Phase-field modeling of two-phase lattice Boltzmann method

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Abstract

In this paper, we introduce a diffuse interface model to simulate multi-component two-phase flow with partial miscibility based on a realistic equation of state (e.g. Peng–Robinson equation of state). Because of partial miscibility, thermodynamic relations are used to model not only interfacial properties but also bulk properties, including density, composition, pressure, and realistic viscosity. As far as we know, this effort is the first time to use diffuse interface modeling based on equation of state for modeling of multi-component two-phase flow with partial miscibility. In numerical simulation, the key issue is to resolve the high contrast of scales from the microscopic interface composition to macroscale bulk fluid motion since the interface has a nanoscale thickness only. To efficiently solve this challenging problem, we develop a multi-scale simulation method. At the microscopic scale, we deduce a reduced interfacial equation under reasonable assumptions, and then we propose a formulation of capillary pressure, which is consistent with macroscale flow equations. Moreover, we show that Young–Laplace equation is an approximation of this capillarity formulation, and this formulation is also consistent with the concept of Tolman length, which is a correction of Young–Laplace equation. At the macroscopical scale, the interfaces are treated as discontinuous surfaces separating two phases of fluids. Our approach differs from conventional sharp-interface two-phase flow model in that we use the capillary pressure directly instead of a combination of surface tension and Young–Laplace equation because capillarity can be calculated from our proposed capillarity formulation. A compatible condition is also derived for the pressure in flow equations. Furthermore, based on the proposed capillarity formulation, we design an efficient numerical method for directly computing the capillary pressure between two fluids composed of multiple components. Finally, numerical tests are carried out to verify the effectiveness of the proposed multi-scale method.

Keywords

Multi-component two-phase flow; Partial miscibility; Multi-scale simulation; Equation of state; Young–Laplace equation; Tolman length.

1. Introduction

Simulation of fluid flow and transport in porous media[1-7] has wide applications in subsurface environmental sciences and petroleum engineering. Numerical modeling and simulation of multi-phase fluid flow with a realistic equation of state (e.g. Peng–Robinson equation of state) is an attractive and challenging research subject in recent years[8-11]. It plays very important role in pore scale modeling and simulation of subsurface fluid flow, especially oil reservoir simulation. Partial miscibility of multiple fluids is a common phenomenon in the experiments and practical applications; actually, the complete miscibility and immiscibility can be viewed as two extremes of partial miscibility according to the thermodynamic theory. Fluids that are completely miscible have been extensively studied in reservoir simulation, for example,[12-14]; there are also many efforts devoted to multiphase immiscible fluid flow in porous media, for example,[15-17]. Many pairs of fluids, however, are only partially miscible, for example, mixing of CO2 and hydrocarbon; in these cases, the degree of miscibility often depends strongly on pressure, temperature and composition of a

mixture. An interface exists between any two immiscible or partially miscible fluids. On the interface, the molecules experience a stronger attractive pull towards the interior of the fluid body, since fluid molecules do not surround the interface molecule equally in all directions. Capillarity effect caused by this anisotropic attractive force significantly impacts the motion of multiple fluids and the shape of the liquid-gas interface. Based on thermodynamics, compositional fluid flow in porous media has been modeled and simulated successfully, for example,[18-20]. However, to our knowledge, at a pore scale, multi-component two-phase fluid flow has not been modeled so far.

In this work, based on thermodynamic relations, for the first time we will introduce a diffuse interface model to simulate multi-component two-phase flow with partial miscibility based on a realistic equation of state (e.g. Peng–Robinson equation of state). In our proposed model, there may exist diffuse interfaces with nonzero thickness between two phases, and the two-phase fluids may mix in these interfaces. So this model reflects the partial miscibility that real fluids always display. Properties of partial miscible fluids are modeled by a unified form for both interfaces and bulk phases. This general framework of multi-component two-phase fluid flow is governed by mass conservation and flow equations based on a realistic equation of state and a consistent viscosity model.

