

GLOBAL IMPLICIT SOLVER FOR MULTIPHASE MULTICOMPONENT FLOW IN POROUS MEDIA WITH MULTIPLE GAS PHASES AND GENERAL REACTIONS

Markus M. Knodel, Serge Kräutle and Peter Knabner

Keywords: PDE reduction method, nested Newton, equilibrium reactions, M++, CO₂.

In order to predict the gas and liquid flow and the efficiency of trapping mechanisms (mineral trapping) for CO₂ storage in deep layers, the system to be solved consists of diffusion-advection-reaction partial differential equations (PDEs), algebraic equations (AEs) and ordinary differential equations (ODEs).

The choice of a suitable formulation of the equations is important for efficient numerical solution. We apply the Kräutle-Knabner PDE reduction method [1] which enables to eliminate the equilibrium reactions based upon specific variable transformations. Separating the resulting remaining PDE/ODE/AE system into a global and a local system, we apply a nested Newton solver method [2] which enables fast and efficient computation of the dynamics of the system by means of the application of parallel solvers to the Finite Element discretized / Finite Volume stabilized PDE system. Our computations of the behavior of the concentrations of the different species of the multiphase multicomponent flow are highly resolved in space and time. We study the mineral trapping scenario [3] using splines derived from experiments for the equations of state (EOS) which describe the interphase mass exchange of CO₂ and the density of CO₂. To this end, we present the work in progress concerning the elaboration and implementation of our methods into the software package M++ for the computation of a recent benchmark which inherits multiple gas phases [4].

References

- [1] S. Kräutle and P. Knabner, *A reduction scheme for coupled multicomponent transport-reaction problems in porous media: Generalization to problems with heterogeneous equilibrium reactions*, Water Resour. Res., 43, W03429, 2007.
- [2] S. Kräutle, *The semismooth Newton method for multicomponent reactive transport with minerals*, Advances Water Res., 34, pp. 137-151. 2011.
- [3] F. Brunner and P. Knabner, *A global implicit solver for miscible reactive multiphase multicomponent flow in porous media*, Computational Geosciences, 23, pp. 127-148, 2019.
- [4] I. Sin, V. Lagneau, L. De Windt and J. Corvisier, *2D simulation of natural gas reservoir by two-phase multicomponent reactive flow and transport - description of a benchmarking exercise*, Mathematics and Computers in Simulation, 137, pp. 431-447. 2017.

M.M. Knodel, S. Kräutle and P. Knabner
Applied Mathematics 1, Universität Erlangen-Nürnberg
markus.knodel@math.fau.de, kraeutle@math.fau.de, knabner@math.fau.de