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Smoothed particle hydrodynamics modeling of viscous liquid drop without tensile instability

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ABSTRACT

Smoothed particle hydrodynamics (SPH), as a Lagrangian meshfree particle method, has been applied to modeling viscous liquid drop with surface tension and wetting dynamics. In the SPH model, the van der Waals (vdW) equation of state is usually used to describe the gas-to-liquid phase transition similar to that of a real fluid. However, the attractive forces between SPH particles originated from the cohesive pressure of the vdW equation of state can lead to tensile instability, which is associated with unphysical phenomena such as particle clustering or blowing away. This paper presents an improved SPH method for modeling viscous liquid drop. The inherent tensile instability in SPH is removed by using a hyperbolic-shaped kernel function which possesses non-negative second derivatives. A single-step approximation for heat flux is used in modeling viscous liquid drop with smoother temperature field. The formations of viscous liquid drops, both in 2D and 3D, are tested and it clearly demonstrates that the tensile instability can be effectively removed. The improved SPH method is also used to model two other numerical examples including the oscillation and binary collision of liquid drops without tensile instability.

1. Introduction

Liquid drop dynamics has been investigated for many years as liquid drops exist widely in nature and industrial production, such as the formation of raindrop, ink-jet printing, fuel injection atomization, droplet-based net-form manufacturing, and many others [1]. Liquid drops were firstly studied quantitatively by Rayleigh [2], and he derived the relation between the period of drop vibration and the surface tension. In the past few decades, Liquid drops have been experimentally investigated and numerical modeled by many researchers. For example, in order to study the rheological properties of liquid drop surfaces, Apfel et al. [3] studied the free oscillations and large deformations of water drops in microgravity. Willis and Orme [1,4] experimentally investigated the viscous binary droplet collisions in a vacuum environment. They quantitatively studied the oscillation cycle of droplets and found that the time period of oblate oscillation is relatively not affected by Weber number and viscosity and that the time period of prolate oscillation is affected by the Reynolds number. In order to understand the impact of a liquid drop into a dry solid surface, Schroll et al. [5] use an axisymmetric volume-of-fluid (VOF) method to simulate the impact at reduced ambient pressure. Bernel et al. [6] experimentally and numerically investigated the drop formation by vortical flows in microgravity. Sun et al. [7] studied the deformation and mass transfer for binary droplet collisions using the moving particle semi-implicit method.

The formation and deformation of liquid drops are associated with evolutionary morphology with changing free surfaces and moving interfaces, which present big challenges to numerical simulations. Over the past decades, interfacial flow simulation has been a formidable topic in computational fluid dynamics and computational physics. In order to deal with free surface and moving interface evolution, different numerical techniques have been proposed to track or capture free surfaces or moving interfaces. Considering the fact that both fluids and solids are composed of particles, the physics related liquid drop dynamics is closely related to the inter particle and intra molecular hydrodynamics interactions of the concerned multiple phase system. Therefore Lagrangian meshfree particle methods can be attractive in modeling liquid drops.

Smoothed particle hydrodynamics (SPH) is a typical meshfree particle method. It was first introduced by Lucy [8] and Gingold and Monaghan [9] for solving astrophysical problems, and later extended to many other problems in engineering and sciences [10–13]. Nugent and Posch [14] firstly studied liquid drops and surface tension for van der Waals (vdW) fluids using SPH as the cohesive pressure part in the vdW equation of state can be used to model surface tension. Tartakovsky and Meakin [15] also developed an SPH method for modeling liquid drop dynamics with surface tension and contact angles for van der Waals fluids using an inter-particle interaction force. Xu et al. [16] developed a diffuse-interface

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SPH model which can also simulating vdW liquid–vapor systems. By introducing a surface tension model in SPH, Zhang [17] simulated binary collisions of liquid drops in two and three dimensions successfully. However, for higher Reynolds number and higher Weber number, the model has to be improved. Viscous droplet has also been studied using SPH method by many other researchers such as Jiang et al. [18] and Meleán et al. [19,20].

It is known that SPH suffers from tensile instability when modeling elastic solids and viscous fluids. The tensile instability is the situation in which when particles are under tensile stress state, the motion of the particle becomes unstable. It could result in particle clustering or particle blowing away in SPH computation. Swegle et al. [21,22] firstly studied the tensile instability and proposed a criterion which states that the instability depends on the sign of the multiplication of the stress and the second derivative of the kernel function. In SPH modeling viscous liquid drops, tensile instability also exist. Meleán et al. [19,20] investigated viscous liquid drops for vdW fluids, and discussed the tensile instability effects. In order to remove the tensile instability of SPH in modeling vdW drops, they applied the artificial stress model which was originally proposed by Monaghan [23] and is associated with an artificial viscous force and energy generation term. It is reported that with optimal coefficients, the artificial viscous stress model can remove tensile instability with sufficiently smoothed density profile.

This paper presents an improved SPH method for modeling viscous liquid drop without tensile instability using a hyperbolic-shaped kernel function which possesses non-negative second derivatives. The paper is organized as follows. In the next section, SPH method for describing van der Waals fluid shall be briefly addressed. In Section 3, the SPH tensile instability shall be discussed and a hyperbolic-shaped kernel function shall be presented to remove tensile instability for SPH modeling viscous liquid drops. In Section 4, three classes of numerical examples shall be provided. The first class involves liquid drop formation both in 2D and 3D, the second class involves oscillation of liquid drops, and the third class involves head-on and off-center binary collisions of two vdW liquid drops. The paper concludes in Section 5 with some discussions.