2. Simulation

In the microscale interfacial model, we have proposed a direct calculation formulation for the capillary pressure of two-phase multicomponent fluids, and relations of this formulation to Young–Laplace equation and Tolman length have also been investigated in theory. Numerical results are presented in this subsection to verify theoretical results.The capillary pressure difference illustrated in Figs. 1

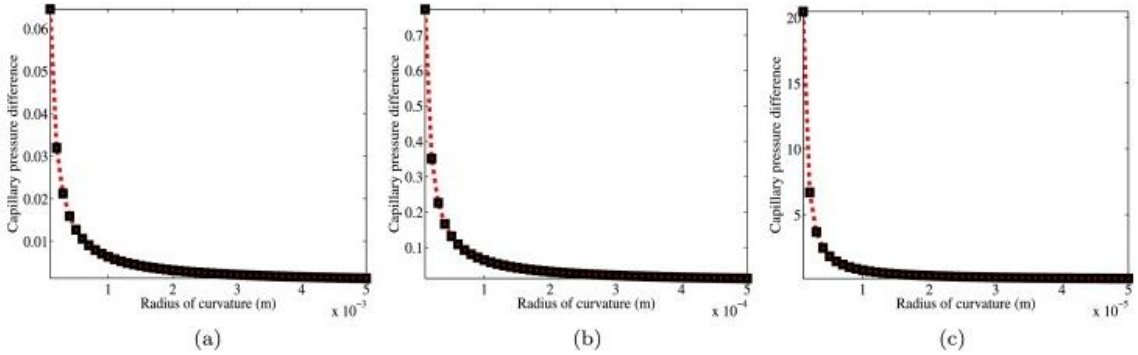


Fig. 1. The capillary pressure difference results at different curvature radiuses.

Figs. 2 illustrate the two-phase interface thickness results, which are computed by (4.14). We can see that the interface thickness will become slightly large as the curvature radius increases, but its magnitude is only near three nanometers. This indicates the necessity of multi-scale numerical modeling and simulation for macroscopical two-phase flow.

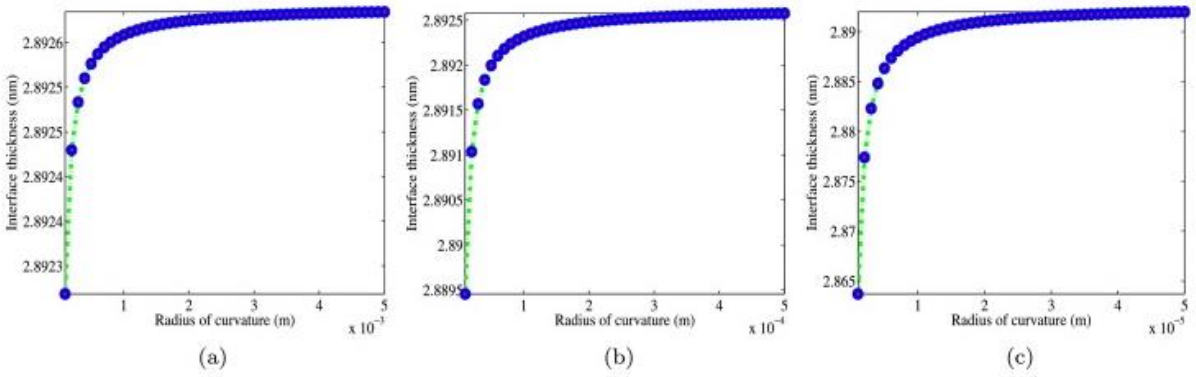


Fig. 2. The interface thickness results at different curvature radiuses.

The simulation domain is a horizontal layer with the square domain dimensions2 cm×2 cm. With domain being horizontal, the effect of gravity is neglected in this example. A uniform rectangular mesh with 20×20 grid cells is applied for simulating the macroscopical motion of fluids, and the no-flow boundary conditions are imposed. In initial conditions, as shown in Fig. 3(a), a droplet having the shape of an ellipse is located at the center of the domain. The grid of the interface is composed of 200 line segments. The simulation time is applied for the interface equation only, and it is set as 0.5 milliseconds.

