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Simulation of Water Droplet on Horizontally Smooth and Rough Surfaces Using Quasi-Molecular Modelling

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***Abstract*—**We developed a method based on quasi-molecular modelling to simulate the fall of water drops on horizontally smooth and rough surfaces. Each quasi-molecule was a group of particles that interacted in a fashion entirely analogous to classical Newtonian molecular interactions. When a falling water droplet was simulated at low impact velocity on both smooth and rough surfaces, the droplets moved periodically (i.e. the droplets moved up and down for a certain period, finally they stopped moving and reached a steady state), spreading and recoiling without splash or break-up. Spreading rates of falling water droplets increased rapidly as time increased until the spreading rate reached its steady state at time $t \sim 0.25$ s for rough surface and $t \sim 0.40$ s for smooth surface. The droplet height above both surfaces decreased as time increased, remained constant after the droplet diameter attained a maximum value and reached its steady state at time $t \sim 0.4$ s. However, rough surface had higher spreading rates of falling water droplets and lower height on the surface than smooth one.

***Keywords*—**Quasi-molecular modelling, particle modelling, molecular aggregate approach.

I. Introduction

SEVERAL studies have investigated the impact of liquid droplets and their interaction with surfaces [1]-[6]. Experimental studies usually use high-speed digital photography to examine the impact of liquid droplets and their spreading on a surface. Examples of experimental studies include investigations of the evolution of fingering patterns at the edges of expanding thin jets travelling along the surface during impact on a glass plate [1], the impact parameter on the droplet impingement [2], the impact of distilled water droplets on a heated wax surface [3], the water droplet spreading phenomena on a glass surface [4], the influence of the surface properties on the dynamics behaviour of impacting water droplet [5], and the influence of surface wettability on droplet spreading [6].

Theoretical studies have been done on droplet spreading [7]-[12] and concluded that theoretical modelling of droplet spreading should account for the following factors: inertia, viscosity, gravitation, capillary forces and wettability [13]. Most numerical simulations of drops impacting on a surface use Navier-Stokes equations in their studies. Navier-Stokes equations are fundamental equations that govern fluid flow and can solve the dynamics of water flow. However, liquid drop modelling encounters a major theoretical difficulty due to the large gradients resulting from surface tension [14]. These large gradients are fundamental to the physics of fluid drops and cannot be solved by Navier-Stokes equations [15].

A numerical approach to particle modelling has been developed for fluid flow modelling based on the attempt to bridge the gap between atomistic and continuum simulations [16]. Unlike the continuum and statistical mechanics approaches, this numerical approach uses a relatively small set of quasi-molecular particles that interact in accordance with classical molecular-type formulas and conserves both mass and normalised energy. This approach concerns non steady state phenomena and variations in dynamical responses due to variation of system parameters.

The dynamics of water drop spreading on flat and rough surface depends on impact velocity, material properties of the surface and surface tension [17]. Droplet spreading is usually characterised by the diameter of the wet area and the drop height above the surface [18]. The way drops spread on a flat surface can be classified into high-speed and low-speed impact spreading. In this study, we used quasi-molecular modelling to simulate a 2-D low-speed impact water droplet on smooth and rough surfaces. The study aimed (1) to simulate water droplet impacting on smooth and rough surfaces by using quasi-molecular modelling, and (2) to investigate and compare spreading rates of falling water droplets and the droplet height through time on smooth and rough surfaces.

II. Materials and Methods

A. Quasi-Molecular Modelling

We used quasi-molecular modelling or particle modelling to simulate the fall of a water drop. The physical response of the fluid was caused by external forces (i.e. gravity and molecular interaction) [16]. Gravity acted uniformly on all

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molecules in the fluid. In the quasi-molecular modelling, interaction forces were considered only between nearest-neighbour particles and assumed to be of the same form as in molecular dynamic (MD) modelling. The interaction force was represented by (1):

$$F(R) = \frac{G}{R^p} + \frac{H}{R^q} \tag{1}$$

Where G, H = parameters in particle structure
p, q = exponential parameter in particle structure
R = equilibrium position in particle structure

G, H, p, q were positive constants with $q > p$ in order to obtain the repulsive effect that was necessarily stronger than the attractive one. Molecular interaction forces had two components: attraction and repulsion. The four parameters G, H, p and q were yet to be determined. If p, q and R_0 were given, then by conditions of mass and energy conservation, G and H were derived. R_0 was the equilibrium distance of the quasi-particle structure.

