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Experimental and computational study of liquid drop over flat and spherical surfaces

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Abstract

Flow of a liquid droplet over a flat plate and a spherical pellet was studied to improve understanding of wetting in trickle bed reactors. High speed imaging system and computational fluid dynamics (CFD) was used for this purpose. Experimental data is reported on dynamics of drop rest on a flat and a spherical surface. Micro-scale motion of liquid droplet on these surfaces was captured with a high-speed CCD camera. Images were analyzed to provide quantitative data of drop dynamics. Drop spread and recoiling velocities were reconstructed from the experimental data. CFD model based on the volume of fluid (VOF) method was used to simulate drop dynamics on flat and spherical surfaces. Surface tension and wall adhesion phenomenon were included in the computational model. Simulated drop dynamics was found to capture key qualitative features observed in the experiments. Numerical simulations with three-dimensional domains are essential for quantitative comparison with experimental data. The experimental results and computational model discussed in this paper would be useful for better understanding of wetting in trickle bed reactors.

Keywords: Droplet dynamics; CFD; VOF; High-speed camera

1. Introduction

Trickle bed reactors, in which gas and liquid phases flow co-currently downward through the packed bed (of catalyst pellets), are used in several chemical industries. Two-phase frictional pressure drop, liquid saturation and degree of wetting are some of the key and essential parameters for design of these reactors. Extensive experimental investigations have been carried out to study these key parameters. In recent years, computational fluid dynamics (CFD) is being used to understand the complex hydrodynamics in more detail (see for example [3,5]). These models, however, require appropriate inter-phase coupling closures. In trickle bed reactors, gas–liquid flow over catalyst pellet is extremely complex and liquid may or may not wet the pellet completely. It is essential to understand the intricacies of gas–liquid flow over a representative single pellet to develop better understanding of inter-phase coupling closures and wetting. As a first step towards this goal, we have studied flow of a liquid droplet on flat and spherical surfaces. Extension to understand influence of gas flow may be straightforward.

Most of the published studies on drop dynamics (see for example [6–8]) considered impact of liquid drops on flat surfaces with high velocities (in the range 1–6 m/s). Such high velocity impact occurs in applications such as spray coating or delivery of agrochemicals. In contrast to this, in trickle bed reactors, liquid droplets interact with solid surfaces with much lower velocity. Such low velocity interaction results in quite different drop dynamics. The other important

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Nomenclature

F_{SF}	continuum surface force ($kg/m^2\,s^2$)
g	gravitational constant (m/s^2)
k	particular phase under consideration
n	unit normal
n_w	normal vector
P	pressure (Pa)
Re	Reynolds number, $\rho V d_p/\mu$
t	time (s)
t_w	tangential vector
V	velocity (m/s)
We	Weber number, $\rho V^2 d_p/\sigma$

Greek letters

α	volume fraction of phase
κ	radius of curvature (m)
μ	viscosity (Pa s)
ρ	density of the fluid (kg/m^3)
σ	surface tension (N/m)

aspect relevant to trickle bed reactors is interaction of liquid droplets with curved surfaces of pellets. Study of such phenomenon has not been reported. Some attempts of numerical simulation of drop dynamics have been made (see for example [2,9]). These attempts, however, cover rather different conditions. Numerical simulations of spreading of liquid droplet on flat and curved surfaces in the operating regime of trickle bed reactors have not been reported.

In this paper we have studied interaction of liquid droplets with flat and spherical surfaces with the help of the high speed imaging technique at drop impact velocities of ~0.2 m/s. Experiments were carried out using high-speed camera to quantitatively measure data on drop spreading and oscillations in drop spreading due to complex interactions of inertial and surface forces. Apart from studying the drop interactions with solid surfaces at low velocities, the objective was also to provide an experimental data to validate and to guide development of computational models to simulate such interactions. A computational flow model based on VOF method was used to simulate the experimental results. The experimental results and computational model discussed in this paper would be useful for better understanding and prediction of wetting in trickle bed reactors.