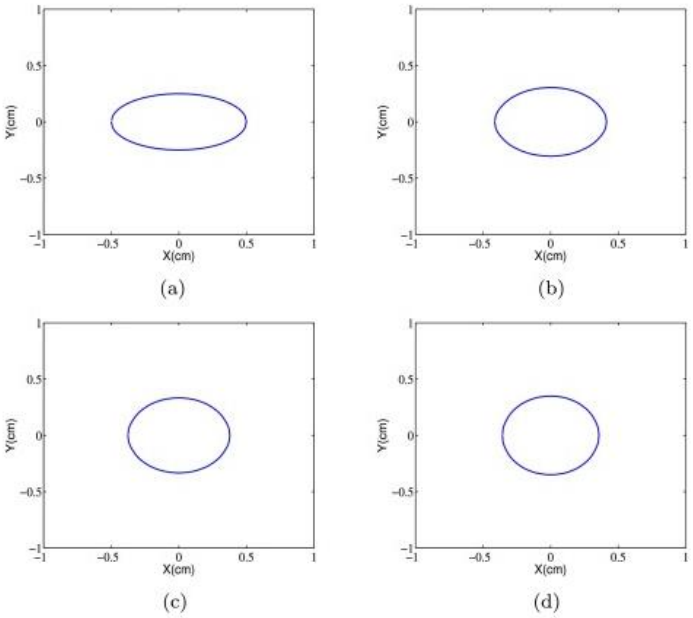


Fig. 3. Droplet deformation problem in steady Stokes flow: the interface shape profiles at the initial time (a), 5th (b), 10th (c) and 20th (d) time step respectively.

The interface shape profiles at the initial time and different time steps are shown in Figs. 3, and the pressure contours and velocity fields at different time steps are illustrated in Figs. 4and Figs. 5.

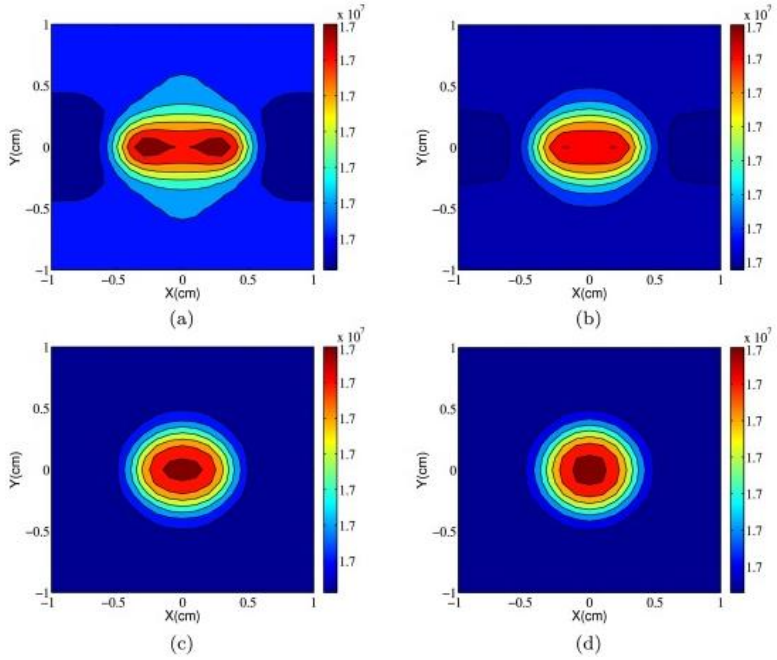


Fig. 4. Droplet deformation problem in steady Stokes flow: the pressure contours at the 1th (a), 5th (b), 10th (c) and 20th (d) time step respectively.