Just as in MD modelling, the dynamical equation of motion for each particle P_i of the system was given by (2):

$$m_i \frac{d^2\vec{R}}{dt^2} = -980\, m_i\vec{\delta} + \alpha \sum_{\substack{j=1 \\ j\neq i}}^{N} \left(\frac{G}{R^p} + \frac{H}{R^q} \right) \frac{\vec{R}_{ij}}{\left|R_{ij}\right|}, \; i \neq j \tag{2}$$

Where m_i = mass of P_i
$\vec{R}_{ij}$ = the vector form of P_j to P_i
α = a normalising constant for P_i
N = the number of particle

α was obtained from (3):

$$\alpha \left| -\frac{G}{\left(\frac{3}{2}R_0\right)^p} + \frac{H}{\left(\frac{3}{2}R_0\right)^q} \right| < 980\, m_i \tag{3}$$

α was used to normalise the interaction force between two particles. After normalisation, the interaction force between two particles was less than the gravitational force (i.e. < 9.8 m/s^2).

For the simulation of a water drop by quasi-molecular modelling, we chose N = 450, p = 1, q = 3, R_0 = 0.03 cm and the distance of local interaction D = 0.06 cm, so the motion of particle P_i was determined by the dynamical (4).

$$\frac{d^2\vec{R}}{dt^2} = -980\,\vec{\delta} + \alpha \sum_{\substack{j=1 \\ j\neq i}}^{540} \left(-\frac{0.014723}{R^p} + \frac{0.000013}{R^q} \right) \frac{\vec{R}_{ij}}{\left|R_{ij}\right|} \tag{4}$$

α where vector $\vec{\delta}$ = (0,1), and the first term on the right-hand side (i.e. $-980\,\vec{\delta}$) was the gravity term. The normalising constant for P_i was $\alpha = 1.40752 \times 10^{-7}$.

For computational convenience, we used the time transformation $T = 10t$ (t in seconds). Equation (4) was reformed as

$$\frac{d^2\vec{R}}{dt^2} = -9.8\vec{\delta} + \sum_{\substack{j=1 \\ j\neq i}}^{540} \left(-\frac{0.763834}{R^p} + \frac{0.000687}{R^q} \right) \frac{\vec{R}_{ij}}{\left|R_{ij}\right|} \tag{5}$$

The model solved this equation simultaneously with a leapfrog numerical scheme.

B. Numerical Solution

In general, $F_i = m_i \ddot{r}_i$ i = 1,2,3, …, N could not be solved analytically from given initial data and had to be solved numerically. The choice of a numerical method was simplified by the physics of quasi-molecular modelling in small time steps. The reason was that the repulsive component H/R^q in (1) could be treated accurately only with small time steps for small R, since H/R^q was unbounded as R went to zero. Therefore, the advantages of using a high order numerical method, which allowed the choice of large time steps in obtaining a high degree of accuracy, were not applicable in Q modelling. The leapfrog formulas relating position, velocity and acceleration for particle P_i were

$$v_{i,1/2} = v_{i,0} + (\Delta t/2)\vec{a}_{i,0}, \qquad \text{(starter formula)} \tag{6}$$

$$v_{i,k+1/2} = v_{i,k-1/2} + (\Delta t)\vec{a}_{i,k}, \quad k = 1,2,3, \ldots \tag{7}$$

$$\vec{r}_{i,k+1} = \vec{r}_{i,k-1/2} + (\Delta t)\vec{v}_{i,k+1/2}, \quad k = 1,2,3, \ldots \tag{8}$$

Where $\vec{v}_{i,k}, \vec{a}_{i,k}$ and $\vec{r}_{i,k}$ were the velocity, acceleration and position vectors of particle i at time $t_k = k\Delta t$, Δt was the time step, $\vec{v}_{i,k+1/2}$ was the velocity of particle i at $t_k = (k+1/2)\Delta t$, and so on.

