Vol 17 No 9, September 2008
1674-1056/2008/17(09)/3185-04

Chinese Physics B

© 2008 Chin. Phys. Soc.
and IOP Publishing Ltd

Simulation solution for micro droplet impingement on a flat dry surface

Sun Zhen-Hai(孙震海)[a)b)c)†] and Han Rui-Jing(韩瑞津)[b)]

[a)] *Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, Shanghai* 200050, *China*
[b)] *Grace Semiconductor Manufacture Corporation, Shanghai* 201203, *China*
[c)] *Graduate School of Chinese Academy of Sciences, Beijing* 100039, *China*

(Received 19 December 2007; revised manuscript received 15 February 2008)

This paper presents a computational fluid dynamics approach for micro droplet impacting on a flat dry surface. A two-phase flow approach is employed using FLUENT VOF multiphase model to calculate the flow distributions upon impact. The contact line velocity is tracked to calculate the dynamic contact angle through user defined function program. The study showed that the treatment of contact line velocity is crucial for the accurate prediction of droplet impacting on poor wettability surfaces. On the other hand, it has much less influence on the simulation of droplet impacting on good wettability surfaces. Good fit between simulation results and experimental data is obtained using this model.

Keywords: droplet impact, wettability, contact line velocity, dynamic contact angle
PACC: 0340G, 4700

1. Introduction

The droplet impact problem has been studied for more than a century, partly due to its relevance to various industrial processes such as spray cooling, spray cleaning, ink jet technology, windshield films, aircraft icing, electronic-component welding, or nebulizers for medical use. The involvement of numerous physical processes in an instationary problem also makes it an attractive academic problem. The difficulties associated with the study of the fluid dynamics of droplet impingement on a flat dry surface are the extreme deformation of the droplet within a very short time and the presence of surface tension and wetting effects.[1]

When an incident droplet impacts on a dry surface, in general, two possible outcomes of the post-impact process may occur. At low impact velocities, the droplet may deposit on the surface in a liquid form; or at faster impact velocities, the droplet may splash and secondary droplets may form. In this paper, situations are considered in which no splashing occurs. For these cases, a lamella is formed when the drop impacts onto the solid surface, which spreads radially on the surface until its spreading diameter reaches a maximum. During this stage, the form of the drop passes from a sphere to a disc-like shape. Then, depending on the wettability of the surface and the impact condition, the liquid recedes, stays at rest or continues to spread further at a much retarded rate.

Theoretically, the droplet impingement prediction is complicated in view of its unsteady character. Several numerical solutions were developed based on approximation.[2−5] The first numerical simulation of the fluid dynamics of droplet impacting was reported by Harlow and Shannon,[6] who neglected all surface tension, viscous and wetting effects in their modelling. Experimental observations have visualized the influence of the wettablity of the system to the spreading progress.[7,8] The contact line velocity and the dynamic contact angle are quite critical for prediction of meniscus shape and maximum spreading diameter. Unlike most numerical models, a computational fluid dynamics simulation solution based on dynamic contact angle tracing is employed in this paper. Reasonable agreement between simulation results and experimental results is found.

2. Droplet impact modelling

Most experimental studies of droplet impact and spreading have been performed using a high-speed camera. For micro-scaled droplet, it is difficult to observe the droplet impact progression experimentally. An accurate numerical simulation approach can pro-

†E-mail: szh000@hotmail.com

vide a detailed insight to the droplet-impacting phenomenon.

In this study, a two-phase flow approach is employed by using FLUENT VOF multiphase model, with droplet as the liquid phase and surrounding air as the gas phase. The model is a three dimensional model which combines a fixed mesh discretization of the Navier–Stokes equations with a piecewise linear volume tracking algorithm to track the droplet free surface. The flow field is computed as unsteady condition under incompressible and isothermal conditions. The heat transfer and solidification are not considered. The liquid droplet is formed by patching the liquid volume fraction with a specified diameter at a specific height from the flat surface. The droplet initial velocity is also introduced through patching.

