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Efficient numerical methods for simulating surface tension of multi-component mixtures with the gradient theory of fluid interfaces☆

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Highlights

- Proposed schemes overcome challenges of the infinite domain and matrix singularity.
- Efficient methods are formulated for surface tension of multi-component mixtures.
- Proposed algorithms are based on a linear transformation and a path function.
- Proposed algorithms are successfully tested using extensive hydrocarbon examples.

Abstract

Surface tension significantly impacts subsurface flow and transport, and it is the main cause of capillary effect, a major immiscible two-phase flow mechanism for systems with a strong wettability preference. In this paper, we consider the numerical simulation of the surface tension of multi-component mixtures with the gradient theory of fluid interfaces. Major numerical challenges include that the system of the Euler–Lagrange equations is solved on the infinite interval and the coefficient matrix is not positive definite. We construct a linear transformation to reduce the Euler–Lagrange equations, and naturally introduce a path function, which is proven to be a monotonic function of the spatial coordinate variable. By using the linear transformation and the path function, we overcome the above difficulties and develop the efficient methods for calculating the interface and its interior compositions. Moreover, the computation of the surface tension is also simplified. The proposed methods do not need to solve the differential equation system, and they are easy to be implemented in practical applications. Numerical examples are tested to verify the efficiency of the proposed methods.

MSC: 65N30; 65N50; 49S05

Keywords: Surface tension; Multi-component mixtures; Euler–Lagrange equations; Gradient theory

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1. Introduction

Subsurface flow and transport often involve multiple fluid phases; that is, subsurface phenomena often come with mixture of immiscible and partially miscible fluids. Subsurface oil and gas reservoirs typically contain oil phase, gas phase and water phase, together with the solid phase (rock or soil) [1]. Modeling and simulation of multiphase fluid systems have been a major effort in reservoir engineering [2]. In addition to oil reservoir management, understanding and modeling of multiphase systems are also crucial to many environment issues [3,4]. For example, one of the most attractive and practical solutions to reduce the CO_2 emission problem is to inject and store CO_2 in the subsurface geological formations [5], such as depleted reservoirs and deep saline aquifers. The large capacity of subsurface storage provides several advantages over other possible alternatives of carbon sequestration. For subsurface carbon sequestration, there are four well-accepted major mechanisms to trap the injected CO_2 for long-term storage, namely, structural (stratigraphic) trapping, residual fluid trapping, solubility trapping and mineral trapping; all of the four major mechanisms are directly or indirectly related to phase behaviors of fluid systems.

At a pore scale, a surface or an interface exists between any two immiscible or partially miscible fluids and between a fluid and a solid. It is well known that at the molecular level of a liquid and gas interface for instance, the interior molecules of the liquid phase experience zero (or negligible) net attractive forces from the surrounding molecules because the molecules are all similar with approximately equal spacing and equal attraction in all directions. However, on the interface, the molecules experience a stronger attractive pull towards the interior of the liquid body, since fluid molecules do not surround the interface molecule equally in all directions. This anisotropic attractive force yields interfacial tension and impacts the shape of the liquid–gas interface. At the Darcy scale, we do not model the liquid–gas interfaces explicitly [6,7], but the existence of these liquid–gas interfaces manifests themselves by many Darcy-scale phenomena.

Capillary effect (or capillarity) is perhaps one of the most important Darcy-scale phenomena arising from the pore-scale liquid–gas interfaces. Capillary effect and its resultant capillary pressure are caused by surface tension between immiscible (or partially miscible) fluids, and it is one of major forces in fluid (oil, gas and water) flow and transport in subsurface [2]. In fact, the capillary effect is frequently the leading mechanism of oil recovery in fractured oil reservoirs. In addition to capillary pressure, surface tension also significantly influences other important parameters of porous medium processes including relative permeability and residual saturations, thus substantially impacts the flow and the transport of the vapor and liquid phases in a porous medium; consequently, it plays important roles in a number of chemical and reservoir engineering problems [8–10].

To simulate the subsurface multiphase flow and transport accurately and efficiently, it is important to model and compute the surface tension of the multiphase mixture properly. There are a few models in the literature for simulating the multicomponent surface, for example, the gradient theory of fluid interfaces [11] and inhomogeneous molecular modeling simulation of multicomponent surface [12–14]. In this paper, we focus on the gradient theory of fluid interfaces, which has been a frequently-used method to model and predict the surface tension [8–11]. In our previous work [15], we have developed an efficient computational scheme to model and calculate the surface tension of single-species two-phase fluid systems based on our rigorous mathematical re-formulation of the gradient theory. In the work presented in this paper, we propose a few efficient computational methods to calculate the surface tension of multiple-species two-phase fluid systems. We note that the work presented here is not a simple extension of our previous work; instead, new computational treatment is proposed to address the challenges of multiple-species systems.

In the gradient theory, the Helmholtz energy density of an inhomogeneous fluid, in the absence of an external potential, is the sum of two contributions: the Helmholtz energy of homogeneous fluid at local composition, and a corrective term, which is function of the local density gradients. By applying the minimum free energy criterion, the compositions in the interface must satisfy the following Euler–Lagrange equations [8,9,15]

$$\sum_{j=1}^{N} c_{ij} \frac{d^2 n_j}{dx^2} = \mu_i^0 - \mu_i, \quad i = 1, \ldots, N, \tag{1.1}$$

where N is the component number of a mixture, $\mathbf{n} = [n_1, n_2, \ldots, n_N]^T$ denotes the molar densities, and the coefficients c_{ij} denote the influence parameters. To describe the definitions of μ_i^0 and μ_i, we first need to define the Helmholtz energy of homogeneous fluid by $f_0(\mathbf{n})$, and its expression is given in Appendix A. From this, the chemical potential of component i is defined by