NUMERICAL STUDY OF DROPLET DYNAMICS ON SOLID SURFACE

M.Z.M.Rody[1], M.A.Salim[2], Sidik.N.C[3], Fudhail.A.M[4], Hassan.M.Z[5]

[1]Department of Automotive,Faculty of Mechanical Engineering, Universiti Teknikal Malaysia Melaka, Melaka, Malaysia

[2]Department of Thermofluid,Faculty of Mechanical Engineering,Universiti Teknologi Malaysia, Skudai, Johor, Malaysia

Email: rody@utem.edu.my

ABSTRACT

This paper presents numerical study of droplet dynamics on solid surface using multiphase model of lattice Boltzmann method. This method is an efficient alternative tool for the numerical simulation of multiphase flow. In this paper, we start by describing a choice of interaction potential that reproduces the attraction force between particles together with the varying contact angles on surface by balancing the adhesive and cohesive force. After showing how the formulation of the particles interaction fits into the framework of lattice Boltzmann simulations, numerical results are presented to highlight the applicability of the approach.

KEYWORDS*: lattice Boltzmann; multiphase; distribution function; droplet; Landau free-energy.*

1.0 INTRODUCTION

Physical properties of droplet dynamics on solid surfaces have attracted considerably growing interest during the last years (S. L. Manzello and J. C. Yang, 2002), (L. O. E. Santos, *et.al*.,2008). The droplet dynamics phenomenon is not only important in many industrial processes such as coating of substances, melting of irons, boiling water reactor (Y. W. Kruijt *et.al*.,2004) etc, but also in everyday situations such as droplet motion on car's front glass, spreading of water on TABLE, hair dryer and so on. Some biological application areas are motions in the tear film on the cornea of the eye (B. Robert and C. Stanley,1974),and flows on liquid covered membranes in the lungs (H. Slama *et.al*,.1973).

The motion of droplets on solid surface also plays an important role in transport phenomena. When a droplet comes into contact with a solid surface, capillary force drive it towards equilibrium. The process of the droplet reaching equilibrium is known as spreading and corresponds to the three phases line between gas, liquid and solid moving over the surface (M. A. Abdullatif *et.al*,.2003).

Considering the significance of these phenomena in theory and applications, many of the researchers have diverted their attention to this type of multiphase flow area. However, experimental investigation on the behaviour of droplet on surface is very difficult if not impossible and high in cost due to complexity of experimental setup. Due to this reason, it is necessary to establish a multiphase numerical model which can exactly simulate the multiphase phenomena especially the droplet motion on a surface. Currently, multiphase lattice Boltzmann method (LBM) is the most suitable numerical tool in predicting multiphase fluid flow problems.

The lattice Boltzmann method, the numerical method that will be used in this study, is the only numerical technique that directly treats the flow behaviour at the microscopic level. LBM utilizes the particle distribution function to describe collective behavior of fluid molecules. This new numerical method, evolved from mathematical statistical approach, has been well accepted as an alternative numerical scheme in computational fluid dynamics field. In comparison with other numerical schemes, LBM is a "bottom up" approach, derives the Navier-Stokes equation from statistical behavior of particles dynamics. The imaginary "propagation" and "collision" processes of fluid particles are reconstructed in the formulation of LBM scheme. These processes are represented by the evolution of particle distribution function, $f(x,t)$ which describes the statistical population of particles at location x and time t.

The advantages of LBM include simple calculation procedure (C. S. N. Azwadi and T. Tanahashi, 1995), suitability for parallel computation (J. Axner *et.al*., 2008), ease and robust handling of multiphase flow (T. Inamuro *et.al*,.2004), complex geometries (M. Gustav and H. Gabor, 2006), interfacial dynamics and others (C. S. N. Azwadi and T. Tanahashi, 2007). A few standard benchmark problems have been simulated by LBM and the results are found to agree well with the corresponding Navier-Stokes solutions (Z. Guo, 2000).

In simulating multiphase flow, the main advantages of LBM lie in the fact that, unlike other numerical scheme, the treatment at the fluid-fluid

or fluid-solid interface is very simple. LBM automatically generate the interface region with no special treatment on the simulation program meaning that no extra computational burdens are needed to track the interface. Application of LBM is expected to increase the efficiency, accuracy and the capability of the current computer performance without sacrificing the need of the detailed behavior of fluid particles in the multiphase phenomena.

