability of an assemblage of complexation models in two cases. In the first case, we tried to predict concentrations of Cd, Cu, Ni, Pb and Zn in soil extracts. We used a large number of soil samples which cover a wide range of soil properties and metal contents. For SOM and DOM, the NICA-Donnan model was used to predict binding of cations, for clay minerals a non-specific Donnan type exchange model, and for metal-(hydr)oxides a two-site DDL model. We found that calculated metal concentrations in the extracts agreed well with measurements, except for Pb where calculations overestimated concentrations by on average one order of magnitude. Also, for some highly Zn contaminated soil samples, concentrations are greatly overestimated. Modeling results also provided the distribution of metals over the different reactive surfaces in the soil solid phase and soil solution. Furthermore, we studied the effects of uncertainties in the concentrations of macro ions and DOM and organic matter composition on the outcome of the modeling. These parameters are often not available in soil studies and then need to be estimated when using advanced complexation and speciation models.

For the second case we applied these models to calculate changes in the soil solution chemistry during a 30-year period at an intensive monitoring plot in Solling, Germany. Partitioning of all elements was calculated within the same framework of speciation and complexation models. This enabled us to calculate the linkage between changes in soil solution chemistry and metal contaminant behaviour. Here, the calculations could be well confirmed by measurements.