Journal of Computational Physics 281 (2015) 421–448

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Direct simulation of drying colloidal suspension on substrate using immersed free surface model

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A R T I C L E   I N F O

Article history:
Received 20 April 2014
Received in revised form 27 September 2014
Accepted 19 October 2014
Available online 24 October 2014

Keywords:
Colloidal suspension
Free surface
Phase change
Immersed free surface model
Immersed boundary method
Level set method

A B S T R A C T

This paper presents a new direct simulation method for a drying colloidal suspension on a substrate. A key issue of the present method is the immersed free surface model proposed by the authors, which enables us to estimate accurately and efficiently capillary forces exerted on particles on a free surface. Using the immersed free surface model along with immersed boundary method and level set method, the present method leads to a three-way coupling of the fluid flow, the free surface motion and the particle motion. In addition, the present method includes a way of curvature estimation using virtual grid differencing to calculate accurately a surface tension. The way of curvature estimation is quantitatively validated through the simulation of a still droplet. The immersed free surface model is quantitatively validated through the simulation of a sphere moving across a free surface and the simulation of two spheres moving along a free surface. Finally, simulations of drying colloidal suspension containing 130 particles are performed to demonstrate the applicability of the present method to actual systems.

1. Introduction

Drying of colloidal suspension on a substrate is a key process to fabricate particulate films that constitute various electronic devices, such as solar cells, flat panel displays and biological/chemical sensors [1]. The colloidal particles in a suspension spontaneously form a variety of microstructures on the substrate during drying [2–8]. The microstructure formation of the colloidal particles is a type of self-organization. Elucidation of the self-organization is crucial to control the microstructures of the colloidal particles. During drying, the colloidal particles are influenced by various non-linear interactions, such as contact interaction, van der Waals interaction, electrostatic interaction, capillary interaction and hydrodynamic interaction including thermal fluctuation of a solvent. A simulation of drying colloidal suspension is a major challenge even though computational fluid dynamics is now well developed. Recently, many researchers have been performed macroscopic simulations of the drying colloidal suspension [9–13], in which the evolution of the solid phase fraction in the suspension has been solved. Although the macroscopic simulations are applicable to systems in actual size, the microstructures of the colloidal particles cannot be obtained. On the other hand, several researchers have addressed direct simulations of the drying colloidal suspension [14,15], in which the motion of each particle has been solved. Although the direct simulation is rather expensive in computation than the macroscopic simulation, it has the advantage of obtaining the microstructures of the colloidal particles during drying.

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http://dx.doi.org/10.1016/j.jcp.2014.10.042

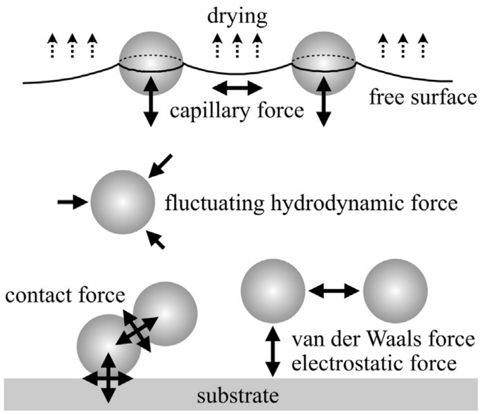

Fig. 1. Forces exerted on colloidal particles that are included in the present simulation method.

For the direct simulation of the drying colloidal suspension, mesoscale gas–liquid–solid three phase flow with phase change should be taken into consideration. The problem can be divided into two issues; mesoscale solid–fluid two phase flow and gas–liquid two phase flow with phase change. Firstly, there are two issues in the mesoscale solid–fluid two phase flow. They are to apply the no-slip boundary condition on the solid–fluid interface and to reproduce the Brownian motion that satisfies the fluctuation–dissipation theorem. The immersed boundary (IB) method [16] is an efficient way to apply the no-slip boundary condition on moving solid objects in a fixed Cartesian coordinate system. Many researchers have applied the IB method to the simulation of particulate flows [17–21]. The fluctuation–dissipation theorem can be satisfied by use of the Landau–Lifshitz Navier–Stokes (LLNS) equations in the fluctuating hydrodynamics [22,23], which includes the stochastic fluctuation stress. Several researchers have simulated the Brownian motion of colloidal particles by use of the LLNS as well as the IB method [24–27]. Secondly, an issue of the gas–liquid two-phase flow is to capture a free surface on which surface tension is exerted. The level set method [28] is one of the most reliable approaches to capture the free surface, because it enables us to calculate accurately the normal vectors and curvatures of the free surface, compared with other capturing methods [29–31]. Many researchers have applied the method to simulations of gas–liquid two-phase flows with phase change [32–37].

Although both colloidal suspension flows and two-phase flows with phase change have been successfully simulated, few direct simulations of the drying colloidal suspension have ever been presented in the literature. A difficulty with the simulation is modeling of the capillary force exerted on the particles protruding from a free surface. In Ref. [15], the capillary force is modeled as the simple spring force that is a function of the immersed height of the particle, in which the free surface is not deformed. In Ref. [14], the capillary force and the deformation of the free surface are calculated through the specified wettability parameter, in which the contact angle on the particle surface cannot be explicitly specified. Most recently, we have developed the immersed free surface (IFS) model to estimate accurately and efficiently capillary forces exerted on many particles at a free surface [38]. The IFS model is used along with the immersed boundary method and the level set method to accomplish a three-way coupling of the fluid flow, the free surface motion and the particle motion. This paper aims to develop a new direct simulation method for a drying colloidal suspension on a substrate using the IFS model. The present simulation method includes the crucial forces exerted on colloidal particles, such as the contact force, the van der Waals force, the electrostatic force, the capillary force, and the fluctuating hydrodynamic force, as shown in Fig. 1. Therefore, the present method enables us to estimate a variety of microstructures of colloidal particles on a substrate during drying.

This paper consists of the following parts. In Section 2, mathematical formulation in the present method is described. Namely, the governing equations of free surface motion, gas–liquid two-phase flow with phase change and particle motion are derived from the conservation laws. The IFS model is introduced into the equation of the free surface motion. In Section 3, numerical solver is described, in which the solution algorithm and the discretization of the governing equations are given in detail. In Section 4, some simulation results are illustrated to stress the capability of the present method. All the simulations in this paper are applied to gas–liquid two-phase flows with density ratio of 1000. Finally, the conclusion of this paper is stated in Section 5.

2. Mathematical formulation

A gas–liquid–solid three phase flow is considered in this paper, in which a liquid and its vapor, spherical solid particles and a substrate exist. Fig. 2 shows a two-dimensional schematic picture of the flow field on a Cartesian grid modeled in the present simulation method. The gas–liquid two-phase flow is treated as a single-field model, in which one set of conservation equations with the variable density and the variable viscosity is adopted. The free surface has a finite thickness, in which the density and the viscosity changes continuously. Each spherical particle is treated as a rigid body, in