There were several works have been done on multiphase flow using LBM, however, only few researches studied droplet dynamics on surface. Therefore, the objective of current study is to demonstrate the capability of LBM in simulating droplet dynamics on solid surface.

The structure of this paper is as follow. To begin, we show the formulation of multiphase lattice Boltzmann model from Landau free energy theory. After showing how the formulation of the particles interaction fits in to the framework of lattice Boltzmann simulations, numerical results of droplet spreading on a solid surface are presented to highlight the applicability of the approach. The final section concludes current study.

2.0 MULTIPHASE LATTICE BOLTZMANN MODEL

The starting points for the lattice Boltzmann simulations is the evolution equation, discrete in space and time, for a set of distribution functions *f*. If a two-dimensional nine-velocity model (D2Q9) is used, then the evolution equation for a given *f* takes the following form

$$f_i(\mathbf{x}+\mathbf{e}_i\Delta t, t+\Delta t)-f_i(\mathbf{x}, t)=-\frac{1}{\tau}\left[f_i(\mathbf{x}, t)-f_i^{eq}(\mathbf{x}, t)\right] \tag{1}$$

where Δt is the time step, e is the particle's velocity, τ is the relaxation time for the collision and i = 0,1,…,8. Note that the term on the right hand side of Equation (S. L. Manzello and J. C. Yang, 2002), is the collision term where the BGK approximation has been applied (P. L. Bhatnagar, 1954). The discrete velocity is expressed as ;

$$\begin{aligned} e_0 &= (0, 0) \\ e_{1,3,5,7} &= \left(cos\frac{(i-1)\pi}{4}, sin\frac{(i-1)\pi}{4}\right) \\ e_{2,4,6,8} &= \sqrt{2}\left(sin\frac{(i-1)\pi}{4}, cos\frac{(i-1)\pi}{4}\right) \end{aligned} \tag{2}$$

f_i^{eq} is an equilibrium distribution function, the choice of which determines the physics inherent in the simulation. In the free-energy two-phase lattice Boltzmann model, the equilibrium distribution is written in the following term

$$f_i^{eq} = A_i + B_i\left(e_{i,\alpha}u_\alpha\right) + C_i\left(e_{i,\alpha}e_{i,\beta}u_\alpha u_\beta\right) + Du^2 + G_{\alpha\beta}e_{i\alpha}e_{i\beta} \tag{3}$$

where the summation, over repeated Cartesion indices, is understood. The coefficients A, B, C, D and $G_{\alpha\beta}$ are determined by placing constraints on the moments of f_i^{eq}. The collision term conserves mass and momentum, and therefore the first and second moments of f_i^{eq} are constrained by

$$\sum f_i^{eq} = \rho \tag{4}$$

$$\sum_i e_{i,\alpha}f_i^{eq} = \rho u_\alpha \tag{5}$$

The continuum macroscopic equations approximated by the evolution equation correctly describe the hydrodynamics of a one-component, non-ideal fluid by choosing the next moment of f_i^{eq}. This gives

$$\sum_i e_{i,\alpha}e_{i,\beta}f_i^{eq} = P_{\alpha\beta} + \rho u_{\alpha\beta} + \upsilon\left[u_\alpha\partial_\beta(\rho) + u_\beta\partial_\alpha(\rho) + u_\gamma\partial_\gamma(\rho)\delta_{\alpha\beta}\right] \tag{6}$$

where $u = \left((t - 1/2)\Delta t\right)/3$ is the kinematic shear viscosity, $P_{\alpha\beta}$ is the pressure tensor, and r is the time relaxation. In order to fully constrain the coefficients A, B, C, D and $G_{\alpha\beta}$, a fourth condition is applied, which is

$$\sum_i e_{i,\alpha}e_{i,\beta}e_{i,\gamma}f_i^{eq} = \frac{\rho c^2}{3}\left(u_\alpha\partial_{\beta\gamma} + u_\beta\partial_{\alpha\gamma} + u_\gamma\partial_{\alpha\beta}\right) \tag{7}$$

