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Identification of Global and Local Parametrization of Material Laws in Fluid Flow and Reactive Transport through Porous Media by Hierarchical and Adaptive Output Least Squares Minimization

*** Michael BLUME[1], Peter KNABNER[2]**

[1] University of Erlangen-Nuremberg, Department of Mathematics
Martensstr. 3, 91058 Erlangen, Germany
blume@am.uni-erlangen.de, http://www1.am.uni-erlangen.de/~blume/

[2] University of Erlangen-Nuremberg, Department of Mathematics
Martensstr. 3, 91058 Erlangen, Germany
knabner@am.uni-erlangen.de, http://www1.am.uni-erlangen.de/members/knabner/

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ABSTRACT

Recent challenges like bioremediation, longterm underground storage of reactive waste or underground carbondioxide sequestration require more and more complex multicomponent reactive transport 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 parameters entering such a model (Monod parameters in multplicative Monod models in conjunction with bioremediation, rate parameters in kinetic mass action law models, ...). 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 parameters show significant improvements in possible accuracy. A second promising application is discudded concerning the identification of a global parametrization (van Genuchten-Mualem form) of soil hydraulic properties from soil column outflow experiments. The approach also can be farourably combined with form free approaches and their hierarchical treatment. Furthermore this approach may 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.