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Global implicit solver for multiphase multicomponent flow in porous media with multiple gas components and general reactions

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In order to study the efficiency of the various forms of trapping including mineral trapping scenarios for CO₂ storage behavior in deep layers of porous media, highly non-linear coupled diffusion-advection-reaction partial differential equations (PDEs) including kinetic and equilibrium reactions modeling the miscible multiphase multicomponent flow have to be solved. We apply the globally fully implicit PDE reduction method (PRM) developed 2007 by Krättele and Knabner for one-phase flow, which was extended 2019 to the case of two-phase flow with a pure gas in the study of Brunner and Knabner. We extend the method to the case of an arbitrary number of gases in gaseous phase, because CO₂ is not the only gas that threatens the climate, and usually is accompanied by other climate killing gases. The application of the PRM leads to an equation system consisting of PDEs, ordinary differential equations, and algebraic equations. The Finite Element discretized / Finite Volume stabilized equations are separated into a local and a global system but nevertheless coupled by the resolution function and evaluated with the aid of a nested Newton solver, so our solver is fully global implicit. For the phase disappearance, we use persistent variables which lead to a semismooth formulation that is solved with a semismooth Newton method. We present scenarios of the injection of a mixture of various gases into deep layers, we investigate phase change effects in the context of various gases, and study the mineral trapping effects of the storage technique. The technical framework also applies to other fields such as nuclear waste storage or oil recovery.

Participation

In-Person

References

Global implicit solver for multiphase multicomponent flow in porous media with multiple gas components and general reactions. Comput Geosci 26, 697-724 (2022). M.M. Knodel, S. Krättele, and P. Knabner. doi.org/10.1007/s10596-022-10140-y

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