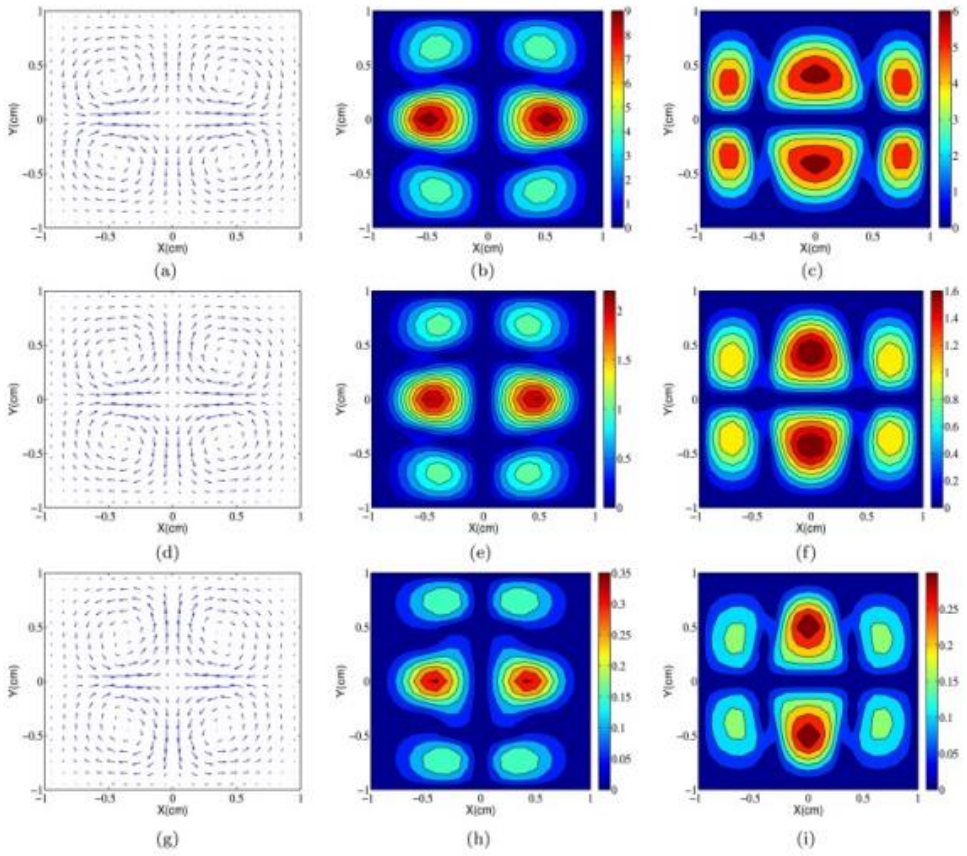


Fig. 5. Droplet deformation problem in steady Stokes flow: the flow quivers (left column), magnitude contours of X-direction velocity component (center column), and magnitude contours of Y-direction velocity component (right column) at the 1th (top row), 10th (center row), and 20th (bottom row) time step respectively.

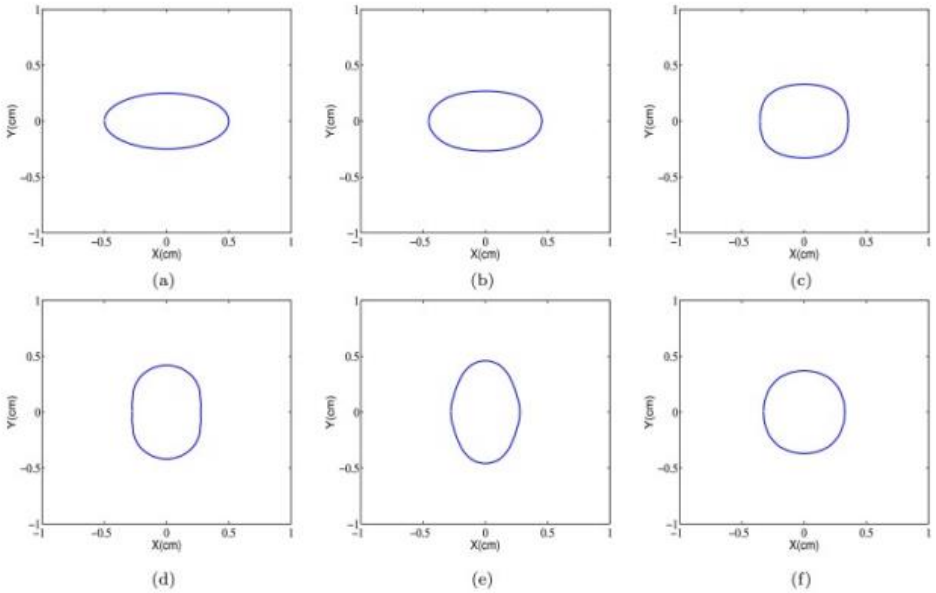


Fig. 6. Droplet deformation problem in unsteady flow: the interface shape profiles at the initial time (a), 5th (b), 10th (c), 15th (d), 25th (e) and 30th (f) time step respectively.

In initial conditions, the velocity is taken to be zero everywhere, and the initial interface position is the same to the problem in the subsection 5.2, which is also shown in Fig. 6(a). The grid of the interface is composed of 200 line segments. The simulation time is 0.21 seconds. The time step size

is uniformly taken to be 0.007 seconds; that is, we use 30 time steps for this simulation. These time settings are applied for both the interface equation and Navier–Stokes equations.

The interface shape profiles at the initial time and different time steps are shown in Figs. 6, while the pressure contours and velocity fields at different time steps are illustrated in Figs. 7and Figs. 8 respectively.

