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# On the dynamic contact angle in simulation of impinging droplets with sharp interface methods

Sashikumaar Ganesan

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**Abstract** Effects of dynamic contact angle models on the flow dynamics of an impinging droplet in sharp interface simulations are presented in this article. In the considered finite element scheme, the free surface is tracked using the arbitrary Lagrangian-Eulerian approach. The contact angle is incorporated into the model by replacing the curvature with the Laplace-Beltrami operator and integration by parts. Further, the Navier-slip with friction boundary condition is used to avoid stress singularities at the contact line. Our study demonstrates that the contact angle models have almost no influence on the flow dynamics of the non-wetting droplets. In computations of the wetting and partially wetting droplets, different contact angle models induce different flow dynamics, especially during recoiling. It is shown that a large value for the slip number has to be used in computations of the wetting and partially wetting droplets in order to reduce the effects of the contact angle models. Among all models, the equilibrium model is simple and easy to implement. Further, the equilibrium model also incorporates the contact angle hysteresis. Thus, the equilibrium contact angle model is preferred in sharp interface numerical schemes.

**Keywords** Dynamic contact angle · Moving contact line · Impinging droplet · Finite elements · ALE approach

# 1 Introduction

A moving contact line is encountered in free surface flows when the free surface moves in contact with a solid surface.

S. Ganesan (🖂)

Numerical Mathematics and Scientific Computing, Supercomputer Education and Research Centre, Indian Institute of Science, Bangalore 560012, India e-mail: sashi@serc.iisc.in Liquid droplet spreading and recoiling on a solid substrate is one of the typical examples of moving contact line problems. Two main challenges in computational fluid dynamics (CFD) simulation of free surface flows are the prescription of the boundary condition on the solid surface, especially at the moving contact line, and to incorporate the wetting effects, i.e., the inclusion of the contact angle into the model equations. This subject has been investigated by several researchers, see for example, Cox (1986), Dussan (1976), Gennes (1985), Haley and Miksis (1991), Hocking (1976), Hocking and Davis (2002), and Huh and Scriven (1971). For a recent review of numerical modeling and methods of multiphase flows, we refer to Wörner (2012).

In the earlier studies, the contact angle is imposed as a boundary condition at the moving contact line in the lubrication theory approximations, see for example, Haley and Miksis (1991), Hocking (1992) and the references therein. However, in CFD simulations of moving contact line flows, the inclusion of the contact angle is not straight forward, see for example, Schönfeld and Hardt (2009). In the volume-of-fluid method (Renardy et al. 2001), the normal vector of the interface at the contact line is defined in such a way that the gradient of the volume fraction coincide with the prescribed contact angle. Alternative to this approach, an additional force term, which contains the contact angle, is added in the vicinity of the contact line in Sikalo et al. (2005). In the level set simulation (Spelt 2005), the contact angle condition is imposed in the re-distance step of the level set function. In the Lagrangian finite element simulation of impinging droplets (Fukai et al. 1995), the contact angle is taken into consideration while determining the curvature at the contact line. In the arbitrary Lagrangian-Eulerian simulation of impinging droplets (Ganesan 2006; Ganesan and Tobiska 2009), the Laplace-Beltrami operator technique is used to handle the curvature term, in which the contact angle has been incorporated at the contact line integral term.

Even though the contact angle can be incorporated in the computational models, prescribing its value in computations is not clear. In general, the angle formed between the free surface and the liquid–solid interface at the contact line is conventionally defined as the contact angle in moving contact line problems. In thermodynamic equilibrium state, the contact angle is related to the interfacial tensions of the free surface  $\sigma$ , solid–liquid  $\sigma_{sl}$  and solid–gas  $\sigma_{sg}$  through the Young's equation

