SIMULATION OF DROPLETS ON INCLINED SURFACES USING SMOOTH PARTICLE HYDRODYNAMICS

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ABSTRACT

Simulation of pendant and sessile droplets has been carried out using the mathematical modelling technique called Smoothed Particle Hydrodynamics (SPH). In this technique, the fluid is represented by SPH particles. The model uses pair-wise particle-particle interactions to simulate surface tension and contact line behavior. The pair-wise forces are different for solid-solid, solid-liquid and liquid-liquid interactions. This allows for the possibility of a very wide variety of solid-liquid pairs that can be simulated, just by altering the relative magnitudes of these interactions. The compressible flow equation has been employed with the concept of artificial compressibility to calculate the pressure. The simulation results for pendant droplets have been validated by experimental results carried out with glycerin droplets placed on cleaned copper surface. The simulation has been carried out for droplets with volumes 5µl, 15µl and 30µl, corresponding to Bond numbers = 1.4, 2.9 and 4.4 respectively, and substrate inclinations ranging from horizontal (0°) to 30°. The droplet was allowed to come to a stable shape at a given angle of inclination. From a macroscopic 'distal' viewpoint, wherein the length scale is of the order of capillary radius, the apparent contact angle has been estimated. However, as we pass through an 'intermediate' or proximal region towards the inner region of the meniscus, there is interplay of viscous and surface tension forces, leading to drastic reduction in the molecular contact angle. The final liquid-solid contact may be manifested as a monolayer thin film wherein it is almost impossible to uniquely define a contact angle at this molecular length scale. The equilibrium apparent contact angle as predicted by the SPH simulations are in excellent agreement with the experimental data.

NOMENCLATURE

$<f(x)>$	Kernel Approximation of function f(x)
Δx	Initial inter-particle spacing (m)
A	Area (m^2)
a	Acceleration (m/s^2)
Bo	Bond Number ($\rho L^2 g / \sigma$)
c	Coefficient of pressure (m/s)
F	Force (N)
g	Acceleration due to gravity (m/s^2)
h	Influence domain of particles (m)
L	Characteristic length (m)
m	Particle mass (kg)
P	Pressure (Pa)
s	Coefficient of surface tension (m/s^2)
t	Time (s)
V	Volume (m^3)
v	Velocity (m/s)
W	Smoothing Function

Greek symbols

σ	Surface tension (N/m)
ρ	Density (kg/m^3)
μ	Dynamic viscosity (Pa.s)
μl	Micro-liter (m^3)
θ	Contact angle (rad)
ε	Normalizing coefficient in XSPH (-)

Subscripts

ad	Advancing angle
i	Particle
ij	Particle 'i' with respect to particle 'j'

j	Particle 'j'
liq	Liquid particles
non-w	Non-wetting solid particles
re	Receding angle
STi	Surface tension on particle 'i'
wet	Wetting solid particles

Abbreviations

CSF	Continuum Surface Force
MD	Molecular Dynamics
SPH	Smoothed Particle Hydrodynamics
NS	Navier-Stokes' equation
SPAM	Smoothed Particles Applied Mechanics

INTRODUCTION

The study of stability of droplets on inclined planes has many applications ranging from green house enclosures, wind shields, solar panels, printing and coating techniques, liquid metal condensation, etc. Stability of droplets is also very important in studying transition from dropwise condensation to film condensation. The shape and stability of droplets on surfaces depend upon an intricate interaction of physical and chemical forces. Many techniques have evolved over time to try and explain all the factors influencing the shape and stability of droplets on inclined planes. Smoothed Particle Hydrodynamics (SPH) is one of the most recent techniques and has been applied here. SPH is a Mesh-free Particle method [1]. It was first used by Lucy [2] to solve astrophysical problems. However, in the past couple of decades its application has been extended to various types of fluid flow problems such as viscous fluid flow [3], low Re-incompressible fluid flow [4], free surface problems [5], etc.

