Lattice Boltzmann Simulations of Inkjet Drop Formation, Propagation, and Impact with Substrates

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Introduction

In this paper, direct numerical simulation (DNS) results for drops striking solid substrates will be presented. Results will be presented for drops striking both flat surfaces and rods. Both the impact of the drop and the subsequent spreading of the drop will be discussed. Results will also be shown for pairs of drops with and without evaporation of the liquid phase. The results were obtained using a formulation of the lattice Boltzmann method (LBM).

Until recently, LBM simulations of two phase flow have been limited to density ratios of order 10 or less. Inamuro et al. (2004) developed a thermodynamically based LBM that permits simulations at density ratios up to 1000 and used it to investigate binary drop collisions in a stationary gas. Their method is a heuristic modification of the "Oxford" formulation of the LBM developed by Swift et al. (1996). The principal modification involves the computation of the pressure from a Poisson equation.

We have used an extension of Inamuro et al.'s LBM that incorporates the physics associated with wetting of a solid substrate to simulate the formation and detachment of drops, their subsequent propagation through the gas phase, and their eventual fate after impacting a solid substrate. The impact may result in splashing or complete deposition on the substrate, followed by wetting of the substrate. By adjusting the humidity of the liquid phase in the gas, the effects of evaporation can be studied.

In what follows, we will first describe the problem formulation. After a brief description of the numerical methods, we will present representative results to illustrate the ability of the method to correctly describe the physical processes.

Formulation

The simulations to be discussed were performed for in a channel formed by two, infinite parallel, smooth walls. Periodic boundary conditions were imposed in two orthogonal directions parallel

to the walls. In describing the system, a Cartesian coordinate system in which the x-coordinate is perpendicular to the walls will be employed, and periodic boundary conditions were imposed in the y and z-directions. In the simulations to be discussed, gravity was neglected. Lattice units will be used in quantifying the problem. The unit of length is the grid spacing, which was uniform.

In one set of simulations, one or two drops were projected toward one of the two bounding walls. The initial velocity of a drop was sufficiently large to enable the drop to reach the wall. In the case in which two drops were projected toward the same wall, the drops had identical initial velocities pointing in the x-direction. In a second set of simulations, drops were projected toward one or more rectangular rods.

Numerical Methods

A formulation of the lattice Boltzmann (LBM) method developed by Inamuro et al. (2004) was used to perform the simulations. This formulation has the advantage that it can be used for density ratios as large as 1000. In the simulations to be discussed, the density ratio was 50; larger density ratios can be used, but more computer time is required for the simulations. The formulation of Inamuro et al. was developed for periodic, unbounded fluids. To impose rigid boundary conditions and the desired wettability, the method described by Briant et al. (2004) was used. Briant et al. used Cahn's (1977) surface free energy formulation to impose the wettability conditions.

A key quantity in the Inamuro et al. formulation is the order parameter, ϕ. The order parameter satisfies a transport equation involving convection and diffusion. The values of the order parameter fall between two limiting values, $\phi_{\min}$ and $\phi_{\max}$, for which two-phase equilibrium with a flat interface is possible. The fluid density is determined as follows:

$$\rho = \begin{cases} \rho_G, & \phi < \phi_G^* \\ \frac{\Delta\rho}{2}\left[sin\left(\frac{\phi - \overline{\phi^*}}{\Delta\phi^*}\pi \right) + 1 \right] + \rho_G, & \phi_G^* \le \phi \le \phi_L^* \\ \rho_L, & \phi > \phi_L^* \end{cases}$$

where $\Delta\rho = \rho_L - \rho_G$, ρ_L is the bulk density of the liquid phase, ρ_G is the bulk density of the gas phase, $\Delta\phi^* = \phi_L^* - \phi_G^*$, and $\overline{\phi^*} = (\phi_G^* + \phi_L^*)/2$. The quantities ϕ_{G}^* and ϕ_{L}^* are chosen to be somewhat different than $\phi_{\min}$ and $\phi_{\max}$ ..

In lattice units, the densities of the gas and liquid were 1 and 50, respectively. The kinematic viscsosities of the gas and liquid were 0.0016, and the surface tension was 0.201. The thickness of the gas-liquid interface was approximately 3.

Results

Let us consider typical results for drops striking a flat wall. In one simulation two identical drops were projected toward a flat, solid wall. The drops struck the wall, spread out and merged into a single drop. The equilibrium contact angle was 90^o. After 41,000 time steps, the dynamic contact angle was 88.6^o , and the footprint of the product drop on the wall was nearly circular. The simulation was done for the following parameter values (in lattice units): initial drop radius = 10; initial drop velocity = 0.05; equilibrium contact angle =90^o. The drops were placed in a $60 \times 60 \times 60$ computational domain. The domain was bounded by two flat, rigid walls at $x = 0$ and $x = 60$. At $t = 0$, one drop was centered at $x = 40, y = 42, z = 30$ and the other drop was centered at $x = 40, y = 18, z = 30$. The initial x-component of velocity of each drop was 0.05, and the other two components were zero. Thus, the initial Reynolds number of each drop was 625, and the initial Weber number of each drop was 12.4. Figure 1 shows a cross-sectional view at $z = 30$. It may be seen from the sequence of images that the drops move gradually apart before striking the wall; this suggests that they exert a repulsive lift force on each other. After striking the wall, the drops spread out, contact each other, and merge. The footprints of the same two drops on the wall are shown in Figure 2 for approximately the same times as the images in Figure 1.