$$\sigma\cos(\theta) = \sigma_{\rm sg} - \sigma_{\rm sl}.$$

The contact angle  $\theta$  in the Young's equation is referred to as the static or equilibrium contact angle ( $\theta_e$ ), i.e.,  $\theta = \theta_e$ . At the equilibrium state, the equilibrium contact angle  $\theta_e$  is unique for the considered gas, liquid and solid material phases. However, when the contact line moves, the contact angle deviates from the equilibrium value, and the difference between the advancing  $\theta_a$  and receding  $\theta_r$  is referred to as a contact angle hysteresis. The advancing contact angle  $\theta_a$  is the largest angle just before the spreading starts and the receding contact angle  $\theta_r$  is the smallest angle just before the recoiling starts. In general, the contact angle that incorporates the hysteresis is called the dynamic contact angle  $\theta_d$ . The evidence for the dynamic behavior of the contact angle can be found in experiments, see for example, Dussan (1979), and Hoffman (1975). Since the dynamic contact is measured away from the contact line in experiments, it is also referred to as the apparent or macroscopic contact angle.

In the volume-of-fluid method (Renardy et al. 2001), a fixed contact angle has been used for moving contact line problems. In the level set computations of flow with multiple moving contact lines (Spelt 2005),  $\theta_a$  and  $\theta_r$  have been used to impose the contact line velocity. In general, the dynamic contact angle is prescribed to vary linearly between  $\theta_a$  and  $\theta_r$ , when the advancing and receding angles are used in computations, see for example, Chen et al. (2009). In the Lagrangian finite element computations of impinging droplets (Fukai et al. 1995), constant values have been used for the dynamic contact angle during the spreading and recoiling stages. In the sharp interface ALE approach, the equilibrium value has been used for the dynamic contact angle in computations of 2D (Ganesan and Tobiska 2005) and 3D-axisymmetric (Ganesan 2006) impinging droplets.

Recently, the effects of different dynamic contact angle models on the flow dynamics in the volume-of-fluid simulation of capillary filling on 2D microchannel have been evaluated by Saha and Mitra (2009). It has been observed by the authors that different models have minimal effect on the meniscus profile. In this paper, we evaluate the robustness and the influence of different contact angle models on the flow dynamics in the ALE simulation of an impinging droplet. The remaining part of the paper is organized as follows. In Sect. 2, the governing equations of a 3D impinging droplet are given. In Sect. 3, the variational form of the equations and the details of the numerical scheme are recalled briefly. Different dynamic contact angle models are described in Sect. 4 The numerical results of a 3D axisymmetric droplet deformation on a horizontal solid surface in Sect. 5 show the influence of different contact angle models on the wetting diameter and the dynamic contact angle. Finally, a short summary is given in Sect. 6

# 2 Mathematical model

We consider a liquid droplet  $\Omega(t) \subset \mathbb{R}^3$  of diameter  $d_0$ impinging on a horizontal solid surface. In our model, we neglected the effect of the surrounding gas-phase, and thus one-fluid case is considered. The sequence of spreading and recoiling of the droplet on the surface is described by the time-dependent incompressible Navier–Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} - \nabla \cdot \mathbb{S}(\mathbf{u}, p) = \frac{1}{Fr}\mathbf{e}, \quad \nabla \cdot \mathbf{u} = 0$$
(1)

in  $\Omega(t) \times (0, I)$  with the initial condition  $\mathbf{u}(\cdot, 0) = 0$ , the kinematic and force balancing conditions

$$\mathbf{u} \cdot \mathbf{v}_{\mathrm{F}} = \mathbf{w} \cdot \mathbf{v}_{\mathrm{F}}, \quad \mathbf{v}_{\mathrm{F}} \cdot \mathbb{S}(\mathbf{u}, p) = \frac{\mathcal{K}}{We} \cdot \mathbf{v}_{\mathrm{F}}$$

on the free surface  $\Gamma_F$ , and the Navier-slip boundary condition

$$\mathbf{u} \cdot \mathbf{v}_{\mathrm{S}} = \mathbf{0}, \quad \beta(\tau_{i,\mathrm{S}} \cdot \mathbb{S}(\mathbf{u}, p) \cdot \mathbf{v}_{\mathrm{S}}) = -\mathbf{u} \cdot \tau_{i,\mathrm{S}},$$

for i = 1, 2, on the solid surface  $\Gamma_S$ . In the above equations, the dimensionless stress tensor  $\mathbb{S}(\mathbf{u}, p)$  for the Newtonian liquid is given by