The thermodynamics of the fluid enters the lattice Boltzmann simulation via the pressure tensor $P_{\alpha\beta}$. The equilibrium properties of a system can

be described by a Landau free energy functional as follow [20]

$$\Psi = \int dx \left[\psi(T,\rho) + \frac{\kappa}{2}(\partial_x \rho)^2 \right] - \int dS \Phi(\rho_s) \tag{8}$$

The right hand side terms of Equation (8) represent free energy density of the bulk phase, free energy from density gradient and contribution from interaction between fluid and solid [21] respectively. *k* is a constant related to the surface tension. Following Gennes [22] and Seppecher (P. Seppecher, 1996), we expand $\Phi(\rho_s)$ as a power series in ρ_s and keep only the first order term since this turn out to be sufficient for the liquid-solid interaction scenarios that we want to consider. Therefore, free energy functional can be rewritten as

$$\Psi = \int dx \left[\psi(T,\rho) + \frac{\kappa}{2}(\partial_x \rho)^2 \right] - \phi_1 \rho_s \tag{9}$$

It then follows that (J. S. Rowlinson and B. Widom, 1982)

$$P_{\alpha\beta}(\mathbf{x}) = \delta_{\alpha\beta} p(\mathbf{x}) + \kappa(\partial_\alpha \rho)(\partial_\beta \rho) \tag{10}$$

with

$$p(\mathbf{x}) = p_0 - \kappa\rho\partial_{\gamma\gamma}\rho - \frac{\kappa}{2}(\partial_\alpha \rho)(\partial_\gamma \rho)^2 \tag{11}$$

where $p_0 = \rho\partial_\rho \psi(T,\rho) - \psi(T,\rho)$ is the equation of state of the fluid.
The Cahn model is used to relate ϕ_1 to θ, the contact angle defined as the angle between the tangent plane to the droplet and the substrate. This gives

$$\phi_1 = 2\beta\tau_p \sqrt{2p_c\kappa}\,\mathrm{sign}\left(\theta - \frac{\pi}{2}\right)\sqrt{\cos\frac{\alpha}{3}\left(1 - \cos\frac{\alpha}{3}\right)} \tag{12}$$

where $\tau_p = (T_c - T)/T_c$, $\alpha = \cos^{-1}\left(\sin^2\theta\right)$ and β is a constant typically equal to 0.1.

3.0 RESULTS AND DISCUSSION

Our first numerical test is the simulation of droplet spreading phenomenon on a horizontal flat plate and compared the 'benchmark' result (F. A. L. Dullien, 1979). Initially, the droplet was set at 180^0 contact angle or in non-wetting conditions. The droplet was then left to spread until it reached the equilibrium contact angle θ_w. FIGURE 1 shows the droplet on flat surface at contact angles of 70^0 and 104^0. In order to verify the simulated results, the graph of the ratio of the droplet wet length a_0 to the droplet height b_0 was plotted and compared with the analytical results and shown in Fig. 2.

$\theta_w = 70^0$ $\theta_w = 104^0$

FIGURE 1: Droplet at equilibrium contact angle

Results of the comparison in Fig. 2 clearly show that the droplet contact angle is in good agreement with theoretical value.

In the next section, the deformation of the droplet under a gravitational force on a horizontal plate will be discussed.

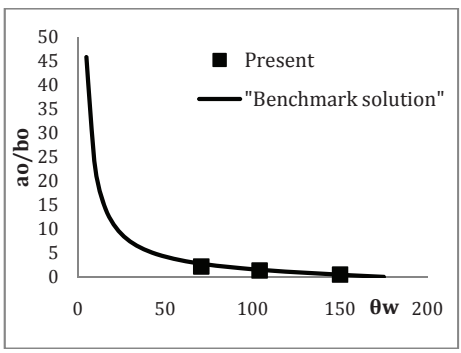

FIGURE 2: Comparison of results for the ratio of droplet wet length to droplet height at various droplet contact angles

4.0 DROPLET SPREADING WITH GRAVITATIONAL EFFECT

The effect of the gravitational force plays a vital role in determining the shape of a droplet for several of Bond numbers. The dimensionless Bond number reflects the balance between the gravitational and capillary forces, given by

$$Bo = \frac{r^2 \rho g}{\sigma} \tag{13}$$

In our simulation, we varied the value of gravitational force g, to obtain various values of the Bond number. Then the simulated droplets at the equilibrium condition were compared quantitatively with those of (K. Murakami *et.al*,.1998) (not shown).

