Modeling the dynamics of liquid drops with SPH

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The method of Smoothed Particle Hydrodynamics (SPH) has been applied in the last 20 years to a wide range of problems involving solution of the continuum fluid-dynamic equations. A variationally consistent SPH formulation has recently been devised which works equally well for both compressible and incompressible fluids. An extension of this method which addresses the tensile instability for a viscous, heat-conducting fluid has been applied to the condensation and binary coalescence collision of liquid drops using the van der Waals equation of state. Here we show and discuss the results obtained for some of these test cases. In particular, the benefits of correcting the tensile instability are described for both the formation of a stable liquid drop and the off-center coalescence of two liquid drops of equal size via a low-energy impact.

Keywords: Computational methods in fluid dynamics; applied fluid mechanics; viscous instability; drops and bubbles.

En los últimos 20 años, el método de Hidrodinámica de Partículas Suavizadas (SPH) ha sido aplicado a un vasto rango de problemas que requieren la solución de las ecuaciones de la dinámica de fluidos. Se ha derivado recientemente una formulación del método SPH que es variacionalmente consistente y que funciona de igual manera para fluidos compresibles e incompresibles. Una extensión de dicha formulación que corrije el problema de la inestabilidad tensional para fluidos viscosos y conductivos ha sido aplicada para simular la condensación y la coalescencia binaria de gotas líquidas usando la ecuación de estado de van der Waals. En este trabajo se muestran y discuten los resultados obtenidos para algunas de estas simulaciones. En particular, se describe el efecto de la corrección de la inestabilidad tensional para la formación de una gota líquida en equilibrio y la coalescencia de dos gotas líquidas de igual tamaño a través de un impacto no frontal y poco energético.

Descriptores: Métodos computacionales en dinámica de fluidos; mecánica de fluidos aplicada; inestabilidad viscosa; gotas y burbujas

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1. Introduction

Smoothed Particle Hydrodynamics (SPH) is a fully Lagrangian technique for solving the partial differential equations of fluid mechanics, in which the fluid elements are represented by particles. In its original form [1,2], the method was invented for applications to astrophysical problems involving compressible flows. Because of its wide range of applicability, SPH has also been employed in model industrial, biological and environmental processes many of which often involve incompressible fluids and their interaction with solid walls. A number of fluid dynamic SPH simulations can be found in the literature, some of which include viscous incompressible flows at low Reynolds numbers [3,4,5], free-surface incompressible flows [6], heat-conducting flows [7,8] and liquid-gas phase transition flows [9].

In SPH the physical properties of a particle are determined from those of a finite number of neighboring particles through kernel interpolation. In this way, the value of any field quantity at a point is represented by a weighted sum over the contribution of all neighboring particles. In the SPH framework, the particles move with the local fluid velocity and in addition to their mass, they carry other fluid properties specific to a given problem. Compared to conventional grid-based schemes, SPH presents several advantages. For instance, it is much easier to incorporate new physics into the formulation, handle moving or deformable boundaries and model the interaction of several fluid phases [10,11].

In this paper, we shall briefly describe a working SPH formulation for solving the equations of a viscous, heat-conducting fluid and apply it to both the condensation and the binary coalescence collision of van der Waals liquid drops.

2. SPH formulation

We have devised an SPH formulation which can be used to model compressible and incompressible fluids alike. Here we shall only describe the salient features of the method and for more details we refer to the reader [5,8]. It is common practice in SPH to estimate the continuous density field at the location of particle i according to

$$\rho_i = \sum_{j=1}^{N} m_j W(\mid \mathbf{r}_i - \mathbf{r}_j \mid, h), \tag{1}$$

where m_j is the mass of particle j, $W(\mid \mathbf{r}_i - \mathbf{r}_j \mid, h)$ is the kernel interpolation function and the sum is taken over N neighboring particles. Here, $\mid \mathbf{r}_i - \mathbf{r}_j \mid$ is the distance between particles i and j, and h is the smoothing length. With the smoothed representation of the fluid variables and their spatial derivatives, the continuum partial differential equations for the momentum and energy are converted into a set of ordinary differential equations for each particle. In order to guarantee variational consistency of the scheme with the use of Eq. (1), the SPH representations of the motion and energy equations must be written in symmetrized form [5,12].