$$\mathbb{S}(\mathbf{u},p) = \frac{2}{Re} \mathbb{D}(\mathbf{u}) - p\mathbb{I}, \quad \mathbb{D}(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}}),$$

where  $\mathbb{D}(\mathbf{u})$  is the velocity deformation tensor. In the above equations,  $\mathbf{u}$  is the fluid velocity, p is the pressure in the fluid,  $\mathbf{w}$  is the moving domain velocity,  $\mathbf{w}$  on  $\Gamma_{\rm F}$  is the free surface velocity, t the time,  $\mathbf{e}$  an unit vector in the opposite direction of the gravitational force,  $v_{\rm F}$ ,  $v_{\rm S}$  and  $\tau_{i,\rm S}$ ,  $\tau_{i,\rm F}$  are the unit normal and tangential vectors, respectively, on their respective surfaces, and  $\mathbb{I}$  is the identity tensor. The symbol  $\nabla$  denotes the gradient operator,  $\nabla \cdot$  denotes the divergence operator,  $\mathcal{K}$  denotes the sum of the principal curvatures and the superscript T denotes the transpose. The dimensionless numbers (Reynolds, Weber, Froude and Slip) are given by

$$Re = rac{
ho UL}{\mu}, \quad We = rac{
ho U^2 L}{\sigma}, \quad Fr = rac{U^2}{Lg}, \quad eta = \epsilon_{\mu} 
ho U$$

where *L* is the characteristic length, *U* the characteristic velocity,  $\rho$  the density,  $\mu$  the dynamic viscosity and *g* the gravitational constant. The unknown numerical slip parameter  $\varepsilon_{\mu}$  in the slip number is equal to the slip length  $\varepsilon$  divided by a parameter with the unit kg m<sup>-1</sup> s<sup>-1</sup>, see for example, Ganesan and Tobiska (2009).

## 3 Numerical scheme

We use the finite element scheme together with the arbitrary Lagrangian–Eulerian approach (ALE-FEM) to solve the model equations. The detailed features of this finite element scheme have been presented in Ganesan (2006) and will not be presented here for brevity. Instead, we briefly summarize the main ingredients of the numerical scheme.

## 3.1 Variational form

Let  $V := (H^1(\Omega(t)))^3$  and  $Q := L^2(\Omega(t))$  be the usual Sobolev spaces. We multiply (1) by test functions  $\mathbf{v} \in V$ and  $q \in Q$ , respectively, and integrate over  $\Omega(t)$ . After integrating by parts and incorporating the boundary conditions, the weak form of (1) reads:

For given  $\Omega(0)$ ,  $\mathbf{u}(0)$  and  $\theta_d$ , find  $(\mathbf{u}(t), p(t)) \in V \times Q$ such that

$$\begin{pmatrix} \frac{\partial \mathbf{u}}{\partial t}, \mathbf{v} \end{pmatrix} + a(\mathbf{u}; \mathbf{u}, \mathbf{v}) - b(p, \mathbf{v}) + b(q, \mathbf{u}) = f(\mathrm{id}_{\Gamma_{\mathrm{F}}}, \mathbf{v}) + c(\theta_{\mathrm{d}}, \mathbf{v}),$$
(2)