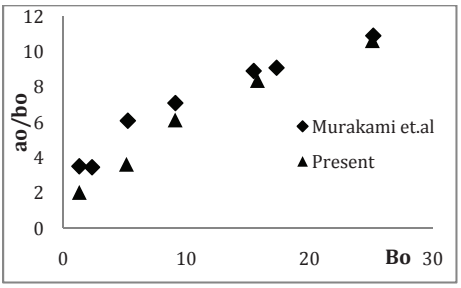

FIGURE 3: Comparison of results for the ratio of the droplet wet length and droplet height at various Bond numbers

The ratio of droplet wet length and droplet height is again plotted with the Bond number. The comparison of results between the present approach and the experimental data by (K. Murakami et al,.1998) is presented in FIGURE 6. Good agreement can be seen between these two approaches.

5.0 CONCLUSION

This paper has shown the capabilities of the lattice Boltzmann method in solving the two-phase system. The advantages of the multiphase lattice Boltzmann approach are not only the capability of incorporating interface deformation and interaction but also the interparticle interactions, which are difficult to implement in traditional methods. The two phase-flow benchmark test showed the relaxation process of the droplet, which is in agreement with the results of other researchers. It is demonstrated that the free energy two-phase lattice Boltzmann model has the capability to simulate the dynamics of droplet on solid surface. These indicate that the two-phase lattice Boltzmann scheme may be applicable for simulating interfacial dynamics in immiscible phases.

6.0 ACKNOWLEDGEMNT

Authors would like to acknowledge Universiti Teknologi Malaysia,Universiti Teknikal Malaysia Melaka and Malaysia Government for supporting this research activity.

7.0 REFERENCES

S. L. Manzello and J. C. Yang, "Experiment study of a water droplet impinging on a liquid surface," Exp. Fluid, vol. 32, May. 2002, pp. 580-589, doi: 10.1007/s00348-001-0401-8.

L. O. E. Santos, F. G. Wolf and P. C. Philippi, "Micro-hydrodynamics of immiscible displacement inside two-dimensional porous media," Microfluid Nanofluid, vol. 4, Apr. 2008, pp. 307-319, doi: 10.1007/s10404-007-0183-2.

P. Raiskinmaki, A. Koponen, J. Merikoski and J. Timonen, "Spreading dynamics of three-dimensional droplets by the lattice Boltzmann method," J. Comp. Mat. Science, vol. 18, Jul. 2000, pp. 18, 7-12, doi: 10.1016/S0927-0256(99)00095-6 .

Y. W. Kruijt, F. N. Vand De Vosse and H. E. H. Meijer, "Droplet behaviour in the presence of insoluble surfactants," Phys. Fluid, vol. 16, Jun. 2004, pp. 2785-2796, doi:10.1063/1.1756168.

A. Moukengue and A. Beroual, "Deformation of water droplets on solid surface in electric field," J. Colloid Interface Science, vol. 298, Jun. 2006, pp. 869-879, doi:10.1016/j.jcis.2005.12.041.

T. Sovorith, "Spreading of a droplet on a solid in the partial wetting and non wetting regime by Monte-Carlo simulation," Colloid Surfaces, vol. 148, Mar. 1999, pp. 223-230, doi:10.1016/S0927-7757(98)00767-5.

B. Robert and C. Stanley, "A surface tension gradient mechanism for driving the pre-corneal tear film after a blink," J. Biomech., vol. 7, May. 1974, pp. 225-228, doi:10.1016/0021-9290(74)90013-X.

H. Slama, W. Schoedel and E. Hansen, "Lung surfactant: Film kinetics at the surface of an air bubble during prolonged oscillation of its volume," Resp. Physio., vol. 19, Nov. 1973, pp. 233-243, doi:10.1016/0034-5687(73)90081-9.