In the present work, simulations of pendant and sessile 2-D microdroplets have been carried out using SPH. At such length scales, surface tension plays a major role in determining the droplet shape and the resulting droplet contact angle. Many techniques have been used by researchers to model the surface tension force. Nugent and Posch [6] used the cohesive pressure of the Van-der-Waal's equation giving rise to an attractive, central force to model surface tension in liquid droplets. Das and Das [7] used a diffuse interface technique to capture the effect of surface tension. Brackbill [8] employed a continuum surface force model (CSF) representing the interface between fluids of different properties or colors as regions of finite thickness, thereby, eliminating the need of interface reconstruction. Tartakovsky and Meakin [9] used a particle-particle interaction method to simulate flow of droplets through fracture junctions. We have employed the particle-particle interaction method as it allows for the simulation of a very wide variety of solid-liquid pairs. Also, we believe that simulating mergers and coalescence of droplets becomes simpler using particle-particle interactions.

MATHEMATICAL MODELLING

The model solves the NS-equation using SPH. Equation (1) represents the particle discretisation of kernel approximation [1] employed in SPH for a function *f(x)*. The code developed uses standard Gaussian kernel as smoothing function, W, to achieve better accuracy, even though it is computationally expensive. Estimation of density has been done using summation density approach Equation (2)

$$f(x_i) \approx \sum_{j=1}^{N} \frac{m_j}{\rho_j} \cdot f(x_j) \cdot W(x_i - x_j, h) \qquad (1)$$

$$\rho_i = \frac{\sum_{j=1}^{N} m_j \cdot W(x_i - x_j, h)}{\sum_{j=1}^{N} \left(\frac{m_j}{\rho_j} \right) \cdot W(x_i - x_j, h)} \qquad (2)$$

This is fairly simple to employ and ensures proper mass conservation. A direct particle-particle interaction term has been coupled with the NS-equation (Equation (3)) to account for the surface tension forces.

$$\frac{dv_i}{dt} = -\frac{\nabla P_i}{\rho_i} + \frac{\mu_i}{\rho_i} \nabla^2 v_i + \frac{Body \quad forces \quad + \quad External \quad forces}{\rho_i} \qquad (3)$$

Standard SPH discretisation [1] of the NS equation has been used to obtain Equation (4)

$$\frac{dv_i}{dt} = -\sum_{j=1}^{N} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \cdot \nabla_i W(r_i - r_j) +$$

$$2\mu_i \sum_{j=1}^{N} m_j \frac{(\vec{v}_i - \vec{v}_j)}{\rho_i \rho_j (\vec{r}_i - \vec{r}_j)^2} (\vec{r}_i - \vec{r}_j) \cdot \vec{\nabla} W(\vec{r}_i - \vec{r}_j, h)$$

$$+ \vec{g} \quad + \quad \frac{\vec{F}_{STi}}{\rho_i} \qquad (4)$$

The pressure calculation has been done using the universal equation of state (Equation (5)), this has been preferred over the more accurate Van-der Waal's equation of state, as it allows for the definition of a clear convergence criterion and provides greater control over density fluctuations.

$$P_i = c^2 \rho_i \tag{5}$$

where c is the pressure coefficient.

Surface tension has been modeled using direct long range attractive and short range repulsive particle-particle interactions [9]. The value of surface tension force on each particle will be the vector sum of the individual force values (Equation (6)).

$$F_{ST_i} = \sum_{j=1}^{N} s_{ij} ST(x) \tag{6}$$

The value for s_{ij} will be different for solid-liquid, solid-solid and liquid-liquid interactions. Also, the value of s_{ij} will be different for solid particles that are being wetted by the liquid particles and those that are not being wetted by the liquid particles.

From the N-S equations we obtain the value of the acceleration of the particles at each time-step. From this we can calculate the new position of each particle using the 'Velocity-Verlet' algorithm [9, 10]. (Equations (7) and (8))

$$r_i(t + \Delta t) = r_i(t) + \Delta t v_i(t) + 0.5 \Delta t^2 a_i(t) \tag{7}$$

and

$$v_i(t + \Delta t) = v_i(t) + 0.5 \Delta t (a_i(t) + a_i(t + \Delta t)) \tag{8}$$

The values obtained from these were then used in the technique of "XSPH" [1, 11] to finally obtain the position and velocity values for each particle

$$\frac{d\vec{x}_i}{dt} = \vec{v}_i - \varepsilon \sum_{j=1}^{N} \frac{m_j}{\rho_j} \vec{v}_{ij} W_{ij} \tag{9}$$

The value of ε can range from 0.0 to 1.0. In this particular case, $\varepsilon = 0.3$ has been used. Normally, for incompressible flows, this value of ε works quite well [1].