C. Coordinate-System Setup

540 particles in two dimensions were used to simulate a regular triangular mosaic. The equilibrium distance was set at R_0 = 0.03 cm. Positions of water particles were set in an x-y coordinate system. The corresponding mesh system was built via the following 1-D storage method:

$$x_1 = 0.5,\; y_1 = 1,\; x_{24} = 0.515, \qquad y_{24} = 1.0259,$$

$$x_{i+1} = 0.03 + x_i, \qquad y_{i+1} = y_1, \qquad i = 1,2, \ldots, 22$$

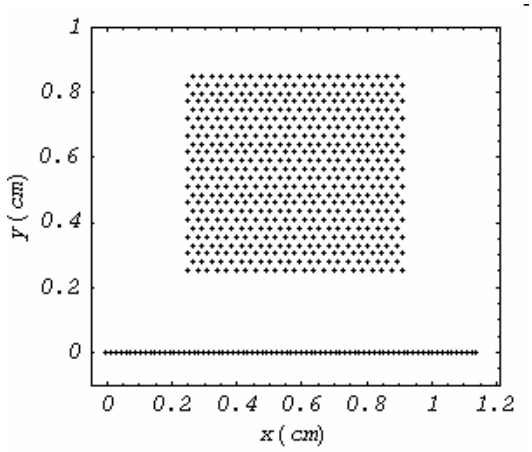
$$x_{i+1} = 0.03 + x_i, \qquad y_{i+1} = y_{24}, \qquad i = 24,25, \ldots, 44$$

$x_{i+1} = x_{i-45}$, $y_i = 2.05196 + y_{i-45}$, $i = 46,47, \ldots, 540$

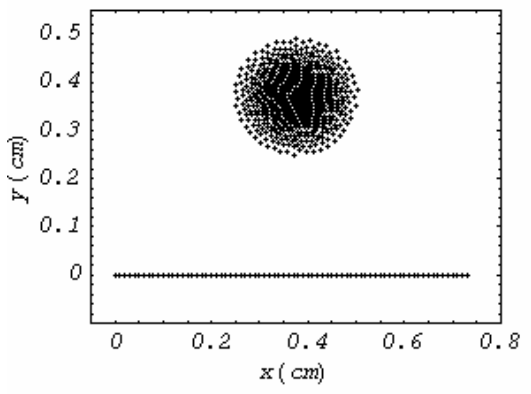
The triangulated particle arrangement was laid in a rectangle that was 0.6600 cm wide and 0.5975 cm high. At each grid point, (x_i, y_i) we set a particle P_i, that is, an aggregate of water molecules (Fig. 1a). The particles in this initial stage were arranged on a regular triangular mosaic. The distance from any P_i to an immediate neighbour was 0.06 cm (i.e. $2R_0$).

D. Simulation of Falling Water Drop

Before the falling water drop was simulated, a single drop needed to be formed as follows. First, let each of the 540 water particles P_i interact with all other particles in accordance with (5), and the numerical solution was generated by the leap-frog formulae with $\Delta t = 0.0005$. Every time step, each velocity was damped by a factor of 10. The effect of the damping was to decrease the total kinetic energy, or internal heat. We imposed a local interaction distance of $D = 0.06$ cm. For simplicity, we assumed that all initial velocities were zero and the interaction during collisions was independent of gravity. We set $g = 0$ in (5). The system allowed interaction through $t = 10$ s, at which time the particles contracted maximally. At this maximal contraction, a stable water drop contained its energy in potential form and no longer oscillated (Fig. 1b). For stable water drops, outer most particles showed lower density than inner particles. This phenomenon was a characteristic of liquid surface tension. The average diameter of stable water drops was approximately 0.42 cm (Fig. 1b). The shape of the water drop depended on the interaction force among water particles.



(a)



(b)

Fig. 1 (a) configuration of 540 water particles and (b) initial stage of water drop formation of 540 water particles on a smooth surface with the initial setting height at 0.25 cm

The stable water drop was used as an initial condition to study the falling water drop (Fig. 1b). We examined the effect of impact velocities on the height ($H(t)$) and the diameter of water drops ($R(t)$). Time was reset to $t = 0$. The system was then allowed to continue its interaction with g reset correctly to $g = 9.8$ m/s^2. If any particle collided with a wall of the basin, then that particle reflected symmetrically.