In particular, for a viscous, heat-conducting fluid, these read as

$$\frac{d\mathbf{v}_i}{dt} = \sum_{j=1}^{N} m_j \left(\frac{\mathbb{T}_i}{\rho_i^2} + \frac{\mathbb{T}_j}{\rho_j^2} \right) \cdot \nabla_i W_{ij}^h, \tag{2}$$

for the momentum equation, and

$$\frac{dU_i}{dt} = \frac{1}{2} \sum_{j=1}^{N} m_j \left(\frac{\mathbb{T}_i}{\rho_i^2} + \frac{\mathbb{T}_j}{\rho_j^2} \right) : (\mathbf{v}_j - \mathbf{v}_i) \nabla_i W_{ij}^h \tag{3}$$

$$- \sum_{j=1}^{N} m_j \left(\frac{\mathbf{Q}_i}{\rho_i^2} + \frac{\mathbf{Q}_j}{\rho_j^2} \right) \cdot \nabla_i W_{ij}^h,$$

for the internal energy equation, where the colon indicates a double dot product, $\mathbf{v}_i$ and U_i are, respectively, the velocity and specific internal energy of particle i, ∇_i is the gradient operator at its location, $\mathbb{T}$ is the stress tensor, $\mathbf{Q} = -\kappa \nabla T$ is the heat flux vector, with κ being the coefficient of thermal conductivity and T the fluid temperature, and $W_{ij}^h = W(|\mathbf{r}_i - \mathbf{r}_j|, h)$.

This scheme has been found to perform well for plane Poiseuille and Hagen-Poiseuille flows at moderate ($Re = 5$) and very low ($Re \ll 1$) Reynolds numbers [5]. Further testing of the method on the formation of a stable van der Waals liquid drop has shown that it is highly susceptible to unstable behavior in the tensile regime [8]. However, the instability is completely removed when Eqs. (2) and (3) are modified by adding to their right-hand sides an artificial viscous force and an artificial viscous heating term, respectively. A complete account of the form of the artificial stress and corrected SPH equations can be found in Ref. 8. The method has also been succesfully applied to the head-on and off-center binary coalescence collision of circular liquid drops [13].

3. Formation of a liquid drop

In this section, we describe the formation of a stable liquid drop at a temperature such that no evaporation of the liquid will take place during the evolution. For this test model, a van der Waals fluid is chosen in which the SPH Eqs. (1)-(3) are closed by the constitutive relations

$$p = \frac{\rho \bar{k}_{\rm B} T}{1 - \rho \bar{b}} - \bar{a} \rho^2 \,, \tag{4}$$

and

$$U = \bar{k}_{\rm B} T - \bar{a} \rho \,, \tag{5}$$

for pressure and specific internal energy, respectively. Here $\bar{k}_{\rm B} = k_{\rm B}/m$, $\bar{a} = a/m^2$ and $\bar{b} = b/m$, where $k_{\rm B}$ is the Boltzmann's constant, m is the particle mass, $a = \bar{\gamma}$ 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. We adopt the same parameters as in Ref. 8. That is, we take $m = 1$, $\bar{a} = 2$, $\bar{b} = 0.5$, and $\bar{k}_B = 1$. In these reduced units, the critical point of the van der Waals fluid occurs for $\rho_{\rm cr} = 2/3$, $p_{\rm cr} = 8/27$ and $T_{\rm cr} = 32/27$. The coefficients of thermal conductivity, shear and bulk viscosity in reduced units are taken to be $\kappa = 5$, $\eta = 1$ and $\zeta = 0.1$, respectively. We choose the (x,y)-plane to represent the fluid and start the evolution from a square array of 1936 SPH particles, of equal mass ($m_i = m = 1$), arranged in a regular Cartesian mesh with length $L_{\rm m} = 32.25$. The particles were given a smoothing length $h = 3$ and an initial temperature $T = 0.2$. At this subcritical value, a condensed, stable circular drop forms as shown in Fig. 1. In Fig. 1a, we show the final configuration obtained without correcting for the tensile instability. A clustering of particles in concentric rings is evident in the drop structure as a result of the tensile instability. When the artificial stress is added, the instability is removed and the drop forms with a more homogeneous structure as displayed in Fig. 1b.