The application of XSPH [1, 11] ensures that the particles move closer to the average velocity of the neighborhood particles and therefore keeps the particle motions more orderly.

RESULTS AND DISCUSSION

The code was run for parameter values corresponding to glycerin droplets on copper surface with volumes 5µl, 15µl and 30µl (Bo = 1.4, 2.9 and 4.4, ρ = 1260 kg/m^3, σ = 0.068 N/m at room temperature). The results have been validated against experimental and simulation (using Young-Laplace equation) results of Bhutani [12] and are found to be in good agreement with the experimental findings. Figure 1 compares the findings of droplet shape using SPH simulations, simulations carried out using Young-Laplace equation and the corresponding experimental observations. In the figure, only the interface particles of the SPH simulations have been shown for ensuring the clarity of representation. From Figure 1, all the three results i.e., experimental, Young-Laplace simulations and SPH simulations follow very closely for droplet volume 5µl. However, as the droplet volume increases the effect of gravity increases and the results show some disparity. This can be attributed to the phenomenon of slipping of the droplet interface. In the case of Young-Laplace simulations, the contact points of the two interfaces at the substrate need to be pinned, i.e., are immobile. However, during the experiments, the advancing contact point need not show local pinning and the advancing contact line usually gets displaced from its position. This leads to a slipping of the advancing contact line of the droplet. This effect is suitably captured in the SPH simulations and thus SPH results are in better confirmation with the experiments than the theoretical Young-Laplace results. Also, in Young-Laplace simulations, the contact angle used is the 'apparent' contact angle which is sharp and well defined. No distinction can be made between 'apparent' contact angle and the 'molecular' contact angle while using Young-Laplace simulations. SPH simulations and careful experimental results [13] however, indicate the presence of a pre-cursor layer leading to the bulk of the liquid. The contact line forms a smooth curve and the apparent contact angle has been defined at the inflection point of the curve. Figure 2 shows the variation of advancing and receding apparent contact angles with inclination of solid substrate. The experimental results of Bhutani [12] are also presented for comparison.

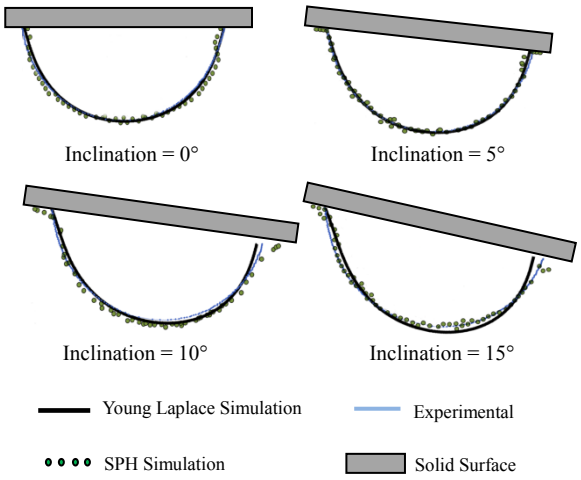

Figure 1(a)

Comparison of the shape of glycerin droplet on a copper surface, volume = 5 µl at different inclinations obtained using Young-Laplace equation, SPH and Experiments.

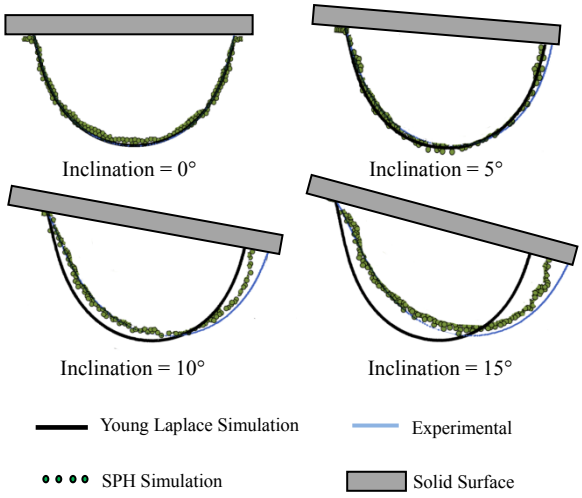

Figure 1(b)

Comparison of the shape of glycerin droplet on a copper surface, volume = 30 µl at different inclinations obtained using Young-Laplace equation, SPH and Experiments.

