Geophysical Research Abstracts, Vol. 9, 02610, 2007
SRef-ID: 1607-7962/gra/EGU2007-A-02610

Evaluation of possible strategies for biogeochemical model calibration

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A large effort has been devoted in recent years to develop numerical models capable of accurately simulating reactive transport phenomena in soils. Certain factors have underpinned this progress, including improved understanding of the biogeochemical processes occurring in the subsurface, the development of more accurate and robust numerical schemes and the increased availability of computer power. These models have thereby become extremely useful for a wide range of applications, such as contaminant hydrogeology and contaminated site remediation design. Nevertheless, major difficulties are still faced when models are applied to real cases; among these, parameter calibration is a particularly challenging task. In the field of hydrology and hydrogeology, inverse modelling has been traditionally performed using gradient-based techniques, such has the Levenberg-Marquardt algorithm. While these methods have been successfully applied to calibrate flow models, experience proved that the performances of such tools are extremely poor in the calibration of biogeochemical models. Attractive alternatives to the gradient-based algorithms are the heuristic methodologies, because they are capable of exploring the parameter space without being diverted to local minima. In this work, we evaluated the performances of different calibration methodologies for a large set of reactions occurring in soils, such as biodegradation, cation exchange and surface complexation. Biogeochemical models were implemented in PHREEQC. We developed a computer code specifically tailored to be used with PHREEQC, where we implemented the simulated annealing and particle swarm optimization (PSO) approaches. We compared the performances of these heuristic methods with those of the Levenberg-Marquardt algorithm, as implemented in the software PEST. Results clearly show that the gradient-based techniques are of-

ten ineffective unless the initial parameter estimate is close to the correct results, and small parameter ranges are provided to the algorithm. Instead, heuristic approaches, and the PSO method particularly, are capable for most of the studied cases to provide good calibrations, even with a large number of model parameters; nevertheless, heuristic methods suffer of a lack in the fine tuning of the parameters.