A NOVEL EULERIAN-LAGRANGIAN FORMULATION FOR COMPOSITIONAL FLOW IN THE SUBSURFACE

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Compositional models describe the simultaneous transport of multiple components flowing in coexisting phases through porous media. Because each component can transfer between different phases, the mass of each phase or a component within a particular phase is no longer conserved. Instead, the total mass of each component among all the phases must be conserved, leading to very large, strongly coupled systems of transient nonlinear advection-diffusion equations. These equations are closely coupled to a very large set of constraining equations, which are strongly nonlinear, implicit functions of phase pressure, phase temperature, and mole fractions and need to be solved on all computational cells at each time step in thermodynamic flash calculations. Additional difficulties include the strong influence of singular sources and sinks, heterogeneities of the porous media, high compressibilities of the fluids, large adverse mobility ratio, anisotropic dispersion in tensor form, and enormous size of field-scale applications. Consequently, these models present severe mathematical and numerical difficulties. Classical second-order methods tend to yield numerical solutions with nonphysical oscillations. In industrial applications, upwind methods with fully coupled and fully implicit temporal discretization have commonly been used to stabilize the numerical approximations. However, these methods often generate excessive numerical dispersion and serious spurious effects due to grid orientation.

Eulerian-Lagrangian methods symmetrize the transport equations and generate accurate numerical solutions even if very large time steps and coarse spatial grids are used. They have shown great performance in the numerical simulations of single-phase flow and immiscible two phase flow. However, there exist serious mathematical and numerical difficulties that hinder the development of such methods for multiphase multicomponent compositional flows in multiple space dimensions: (1) Eulerian-Lagrangian methods require the governing equations to have a well-defined transport velocity in terms of their primary unknowns. The molar mass balance equations in compositional flows are expressed as a weighted sum of mole fractions and phase velocities in different phases. (2) Although the excessive numerical diffusion present in upwind methods severely smears the moving steep fronts and introduces grid orientation effect, it firmly subdues and hides various numerical difficulties. Eulerian-Lagrangian methods minimize numerical diffusion in upwind methods, leading to significantly improved accuracy. However, the numerical difficulties subdued by the excessive numerical diffusion in upwind methods reoccur. Moreover, the use of Lagrangian coordinates in Eulerian-Lagrangian methods introduces extra difficulties. All these numerical difficulties are in addition to the mathematical and numerical difficulties of compositional modeling.

In this talk, we present a novel Eulerian-Lagrangian formulation for multiphase and multicomponent compositional flow. Our preliminary numerical experiments show that the resulting numerical scheme generates stable and physically reasonable numerical solutions even if extremely large time steps (of more than 0.1 pore volume injected) is used. This shows that the strong potential of the proposed mathematical formulation.