International Journal of Multiphase Flow 81 (2016) 54–66

Contents lists available at ScienceDirect

International Journal of Multiphase Flow

journal homepage: www.elsevier.com/locate/ijmultiphaseflow

On dual-grid level-set method for contact line modeling during impact of a droplet on hydrophobic and superhydrophobic surfaces

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ARTICLE INFO

Article history:
Received 17 August 2015
Revised 6 November 2015
Accepted 11 January 2016
Available online 21 January 2016

Keywords:
Dual-grid level-set method
Traditional level-set method
Droplet impact
Contact line modeling
Non-bouncing
Bouncing

ABSTRACT

In this paper, a numerical methodology for modeling contact line motion in a dual-grid level-set method (DGLSM) – solved on a uniform grid for interface which is twice that for the flow equations – is presented. A quasi-dynamic contact angle model – based on experimental inputs – is implemented to model the dynamic wetting of a droplet, impacting on a hydrophobic or a superhydrophobic surface. High-speed visualization experiments are also presented for the impact of a water droplet on hydrophobic surfaces, with non-bouncing at smaller and bouncing at larger impact velocity. The experimental results for temporal variation of the droplet shapes, wetted-diameter and maximum height of the droplet match very well with the DGLSM based numerical results. The validation of the numerical results is also presented with already published experimental results, for the non-bouncing on a hydrophobic and bouncing on a superhydrophobic surface, at a constant impact velocity. Finally, a qualitative as well as quantitative performance of the DGLSM as compared to the traditional level set method (LSM) is presented by considering our experimental results. The accuracy of the partially refined DGLSM is close to that of the fine-grid based LSM, at a computation cost which is close to that of the coarse-grid based LSM. The DGLSM is demonstrated as an improved LSM for the computational multi-fluid dynamics (CMFD) simulations involving contact line motion.

Introduction

Droplet impact dynamics on hydrophobic and superhydrophobic surfaces is both scientifically exciting as well as relevant to many practical applications. The potential applications are in the design and manufacturing of effective spray coating (Bergeron et al., 2000), self-cleaning surfaces (Blossey, 2003), drag reduction for fluid flow (Truesdell et al., 2006), anti-snow adhesion surfaces in aviation applications (Cao et al., 2009) and hot surface cooling (Betz et al., 2010; Patil and Bhardwaj, 2014). The impact of droplet is a highly transient process which depends on forces due to surface tension, inertia, viscosity, gravity and solid surface wettability. The interplay of these forces determines spreading, bouncing, non-bouncing or splashing of the droplet (see review by Yarin, 2006; Marengo et al., 2011). The wetting at the solid–liquid–gas contact line plays an important role during the impact dynamics. The dynamics at the wetting line is mainly governed by the equilibrium, advancing and receding contact angles of the droplet on a surface. The equilibrium contact angle value characterizes the surface property, *i.e.*, hydrophilic or hydrophobic. The equilibrium contact angle varies between 0 and less than 90°, for hydrophilic; 90 and less than 150°, for hydrophobic; and 150 and 180° for superhydrophobic surfaces. The hydrophobic/superhydrophobic surfaces exhibit larger equilibrium contact angle and lower contact angle hysteresis as compared to the hydrophilic surfaces; thus, such surfaces when inclined leads to rolling of the water droplets – taking away the dirt particles and clean up the surfaces (Blossey, 2003).