for all  $\mathbf{v} \in V$  and  $q \in Q$ . Here,

$$\begin{split} a(\hat{\mathbf{u}};\mathbf{u},\mathbf{v}) &= \frac{2}{Re} \int_{\Omega(t)} \mathbb{D}(\mathbf{u}) : \mathbb{D}(\mathbf{v}) dx + \int_{\Omega(t)} (\hat{\mathbf{u}} \cdot \nabla) \mathbf{u} \cdot \mathbf{v} dx \\ &+ \frac{1}{\beta} \int_{\Gamma_{\mathrm{S}}(t)} (\mathbf{u} \cdot \tau_{i,\mathrm{S}}) (\mathbf{v} \cdot \tau_{i,\mathrm{S}}) d\gamma_{\mathrm{S}}, \\ b(q,\mathbf{v}) &= \int_{\Omega(t)} q \nabla \cdot \mathbf{v} dx, \\ f(\mathrm{id}_{\Gamma_{\mathrm{F}}},\mathbf{v}) &= \frac{1}{Fr} \int_{\Omega(t)} \mathbf{e} \cdot \mathbf{v} dx - \frac{1}{We} \int_{\Gamma_{\mathrm{F}}(t)} \frac{\Gamma_{\mathrm{F}}}{\Gamma_{\mathrm{F}}} \cdot \underline{\nabla} \mathbf{v} d\gamma_{\mathrm{F}}, \\ c(\theta_{\mathrm{d}},\mathbf{v}) &= \frac{1}{We} \int_{\zeta_{t}} \cos(\theta_{\mathrm{d}}) \mathbf{v} \cdot \tau_{\mathrm{S}} d\zeta, \end{split}$$

where  $\zeta_t$  is the contact line,  $\underline{\nabla}$  is the tangential (surface) gradient operator and  $id_{\Gamma_F}$  is an identity mapping. The

dynamic contact angle  $\theta_d$  in the above equation has been incorporated by replacing the curvature  $\mathcal{K}$  in the free surface integral with the Laplace–Beltrami operator,  $\underline{\Delta}(:= \underline{\nabla} \cdot \underline{\nabla})$  and then integration by parts, see Dziuk (1991), Ganesan and Tobiska (2009) for more details.

To track the moving boundary, the variational form of the Navier–Stokes equation (2) is rewritten into the ALE form, which reads:

For given  $\Omega(0)$ ,  $\mathbf{u}(0)$ ,  $\mathbf{w}(0)$  and  $\theta_d$ , find  $(\mathbf{u}(t), p(t)) \in V \times Q$  such that

$$\begin{pmatrix} \frac{\partial \mathbf{u}}{\partial t}, \mathbf{v} \end{pmatrix} + a(\mathbf{u} - \mathbf{w}; \mathbf{u}, \mathbf{v}) - b(p, \mathbf{v}) + b(q, \mathbf{u})$$
  
=  $f(\mathrm{id}_{\Gamma_{\mathrm{F}}}, \mathbf{v}) + c(\theta_{\mathrm{d}}, \mathbf{v}),$  (3)

for all  $\mathbf{v} \in V$  and  $q \in Q$ .

#### 3.2 Axisymmetric formulation

The considered liquid droplet deformation is axisymmetric, and thus we derive the 3D-axisymmetric form from the variational form of the 3D equations. The main advantage in this approach is that the same equations (2) can be used for 2D, 3D-axisymmetric and 3D models. Further, we do not need boundary conditions in cylindrical coordinate systems, since all boundary conditions are already incorporated in the variational form (2).

## 3.3 Discretization and solution

For the time discretization we use the second order, strongly A-stable fractional-step-9 scheme (Bristeau et al. 1987; Rannacher 2004; Turek 1999). The non-linear convection term is linearized by an iteration of fixed point type. The meridian domain is triangulated by a boundary resolved triangular mesh. For the spatial discretization we use the "inf-sup" stable second-order finite element pair  $P_2^{\text{bubble}}$ /  $P_1^{\text{disc}}$ , where the velocity space is enriched with a cubic bubble function (Crouzeix and Raviart 1973). This finite element pair guarantees an excellent mass conservation, since it satisfies the divergence constrain cell-wise. Finally, the obtained system of linear algebraic equations is solved by a direct solver. We could use more sophisticated multigrid solvers. However, constructing a hierarchical mesh during the remeshing needs special attention. Since the system is small and sparse in 3D-axisymmetric configuration, we preferred the direct solver. Nevertheless, a sophisticated iterative solver is preferred in 3D computations.