Two different wetting conditions are discussed here: hydrophilic surface with a lower static contact angle and a hydrophobic surface with a higher static contact angle. While during spreading, the dynamic contact angle must be considered. The contact angle between the liquid and the flat surface needs to be treated with care. Three important facts that should be considered in the modelling of the wetting are the following: (1) the value of the dynamic contact angle depends on the velocity of the contact line; (2) the advancing contact angle is larger than the receding contact angle; (3) more than one values of the contact angle are possible for a stationary contact line. In our study, a dynamic contact angle approach is used to set the contact angle at fluid advancing and receding stages. This is achieved through a user defined function (UDF) program, which calculates the contact line velocity using Blake's model.[9]

According to this model, it supposes that for the wetting line to advance across the solid surface, molecules already adsorbed at localized sites on the initial solid/fluid interface must be displaced by molecules from the advancing fluid. Dynamic contact angle θ and contact line velocity v can be linked through the expression below:

$$v = 2\kappa_{\mathrm{w}}^{0}\lambda \sinh\left[\frac{\gamma_{12}(\cos\theta^{0} - \cos\theta)}{2nkT}\right], \qquad (1)$$

where κ_{w}^{0} is called equilibrium frequency of molecular displacements, λ is the average length of each molecular displacement, γ_{12} is the liquid/gas interfacial tension, n is the number of adsorption sites per unit area, k is the Boltzmann constant and T is the temperature.

Two simulation cases are performed based on the data published in Ref.[10]. Detail conditions are listed in Table 1. The dimensionless groups (Reynolds and Weber numbers) listed in Table 1 are defined as follows:

$$R_{\mathrm{e}} = \frac{V_0 D_0}{\gamma}, \quad W_{\mathrm{e}} = \frac{\rho D_0 V_0^2}{\sigma}, \qquad (2)$$

where V_0 is the initial velocity of droplet, D_0 is the diameter of droplet, γ is the liquid kinematic viscosity, ρ is the liquid density and σ is the liquid surface tension coefficient.

Table 1. Detail conditions for two simulation cases.

	case 1	case 2
droplet diameter, D_0/μm	85	66
initially velocity, V_0/(m/s)	5.1	11.4
static contact angle, $\theta/(^\circ)$	35	15
R_{e}	434	752
W_{e}	30	118

A 45-degree section of a cylinder is used as the computation domain. Figure 1 shows the configuration of the computation domain. Liquid water is used as the droplet material, and air is used as the gas phase material. Figure 2 shows the computation meshes used for the simulation. The number of computation meshes ranges from 50,000 to 90,000. The time step used in the computation is 0.05 μs. The calculation time ranges from 20 to 30 hours for each case with 4 CPUs on a 64-bit Linux Cluster.

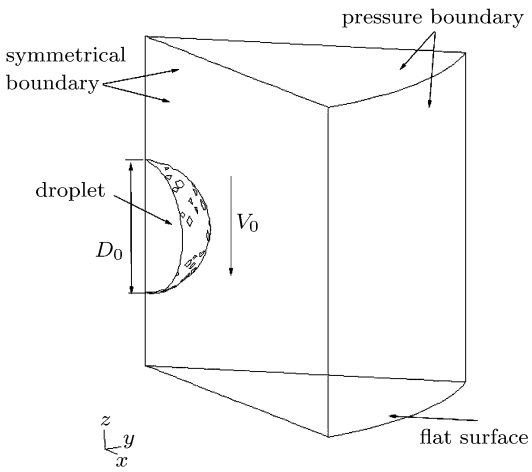


Fig.1. Computation domain of simulation cases.

