

Simulating Compositional Two-Phase Fluid Systems using a Diffusive Interface Model

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In this talk, we report our recent work in simulating partially miscible, compositional two-phase fluid systems using a diffusive interface model together with a cubic Equation of State (EOS). It is our hope that this research will lead to the eventual goal of simulating two-phase systems consisting of hydrocarbon components at a pore scale with realistic oil/gas applications. In the presentation, a partial difference equation system is proposed to model the compositional two-phase system, and the spatial discretization is then established with a finite volume-based method. We first computationally decouple the resultant ordinary differential equation system by using a splitting scheme, and we integrate in time using a semi-implicit marching scheme. Most fully implicit methods surprisingly fail to have the desired stability, while a properly designed semi-implicit time marching scheme works reasonably well. This proposed semi-implicit time scheme is based on a convex splitting idea, and it is unconditionally energy stable. The proposed algorithm is able to solve successfully the spatially heterogeneous two-phase systems with varied molar density profiles in multiple dimensional domains. We also compare our computational results with laboratory experimental data reported in the literature.