In the literature, several numerical investigations for the droplet impact on various solid surfaces are found. These simulations were performed on two types of grid: fixed (Renardy et al., 2001; Pasandideh-Fard et al., 2002; Gunjal et al., 2005; Yokoi et al., 2009) and moving (Fukai et al., 1995; Bhardwaj and Attinger, 2008). The former one corresponds to marker and cell (MAC) (Harlow and Shannon, 1967; Unverdi and Tryggvason, 1992), volume of fluid (VOF) (Gunjal et al., 2005; Dupont and Legendre, 2010; Malgarinos et al., 2014), level-set method (LSM) (Ding and Spelt, 2007; Caviezel et al., 2008; Lee and Son, 2011), and combined LS-VOF (Yokoi et al., 2009) methods, and the latter corresponds to the finite element method (FEM) (Fukai et al., 1995; Bhardwaj and Attinger, 2008). In recent times, the Lattice–Boltzmann method (Mukherjee and Abraham, 2007; Tanaka et al., 2011) is also used for the simulation of the droplet impact

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http://dx.doi.org/10.1016/j.ijmultiphaseflow.2016.01.005
0301-9322/

problem. VOF and LSM based formulations can handle severe interface deformations easily, and have been comprehensively employed for the droplet dynamics simulations.

There are numerous works on the improvement of the biggest disadvantage of LSM – mass-error. One such method involves improvement in the accuracy of capturing interface, by solving level-set equations on a finer grid resolution as compared to the grid used for solving Navier–Stokes (NS) equations for the flow, proposed by Gómez et al. (2005) and called as Dual Resolution LSM (DR-LSM). The LS/advection equations take much less computational time as compared to the nonlinear coupled NS/flow equations, leading to a slight increase in the total computational time for DR-LSM as compared to LSM; however, there is a substantial improvement of the accuracy/mass-error of the results.

The initial work on DR-LSM – by Gómez et al. (2005) for structured/Cartesian and by Herrmann (2008) for unstructured grid – was on *locally-refined* adaptive grid; the grid-refinement was restricted to a narrow band near the interface. However, to avoid dynamic adaption of the locally refined grid, a *globally-refined* DR-LSM was proposed by Gada and Sharma (2011) – on a uniform Cartesian grid. They called it a Dual-grid level-set method (DGLSM), with a built-in grid refinement everywhere in the domain; one additional grid for the level-set function in-between two uniformly spaced grid points for velocity/pressure/temperature is used. The partially refined DGLSM takes slightly more computational time (as compared to completely coarse-grid based LSM), to achieve a computational accuracy slightly less than that obtained by a completely refined-grid based LSM. This was demonstrated – qualitatively as well quantitatively – for various two-phase flow problems in Cartesian coordinates by Gada and Sharma (2011), and recently for two fluid electro-dynamic axisymmetric flow by Lakdawala et al. (2015a). The globally-refined DGLSM is much easier to implement as compared to the locally-refined adaptive-grid DR-LSM. The extension of the globally-refined dual-grid strategy for the volume-of-fluid method – DR-VOFM – was proposed recently by Ding and Yuan (2014). A review on LSM based development, application and analysis for multi-phase flow was reported recently by Sharma (2014).

The challenging task in the various numerical models used for the droplet impact simulations is the implementation/modeling of the moving three phase (solid-liquid-gas) wetting/contact line which characterizes the droplet fate. The difficulty arises due to the presence of hydrodynamic stress singularity at the moving contact line because of no-slip boundary conditions at the solid surface (Huh and Scriven, 1971; Shikhmurzaev, 2006). Thus, at the contact point, a slip BC is required to move the contact line (Shikhmurzaev, 2006). Several numerical studies can be found for the modeling of moving contact line (see review by Bonn et al., 2009 and Sui et al., 2014). The correct implementation of dynamic contact angle models is prominent factor for the accuracy of the results. At the contact line, dynamic contact angle (θ_d) and contact line velocity (U_{CL}) are interdependent parameters, which are responsible for the droplet spreading as well as receding/rebounding (Ngan and Dussan, 1989). Till date, there is a scarcity of universal contact line boundary condition at the contact line. Therefore, the experimentally measured equilibrium (θ_{eq}), advancing (θ_{adv}) and receding (θ_{rec}) contact angles are used in the contact line model.

