The Hong Kong Polytechnic University
Department of Applied Mathematics

Colloquium

A robust and convergence-guaranteed iterative algorithm for simulating two-phase equilibria of multi-component fluids at constant moles, volume and temperature

by

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Abstract

Phase behavior of partially miscible two-phase or multi-phase fluid mixture is a key to understand subsurface multi-phase flow, especially in a petroleum reservoir. Accurate modeling and robust computation of the phase behavior is essential for optimal design and cost-effective operations in a petroleum processing plant. A typical problem formulation in phase behavior is two-phase constant volume flash, i.e. the two-phase phase-split under the constant temperature, moles, and volume, which is stated as follows. Consider a closed system of constant volume V in which there is a mixture of c components with mole numbers n1, ..., nc at temperature T. Assuming that the system is in two-phase, we want to establish compositions and amounts of both phases. One motivation for constant volume flash (or NVT flash) is the equilibrium calculation in a mixing cell when two non-equilibrium phases are introduced. Conventional algorithms for flash calculation are based on fixed-point iteration, Newton-type iteration, or their combination, and the convergence has never been guaranteed. In this work, we propose an energy-stable iterative method for the calculation of the phase equilibria under given volume, temperature, and moles (NVT-flash). An iterative algorithm for describing the dynamics of two-phase fluid system is based on Fick's law of diffusion for multi-component fluids and the Peng-Robinson equation of state. The mobility is obtained from diffusion coefficients by relating the gradient of chemical potential to the gradient of molar density. The evolutional equation for moles of each component is derived using the discretization of diffusion equations, while the volume evolutional equation is constructed based on the mechanical mechanism and the equation of state. By using the Euler time scheme to discretize this evolutional system, we develop an energy stable algorithm with an adaptive choice strategy of time steps, which allows us to calculate the suitable time step size to guarantee the physical properties of moles and volumes, including positivity, maximum limits and correct definition of the Helmholtz free energy function. The proposed iterative procedure is also proven to be energy stable under the proposed time step choice. Numerical examples are tested to demonstrate efficiency and robustness of the proposed method.

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