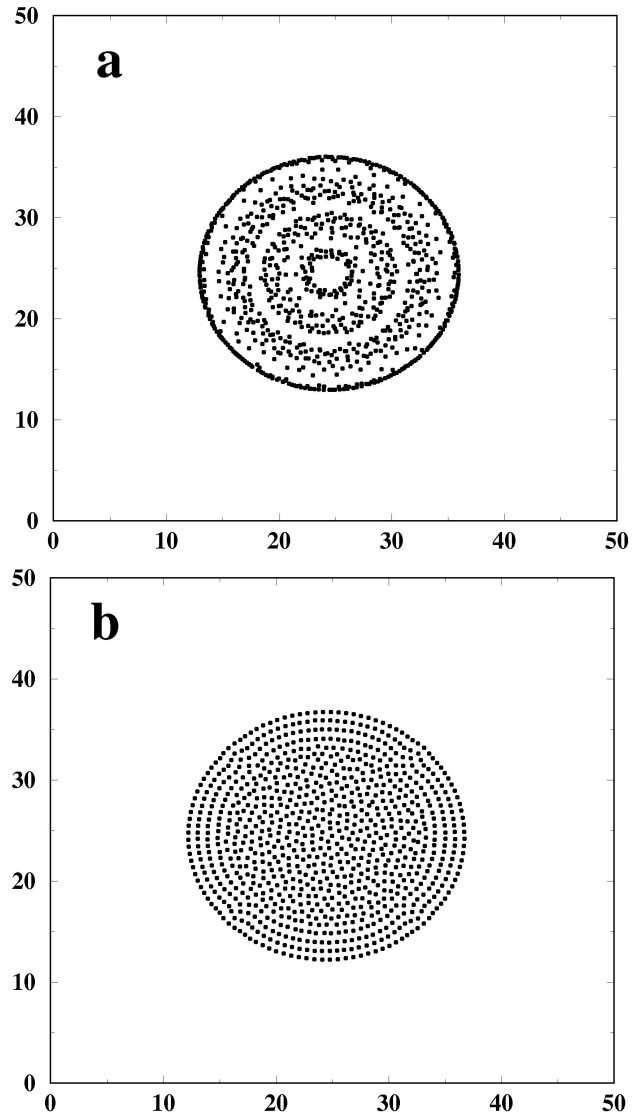

FIGURE 1. Particle positions in the (x, y)-plane showing the stable van der Waals liquid drop obtained a) when the tensile instability is present and b) when it is removed by adding an artificial stress.