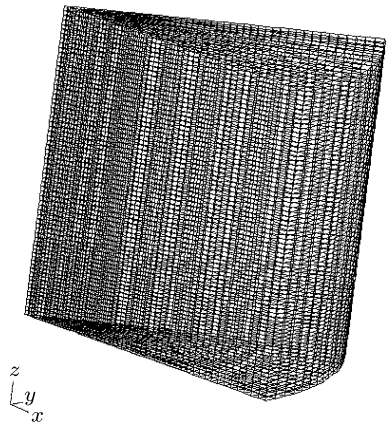


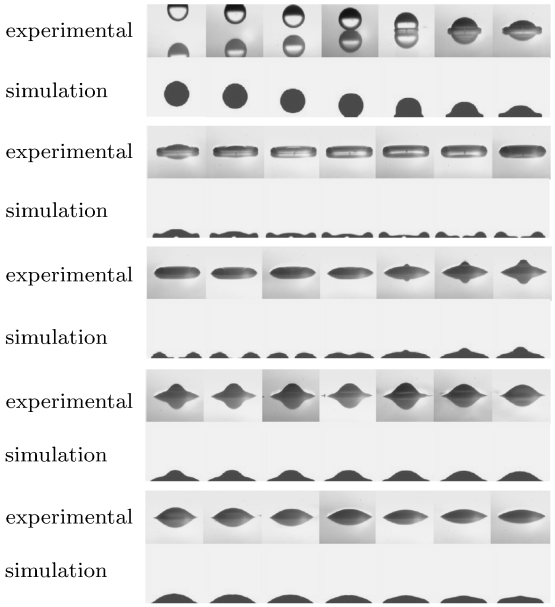
Fig.2. Computation meshes.

3. Results and discussion

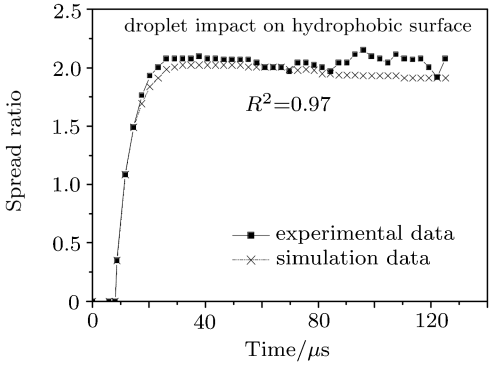
Liquid volume fraction contour plots and video images captured during impact progress are compared in frame-by-frame fashion. Results of case 1 are showed in Fig.3. The frame time interval is 3 μs. With the implementation of the UDF program, the contour plots of the droplet liquid volume fraction show that the shape of the droplet spreading compares fairly well with the video images. Recoil and oscillation are observed due to the surface poor wettability. The liquid spread ratio, which is defined as $r = d/D_0$ (where d is the liquid spread diameter and D_0 is the droplet initial diameter) is used as the criteria when comparing between numerical results and experimental images. R square, coefficient of determination, is used to evaluate the goodness of curve fit. The R square of case 1 is 0.97 (Fig.3(b)) which indicates the good fitness between simulation and experiment.

At the last stage of oscillation, the spread ratio curve shows a little discrepancy which can be seen in Fig.3(b). The spreading droplet is about to reach an equilibrium contact angle and the contact line velocity is relatively small. In the prediction of Blake's model, the contact line becomes pinned at the solid surface at low rates of wetting. So the measured spread diameter cannot reflect the contact angle vibration. That is why discrepancy between numerical prediction and experimental data occurs at the last stage of vibration.

The gas bubble seen at the centre of impinging droplet on the video images is also reflected on the simulation results (Fig.4). Air is trapped between the droplet and flat surface due to poor wettability.

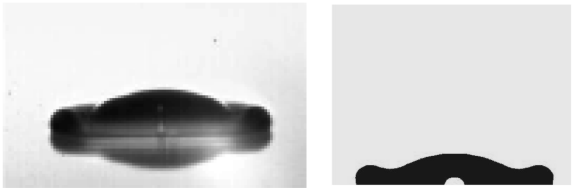


(a) frame-by-frame comparison



(b) spread ratio curves comparison

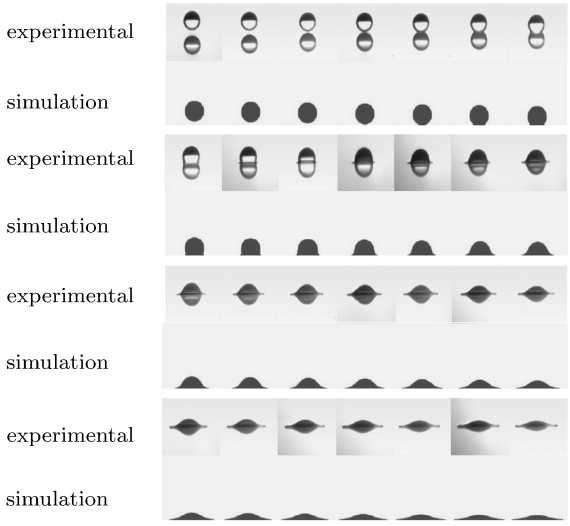
Fig.3. Droplet impact on a higher contact angle surface. Time interval between frames is 3 μs. Impacting condition: droplet size 85 μm, initial velocity 5.1 m/s, static contact angle 35°.