2. Experimental set-up

Experimental set-up used for studying interaction of falling drop with a flat plate and a spherical pellet is shown in Fig. 1. It consists of a dropper for drop generation, high-speed CCD camera (Red Lake Imaging, USA) with the maximum frame rate of 500 frames per second, flashlight and image processing software. Dropper tip was held 8 mm apart from the objective surface. The size of the drop formed at the tip was found to be about 4.2 mm. Spherical pellet of diameter 10.4 mm was held under the dropper with an offset of 1 mm from the centerline of pellet (see Fig. 1b). Droplets were generated using dropper of inner diameter 3 mm. Distilled water was used for generating a drop on a smooth and non-porous glass flat plate and a spherical pellet. Porosity and roughness of solid surface would affect contact angle and its dynamic behavior. At present, however, adequate understanding of time varying contact angle and their interaction with surface porosity/roughness is not available. The present work was therefore restricted to the non-porous and smooth solid surfaces. Before the start of the each experiment, surface of the plate and pellet were washed with the hot water, dried at temperature of 80 °C and cooled to room temperature. This procedure was followed to ensure that the surface is free from any contamination and is dry. Drop impact behavior and dynamics was recorded with the help of the charged couple device (CCD) camera. Recording was carried out at frame speed of 250 frames/s ensuring that the there was no loss of

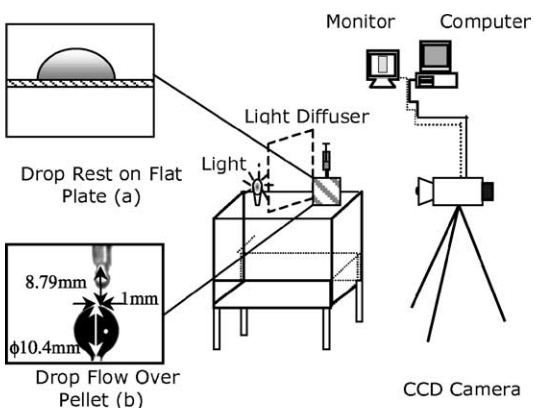

Fig. 1. Experimental set-up for high speed imaging of droplet flow.

critical information between two consecutive frames. Camera was located at 15 cm from the dropper and lens 18-180/2.5 was used for recording. Focus was made upon 15 mm × 15 mm area about the object. Recorded images were further processed with the help of the image analysis software Image Pro Plus (Media Cybernetics, USA). For calibration, a test material of known dimension was recorded during each set of conditions. Contact angle for water and glass material was measured and was found to be 45° with ±5% error. The experimental results were analyzed to determine the spreading of the droplet, height variation with respective time and drop front velocity.

3. Computational model

Simulations of drop impact/flow were performed using the volume of fluid (VOF) method [4]. Gas and liquid phases were modeled as incompressible fluids with constant value of viscosity and surface tension. Flow was assumed to be Newtonian and laminar. Surface stress of liquid phase was assumed to be one dimension, i.e. across normal to the surface and tangential stresses were neglected.

The mass and momentum conservation equations for each phase is given by:

$$\nabla V = 0 \tag{1}$$

$$\frac{\partial V}{\partial t} + \nabla(VV) = -\frac{1}{\rho}\nabla P + \nu\nabla^2 V + g + \frac{1}{\rho}F_{\mathrm{SF}} \tag{2}$$

This single set of flow equations were used throughout the domain and mixture properties as defined below were used.

$$\rho = \sum \alpha_k \rho_k \tag{3}$$

and for any variable,

$$\phi = \frac{\sum \alpha_k \rho_k \phi_k}{\sum \alpha_k \rho_k} \tag{4}$$

Thus, when in a particular computational cell, $\alpha_k = 0$ then the cell is empty (of the kth fluid). $\alpha_k = 1$, the cell is full (of the kth fluid). $0 < \alpha_k < 1$, the cell contains the interface between the kth fluid and one or more other fluids.

