SPH Modeling of Multiphase Drop Dynamics

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***Abstract*—This paper presents an SPH (smoothed particle hydrodynamics) model for numerical simulation of multiphase drop dynamics including liquid drop formation and deformation, coalescence and separation, liquid drop impacting, spreading and splashing. SPH is a Lagrangian, meshfree particle method. It has special advantages in modeling multiphase drop dynamics. Surface tension effects are modeled using a particle-particle interaction force, which avoids the calculation of surface and interface curvature. Solid boundaries are modeled using a coupled dynamic boundary treatment algorithm, which ensures the accuracy and flexibility of the SPH method. Numerical investigations of a liquid drop oscillation and a single liquid drop impacting onto a liquid film are conducted. The inherent physics of multiphase drop dynamics are well described.**

Keywords- liquid drop, drop dynamics, smoothed particle hydrodynamics，surface tension

I. INTRODUCTION

Multiphase drop dynamics is a significant aspect of complex multiphase flows. Phenomena related to multiphase drop dynamics exist widely in nature and industrial production, such as ink-jet printing, enhanced oil recovery, soil erosion, and fuel injection atomization. Multiphase drop dynamics is associated with complex physics such as liquid drop formation and deformation, coalescence and separation, liquid drop impacting, spreading and splashing with rapidly changing free surfaces and morphology evolution. Surface tension and wetting effects can be very important in multiphase drop dynamics, especially when the spatial scale reduces.

Many researchers have used different methods to study problems with multiphase drop dynamics, either by experimental observations or numerical simulations [1-3]. These approaches have demonstrated success with limitations. Smoothed particle hydrodynamics (SPH) is a Lagrangian, particle-based meshfree method [4, 5]. In SPH, the state of a system is represented by a set of particles, which possess material properties and interact with each other within the range controlled by a weight function or smoothing function. An important advantage of SPH is that in SPH, there is no explicit interface tracking for multiphase or free surface flows – the motion of the fluid is represented by the motion of the particles, and fluid surfaces or fluid-fluid interfaces move with particles representing their phase defined at the initial stage. Since its invention, the SPH method has been comprehensively investigated and widely applied to different areas in engineering and sciences [6-10].

In this paper, multiphase drop dynamics is modeled using an SPH method. Surface tension effects are modeled using a particle-particle interaction force, which avoids tremendous efforts in calculating of surface and interface curvature. Physics inherent in multiphase drop dynamics is investigated and compared with results from other sources.

II. SMOOTHED PARTICLE HYDRODYNAMICS

A. *SPH methodology*

In conventional SPH method, the values of a particular variable at any point can be obtained using following equations:

$$< f(\mathbf{x}_i) >= \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(\mathbf{x}_j) W(\mathbf{x}_i - \mathbf{x}_j, h) , \qquad (1)$$

$$< \nabla \bullet f(\mathbf{x}_i) >= \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(\mathbf{x}_j) \nabla_i W_{ij} , \qquad (2)$$

where, $< f(\mathbf{x}_i) >$ is the approximated value of particle *i*, $f(\mathbf{x}_j)$ is the value of $f(\mathbf{x})$ associated with particle *j*, $\mathbf{x}_i$ and $\mathbf{x}_j$ are the positions of corresponding particles. m and ρ denote mass and density respectively. h is the smooth length, N is the number of the particles in the support domain. W is the smoothing function, and represents a weighted contribution of particle *j* to particle *i*. The smoothing function is sometimes referred to as kernel or kernel function, and it should satisfy some basic requirements, such as normalization condition, compact supportness, and Delta function behavior.

B. *SPH equations of motion*

For incompressible viscous hydrodynamic problems, the Lagrangian form governing Navier-Stokes (N-S) equation can be written as

$$\frac{d\rho}{dt} = -\rho \nabla \bullet \mathbf{v} , \qquad (3)$$

$$\frac{d\mathbf{v}}{dt} = -\frac{1}{\rho} \nabla p + \frac{\mu}{\rho} \nabla^2 \mathbf{v} + \mathbf{g} , \qquad (4)$$

where $\mathbf{v}, p, \mathbf{g}$ and μ denote velocity vector, pressure, gravity and dynamic viscosity respectively. According to equations (1) and (2), the SPH equations of motion for the N-S equation can be obtained as follows