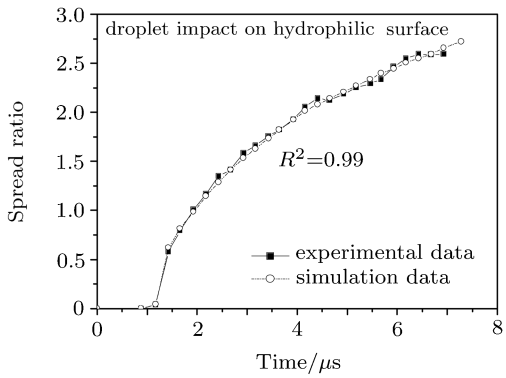
(a) experimental image (b) simulation contour plot

Fig.4. Air bubble at the centre of the droplet upon impact.

For low contact angle case 2, the simulation result is also compared with experimental images (Fig.5).



(a) frame-by-frame comparison



(b) spread ratio curves comparison

Fig.5. Droplet impact on lower contact angle surface. Time interval between frames is 0.25 μs. Impacting condition: droplet size 66 μm, initial velocity 11.4 m/s, static contact angle 15°.

No recoiling is observed during the whole computation time due to good wettability. The R square is 0.99, which indicates a perfect match between simulation and experiment.

Due to its good wettability and higher impacting velocity comparing with case 1, it shows less dependence on the UDF program. The same fitness can be achieved without the UDF program. That is to say, the contact line velocity has much less influence on contact angle when droplet impacts on a good wettability surface. This keeps the same conclusion with Podvysotskii and Shraiber (1993).[11]

4. Summary

In this paper we presented a computational fluid dynamics (CFD) simulation solution for droplet impacting on a flat dry surface. The simulation model does not consider heat transfer and solidification. It accounts for the wetting effects. The contact line velocity is tracked to calculate the dynamic contact angle through UDF program based on the Blake's model. The study showed that the treatment of contact line velocity is crucial for the accurate prediction of droplet impacting on poor wettability surfaces. While on good wettability surface, the contact angle changes less during spreading. So the simulation prediction can be more accurate. For both cases, the simulation model predicts well the deformation of the impacting droplet, not only in the spreading phase, but also during recoiling and oscillation.

Acknowledgment

The authors are grateful for the financial support from Grace Semiconductor Manufacturing Corporation.

References

[1] Jian Y J, E X Q, Zhang J and Meng J M 2004 *Chin. Phys.* **13** 2013
[2] Fukai J, Shiiba Y, Yamamoto T, Miyatake O, Poulikakos D, Megaridis C M and Zhao Z 1995 *Phys. Fluids* **7** 236
[3] Tsurutani K, Yao M, Senda J and Fujimoto H 1990 *JSME Int. J. Ser.* **II 33** 555
[4] Trapaga G and Szekely J 1991 *Metall. Trans.* B **22** 901
[5] Elyousfi A B A, Chesters A K, Cazabat A M and Villette S 1998 *J. Colloid Interface Sci.* **207** 30
[6] Harlow F H and Shannon J P 1967 *J. Appl. Phys.* **38** 3855
[7] Rioboo R, Marengo M and Tropea C 2002 *Experiments in Fluids* **33** 112
[8] Heinig P, Wurlitzer S and Fischer T M 2004 *Eur. Phys. J.* E **14** 293
[9] Blake T D in: Berg J C (ed) 1993 *Wettability* (New York: Dekker) pp251–302
[10] Dirkjan B van Dam and Christophe Le Clerc 2004 *Physics of Fluids* **16** 3403
[11] Podvysotskii A M and Shraiber A A 1993 *Fluid Dynamics* **28** 203