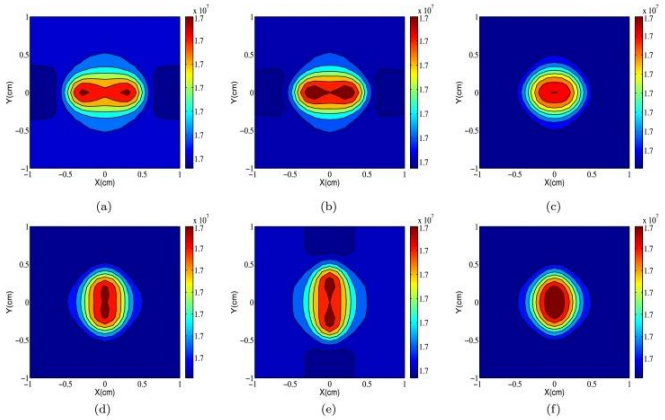


Fig. 7. Droplet deformation problem in unsteady flow: the pressure contours at the 1th (a), 5th (b), 10th (c), 15th (d), 25th (e) and 30th (f) time step respectively.

The simulation domain is a vertical layer with the domain dimensions 9 mm×9 mm. This domain is divided by a uniform rectangular mesh with 30×30 grid cells. The no-flow boundary conditions are used for the Navier–Stokes equations. In the initial conditions, the velocity is taken to be zero everywhere, and the initial interface is a circle, which is shown inFig. 9(a). The grid of the interface is composed of 1000 line segments. The simulation time is 60 milliseconds.

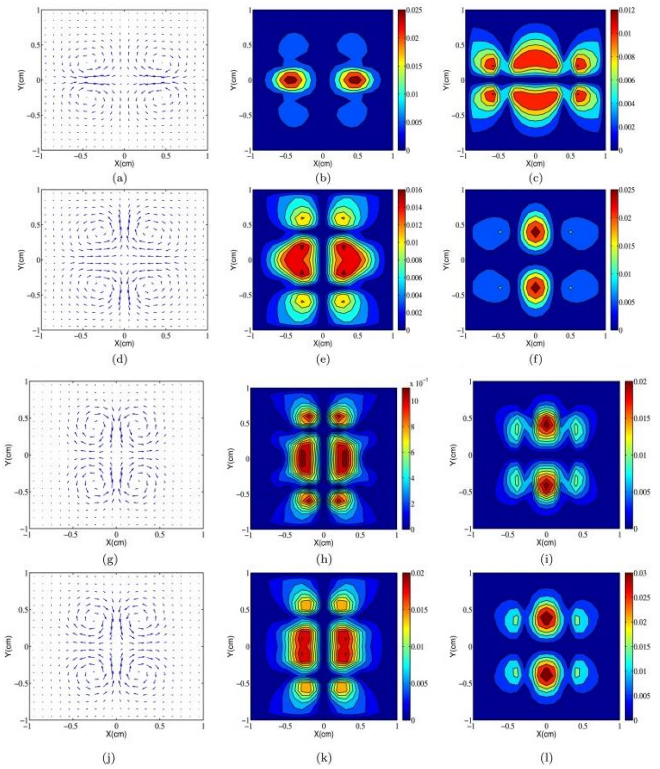


Fig. 8. Droplet deformation problem in unsteady flow: the flow quivers (left column), magnitude contours of X-direction velocity component (center column), and magnitude contours of Y-direction velocity component (right column) at the 5th (the first row), 15th (the second row), 25th (the third row), and 30th (the last row) time step respectively.

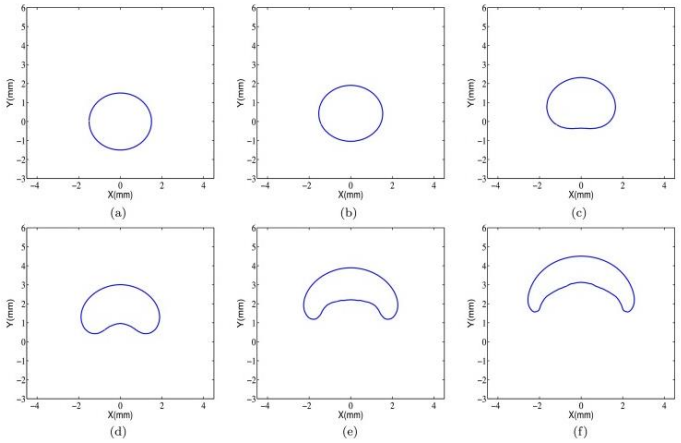


Fig. 9. Bubble rising problem: the bubble interface shape profiles at the initial time (a), 20th (b), 30th (c), 45th (d), 65th (e) and 80th (f) time step respectively.