2. SPH method for van der Waals fluid

In general, SPH is a numerical method for solving partial differential equations of continuum dynamics by replacing the continuum with a set of particles. In this section, we will briefly describe the governing equations of van der Waals (vdW) fluid and the corresponding SPH formulations.

In vdW flow, the effect of heat conduction is very important, so an internal energy equation should be considered. The general equations governing the motion of heat conducting and viscous fluid can be written as

$$\frac{d\rho}{dt} = -\rho\nabla\cdot\boldsymbol{u} \tag{1}$$

$$\frac{d\boldsymbol{u}}{dt} = \frac{1}{\rho}\nabla\cdot\boldsymbol{S} + \boldsymbol{g} \tag{2}$$

$$\frac{de}{dt} = \frac{1}{\rho}\boldsymbol{S}:\nabla\boldsymbol{u} - \frac{1}{\rho}\nabla\cdot\boldsymbol{q} \tag{3}$$

where t is time instant, ρ is the density, $\boldsymbol{u}$ is the velocity, $\boldsymbol{S}$ is the stress tensor, $\boldsymbol{g}$ is the body force per unit mass, e is the specific internal energy, and $\boldsymbol{q}$ is the heat flux vector.

The stress tensor $\boldsymbol{S}$ is written as

$$\boldsymbol{S} = -p\boldsymbol{I} + \sigma \tag{4}$$

where p is the internal pressure, $\boldsymbol{I}$ is the unit tensor, and σ is the viscous stress tensor given by

$$\sigma = \eta(\nabla\boldsymbol{u} + \boldsymbol{u}\nabla) + \left(\zeta - \frac{2}{d}\eta\right)(\nabla\cdot\boldsymbol{u})\boldsymbol{I} \tag{5}$$

where η and ζ is the coefficients of shear and bulk viscosity, respectively. The parameter d is the spatial dimension, with $d = 2$ and 3 for two- and three-space dimensions, respectively [20,24].

The heat flux vector is written as

$$\boldsymbol{q} = -\kappa\nabla T \tag{6}$$

where κ is the coefficient of thermal conductivity and T is the fluid temperature.

Eqs. (1)–(3) are closed by the mechanical and caloric equations of state for the pressure and the internal energy, respectively. For vdW fluid, the governing equations are closed by

$$p = \frac{\rho\bar{k}T}{1-\rho\bar{b}} - \bar{a}\rho^2 \tag{7}$$

and

$$e = \bar{k}T - \bar{a}\rho \tag{8}$$

where $\bar{k} = k_B/m$, $\bar{a} = a/m^2$, and $\bar{b} = b/m$, here k_B is the Boltzmann's constant, m is the particle mass, a is the cohesive action responsible for the short-range attractive forces between neighboring molecules, and b is a constant parameter due to the finite size of the molecules. The cohesive part of the pressure in Eq. (7) gives rise to an attractive, central force between particles with an interaction range which is assumed to exceed that of all other smoothed forces appearing in Eq. (10). With this assumption, stable drops can be formed [20].

In SPH method, a continuous field is represented by a set of particles. The particles carry physical properties such as mass m, density ρ, velocity $\boldsymbol{u}$, and energy e. The governing equations are solved on particles and they can be written in SPH as [14,19,20]

$$\frac{d\rho_a}{dt} = \sum_b m_b(\boldsymbol{u}_a - \boldsymbol{u}_b)\cdot\nabla_a W_{ab} \tag{9}$$

$$\frac{d\boldsymbol{u}_a}{dt} = \sum_b m_b\left(\frac{\boldsymbol{S}_a}{\rho_a^2} + \frac{\boldsymbol{S}_b}{\rho_b^2}\right)\cdot\nabla_a W_{ab} + \boldsymbol{g}_a \tag{10}$$

$$\frac{de_a}{dt} = \frac{1}{2}\sum_b m_b\left(\frac{\boldsymbol{S}_a}{\rho_a^2} + \frac{\boldsymbol{S}_b}{\rho_b^2}\right) : (\boldsymbol{u}_a - \boldsymbol{u}_b)\nabla_a W_{ab} - \sum_b m_b\left(\frac{\boldsymbol{q}_a}{\rho_a^2} + \frac{\boldsymbol{q}_b}{\rho_b^2}\right)\cdot\nabla_a W_{ab} \tag{11}$$

where subscripts a and b denote particle indexes, $W_{ab} = W(\boldsymbol{r}_b - \boldsymbol{r}_b, h)$ is a kernel function (also referred to as smoothing function, or simplified as kernel), h is a smoothing length which determines the range of the interaction of particles, $\nabla_a W_{ab}$ denotes the gradient of the kernel function taken with respect to the coordinate of particle a. The summation is taken over all the neighboring particles determined by the smoothing length. Note that the spatial derivative in the governing equations has been transformed to the derivative of the kernel function which can be obtained analytically. The kernel function should satisfy some conditions which will be introduced in the following section.

In SPH, an alternative method to approximate the density of a particle is

$$\rho_a = \sum_b m_b W_{ab} \tag{12}$$

There is a disadvantage that the density of the particles near free surface obtained by Eq. (12) always less than the reasonable value,