Interface between the two phases was tracked by solution of continuity equation for volume fraction function:

$$\frac{\partial \alpha_k}{\partial t} + (V_k \nabla)\alpha_k = 0 \tag{5}$$

where α_k is the volume fraction of the kth fluid. Volume fraction for the primary phase (gas) was not solved and was obtained from the following equation:

$$\sum_k \alpha_k = 1 \tag{6}$$

In addition to the mass and momentum balance equations, surface tension and wall adhesion were needed to specify at the interface. Surface tension was modeled as the smoothed variation of capillary pressure across the interface. Following Brackbill et al. [1], it was represented as a continuum surface force (F_{ST}) and was specified as a source term in momentum equation as:

$$F_{\mathrm{SF}} = 2\sigma\alpha_2\kappa n \tag{7}$$

$$n = \nabla\alpha_2 \tag{8}$$

$$\kappa = \frac{1}{|n|}\left[\left(\frac{n}{|n|}\nabla\right)|n| - (\nabla n)\right] \tag{9}$$

where n is the surface normal and k the radius of the curvature. Wall adhesion was included in the model through contact angle as:

$$n = n_{\mathrm{w}}\cos\theta_{\mathrm{w}} + t_{\mathrm{w}}\sin\theta_{\mathrm{w}} \tag{10}$$

where n_{w} and t_{w} are the unit vector normal and tangential to the wall. Surface normal obtained from one cell above the wall and near the wall (from Eq. (10)) were used to obtain the body surface force from the surface tension. Geometrical reconstruction scheme, which was found to be the more accurate, was used for obtaining the interface position within the computational cell. Once interface position was updated, flux across the cell was computed, which gives the normal and tangential velocity distribution on the face.

Simulation set-up consists of two steps (1) meshing the solution domain and providing the appropriate boundary conditions and (2) mapping the case onto the commercial software Fluent 6.0 (Fluent, USA). The solution domain and the grid used for simulation of the single drop falling on a flat plate is shown in Fig. 2a. Experimental studies of drop fall (see Fig. 3) and its subsequent spreading and recoiling was found to be symmetric. Therefore, only half of the domain was considered for simulation and quadrilateral grid

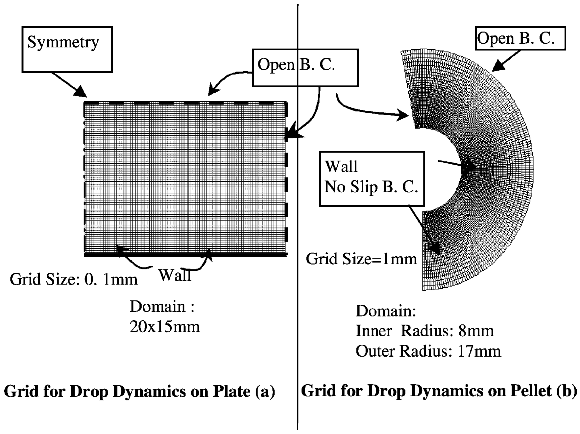

Fig. 2. Computational domain and grid mapping for flat plate and spherical domain.

was mapped in the 20 cm × 15 cm domain with grid spacing of 0.2 mm. Axis-symmetric boundary condition was provided at the axis and no slip boundary condition was provided at wall. Rest of the edges were defined as the pressure inlet for providing the open boundary conditions. Half domain was selected for drop spreading over the spherical pellet surface as well (see Fig. 3b). The computational domain over the spherical surface was divided into two sections: (1) inner section of 12.5 mm radius of the spherical domain which contain the pellet surface of 5.2 mm radius. This domain was mapped with quadrilateral meshes with uniform grid spacing of 0.2 mm; (2) outer domain of 17.5 mm radius was mapped with non-uniform grid of spacing 0.4 mm grid spacing with weighting factor 1.06. At the outer face of this domain, pressure inlet boundary condition was provided. Unsteady simulations were performed with patching initial volume fraction of liquid in the domain at time $t = 0$ s. Care was taken to ensure that simulated results are not functions on numerical parameters (grid size, time step, discretization scheme).