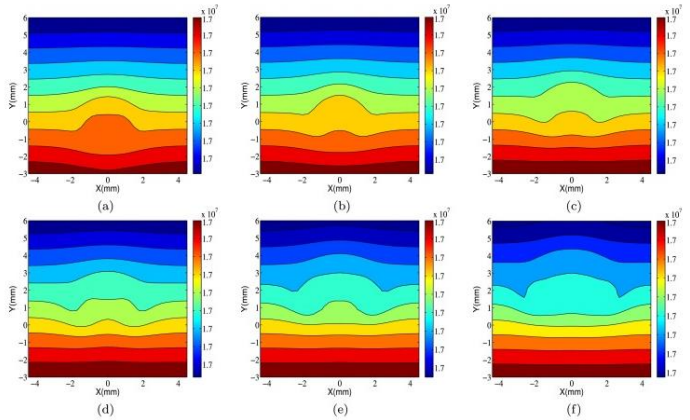
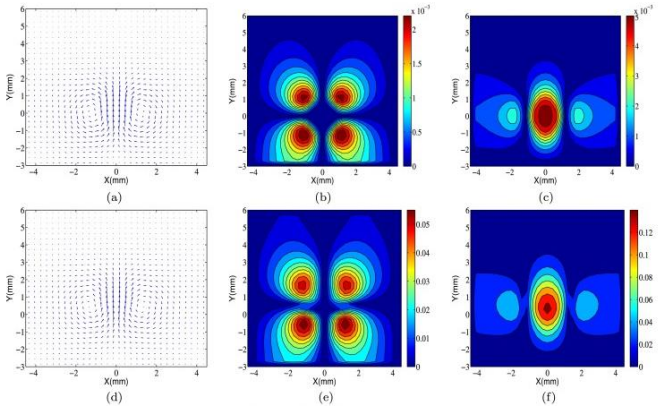


Fig. 10. Bubble rising problem: the pressure contours at the 1th (a), 20th (b), 30th (c), 45th (d), 65th (e) and 80th (f) time step respectively.

Figs. 11 show the velocity fields and magnitude contours of velocity components at different time steps, respectively.From Figs. 10, we can see that although the gravity has effect on the pressure fields, the pressures are also close to the bulk-phase pressure 170 bar, and thus, the phase splitting exists stably in this multi-component mixture.



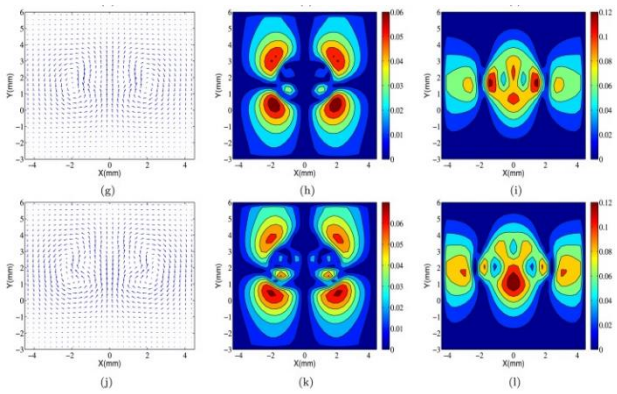


Fig. 11. Bubble rising problem: the flow quivers (left column), magnitude contours of X-direction velocity component (center column), and magnitude contours Y-direction velocity component (right column) at the 1th (the first row), 30th (the second row), 65th (the third row), and 80th (the last row) time step respectively.

3. Conclution

A diffuse interface model has been introduced to simulate multi-component two-phase flow with partial miscibility based on a realistic equation of state (e.g. Peng–Robinson equation of state) and a consistent viscosity model. In order to simulate this model problem, we develop a multi-scale simulation method, which can resolve the scale contrast between the nanoscale interface and macroscale bulk fluid motion. In the macroscale flow, two fluids are separated by the sharp interfaces, and the capillary pressure is straightforwardly incorporated into Navier–Stokes equations instead of a combination of surface tension and Young–Laplace equation. A compatible condition is also derived for the pressure in flow equations. In the microscopic interface, in order to establish the coupling relation with macroscale flow equations, we deduce a formulation of capillary pressure from a reduced interfacial equations. Moreover, Young–Laplace equation is viewed as an approximation of this capillarity formulation, and this formulation also matches the concept of Tolman length. For numerical methods, the front-tracking method is applied to simulate the macroscale fluid flow, and based on the proposed capillary pressure formulation, we propose an efficient numerical method for directly computing the capillary pressure between two fluids composed of multiple components. Numerical results are provided to verify the effectiveness of the proposed multi-scale method.

Acknowledgements

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