Comparison of results for pendant and sessile droplets has also been done and the results have been presented in Figure (3). It was observed that the particle density for sessile droplets was slightly higher near the solid interface than for pendant droplets. This can be attributed to the effect of gravity. However, the apparent contact angle for the two cases is nearly the same for small droplet volumes, thereby, confirming the applicability of the method to both pendant and sessile droplets.

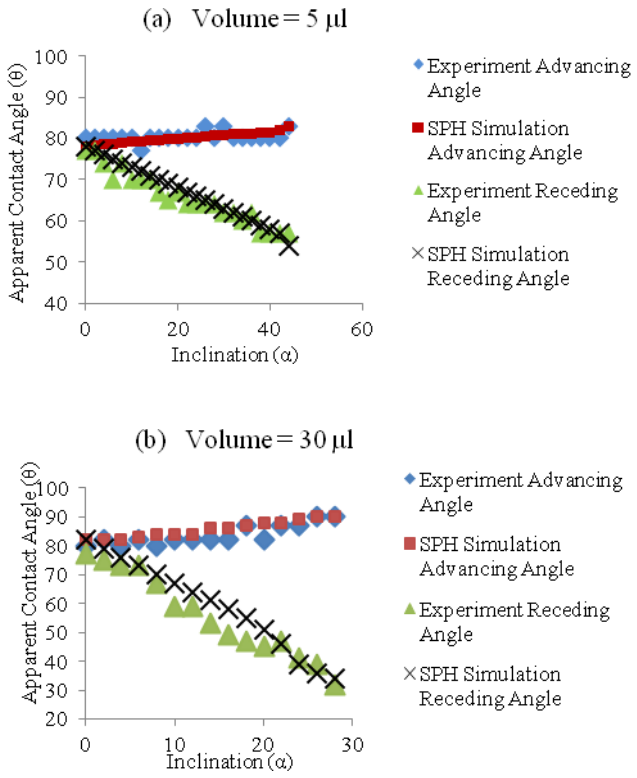

Figure 2

Comparison of apparent contact angle (Advancing/ Receding) data for glycerin droplet on copper surface plotted against angle of inclination of the surface for volume a) 5µl, and, b) 30 µl.

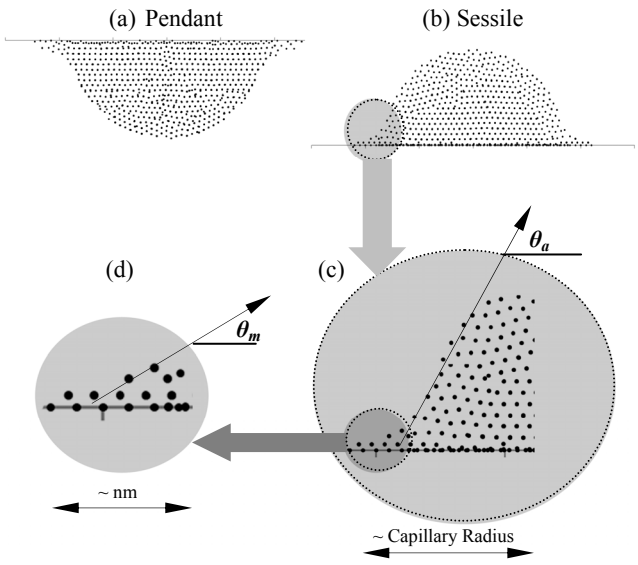

Figure 3

Simulation of a) Pendant and b) Sessile droplet carried out using SPH for Glycerin on a cleaned copper surface at room temperature. c) "Intermediate region"; apparent contact angle measured at inflection point. d) "Inner region"; molecular or the actual contact angle.

It can be seen that these results obtained from the SPH simulations are very well in agreement with the experimental results. In order to extend the analysis to other liquid-solid pairs, the value of computational parameters needs to be suitably altered. This presents a limitation on the method as these computational parameters cannot be calculated using any physical techniques. However, we can lay down certain general guidelines to choose their respective values.

