Geophysical Research Abstracts,
Vol. 11, EGU2009-3037, 2009
EGU General Assembly 2009

Recursive and Hierarchical Identification of Reactive Transport and Fluid Flow Parametrization

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Recent challenges like bioremediation, longterm underground storage of reactive waste or underground carbon-dioxide sequestration require more and more complex multicomponent reactive transport and fluid flow models. Although being demanding concerning their efficient numerical approximation, the decisive bottleneck in using such models seems to lie in the availability of the increasing range of reaction and hydraulic flow parameters entering such a model (Monod parameters in multiplicative Monod models in conjunction with bioremediation and rate parameters in kinetic mass action law models as well as van Genuchten parameters for the modelling of hydraulic properties ...). We address the reliable and accurate identification of such parameters from one of most controlled experimental set ups, namely from soil column breakthrough curves (letting the upscaling issue aside), but the following methology can also applied to field experiments. It is wellknown that the (missing) sensitivity and the correlation of parameters prevent a reliable reconstruction from naive history matching (output least squares minimization). For a fixed experimental setup we propose a systematic use of the singular values of the sensitivity matrix in the definition of the error functional to design an adaptive approach in which after each termination in a (local) minimum the error functional is changed. Applications to the identification of Monod and van Genuchten parameters show significant improvements in possible accuracy. Furthermore, a favourable form free approach with hierarchical treatment for the global parametrization of one- or multidimensional nonlinearities are used. Thereby, because of the so called *curse of dimensionality* sparse grids are applied in case of higher dimensional problems to decrease the degree of freedom significantly. In addition the presented methods can also be combined with a hierarchical concept to filter out the most sensitive parameters and identify them first. In a further step these approaches can be used also within experimental design to find more appropriate sequences of experiments which can be taken into account into an multiexperiment identification approach.