Journal of Computational Physics 318 (2016) 349–372

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Multi-scale diffuse interface modeling of multi-component two-phase flow with partial miscibility ☆

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ARTICLE INFO

Article history:
Received 15 November 2015
Received in revised form 27 April 2016
Accepted 27 April 2016
Available online 10 May 2016

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

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.

☆ This work is supported by National Natural Science Foundation of China (No. 11301163), and KAUST research fund to the Computational Transport Phenomena Laboratory.

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http://dx.doi.org/10.1016/j.jcp.2016.04.055
0021-9991/

1. Introduction

Simulation of fluid flow and transport in porous media [6,10,13,30,38–40] 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 [20–22,35]. 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, [8,32,44]; there are also many efforts devoted to multiphase immiscible fluid flow in porous media, for example, [4,17,23]. Many pairs of fluids, however, are only partially miscible, for example, mixing of CO_2 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, [18,29,33]. 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.

For simulating the proposed model problem, we will develop a multi-scale numerical simulation method. As shown in [20,21], the gas and liquid interface has a nanoscale thickness, and as a result, the interfacial structure and behavior must be simulated at a microscopic scale. However, numerical simulation at a macroscopic scale is required to meet the needs of many practical applications, for example, subsurface flow simulation at the pore scale. Thus, the contrast between these two spatial scales is the primary challenge encountered in simulation of multi-phase fluid flow with a realistic equation of state. The direct numerical simulation of this problem needs to locally refine the mesh around the interfaces; even so, it will still lead to enormous computation cost and memory requirements, so it is not a preferable choice. Multi-scale concept has been extensively used in fundamental and practical problems, for example, [9,12,19,37]. For multi-scale simulation for multi-phase flow, we refer to the references [7,14,45,46] for instance. In these reported works, however, a realistic equation of state has not been included, and a realistic capillarity has also not been modeled and simulated at the microscopic interfacial scale. In this work, following a multi-scale concept, we will develop a multi-scale numerical simulation method for multi-component two-phase fluid flow with partial miscibility based on the Peng–Robinson equation of state.

At a macroscopic scale, due to the measure contrast between bulk fluids and their interfaces, the gas–liquid interfaces will be treated sharply; that is, the interfacial thickness is assumed to be zero. The motion of the bulk fluids is dominant at this scale. The force effect arising on the interface is characterized by capillarity between immiscible fluids, which is actually one of major forces in fluid motion. Physical properties such as fluid composition, density and viscosity have discontinuous values at this sharp interface. A number of numerical methods have been developed to simulate similar problems of multi-phase flow, for example, level set methods [31], volume of fluid (VOF) method [2,16]. The front tracking method [41,43] is a natural and straightforward simulation method for the macroscopic scale problem. In this method, a fixed grid is used to simulate the fluid motion governed by Navier–Stokes equations, while the interface is represented by curves in two dimensions and surfaces in three dimensions. In this work, we directly incorporate capillarity into Navier–Stokes equations instead of the conventional treatment that incorporates surface tension using Young–Laplace equation. The capillarity effect will be evaluated by a microscopic interfacial model derived in this work.

At a microscopic scale, we will model partial miscibility of two-phase fluids on the interfaces. Physical properties of fluids continuously vary from the one phase to the other phase within diffuse interfaces. This partial miscibility leads to inhomogeneous compositions on the interfaces, and it is also the leading mechanism of surface tension and its resulted capillary pressure. In the conventional method, the surface tension is first calculated based on the interfacial composition, and then the capillary pressure is obtained using Young–Laplace equation. However, the surface tension of a small liquid droplet or bubble generally deviates from its planar value [1]. Indeed, the Tolman length is introduced to measure the extent of this deviation, but its expression contains tuned or adjustable parameters and it is not easy to be evaluated in practice [1]. The interfacial numerical simulation methods in one dimension, for example [20,27,28], are not perfect choices for our microscopic problem. On the other hand, the interface is treated as a discontinuous surface without interfacial thickness at the macroscopic scale, and as a result, its geometrical shape can not be clarified at the microscopic scale. This means that at a microscopic scale, we also can not use the numerical modeling and simulation based on general multi-dimensional domain, for example [21,22,35]. To address this challenge, in this work we will derive a new formulation of capillarity based on a realistic equation of state, and also design an efficient numerical calculation method.