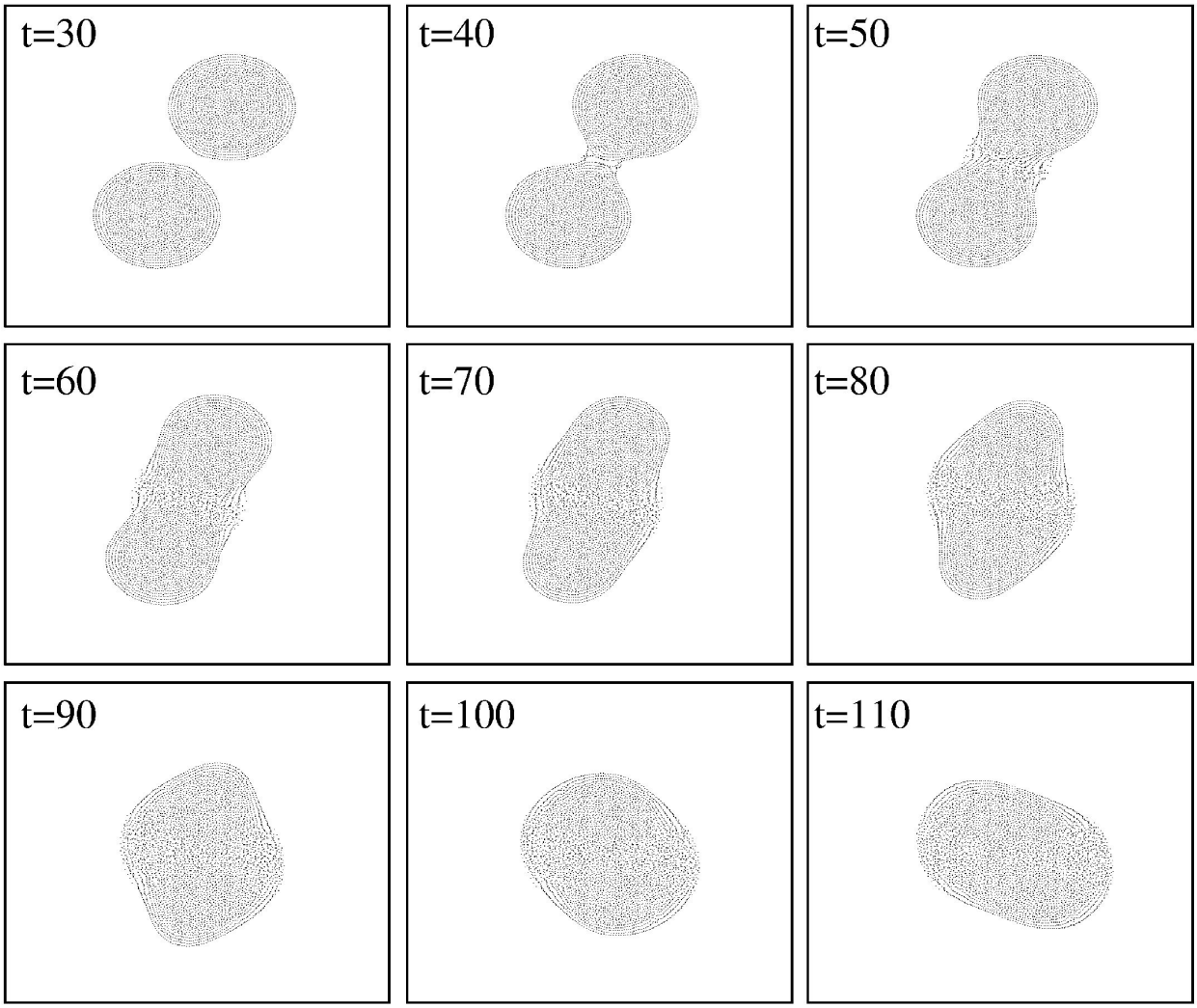

FIGURE 2. Time resolved shape evolution of the grazing collision of two equal-size drops. The time is given in dimensionless units. The sides of the boxes are twice as long as those shown in Fig. 1.

4. Off-center binary drop coalescence collision

We now describe the results obtained for the grazing collision of two liquid drops of equal size. The colliding drops are physically identical and in thermo-mechanical equilibrium. The drop model configuration corresponds to that shown in Fig. 1b. The binary drop collision is fully described by the density ρ, the shear viscosity η, the surface tension σ, the diameters ($D_1 = D_2 = D \approx 36$) of the colliding drops and their relative velocity U [14]. A further important quantity is the impact parameter X, defined as the distance from the center of one drop to the relative velocity vector placed at the center of the other drop. These quantities can be combined to produce the following dimensionless numbers

$$Re = \frac{\rho U D}{\eta}, \qquad We = \frac{\rho U^2 D}{\sigma}, \qquad x = \frac{X}{D}, \qquad (6)$$

where Re is the Reynolds number, We the Weber number and x the dimensionless impact parameter. The drops have a central density $\rho_c \approx 1.8$ and surface tension $\sigma \approx 7.1$, as determined using the Laplace equation. With the choice of a constant relative velocity $U \approx 0.26$ and $X = D$, we get $Re \approx 17$, $We \approx 0.62$ and $x = 1$, corresponding to a low energy collision with a high impact parameter.

At low Weber numbers, we expect the impact to result in the permanent coalescence of the drops into a single one as shown in Fig. 2 for the temporal evolution of the collision. The early stages ($t < 90$) are mainly governed by the initial kinetic energies of the colliding drops and the presence of very large surface curvatures at the interface between them. The former results in uniform motion of the drops toward each other, while the latter causes a fast outward motion of the surface perpendicular to the line of contact. In this region, the viscous effects become important because of the high velocity gradients generated there. Further outward motion is, however, impeded by the high surface energies involved which ultimately reverse the flow making the combined drop configuration oscillate. The evolution is followed up to $t = 290$ at which time the coalesced drops have already completed a full revolution ($t \approx 230$).

A more detailed description of the models and physics involved in the permanent coalescence of equal-size drops colliding head-on ($x = 0$) and off-center ($x = 0.5$ and 1.0) for varied Re and We (up to $We = 10$) is given in Ref. 13.

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