Preface

Special issue on simulations of reactive transport: results of the MoMaS benchmarks

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This special issue of Computational Geosciences is dedicated to a selection of papers presented at the international workshop ‘Reactive Transport Modelling’. This meeting was organized in January 2008, in Strasbourg (France) by the MoMaS group and the University of Strasbourg. The research activities of the group MoMaS (Mathematical Modeling and Numerical Simulation for Nuclear Waste Management Problems - 2008–2011) are centred around scientific computing, design of new numerical schemes and mathematical modelling (upscaling, homogenization, sensitivity studies, inverse problems ...).

The selected papers are dedicated to the simulations of benchmarks which were designed to evaluate the performance of numerical models devoted to the simulation of reactive transport in saturated porous media. In numerical mathematics, benchmarking is one of the most popular ways of evaluating the quality of different numerical methods. This special issue gathers the results of simulations obtained by different numerical codes based on different numerical methods (finite volume, finite elements, discontinuous finite elements) and different ways of coupling the transport equations with the equations used to describe the chemistry: operator splitting approaches (iterative or non itera-

tive) or global methods (direct substitution approach, differential and algebraic equations).

The benchmarks deal with reactive transport problems in 1 or 2 dimensions, with advective or diffusive dominant transport. The parameters were chosen to highlight expected numerical problems such as oscillations, numerical diffusion and convergence. These benchmarks are presented in the first paper of this issue. The following papers are dedicated to a detailed presentation of the numerical codes and their related simulations. Finally, the last paper is devoted to the comparison of the different results.

In terms of performance, it appears that a single ‘best method’ could not be identified by these benchmarks. This exercise also clearly demonstrates that more researches on numerical methods are necessary to improve the efficiency of the numerical codes (only a few codes were able to solve the 2D problem ...). Furthermore, benchmark collections (synthetic examples or well designed laboratory experiments) should be created in order to perform fair evaluations and comparisons of methods and software.

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