In the literature, two types of contact line models are found namely, hydrodynamic (Dussan and Davis, 1974; Cox, 1986) and molecular-kinetic (Blake and De Coninck, 2002) models. In the former (used in the present paper), the growth of an apparent dynamic contact angle is accounted by the hydrodynamic deformation of the interface at the contact line (Cox, 1986). Such approach can be found in Fukai et al. (1995), Bussmann et al. (2000), Spelt (2005), Liu et al. (2005), Ding and Spelt (2007), Shin and Juric (2009) and Lee and Son (2011). They treated contact line boundary condition mainly by prescribing the dynamic contact angle as a function of θ_{adv} and θ_{rec} based on the sign of the contact line velocity; for example, one of the first such model – by Fukai et al. (1995) – is $\theta_d = \theta_{adv}$ for $U_{CL} \geq 0$ and $\theta_d = \theta_{rec}$ for $U_{CL} < 0$. The droplet impact simulations by Ngan and Dussan (1989), Spelt (2005), Mukherjee and Abraham (2007), Shikhmurzaev (2006), Yokoi et al. (2009) and Griebel and Klitz (2013) calculated the dynamic contact angle as a function of several parameters such as equilibrium contact angle, dynamic advancing and receding contact angle, Capillary number (*Ca*), Weber number (*We*) or substrate material related constants (k_{adv} and k_{rec}). Earlier, Pasandideh-Fard et al. (1996) implemented contact angle effects by measuring its temporal variation from the experiments and using these data as boundary conditions for the numerical simulations. Furthermore, Renardy et al. (2001) and Caviezel et al. (2008) used a constant equilibrium contact angle value throughout the droplet impact simulations and also found good agreement with measurements. In the molecular-kinetic approach, the molecular movement at the wetting line is accounted. The model is developed by Blake and De Coninck (2002). They explained that in the vicinity of a moving contact point the interfacial inertial and surface tension forces are present which favor the motion of molecules in a advancing and receding direction. This model can be found in the works of Ren and Weinan (2007), Bhardwaj and Attinger (2008) and Bhardwaj et al. (2010). They treated contact line boundary condition by prescribing the contact line velocity dependent on the value of dynamic contact angle.

From the literature survey, it is found that most of the numerical studies are reported for non-bouncing cases on hydrophilic surfaces; there is scarcity of numerical investigation (except Mukherjee and Abraham, 2007; Caviezel et al., 2008; Sprittles and Shikhmurzaev, 2012) for the impact of a droplet on hydrophobic and superhydrophobic surfaces which results in bouncing or non-bouncing fate. Thus, with a long term objective of a numerical impact-dynamics study for the hydrophobic and superhydrophobic surfaces, the present paper was initiated with three objectives as follows:

i. To incorporate the modeling of contact line motion (as an extension to a series of work, Gada and Sharma, 2011, 2012; Lakdawala et al., 2014, 2015a, 2015b; in our research group) in the DGLSM based in-house code in the 2D axisymmetric cylindrical coordinate system developed by Gada (2012).
ii. To perform the experiments on the impact of a droplet on hydrophobic and superhydrophobic surfaces, at various droplet impact velocities, and use them for the validation and a performance study of our numerical results.
iii. To demonstrate an effectiveness of the DGLSM as compared to the traditional LSM for the present problem.

In the present paper, a quasi-dynamic contact angle model of Fukai et al. (1995) is implemented and experimentally recorded advancing and receding contact angles are used as inputs in the model.

Physical and computational description of the problem

In the present study on the level-set method for the contact line modeling, the problem considered is a gravity induced impact of a spherical droplet on a flat or micropillared surface, shown in Fig. 1. The figure shows a water droplet (of initial diameter d_0) impacting the surface with a velocity v_0 in air. For the present non-dimensional study, d_0 is the characteristic length and v_0 is the velocity scale, and water (fluid 1) is considered as the reference fluid. A time wise variation of non-dimensional maximum droplet height and wetted radius is shown as H_{max} (defined at the axis) and R_{wetted}, respectively; D_{wetted} is the wetted diameter (Fig. 1b).