## 3.4 Free surface tracking

In order to find the new shape of the droplet for the next time step  $t = t^n$ , we solve first the Eq. (3) and move the free surface vertices using fluid velocity  $\mathbf{u}^n$ . Let  $\Psi_F^n$  be the

resulting displacements of the free surface vertices. Now, we compute the displacement of the inner vertices by solving the linear elasticity problem (elastic mesh update Ganesan and Tobiska 2008, Johnson and Tezduyar 1994)

$$\nabla \cdot \mathbb{T}(\Psi^n) = 0 \quad \text{in } \Omega(t^{n-1}),$$
  

$$\Psi^n = \Psi^n_F \quad \text{on } \Gamma_F(t^{n-1}),$$
  

$$\Psi^n = 0 \quad \text{on } \partial\Omega(t^{n-1}) \setminus \Gamma_F(t^{n-1}).$$

Here, the stress tensor  $\mathbb{T}$  is given by

$$\mathbb{T}(\phi) = \lambda_1 (\nabla \cdot \phi) \mathbb{I} + 2\lambda_2 \mathbb{D}(\phi),$$

where  $\lambda_1$  and  $\lambda_2$  are the Lame constants (chosen to be  $\lambda_1 = \lambda_2 = 1$  in our numerical tests). Then, the new shape of the droplet is obtained by moving the inner vertices using the displacement vector  $\Psi^n$ . Also, the mesh velocity is computed form the displacement vector by  $\mathbf{w}^n \approx \Psi/(t^n - t^{n-1})$  at time  $t = t^n$  in  $\Omega(t^n)$ , which is needed in (3).

Next, we have observed a rolling motion of the droplet while spreading. It is handled by changing the boundary description of the edge that arrives from the free surface to the solid surface. In computations, a few vertices on the free surface accumulates at a position or the resolution at some parts of the free surface becomes inadequate after several time steps. We overcome this challenge by redistributing the free surface vertices using the interpolated cubic spline when needed. Occasionally, the distortion of the mesh may become very large when the deformation of the domain is large. In such situations, we remesh the domain and interpolate the solution from the old mesh to the newly generated mesh. Since we use the ALE approach with the elastic mesh update technique, remeshing and interpolation are not needed often.

## 4 Dynamic contact angle

In order to approximate the solution of the Eq. (2), the dynamics contact angle  $\theta_d$  in the contact line integral  $c(\theta_d, \mathbf{v})$  has to be prescribed. Both in theoretical models and in empirical correlations, it is common to relate the dynamic contact angle  $\theta_d$  to the dynamic capillary number  $Ca_{cl}$  and the static contact angle ( $\theta_0$ ), *i.e.*,

$$\theta_{\rm d} = \mathcal{F}(Ca_{\rm cl}, \theta_0). \tag{4}$$

Here,

$$Ca_{\rm cl} = \frac{\mu |u_{\rm cl}|}{\sigma} = \frac{\mu U}{\sigma} |\hat{u}_{\rm cl}| = Ca |\hat{u}_{\rm cl}|,$$

where Ca(=We/Re) is a fixed capillary number and  $\hat{u}_{cl}$  is the nondimensional relative velocity between the solid surface and the contact line. Apart form the parameters in the Eq. (4), obviously there are other parameters such as the surface roughness, the surface inhomogeneities, surfactant, polymers, etc., that will influence the dynamic contact angle, see for example, Gennes (1985) and Kistler (1993). Thus, the choice of an universal relation for the dynamic contact angle is almost impossible.

For a perfectly wetting liquid it is obvious to take  $\theta_0 = 0$ , since  $\theta_e \approx 0$ . However, the choice of an appropriate contact angle value for partially wetting liquids is not simple. Either the equilibrium contact angle ( $\theta_e$ ) or the advancing/receding contact angle ( $\theta_a/\theta_r$ ) or any other relevant value can be used. In this paper we consider the following four contact angle models. The first model

M1: 
$$\theta_d = \theta_e$$
 (5)

is the simplest of all models from the implementation point of view. In this model, it does not mean that the dynamic contact angle is fixed to the equilibrium value during the computations. Since the contact angle is included in a weak sense without imposing any condition on the geometry or on the contact-line velocity, the movement of the free surface in computations induces the hysteresis behavior of the contact angle. Next, we consider