Selection of $h/\Delta x$: A theoretical analysis for the error term in SPH was given by Fulk and Quinn [14]. It was found that the error term was inversely proportional to the value of $h/\Delta x$. Thus, higher the value of this term, lesser the error that propagates in the solution. However, higher the value of $h/\Delta x$, greater will be the computational requirements. A high value of $h/\Delta x$ also leads to a thicker interface with a higher density gradient and can be a cause of numerical instability. In the present code, the value for $h/\Delta x$ has been set at 1.20 as this gives good results.

Effect of s_{ij}: The different values of s_{ij} for wet solid particles, non-wet solid particles and liquid particles are responsible for the formation of different contact angles. One can estimate the value of contact angle from the force balance at the contact line. For 2-dimensions we have the formula:

$$s_{ij,non-w} = s_{ij,wet} + s_{ij,liq}\cos\theta \tag{10}$$

$$\cos\theta = \frac{s_{ij,non-w} - s_{ij,wet}}{s_{ij,liq}} \tag{11}$$

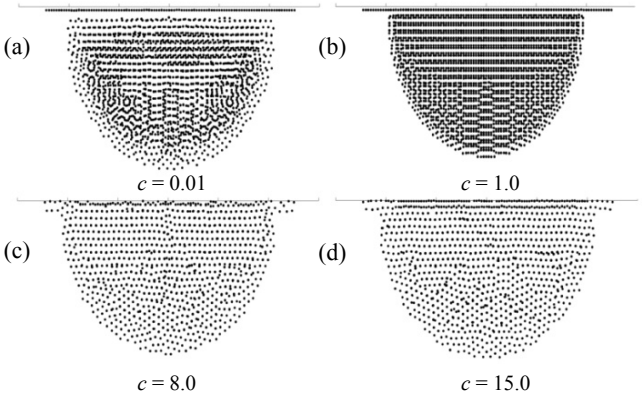

Figure 4
The impact of pressure coefficient on the density distribution in liquid bulk and droplet clamping to solid surface.

We can notice that the value of the contact angle depends on the *difference* between the s_{ij} values for the non-wetting and the wetting solid particles. If the two values were to change correspondingly, the apparent contact angle would still remain the same but the molecular contact angle and hence the shape of local meniscus will be slightly changed. The selection of these two coefficients is also required to clamp the droplet properly to the solid surface. Using a high value of $s_{ij,liq}$ leads to a compression in the bulk and the average density is found to be slightly lower than the expected density and vice-versa.

Effect of Pressure Co-efficient: The pressure coefficient ensures uniform density distribution throughout the bulk of the fluid. Any density differences lead to a density gradient and hence a pressure force is created. Higher the value of the pressure coefficient, greater the restoring force hence smaller the density variations. Also, a high pressure coefficient ensures greater clamping of the droplet to the surface. However, a high pressure term imposes limitation on time step and a higher value needs significantly higher computational power.

In the present code, a pressure coefficient of 8.0 has been used. This allows for reasonably acceptable variation in density (~5%). The effect of pressure coefficient on the density distribution and clamping to solid surface can be seen in the Figures [4(a)-4(d)]. It can be seen that the droplet is poorly clamped to the solid surface for c = 0.01; also the density variation is high. However, as the pressure coefficient is increased, the density becomes more uniform and so does the clamping.

CONCLUSIONS

The application of particle-particle interaction term to standard SPH equation suitably captures the behavior of sessile and pendant droplets on inclined surfaces. The apparent contact angle and the droplet shape predicted from the SPH simulations are in excellent agreement with those obtained from experiments. Thus, we can conclude that particle-particle interaction method using SPH can be employed to simulate droplets on inclined surfaces. A very large combination of liquid-solid pairs can be simulated by changing the respective mutual interaction values between SPH particles. Initial benchmark experiments are needed for fine tuning of

the model parameters. Shape of the droplet and the advancing and receding angles for a given pair of liquid-solid can then be calculated using the simulation technique.

KEYWORDS

Smoothed Particle Hydrodynamics (SPH), Interfacial phenomenon, Young's equation, Static droplet shape, Apparent Contact Angle

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