M. A. Abdullatif, S. Dalia and M. Abdelsamie, "Interfacial effect in the spreading kinetics of liquid droplets on solid substrate," J. Colloid and Interface Science, vol. 264, Aug. 2003, pp. 221-227, doi:10.1016/S0021-9797(03)00443-0.

C. S. N. Azwadi and T. Tanahashi, (1995), "Simplified finite difference thermal lattice Boltzmann method," Intl. J. Mod. Phys. B, vol. 22, Sep. 2008, pp. 3865-3876, doi: 10.1142/S0217979208048619.

J. Axner, J. Bernsdorf, T. Zeiser, P. Lammers, J. Linxweiler and A. G. Hoekstra, "Performance evaluation of a parallel sparse lattice Boltzmann solver," J. Comp. Phys., vol. 227, May. 2008, pp. 4895-4911, doi:10.1016/j.jcp.2008.01.013.

T. Inamuro, T. Ogata and F. Ogino, "Numerical simulation of bubble flows by the lattice Boltzmann method," Fut. Gen. Comp. Syst., vol. 20, Aug. 2004, pp. 959-964, doi:10.1016/j.future.2003.12.008.

M. Gustav and H. Gabor, "Direct numerical and large eddy simulation of longitudinal flow along triangular array of rods using the lattice Boltzmann method," Math Comp. Simulation, vol. 72, Sep. 2006, pp. 173-178, doi:10.1016/j.matcom.2006.05.011.

C. S. N. Azwadi and T. Tanahashi, "Three dimensional thermal lattice Boltzmann simulation of natural convection in a cubic cavity," Intl. J. Mod. Phys. B, vol. 21, Jan. 2007, pp. 87-96, doi: 10.1142/S0217979207035911.

X. Shan and G. Doolen, "Diffusion in a multicomponent lattice Boltzmann equation model," Phys. Rev. E, vol. 54, Oct. 1996, pp. 3614-3620, doi: 10.1103/PhysRevE.54.3614.

Z. Guo, E. Baochang and W. Nengchao, "Lattice BGK model for incompressible Navier-Stokes equation," J. Comp. Phys., vol. 165, Nov. 2000, pp. 288-306, doi: 10.1006/jcph.2000.6616.

C. S. N. Azwadi and T. Tanahashi, "Simplified thermal lattice Boltzmann in incompressible limit," Intl. J. Mod. Phys. B, vol. 20, Jul. 2006, pp. 2437-2449, doi: 10.1142/S0217979206034789.

R. G. McNamara, L. G. Alejandro and J. A. Berni, "A hydrodynamically correct thermal lattice Boltzmann model" J. Stat. Phys., vol. 87, Jun. 1997, pp. 1111-1121, 10.1007/BF02181274.

P. L. Bhatnagar, E. P. Gross and M. Krook, "A model for collision processes in gasses; Small amplitude in charged and neutral one-component system," Phys. Rev., vol. 94, May. 1954, pp. 511-525, 10.1103/PhysRev.94.511.

L. D. Landau and E. M. Lifshitz, "Statistical physics," London: Pergamon Press, 1958, pp. 48-51.

J. W. Cahn, "Critical point wetting," J. Chemical Phys., vol. 66, Apr. 1977, pp. 3667-3672, doi:10.1063/1.434402.

P. G. De Gennes, "Wetting: statics and dynamics," Rev. Mod. Phys., vol. 57, Jul. 1985, pp. 827-863, doi: 10.1103/RevModPhys.57.827.

P. Seppecher, "Moving contact lines in the Chan-Hilliard theory," Intl. J. Eng. Science, vol. 34, Jul. 1996, pp. 977-992, doi:10.1016/0020-7225(95)00141-7.

J. S. Rowlinson and B. Widom, "Molecular theory of capillarity," Oxford: Clarendon Press, 1982, pp. 1-80

F. A. L. Dullien, Porous media : fluid transport and pore structure, New York : Academic Press, 1979, pp. 1-396.

K. Murakami, S. Nomura and M. Shinozuka, "Numerical analysis of shape of liquid droplet on solid surface with SOLA-VOF method," Jap. J. Multiphase Flow, vol. 12, Dec. 1998, pp. 56-58.