M2: 
$$\theta_d^3 = \theta_e^3 + 9 Ca_{cl} \ln(1/\beta)$$
 (6)

as the second model, where  $\beta$  is the dimensionless slip number. It has been proposed by Hocking (1995) based on the earlier theoretical model (Hocking 1983). Different variants of expressions have been proposed for the constant (9 *Ca* ln(1/ $\beta$ )) in (6), see Hocking (1983). However, the exponent in (6) is widely believed to be the correct one, since it is consistent with the Tanner's power law from hydrodynamic theory for the spreading of a droplet. Next, we consider

M3: 
$$\frac{\cos(\theta_{e}) - \cos(\theta_{d})}{\cos(\theta_{e}) + 1} = \tanh(4.96Ca_{cl}^{0.702})$$
 (7)

as the third model, and it is one of the first empirical correlations proposed by Jiang and Slattery (1979). It is based on the Hoffman's data (Hoffman 1975) for silicone oil spread through a glass capillary tube. Finally, we consider another empirical correlation

M4: 
$$\frac{\cos(\theta_{\rm e}) - \cos(\theta_{\rm d})}{\cos(\theta_{\rm e}) + 1} = 2\sqrt{Ca_{\rm cl}}$$
(8)

proposed by Bracke et al. (1989) as the fourth model.

In the empirical correlations (7) and (8), the contact line velocity  $u_{cl}$ , which is a prior unknown, is an input for the trigonometric function, and it is treated explicitly in computations. Further, these models cannot be used for arbitrarily large values of  $\hat{u}_{cl}$ . To demonstrate their limitations, the dynamic contact  $\theta_d$  obtained from these empirical models are presented in Fig. 1 as a function of  $u_{cl}$  for





different values of  $\theta_e$  and *Ca*. The behavior of the empirical model (7) is similar in both  $\theta_e = 10^\circ$  and  $100^\circ$  cases. Further,  $\theta_d$  reaching the maximum value (180°) rapidly even for a small value of  $u_{cl}$  when Ca > 0.1. It is clear from Fig. 1 that the empirical model (8) can only be used if Ca < 0.1. Further, it should be noted that both these empirical models have been validated for spreading liquids. Thus, the validity of these empirical models in the receding stage of the droplet is not clear. Apart from these contact angle models, a number of theoretical and empirical contact angle models have been proposed in the literature, see for example, Cox (1986), Kistler (1993), Hocking (1995), Bayer and Megaridis (2006) and the references therein.

# **5** Numerical results

In this section, we study the influence of different contact angle models on the flow dynamics of an impinging axisymmetric liquid droplet on a horizontal surface. We consider the water and glycerin liquid droplets with different impinging velocities on the glass and wax surfaces. We use  $\rho = 996$  kg m<sup>-3</sup>,  $\mu = 10^{-3}$  N s m<sup>-2</sup> and  $\sigma =$ 0.073 N m<sup>-1</sup> for the water, and  $\rho = 1,220$  kg m<sup>-3</sup>,  $\mu = 0.116$ N s m<sup>-2</sup> and  $\sigma = 0.063$  N m<sup>-1</sup> for the glycerin. Further, we take  $U = u_{imp}$ ,  $L = d_0$  and g = 9.8 m s<sup>-2</sup>. The corresponding

Table 1 Dimensionless numbers of different cases used in this work

Case	Liquid	Re	Ca	We	Fr	$\theta_{\rm e}$	β
1	Glycerin	106	7.5	798	700	94	10
2	Glycerin	106	7.5	798	700	15	1,000
3	Glycerin	36	2.6	94	83	94	10
4	Glycerin	36	2.6	94	83	15	1,000
5	Water	4,002	0.023	90	112	100	5
6	Water	4,002	0.023	90	112	10	5
7	Water	2,440	0.014	34	42	135	1

The initial diameter of the droplet in all cases is 2.45 mm

dimensionless numbers obtained using these parameters are given in Table 1. We compare the computationally obtained dimensionless wetting diameter  $(d/d_0)$  and the contact angle  $(\theta_c)$  with their corresponding experimental values provided in Šikalo et al. (2005). The first four cases in Table 1 are the first four experiments in Šikalo et al. (2005), where as case 5 is the seventh experiment. Further, we examine the effect of different contact angle models on the height of the droplet at the center, i.e., at r = 0. The contact angle models M2, M3 and M4 are treated explicitly, i.e, the previous time step fluid velocity is used to calculate  $Ca_{cl}$ . Further, the slip number ( $\beta$ ) is considered as a numerical model parameter, and the values of  $\beta$  for different cases are determined by comparing the computationally obtained wetting diameter with their corresponding experimental observation. We observed that the  $\beta$  should be large in general for droplets with the small  $\theta_e$  in order to match the experimental values.