4. Results and discussion

4.1. Interaction of a liquid droplet with the flat plate

Dynamics of drop spreading on the flat surface depends on impact velocity, viscosity, material properties of the surface and surface tension. During the impact, kinetic energy of the drop is utilized for viscous dissipation and new surface creation. After impact of the

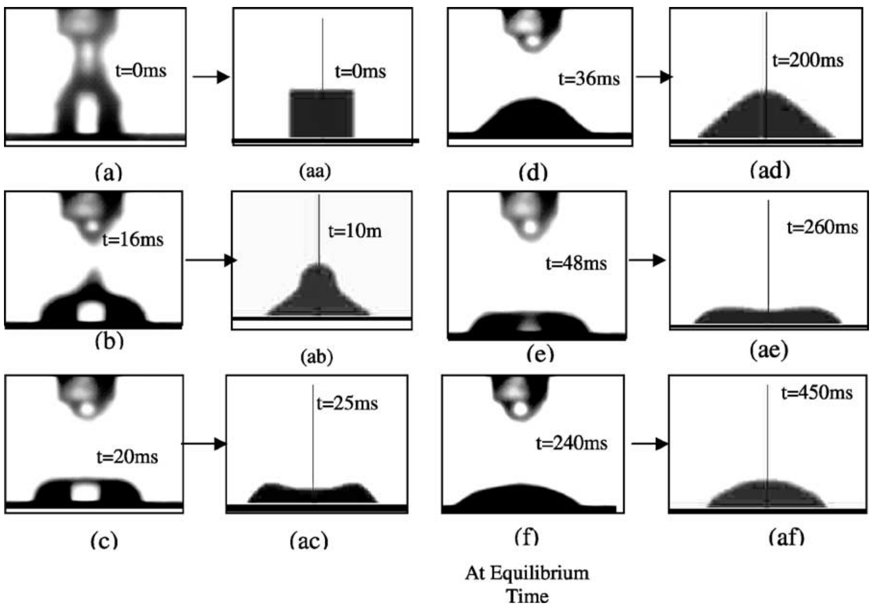

Fig. 3. Experimental and simulated results of the drop dynamics over the flat plate.

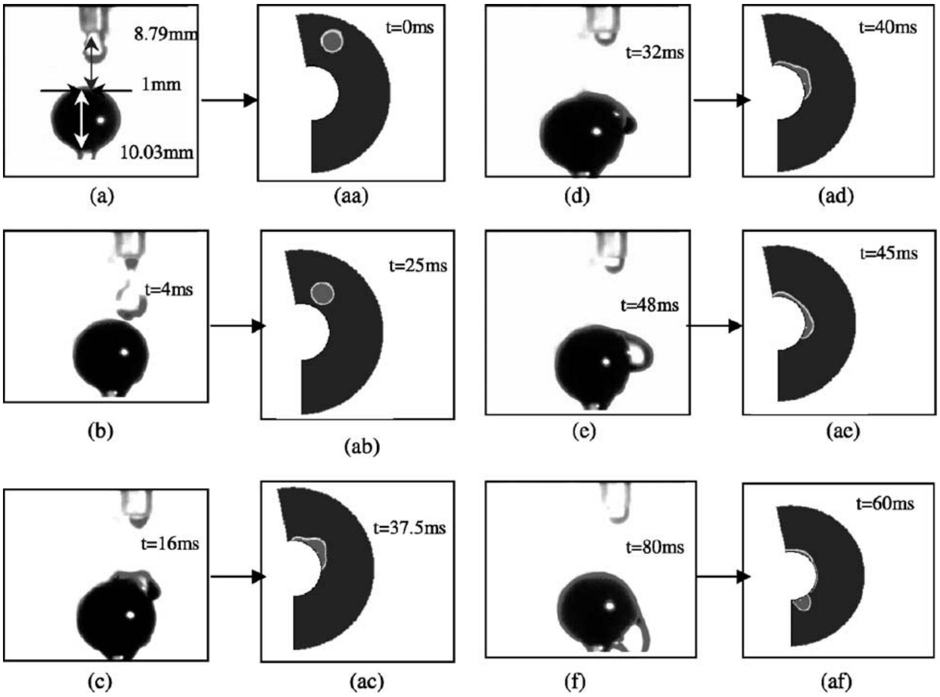

Fig. 4. Drop rise and fall velocities during oscillations (fluid: water; initial drop diameter = 4.2 mm).

