


219-12 Modeling of Trace Element Partitioning in Soil: Validation and Comparison of Predictive Power Between a Mechanistic Multisurface and An Empirical Regression Based Modeling Approach.

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Solid solution partitioning of trace elements in soils is one of the key factors which determine their leaching to ground water and runoff to surface water. Within reactive transport models two clearly distinct concepts are used to compute trace element partitioning i.e. the use of (i) regression based empirical models or (ii) mechanistic process based models. Numerous regression based models are available in literature. These models either directly relate solution concentrations to solid phase concentrations and soil properties (e.g. soil organic matter and pH) or they relate adsorption constants (Kd or Freundlich adsorption parameters) to soil properties. Regression based models are used very frequent because of their easiness of use, short runtime and low demand for input data. This makes these models attractive to be used in large scale applications (regional scale models) and simple web based applications. Most recent examples of mechanistic solid solution partitioning models are multi surface models which combine separate adsorption models for different reactive soil phases: clay, dissolved and particulate organic matter and Al and Fe (hydr)oxides. Although these models have a high input demand for model parameters, the availability of data sets with generic model parameters largely increases the applicability of these models. Here we test both model concepts on (independent) data of soil solution extracts for a large number of soil samples and on pH titration data of soil samples for the elements As, Ba, Cd, Co, Cr, Cu, Mo, Ni, Pb, Sb, Se, Sn, V and Zn.

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