To simulate the spreading of water droplet on rough surface, we used the falling water drop (Fig. 1b) as an initial condition and a rough surface of 131 additional particles was added via the following 1-D storage method (see Fig. 2):

$x_i = 0.2 + 0.015(i - 540)$, $y_i = 0$, $i = 541,542, \ldots, 605$

$x_i = 0.2 + 0.030(i - 605)$, $y_i = 0.005$, $i = 606,607, \ldots, 638$

$x_i = 0.2 + 0.030(i - 638)$, $y_i = 0.01$, $i = 639,640, \ldots, 671$

The quasi-molecules of the rough surface were fixed, that is they were not allowed to move, and were called solid particles. However, they were allowed to interact with the fluid particles with a force given by (9).

$$F(R) = -\frac{0.627200}{R^p} + \frac{0.000141}{R^q} \qquad (9)$$

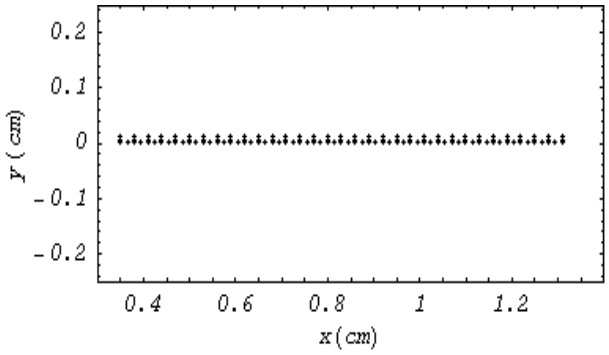


Fig. 2 Configuration of 131 particles of a rough surface

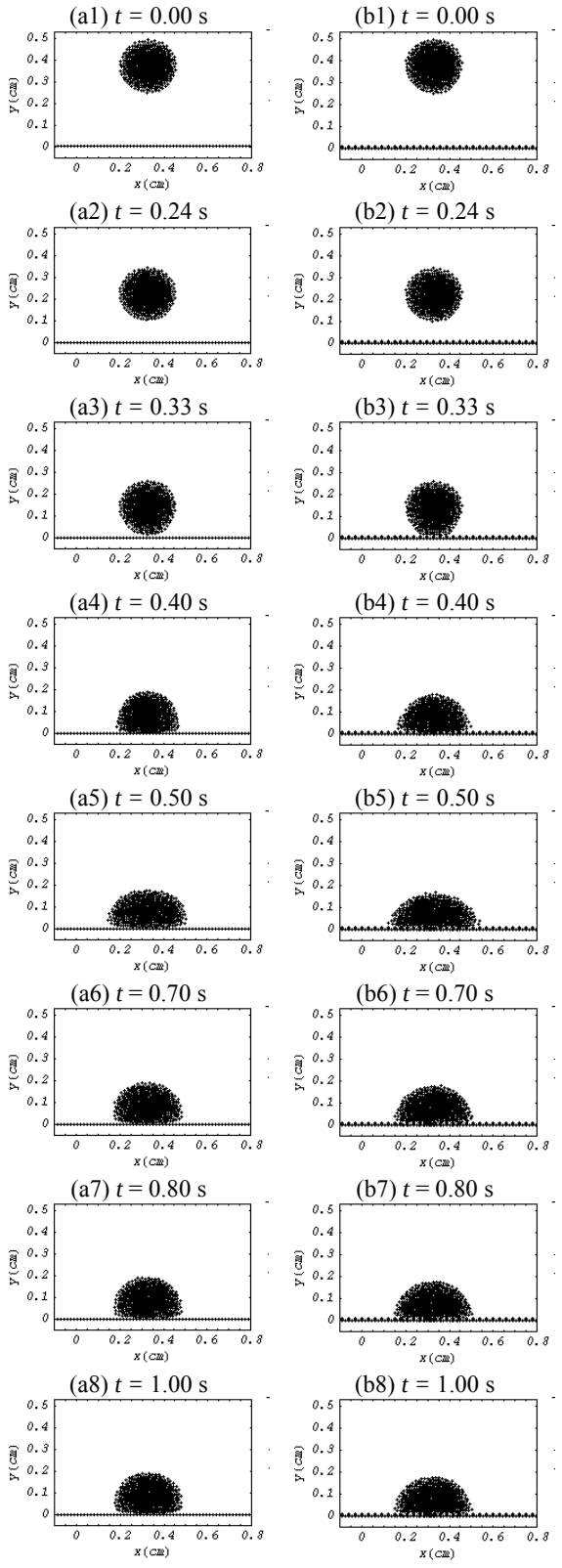


Fig. 3 Time sequence of droplet impact on a smooth surface (a1-a8)
and a rough surface (b1-b8). (1) t = 0.00 (s), (2) t = 0.24 (s), (3) t = 0.33 (s), (4) t = 0.40 (s), (5) t = 0.50 (s), (6) t = 0.70 (s),

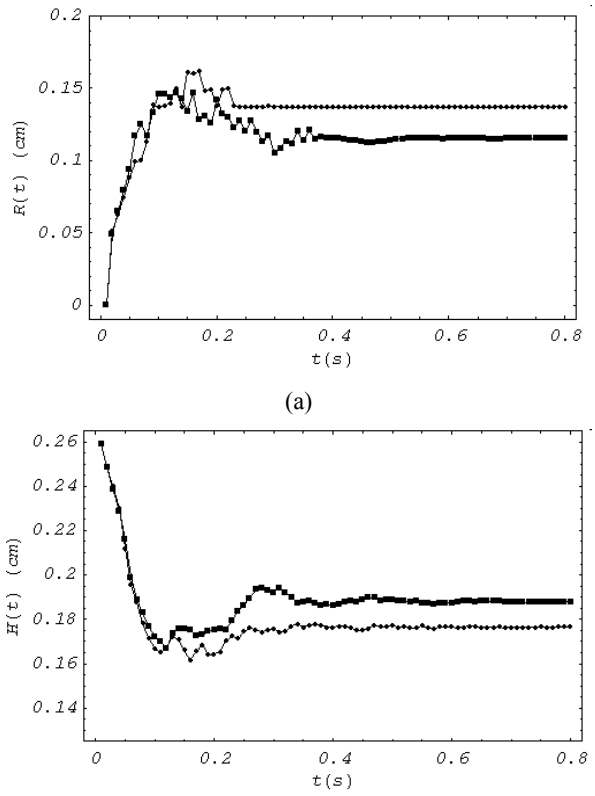


Fig. 4 (a) spreading rate ($R(t)$), and (b) Water drop height ($H(t)$) above the smooth (—■—) and rough (—●—) surfaces versus time for a water drop impacting on a surface

III. Results and Discussion

Time sequences of water droplet impact on smooth surface and rough surfaces at the released height of 0.25 cm from time t = 0.00 to t = 1.00 s were shown in Fig. 3a1-a8 and Fig. 3b1-b8. When a falling water droplet was simulated at low impact velocity, the water droplets moved up and down periodically, spreading and recoiling without splash or break-up on