drop, drop spreads on the flat surface till the inertial forces are dominant over surface forces. When surface forces overcome to the inertial forces, drop start recoiling. Thus surface tension and liquid–solid contact angle play an important role in spreading and recoiling of the drop. In our experiment, drop (4.2 mm diameter, 0.2 m/s impact velocity) spread on flat plate was studied with the help of the high-speed imaging and snaps drop dynamics is shown in Fig. 3. Reynolds number for impacting drop was 84 and Weber number was 2.3. One can clearly see the drop oscillations due to spreading and recoiling in Fig. 3a–e. In the first cycle, drop spreads ~2 times its initial diameter (4.2 mm) and after recoiling drop height become almost double the equilibrium height (Fig. 3f). Drop height and drop diameter were measured during spreading and recoiling and plotted with time (Fig. 4). Drop takes several oscillations before it comes to rest (~260 ms). Mean oscillation time of the drop dynamics is ~25 ms, which confirms that the frame rate (250 frames/s) used in the present work was adequate.

Velocity of the drop-rise and fall after each period was reconstructed from the captured snapshots. Fig. 5 shows the drop fall and drop rise velocities as a function of the time. It can be seen that drop rise and fall velocities are almost the same. Fig. 6 shows the variation of the drop spreading and recoiling velocities with time. In the initial period (60 ms),

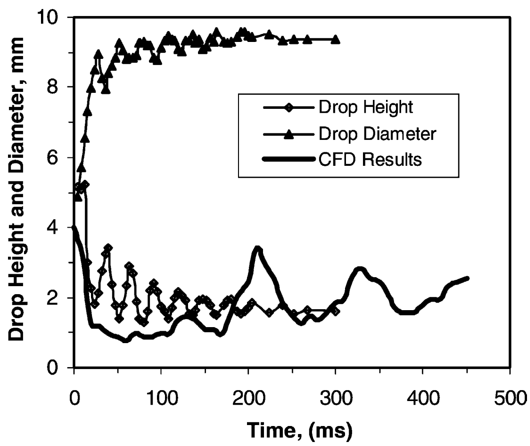

Fig. 5. Drop spread and recoil velocity during oscillations (fluid: water; initial drop diameter = 4.2 mm).

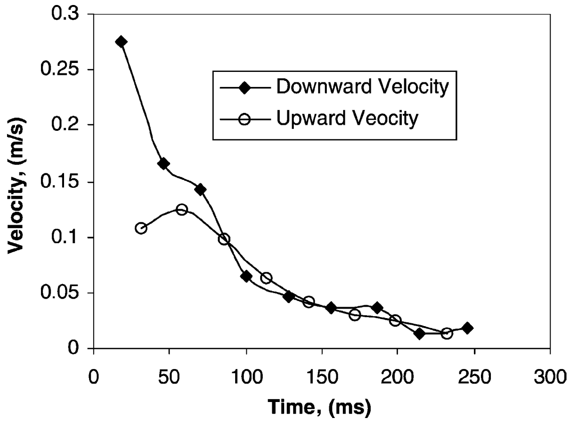

Fig. 6. Experimental and simulated results of the drop dynamics over the spherical pellet.

drop-spreading velocities are lower than the rising velocities. This may be due to initially liquid droplet was spreading on a non-wetted surface (see Fig. 4, time required to achieve maximum diameter was approximately 65 ms). While recoiling, however, the surface was wet and hence rise velocities were higher than the fall velocities. For consecutive cycles of the oscillations, this was not true (Fig. 6, after 70 ms) and recoil velocities were found to be lower than the spread velocities.

