Numerical Simulation of Compositional Two-Phase Flow in Porous Media with Applications in CO₂ Sequestration High Performance Scientific Computing

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Abstract: We deal with the numerical modeling of compressible multicomponent two-phase flow in porous media with species transfer between the phases. The mathematical model is formulated by means of the extended Darcy's laws for all phases, components continuity equations, constitutive relations, and appropriate initial and boundary conditions. The splitting of components among the phases is described using a formulation of the local thermodynamic equilibrium which uses volume, temperature, and moles as specification variables.

The problem is solved numerically using a combination of the mixed-hybrid finite element method for the total flux discretization and the finite volume method for the discretization of continuity equations. These methods ensure the local mass balance. The resulting system of nonlinear algebraic equations is solved by the Newton-Raphson iterative method. The numerical flux is discretized in a way that no phase identification nor determination of correspondence between the phases on adjacent elements is required in contrast to the traditional approaches. This is very important for the simulations of CO_2 sequestration because, typically, the CO_2 is injected into a reservoir in the supercritical state at which the phase distinction is ambiguous. Moreover, our model performs well in situations where a phase appears or disappers and no switching of variables is needed.

We briefly describe the numerical method and provide several 2D simulations, e.g. CO_2 injection into water saturated reservoir, to show advantageous features of our approach. The simulation of the CO_2 and water mixture is also compared with experimental data to verify our numerical model.

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