Geophysical Research Abstracts,
Vol. 11, EGU2009-10623, 2009
EGU General Assembly 2009

Illuminating a black box – determination of rates of reactive transport by combining numerical tools with optimized experiments

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Only the combination of physical models and experiments can elucidate the processes of reactive transport in porous media. Column scale experiments offer a great opportunity to identify and quantify processes of reactive transport. In contrast to batch experiments, approximately natural flow dynamics can be realized. However, due to the complexity of interactions and wide range of parameters the experiment can be insensitive to the wanted process and misinterpretation of the results is likely. In the proposed talk we want to give examples how numerical tools can be applied for thorough planning and evaluation of experiments. In a first phase, we performed systematical numerical experiments to optimize the experimental conditions, which allow the quantification of (de-)sorption kinetics under percolation conditions. For short term column experiments we found, that the application of flow interruptions along with two different flow velocities can be applied to avoid uniqueness problems with respect to identification of partitioning coefficient and mass transfer rate. By a sensitivity analysis the parameter space was divided into regions where physical reasonable parameter estimates can be expected and where equifinal solutions are likely. In a second phase we conducted column experiments to test this optimized experimental design for its suitability for the identification and quantification of rate-limited contaminant release. We used materials polluted with organic and inorganic contaminants originating from different soils, sites and materials (Coke oven sites, abandoned industrial sites, destruction debris, municipal waste incineration ash). Repacked soil columns were percolated under saturated and unsaturated conditions and were subjected to multiple flow interruptions and different flow velocities. The third phase consisted of data evaluation and process quantification applying numerical inversion of a physical transport model. The parameter sets were evaluated against the results of the sensitivity analysis, which allowed to seperate physical reasonable models from equifinal parameter sets. The drawbacks of the model could be identified and gave valuable hints on the actual processes.