# 5.1 Glycerin droplets

In Fig. 2, the computationally obtained dimensionless wetting diameter, the contact angle and the height of the droplet at r = 0 with different contact angle models are presented for cases 1 and 2. Note that the flow configurations are same in both cases but the only difference is the equilibrium contact angle, i.e.,  $\theta_e = 94^\circ$  and  $\theta_e = 15^\circ$  in case 1 and case 2, respectively. Since the capillary number is large in these cases, the empirical contact angle model M4 is not applicable to these cases. In case 1, the dimensionless wetting diameter obtained from different contact angle models are in good agreement with the experimentally observed values during the spreading stage. However, all three contact angle models induce different recoiling dynamics, and it can clearly be seen in Fig. 2b. Since different contact angle models provide different dynamic contact angle values during the recoiling stage, the recoiling dynamics is not uniform. During the spreading, the contact angle  $\theta_c$  increases initially, and then approach the dynamic value given by different contact angle models. Initially, the increase in the contact angle obtained in computations is large in comparison with the experimental values. The rolling motion in the boundary fitted mesh could be one of the reasons for it. In computations, the contact angle is evaluated between the solid surface and the first vertex on the free surface. Therefore, the evaluated contact angle will be very oscillatory when the droplet rolls, i.e., the first free surface vertex reaches the solid surface. Initially, i.e., immediately after the impact, the droplet spreading is dominated by the rolling motion, and it is the main reason for the large scattering in the evaluated contact angle in Fig. 2b and in later cases. Though we do not have experimental values for the height of the droplet at r = 0, there is almost no difference among the computed values obtained with these three contact angle models. The recoiling is not observed in case 2, since the equilibrium contact angle is small, i.e.,  $\theta_{\rm e} = 15^{\circ}$ . Further, all computed values are in very good agreement with the experimental observations in case 2. Even though the obtained contact angle  $\theta_{\rm c}$  in all cases is far from the equilibrium value, it approaches the equilibrium value asymptotically. The height of the droplet at r = 0obtained with the three contact angle models in case 2 is also similar.

Next, the dimensionless wetting diameter, the contact angle and the height of the droplet at r = 0 obtained for cases 3 and 4 with different contact angle models are presented in Fig. 3. In case 3, the dimensionless wetting diameter obtained with different models are in good agreement with the experimental observations only during the initial spreading stage. Later, the wetting diameter obtained with different models are different from each other. Further, the maximum wetting diameter also differs between different contact angle models. The numerical results obtained with model M1 fits closely with the experimental data. During the recoiling stage, significant differences are observed in the obtained wetting diameter among all models. It is more visible in Fig. 3b, where the computationally obtained contact angle with all models are presented. In model M3, the droplet recedes quickly in comparison with other two models. Due to fast receding, the height of the droplet at r = 0 also increases rapidly, see Fig. 3c. Even though the equilibrium contact angle  $\theta_e =$ 94°, the apparent contact angle decreases below 65° in experiments, whereas the computationally obtained contact angles with models M1 and M2 are close to the equilibrium value during the entire receding stage. In case 4, the droplet receding is not observed, and it is due to the small equilibrium contact angle  $\theta_e = 15^\circ$ . In this case, the flow dynamics of the droplet obtained from the M2 and M3 models are similar, whereas the droplet keeps spreading in model M1. The obtained contact angle in both M2 and M3 models remain  $60^{\circ}$ , whereas the contact angle approaches the equilibrium value in model M1.