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$$\frac{d\rho_i}{dt} = \sum_{j=1}^{N} m_j \mathbf{v}_{ij} \nabla_i W_{ij} , \quad (5)$$

$$\frac{d\mathbf{v}_i}{dt} = -\sum_{j=1}^{N} m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right) \bullet \nabla_i W_{ij} + \sum_{j=1}^{N} \frac{4m_j\left(\mu_i+\mu_j\right)\mathbf{x}_{ij} \bullet \nabla_i W_{ij}}{\left(\rho_i+\rho_j\right)^2\left(x_{ij}^{\ 2}+0.01h^2\right)} \boldsymbol{v}_{ij} + \mathbf{g} . \quad (6)$$

C. Surface tension

Surface tension effects are very important for liquid drop dynamics especially when the spatial scale reduces. For particle methods such as SPH, there are basically two approaches to model multiphase contact line dynamics with SPH method [11] . The first approach is to incorporate the continuum surface force (CSF) model and introduced directly surface tension force into the momentum equation as expressed in equation (6). This approach is straightforward, and physical parameters are used in numerical simulation. Surface curvature needs to be calculated, and this is quite troublesome for SPH method. Therefore in this paper, we used another approach, i.e., to introduce an inter-particle interaction force (IIF) in the SPH equations. The inter-particle interaction force can contain short-distance repulsion and long-range attraction, and the attractive force between every pair of SPH particles contribute to the surface tension. For example, Tartakovsky and Meakin [12] proposed following inter-particle interaction force between particle j and particle i

$$\mathbf{f}_{ij} = s_{ij} \cos\left(\frac{1.5\pi}{3h}\left|\mathbf{x}_j-\mathbf{x}_i\right|\right)\frac{\mathbf{x}_j-\mathbf{x}_i}{\left|\mathbf{x}_j-\mathbf{x}_i\right|}, \quad \left|\mathbf{x}_j-\mathbf{x}_i\right| \le h . \quad (7)$$

Here s_{ij} is taken as 0.001. Therefore the summation of such IIF on particle i leads to

$$\mathbf{f}_i = \sum_{j=1}^{N} \mathbf{f}_{ij} \quad (8)$$

The force obtained from equation (8) vanishes for interior particles with possible small fluctuation. For surface or interface particles, e.g., particles near the gas-liquid interface, a surface force is produced from equation (8), and it can be added to equation (6) as

$$\frac{d\mathbf{v}_i}{dt} = -\sum_{j=1}^{N} m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right) \bullet \nabla_i W_{ij} + \sum_{j=1}^{N} \frac{4m_j\left(\mu_i+\mu_j\right)\mathbf{x}_{ij} \bullet \nabla_i W_{ij}}{\left(\rho_i+\rho_j\right)^2\left(x_{ij}^{\ 2}+0.01h^2\right)} \boldsymbol{v}_{ij} + \mathbf{g} + \frac{1}{m_i}\mathbf{f}_i . \quad (9)$$

D. Solid boundary treatment

In this work, we used a coupled dynamic solid boundary treatment (SBT) algorithm. In this coupled SBT algorithm, two types of virtual particles, repulsive particles and ghost particles (as shown in Figure 1), are used to represent the solid boundary. The repulsive particles produce a suitable repulsive force to the approaching fluid particles near the boundary, and they are located right on the solid boundary. Ghost particles are located outside the solid boundary area. It should be noted that, in conventional SBT algorithms, ghost particles are generated from mirroring or reflecting fluid particles onto solid boundary areas, and need to adapt with the fluid particles at each time step. In contrast, this new SBT algorithm can generates ghost particles in a regular or irregular distribution at the first time step, while ghost particle positions do not need to change during following steps.

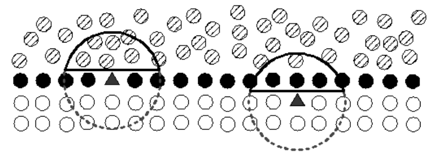

Figure 1. Illustration of the coupled dynamic SBT algorithm.