both types of surface (Fig. 3a1-a8 and Fig. 3b1-b8). Similar observations have been shown in many studies including dynamic behaviour of single droplets impacting on a flat surface, and dynamics of water spreading on a glass surface, horizontal surface, and solid surface [3], [7], [8], [17].

Droplet spreading was characterised by the diameter of the wetted area (i.e., the spreading rate ($R(t)$) and the droplet height above the surface ($H(t)$). Spreading rates of falling water droplets increased rapidly as time increased until the spreading rate reached its steady state at time $t \sim 0.25$ s for rough surface and $t \sim 0.40$ s for smooth surface (Fig. 4a). The droplet height above the surface decreased as time increased, remained constant after the droplet diameter attained a maximum value and reached its steady state at time $t \sim 0.40$ s on both surfaces (Fig. 4b). However, rough surface had higher

spreading rates of falling water droplets and lower droplet heights on the surface than smooth one (Fig. 4a,b). Similar observations have been shown in the studies including of [5], [6].

In summary, this study is the first to develop a new method based on a quasi-molecular modelling to simulate the fall of water drops. Our results show that a quasi-molecular modelling could be used to study the flow dynamics during the spreading on both smooth and rough surfaces, spreading rates of falling water droplets through time and the droplet height above the surface. Future studies should be conducted on 3-D falling water drop simulations in order to gain a better understanding of falling water drop dynamics.

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