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Cahn-Hilliard vs Singular Cahn-Hilliard Equations in Phase Field Modeling

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Abstract. The Cahn-Hilliard equation is often used to describe evolution of phase boundaries in phase field models for multiphase fluids. In this paper, we compare the use of the Cahn-Hilliard equation (of a constant mobility) for the phase variable with that of the singular or modified Cahn-Hilliard equation (of a variable mobility) in the context of physical derivation of the transport equation and numerical simulations of immiscible binary fluids. We show numerically that (i). both equations work fine for interfaces of small to moderate curvature in short to intermediate time scales; (ii) the Cahn-Hilliard equation renders strong dissipation in simulations of small droplets leading to dissolution of small droplets into the surrounding fluid and/or absorption of small droplets by larger droplets nearby, an artifact for immiscible binary fluids; whereas, the singular Cahn-Hilliard equation can significantly reduce the numerical dissipation around small droplets to yield physically acceptable results in intermediate time scales; (iii) the size of droplets that can be simulated by the Cahn-Hilliard equations scale inversely with the strength of the mixing free energy. Since the intermediate timescale is the time scale of interest in most transient fluid simulations, the singular Cahn-Hilliard equation proves to be the more accurate phase transporting equation for immiscible binary fluids.

AMS subject classifications: 65M06, 76D05, 76A05, 76T30, 76Z05, 92C05

Key words: Cahn-Hilliard equation, phase field, finite difference method, immiscible multiphase flow, singular Cahn-Hilliard equation.

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1 Introduction

Modeling and simulating immiscible multiphase fluid flows has been challenging both mathematically and technically. Over the years, various mathematical theories and computational technologies have been developed to tackle the problem. The front tracking method [8], boundary integral method [12], level-set method [16, 19], volume-of-fluid method [11], immersed-boundary method [14,18], and phase field method [1,20–22] have all been proposed, implemented and refined, each of which has shown effectiveness in designated applications. Some of the methods are interconnected while others can be combined to yield more effective computational technologies [13]. Among all above, the phase field method for multiphase fluid flows is perhaps the simplest to implement, given that the phase boundary is embedded in a level set of the phase variable governed by a dissipative evolutionary equation, and physically the most relevant. Because of the ease of use and simplicity, refined details in the formulation of the phase field equation must be well thought out and the free energy, especially, the interfacial free energy for the multiphase fluid must be devised properly to ensure accuracy in numerical computations and fidelity in physical modeling.

In an immiscible binary fluid, the phase field method employs a phase variable $0\leq\phi\leq 1$ to track each phase in the binary fluid: $\phi=1$ describes the region occupied by fluid 1 and $\phi=0$ denotes the one occupied by fluid 2 while $0<\phi<1$ describes the interfacial region. The phase variable is also known as the labeling function by some. The time evolution of the phase variable ϕ is governed according to the Cahn-Hilliard equation [4, 5]

$$\frac{d\phi}{dt}=\nabla\cdot(\lambda\nabla\mu), \tag{1.1}$$

where λ is the mobility and μ is the chemical potential of the multiphase fluid system, a functional of the phase variable ϕ. The phase variable ϕ can be identified with the volume fraction of fluid 1; so, $1-\phi$ serves as the volume fraction of fluid 2. In this formulation of the transport equation for ϕ, the flux of ϕ is assumed to be proportional to the force due to the prescribed chemical potential. However, a more physically appropriate assumption is to assume the transporting velocity of ϕ is proportional to the force due to the chemical potential, a consequence of the friction dynamics [3, 6]. This leads to the singular or modified Cahn-Hilliard equation

$$\frac{d\phi}{dt}=\nabla\cdot(\lambda_s\phi\nabla\mu), \tag{1.2}$$

where λ_s is the mobility. The effective mobility is $\lambda=\lambda_s\phi$ in the singular Cahn-Hilliard equation. It vanishes in fluid 2. If we assume mixing only goes on in the interfacial layer, it would be reasonable to assume $\lambda_s=\lambda_s^1(1-\phi)$, where λ_s^1 is a constant. Hence, the effective mobility is $\lambda=\lambda_s^1\phi(1-\phi)$. In the classical Cahn-Hilliard equation, the mobility is a constant, whereas it is a phase variable dependent function in the modified case.