Available online at www.sciencedirect.com

ScienceDirect

Journal of Computational Physics 226 (2007) 2078–2095

JOURNAL OF COMPUTATIONAL PHYSICS

www.elsevier.com/locate/jcp

Diffuse interface model for incompressible two-phase flows with large density ratios

Hang Ding [a,*], Peter D.M. Spelt [a], Chang Shu [b]

[a] Department of Chemical Engineering, Imperial College London SW7 2AZ, UK
[b] Department of Mechanical Engineering, National University of Singapore, Singapore 119260, Singapore

Received 30 October 2006; received in revised form 6 June 2007; accepted 27 June 2007
Available online 5 July 2007

Abstract

We investigate the applicability of an incompressible diffuse interface model for two-phase incompressible fluid flows with large viscosity and density contrasts. Diffuse-interface models have been used previously primarily for density-matched fluids, and it remains unclear to what extent such models can be used for fluids of different density, thereby potentially limiting the application of these models. In this paper, the convective Cahn–Hilliard equation and the condition that the velocity field is divergence-free are derived from the conservation law of mass of binary mixtures in a straightforward way, for fluids with large density and viscosity ratios. Differences in the equations of motion with a previously derived *quasi-incompressible model* are shown to result from the respective assumptions made regarding the relationship between the diffuse fluxes of two species. The convergence properties of the model are investigated for cases with large density ratio. Quantitative comparisons are made with results from previous studies to validate the model and its numerical implementation. Tests show that the variation in volume during the computation is of the order of machine accuracy, which is consistent with our use of a conservative discretization scheme (finite volume methods) for the Cahn–Hilliard equation. Results of the method are compared with previous work for the change in topology of rising bubbles and Rayleigh–Taylor instability. Additional results are presented for head-on droplet collision and the onset of droplet entrainment in stratified flows.

Keywords: Diffuse interface; Large density ratio; Multiphase flow; Bubbles; Rayleigh–Taylor instability; Droplet collision; Stratified flow

1. Introduction

Amongst interface tracking methods such as volume-of-fluid (VOF) [1,2], level-set (LS) [3,4] and front-tracking [5], diffuse interface (DI) methods [6–8] provide a useful alternative that does not seem to suffer from problems with either mass conservation or the accurate computation of surface tension. In DI methods, the sharp fluid-fluid interface is replaced by a narrow layer in which the fluids may mix. The concept of a diffuse

* Corresponding author. Tel.: +44 (0) 207 594 1455.
E-mail address: h.ding@imperial.ac.uk (H. Ding).

0021-9991/$ - see front matter
doi:10.1016/j.jcp.2007.06.028

interface was proposed by van der Waals long ago [9], but it has gained popularity only in recent years as a tool for numerical simulations of two-phase flows. The resulting DI method has been used for the simulation of a wide range of two-phase flow problems including vesicle dynamics [10], Hele–Shaw flows [11], head-on droplet collision [12] and moving contact lines [13,14] (see [7] for an extensive review). Of the DI models for incompressible, immiscible two-phase flow, which is the focus of our work, Model H [15] has attracted much attention in the context of the simulation of matched-density fluids. In this model, the governing equations are the continuity and momentum equations for a divergence-free velocity field, in conjunction with the convective Cahn–Hilliard equation for the order parameter. Jacqmin [14] and the present authors [16] showed that an analysis of the flow near a moving contact line based on the H Model leads to results that are directly comparable to results of the Navier–Stokes equations with a sharp interface. Kim [17] presented a comparison of (two-dimensional) numerical results obtained from the H Model for density-matched fluids with analytical results from the Navier–Stokes equations with a sharp interface for a capillary wave, and for a deformed droplet in a shear flow.

The issue whether the H Model can be applied to two-phase flows with a density contrast has received little attention, but is obviously crucial in applications. A straightforward extension of the H model would be to replace the constant density ρ_0 with a variable density $\rho(C)$ and to continue to take the velocity field to be divergence-free. This so-called *modified H Model* would be an appealing computational method for general two-phase flows, primarily because of the smooth variation of the order parameter across interfaces. It has been used previously by Jacqmin [6], for the simulation of Rayleigh–Taylor instability as well as for flows with moving contact lines [14,16,18]. Test cases using this model for fluids with a large density contrast are rare, however. An exception is a case run by Kim [17], who primarily tested his new surface tension formulation, but a detailed comparison with previous work was not provided and this single test was only qualitative. One of the main aims of the present paper is therefore to perform extensive numerical tests for a variety of problems.

In addition to the performance of the modified H model in numerical validation tests, the theoretical basis of the model for flows of fluids with a density contrast is unclear at present. Most rigorous work to justify the use of the modified H Model has focused on the stresses arising from gradients in the order parameter, with emphasis on showing that these strictly dissipate energy [6]. But a full derivation of these equations of motion is not available, to our knowledge. Jacqmin [14] merely stated that this is the simplest possible Navier–Stokes–Cahn–Hilliard DI model, and that effects of compressibility are neglected in this model. This is also borne out by more rigorous derivations of DI models for fluids with a density contrast, as these do not recover the (modified) H model. Antanovskii [19] derived a quasi-incompressible DI model for binary mixtures, wherein the immiscible liquids can mutually penetrate into each other in such a way that the sum of the *mass diffusive flow rates* of the two fluids equals zero (as discussed in more detail in the next section). As a result he obtained the conventional compressible continuity equation

$$\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{1}$$

such that the velocity field is only solenoidal if the bulk densities are equal. Lowengrub and Truskinovsky [20] extended Antanovskii's model by presenting a new formulation of the chemical potential, in which the kinetic fluid pressure and fluid density were introduced. An important issue here is that, in order for results of DI simulations to be comparable to solutions of the incompressible Navier–Stokes equations, the volume of each fluid should remain constant in time: it should not be allowed to change because of diffuse fluxes. It is anticipated that this is a concern if the velocity field is not divergence-free. A further aim of this paper is therefore to investigate the origin of the differences with the modified H Model.

We therefore first investigate in this paper the origins of the differences between the H and other DI models. In Section 2, it is shown that either the H Model or a quasi-incompressible DI model can be recovered by using different choices of definition of the diffusive fluxes. We start from the continuity equations for the binary mixtures of two fluids, and use the volume fraction of one of the fluids as the order parameter. The convective Cahn–Hilliard equation and the continuity equation for a divergence-free velocity field are then derived in a straightforward way with the assumption of incompressibility of the two-fluid mixture. Also investigated in Section 2 is whether the H Model conserves mass. Results of detailed numerical validation studies that have been carried out for various test cases are presented in Section 4. Comparisons with previous work are made