The new SBT algorithm consists of a new repulsive force for repulsive particles, and a new numerical scheme to approximate the information of the virtual particles. The new repulsive force is a distance-dependent repulsive force with finite magnitude on fluid particles approaching solid boundaries

$$\mathbf{F}_{ij} = 0.01c^2 \bullet \chi \bullet f(\eta) \bullet \frac{\mathbf{x}_{ij}}{r_{ij}^{\ 2}} , \quad (10)$$

$$\chi = \begin{cases} 1-\dfrac{r_{ij}}{1.5\Delta d} & 0<r_{ij}<1.5\Delta d \\ 0 & otherwise \end{cases} , \quad (11)$$

$$\eta = r_{ij} / (0.75h_{ij}) \quad (12)$$

$$f(\eta) = \begin{cases} 2/3 & 0<\eta\le 2/3 \\ (2\eta-1.5\eta^2) & 2/3<\eta\le 1 \\ 0.5(2-\eta)^2 & 1<\eta<2 \\ 0 & otherwise \end{cases} . \quad (13)$$

Here, Δd is the initial distance of two adjacent particles.

In this coupled dynamic SBT algorithm, field variable of the virtual particles (both repulsive particles and ghost particles, see Figure 1) can be dynamically evolved and obtained from SPH approximation of neighbor fluid particles within the support domain. To restore the particle consistency, Shepard filter method or moving least square (MLS) method can be used in the coupled dynamic SBT algorithm for approximating both the fluid and virtual particles.

It has been demonstrated that improved SPH particle approximations with Shepard filter or moving least square correction can lead to much better results than conventional SPH particle approximation schemes [13]. It should be noted that existing modifications in SPH particle approximations with Shepard filter or MLS are only used for approximating information of fluid particles. It is natural to extend Shepard filter or MLS for approximation information of virtual particles for better accuracy.

E. Other numerical aspects

The conventional SPH method is usually baffled for poor computational accuracy. In this paper, we used an improved version of SPH, which uses modified schemes for approximating density (density correction) and kernel gradient (kernel gradient correction, or KGC) to achieve better accuracy with smoother pressure field. Accuracy [6]. An artificial compressibility technique is used to model the incompressible flow as a slightly compressible flow. Besides, To overcome possible tensile instability, an artificial stress is added into SPH equations of motion [14].

III. NUMERICAL EXAMPLES

A. Liquid drop oscillation

In this numerical example, the large-amplitude oscillations of an initially oblate liquid drop were studied. SPH simulation was conducted for an initially oblate liquid drop with an aspect ratio of 5 using the van der Waals (vdW) equation of state. Figure 1 shows snapshots of the liquid drop morphology evolution, which experiences whole oscillation process with liquid drop deformation compression, necking and elongation. It is clear that in SPH simulations, the liquid drop underwent oscillations that closely resemble the oscillations of a large ball of water under micro gravity conditions observed experimentally in the space shuttle Columbia [17].

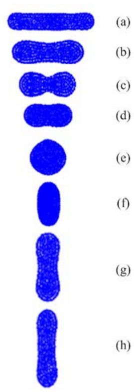

Figure 2. SPH simulation of the large-amplitude oscillations of a vdW fluid drop with an initial aspect ration of 5 at 8 representative instants.

B. Liquid drop impacting

To again demonstrate the effectiveness of the SPH method, the complete process of a drop impacting onto a thin liquid film is modeled (see Figure 3), while Wang and Chen [15] had experimentally investigated the same case.

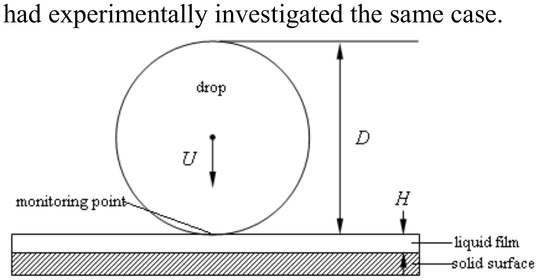

Figure 3. Schematic illustration of a drop impacting onto a thin film.

The diameter D of the initial drop is $4.2\ \text{mm}$. The density ρ of the glycerol–water solution used in the numerical simulation is $1200\,\text{kg}/\text{m}^3$. The viscosity μ is $0.022\ \text{N}\cdot\text{s}/\text{m}^2$. The initial impact speed U is 2.22 m/s. The surface tension coefficient σ is $0.0652\ \text{N}/\text{m}$. The Ohnesorge number ($Oh = \mu/(\sigma\rho D)^{1/2}$) is 0.0384. The We number is 381, and the dimensionless film thickness (the ratio of target liquid film thickness to drop diameter) is 0.05.