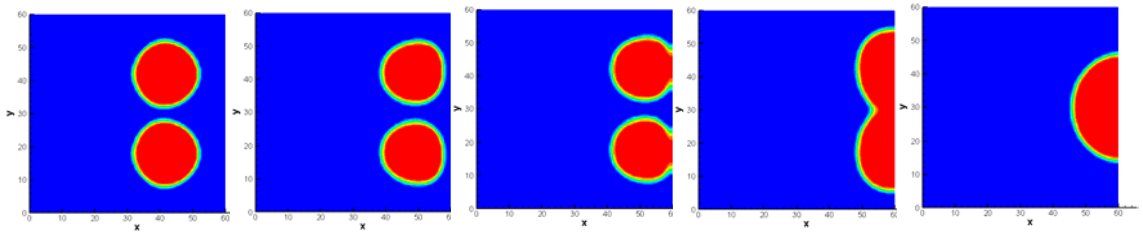

Fig. 1. A sequence of images showing a cross-sectional view of two identical drops having identical initial velocities that strike a wall and merge.

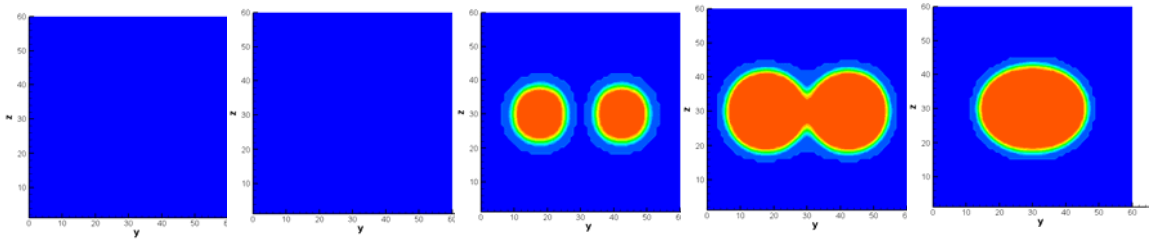

Figure 2. Footprints of the two evaporating drops shown in Fig. 2.

To relate the above results to real physical systems, let us assume that the dynamic viscosity of the drops is 30cP, the drop density is 1 g/cm^3 , and the surface tension is 40 g/s^2 , and determine the velocity and size of the drops from the Reynolds number and Weber number. The drop velocity is $v = (\sigma / \mu_L)(We / Re)$ where σ is the surface tension and μ_L is the dynamic viscosity of the liquid. For the assumed values of σ and μ_L , the velocity is 6.7 m/s. The corresponding drop diameter is 2.8 mm. For an inkjet, Re=20, We=0.5 might be appropriate. We can achieve these values by using an initial drop velocity roughly equal to 0.0125 and a kinematic viscosity equal to 0.0125.

Evaporating Drops. To cause evaporation, the initial value of the order parameter was set to values lower than ϕ_{min} (the minimum value of the order parameter that is determined from the

conditions that the chemical potential and the thermodynamic pressure should be the same in the liquid and gas phases.) In one run, the initial value of ϕ was $0.5\phi_{\min}$. At the completion of the run (4000 time steps), 47% of the liquid had evaporated. There was no qualitative difference between this run and the non-evaporating drops run; the drops struck the surface and merged. In the second run, the order parameter vanished outside the drops in the initial condition. In this run, 72% of the liquid evaporated in 4000 time steps. The sequence of events was qualitatively different; the drops struck the surface and spread out, but they did not merge. The shrinkage of the drops with time can be clearly seen in Figure 3. The dynamic contact angle at the end of the simulation was 96.2^{o}. The fact that the contact angle was farther from the equilibrium angle than for the non-evaporating drops is attributable to contact line motion caused by evaporation. Although we set the order parameter to zero in the second run, this does not mean that the drops were initially moving through a vacuum. The density and viscosity of the gas phase are fixed in the Kyoto formulation. Setting the order parameter to zero corresponds to setting the humidity to zero.

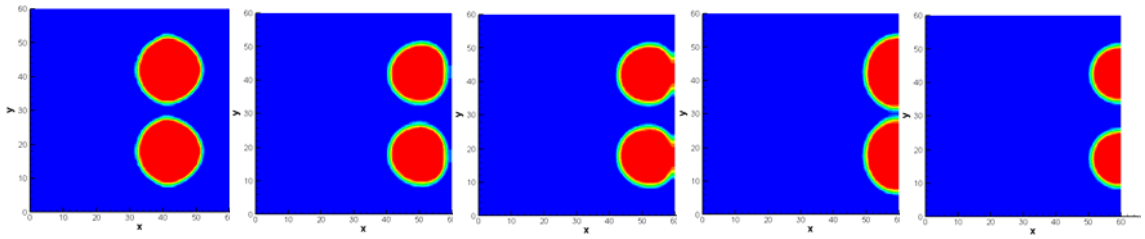

Figure 3. Cross-sectional view of two evaporating drops striking a wall.

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