Simulations of a drop falling on a flat surface were carried our with a two-dimensional solution domain. In these simulations, a rectangular liquid drop (4.2 mm × 5 mm, based on measurements shown in Fig. 3a) was considered at the beginning ($t = 0$). The simulated spreading of a drop is shown in the form of contours of liquid phase volume fraction in Fig. 3. Numerical simulations also show consecutive spreading and recoil, which is qualitatively similar to the experiments. Simulated variation of drop height with time is plotted and compared with the experimental data in Fig. 4. It is clear from this figure that simulated oscillation time is much larger than that observed experimentally (almost five times larger). It must be noted that numerical simulations consider two-dimensional system, which is equivalent to falling of a cylinder of liquid on a flat surface. Therefore, though VOF method can capture the oscillations qualitatively, there is a significant disagreement between simulated and experimental results. Assumption of two-dimensional domain leads to consideration of significantly more liquid volume per unit surface in simulations. This invariably results in larger values of oscillation time. Simulations with smaller initial liquid drop with two-dimensional domain and preliminary simulations with three-dimensional domain confirm this observation. Further work with three-dimensional solution domain is in progress. Despite the absence of quantitative agreement with experimental data, two-dimensional simulation may provide valuable insights into interaction of droplet with solid surfaces. The present computational model was therefore applied for simulating interaction of liquid droplets with spherical surfaces.

4.2. Interaction of a liquid droplet with the spherical pellet

In order to capture a clear image, liquid droplet was dropped with 1 mm offset from the center to ensure that the drop falls on one side of the pellet. Drop was dropped from 6 mm above the pellet surface and the time at which drop get detached from the dropper was considered as a starting time. As discussed in the earlier section, drop takes more time to spread on the non-wetted surface than on the pre-wetted surface. Therefore, two cases were studied experimentally: (1) drop spread on non-wetted surface and (2) drop spread on wetted surface. The second case was studied several times to ensure the reproducibility. Experimental snapshots of the drop dynamics for the second case, where pellet surface was wetted by preceding drop, are shown in Fig. 7. From the experimental images, drop retention time was measured and compared with the non-wetted and pre-wetted surface. It was found that for non-wetted surface, drop retention time is three times more than the pre-wetted drop (80 ms). Drop flow over the spherical surface was simulated by considering the two-dimensional solution domain. The predicted contours of the liquid phase volume fraction are compared with the experimental results (for Case 2) in Fig. 7. Experimental images indicate that the fallen drop initially oscillates upon impact (see Fig. 7c–e) without moving and then starts flowing from the side. Simulations, however, fail to capture the oscillations on the surface of the pellet. Therefore, the simulated drop retention time (60 ms) over the pellet surface is less than the experimental value. Much

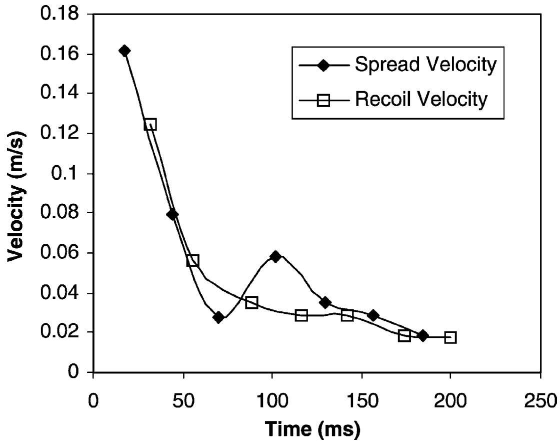

Fig. 7. Variation of the drop height and diameter with time (material: water; initial drop diameter = 4.2 mm).

finer grid resolution may be needed to capture oscillations observed in the experiments. Further work with refined grid and three-dimensional solution domain is in progress.

5. Conclusions

Flow of a liquid droplet over a flat plate and a spherical pellet was studied to improve understanding of wetting in trickle bed reactors. Interactions of liquid droplets with flat and spherical surfaces at low impact velocities (less than 0.25 m/s) were studied using high-speed camera. Even at such a low impact velocities, the complex interactions of inertial and surface forces found to result into oscillations of liquid droplet. Quantitative information about the drop spread and recoiling velocities were reported. CFD model based on the VOF method was used to simulate drop dynamics on flat and spherical surfaces. Surface tension and wall adhesion phenomenon were included in the computational model. Simulated drop dynamics was found to capture key qualitative features observed in the experiments. Detailed quantitative comparisons indicate that numerical simulations with three-dimensional domains are essential for quantitative simulation of experimental data. The present work may be extended to porous surfaces by incorporating time varying contact angle in the developed framework, which will be useful for better understanding and prediction of wetting in trickle bed reactors.

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