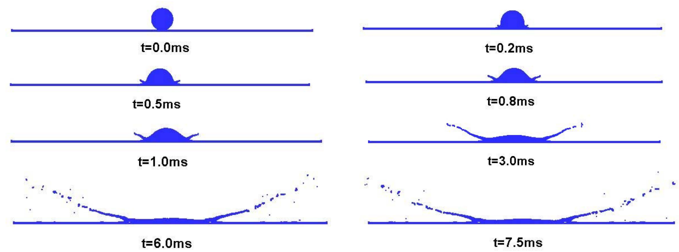

Figure 4. Drop impacting process.

Figure 4 shows the complete process of the drop impacting onto the liquid film at different instants. It can be seen that a small rim forms in the contact area between the drop and films immediately after the drop attacks onto the liquid film. In the contact area, parts of the splashed drop particles integrate with parts of the liquid film particles, producing two liquid jets, and then generating two rims. As more particles impact onto liquid film (Figure 5), we can observe clearly that parts of liquid film spread to both sides along the solid wall because of the drop impacting. The other parts integrate with drop particles, two rims gradually expand and move outwards, generating two crown-line liquid column. The evolution process of the two continuous rims is consistent with both experimental observation and physical phenomena. The rim extension will lead to sharper edges and bigger curvatures, and therefore bigger surface tension forces. This eventually prevents the continued expansion of the liquid rim. With the interplay of inertial force, viscous force, surface tension force and gravity, the formed crown move downward and integrate with liquid film. In later movement, some particles on the top of the formed crown will fall downwards, separate from edge, and then produces many smaller drops, which leads to splashing.

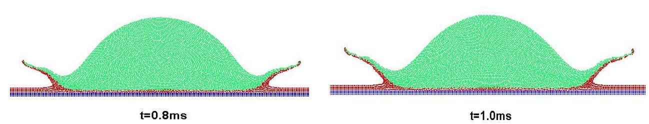

Figure 5. Particle evolution during drop impacting.

In Reference [16], it is found that the radius, x_c, of the crown formed by impact can be well described by a square-root function of time t, i.e., $x_c = \left[c\left(t - t_0\right)\right]^{1/2}$, where c and

t_0 are constants. Based on obtained SPH numerical results as shown in Figure 6, the crown radius y is fitted as $y = \left[0.0001089 \left(t - 0.40385 \right) \right]^{1/2}$ (unit of y is m and unit of t is ms). It is clear that the obtained kinematics of the crown with agree well with analytical predictions.

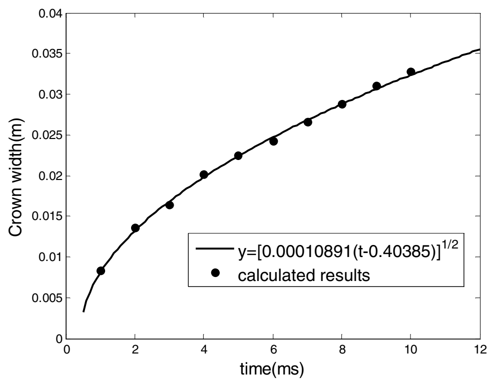

Figure 6. Kinematics of the crown radius.

IV. CONCLUDING REMARKS

This paper presents an SPH model for numerical simulation of multiphase drop dynamics. Numerical investigations of a liquid drop oscillation and a single liquid drop impacting onto a liquid film are conducted. For liquid drop oscillation, the SPH model can well describe the whole process of liquid drop deformation, compression, necking and elongation. For liquid drop impacting, the SPH model can effectively simulate the complete process of crown conformation and evolution, drop breaking-up and aggregation, film splashing and spreading. Free surface shapes of drop impacting onto liquid film obtained from SPH modeling are consistent with available sources. It is concluded that the SPH model is effective in simulating multiphase drop dynamics with complex physics including liquid drop formation and deformation, coalescence and separation, liquid drop impacting, spreading and splashing.

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