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An adaptive finite element method for simulating surface tension with the gradient theory of fluid interfaces

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ABSTRACT

The gradient theory for the surface tension of simple fluids and mixtures is rigorously analyzed based on mathematical theory. The finite element approximation of surface tension is developed and analyzed, and moreover, an adaptive finite element method based on a physical-based estimator is proposed and it can be coupled efficiently with Newton's method as well. The numerical tests are carried out both to verify the proposed theory and to demonstrate the efficiency of the proposed method.

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1. Introduction

A number of chemical and reservoir engineering problems strongly depend on surface tension, such as capillary pressure, relative permeabilities, and the parameters characterizing the transport of the vapor and liquid phases in a porous medium [1–3]. The gradient theory of fluid interfaces [4] is a popular method to model and predict the surface tension. One main input of the gradient theory is the Helmholtz free energy density of a homogeneous fluid, which can be computed by a thermodynamic model. By the minimum free energy criterion, we can derive the corresponding Euler–Lagrange equations to calculate the molar densities of components at the liquid–vapor interface, and based on the density distributions, we can further calculate the magnitude of surface tension at the interface [1,2]. The gradient theory of fluid interfaces has been successfully utilized in chemical and reservoir engineering applications, but usually without the rigorous mathematical fundamentals. In this paper, we will analyze this theory rigorously by a combination of thermodynamics and mathematical theory of variational calculus [5].

When the gradient theory is applied to calculate the surface tension, one key problem is to solve the nonlinear Euler–Lagrange equations for capturing component density distributions at the interfaces. Adaptive finite element methods have been developed currently as a fundamental numerical instrument to approximate partial differential equations in scientific and engineering problems [6–12]. For the surface tension computation considered here, the adaptive technique is capable of adaptively capturing the location of interface between two phases. We need to design a preferable *a posteriori* error estimator that is an essential ingredient of adaptivity [13]. Following the pioneering work of Babuška [6,7], a great deal of effort has been devoted to the design of *a posteriori* error estimators, and now these are computable quantities depending

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on the computed solutions and data, and thus they can be used to make judicious mesh modifications. With the perfect error estimators, we can make local mesh modifications by refinement, and the approximation errors will eventually decrease fast with the less computational effort. Although the most computation is costed in the solutions of Euler–Lagrange equations, the ultimate purpose is to calculate surface tension, so the error estimator should be designed based on the contribution to the surface tension. Moreover, because of the nonlinearity of the Euler–Lagrange equations considered in this paper, Newton's method [14] is utilized to solve the system of nonlinear algebraic equations obtained from finite element discretization, and naturally, we hope that the adaptive finite element method can be coupled with Newton's method to guarantee the robustness and convergence of the entire numerical algorithm.

The rest of this paper is organized as follows. In Section 2, we will state the gradient theory of fluid interfaces and carry out rigorous mathematical derivations of Euler–Lagrange equations. In Section 3, the finite element method is applied to solve nonlinear Euler–Lagrange equations, and the error estimates of the corresponding approximate surface tension is also analyzed. Furthermore, we will propose an adaptive finite element method based on a physical-based estimator and combine it well with Newton's method. In Section 4, the proposed method is applied to predict surface tension of a hydrocarbon fluid system and the numerical results are provided as well. Finally, concluding remarks are provided in Section 5.

2. The gradient theory for multicomponent mixtures

2.1. Basic description of the gradient theory

We now outline the gradient theory, which has been described extensively by several authors, see [1–4]. For a mixture composed of N components, we denote by n_i the molar density of the component i , and let $\mathbf{n} = (n_1, n_2, \dots, n_N)^T$ and $n = n_1 + n_2 + \dots + n_N$. The gradient theory states that the Helmholtz energy density of an inhomogeneous fluid, in the absence of an external potential, is the sum of two contributions: the Helmholtz energy $f_0(\mathbf{n})$ of a homogeneous fluid at local composition \mathbf{n} , and a corrective term which is function of the local density gradients:

$$F(\mathbf{n}) = \int_{\Omega} \left(f_0(\mathbf{n}) + \frac{1}{2} \sum_{i,j} c_{ij} \nabla n_i \cdot \nabla n_j \right) d\mathbf{x}, \quad (2.1)$$

where ∇n_i represents the local gradient in density of component i and the coefficients c_{ij} denote the influence parameters. The corresponding functional without gradient contribution (thus not to model phase interface) is defined by

$$F_B(\mathbf{n}_B) = \int_{\Omega} f_0(\mathbf{n}_B) d\mathbf{x}, \quad (2.2)$$

where \mathbf{n}_B is the molar density in the equilibrium bulk phases. The Helmholtz energy $f_0(\mathbf{n})$ of a Peng–Robinson homogeneous fluid is given by

$$f_0(\mathbf{n}) = f_0^{ideal}(\mathbf{n}) + f_0^{excess}(\mathbf{n}), \quad (2.3)$$

$$f_0^{ideal}(\mathbf{n}) = RT \sum_{i=1}^N n_i (\ln n_i - 1), \quad (2.4)$$

$$f_0^{excess}(\mathbf{n}) = -nRT \ln(1 - bn) + \frac{a(T)n}{2\sqrt{2}b} \ln \left(\frac{1 + (1 - \sqrt{2})bn}{1 + (1 + \sqrt{2})bn} \right), \quad (2.5)$$

where T is the temperature of the mixture and R is the universal gas constant. Here, b is the covolume and $a(T)$ is the energy parameter. For a mixture, these parameters are related to the ones of pure fluids by mixing rules.

We now describe the computations of parameters $a(T)$ and b in (2.5). Let P be the pressure of the mixture and let T_{c_i} , P_{c_i} and ω_i be the critical temperature, pressure and acentric factor, respectively, of component i . For each component, we define the reduced pressure as $P_{r_i} = P/P_{c_i}$ and the reduced temperature as $T_{r_i} = T/T_{c_i}$, and furthermore, we define the mole fraction $y_i = n_i/n$. Then $a(T)$ and b are calculated by

$$a(T) = \sum_{i=1}^N \sum_{j=1}^N y_i y_j (a_i a_j)^{1/2} (1 - k_{ij}), \quad b = \sum_{i=1}^N y_i b_i, \quad (2.6)$$

where

$$a_i = 0.45724 \frac{R^2 T_{c_i}^2}{P_{c_i}} \left[1 + m_i (1 - \sqrt{T_{r_i}}) \right]^2, \quad b_i = 0.07780 \frac{R T_{c_i}}{P_{c_i}}. \quad (2.7)$$

In addition, k_{ij} are the given binary interaction coefficients for the energy parameters. The coefficient m_i is function of the acentric factor ω_i as

$$m_i = 0.37464 + 1.54226\omega_i - 0.26992\omega_i^2, \quad \omega_i \leq 0.49, \quad (2.8)$$

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