Irrespective of the contact angle model, all these calculated flow parameters should reach a steady state value when the droplet reaches the equilibrium stage. To examine this, we consider case 1 and performed the computations for different contact angle models for a longer period of dimensionless time. The obtained results are presented in Fig. 6. The wetting diameter obtained from both the M1 and M2 models reached the steady state value before the dimensionless time 125, whereas in M3 it is slowly approaching the steady state value. In experiments, the recoiling is very slow and the droplet is far from the equilibrium stage even at the dimensionless time 125. The obtained contact angles ( $\theta_c$ ) in both the M1 and M2 models have reached the equilibrium contact angle ( $\theta_{e}$ ) value, whereas  $\theta_{\rm c}$  is far from the  $\theta_{\rm e}$  value in the experiment. However, the droplet recoiling speed in computations can be reduced by choosing larger value for  $\beta$  than the used value  $\beta = 1,000$ . But the purpose of this computations is to show that the computed flow parameters in all contact angle models will reach a steady state value when the droplet reaches the equilibrium state, and it is shown in Fig. 6.

## 5.2 Water droplets

Figure 4 represents the dimensionless wetting diameter, the contact angle and the height of the droplet at r = 0 obtained from computations of cases 5 and 6 with different contact angle models. The top and bottom rows in Fig. 4 represent the numerical results for  $\theta_e = 10^\circ$  and  $\theta_e = 10^\circ$ , respectively.



Fig. 2 Computationally obtained dimensionless wetting diameter (a, d), the contact angle (b, e), the height of the droplet at r = 0 (c, f) with different contact angle models for cases 1 and 2, respectively, are compared with the experimentally observed values



Fig. 3 Computationally obtained dimensionless wetting diameter (a, d), the contact angle (b, e), the height of the droplet at r = 0 (c, f) with different contact angle models for cases 3 and 4, respectively, are compared with the experimentally observed values



Fig. 4 Computationally obtained dimensionless wetting diameter (a, d), the contact angle (b, e), the height of the droplet at r = 0 (c, f) with different contact angle models for cases 5 and 6, respectively, are compared with the experimentally observed values

In these cases, the capillary number is small (Ca = 0.023). Hence, we were able to obtain results using M4 model (8) also. The wetting diameter obtained with all contact angle models are in good agreement with the experimental values when the equilibrium contact angle value is large. More interestingly, computational results agree well with the experimental values even during the recoiling stage, see the top row in the Fig. 4. Though the maximum wetting diameter is slightly high in M1 and M2 models, the contact angle and the height of the droplet at r = 0 obtained in all contact angle models are comparable. By contrast, the wetting diameters obtained with different contact angle models are different when small equilibrium contact angle value is used, see the bottom row in the Fig. 4. However, the contact angles and the height of the droplet at r = 0 obtained with different contact angle models are not varied as in case 3.

Next, the dimensionless wetting diameter, the contact angle and the height of the droplet at r = 0 obtained from computations of case 7 with different contact angle models are presented in Fig. 5. Similar to the previous case, the capillary number is small (Ca = 0.014) in case 7. Further, note that the equilibrium contact angle in this case is 135°. Though the experimental values are not available for this case, the computationally obtained values with all models are almost same, at least there is no visible difference between the wetting diameter curves (Fig. 5a). The contact angle and the height of the droplet at r = 0 obtained with different contact angle models are also in good agreement. Note that the droplet height at r = 0 becomes zero, i.e., "dry out" at the center of the droplet in this case.

Overall, the contact angle model M1 agrees well with the experimental results, and the flow dynamics obtained with models M1 and M2 are similar. The M4 model is applicable only for droplets with small capillary numbers. The wetting diameter, the contact angle ( $\theta_c$ ) and the height of the droplet at r = 0 obtained with the M3 model are comparable with the other models only during the spreading stage. Interestingly, the flow dynamics obtained with all contact angle models are similar when the equilibrium contact angle ( $\theta_e$ ) is large, for e.g., in case 7. In the numerical study, it is observed that the different contact angle models induce different flow dynamics, especially during the recoiling stage, when the equilibrium contact angle is small. In the next section, we examine the influence of equilibrium contact angle further.

# 5.3 Influence of equilibrium contact angle

In the previous section, we have observed that different contact angle models induce different flow dynamics when the equilibrium contact angle is small. To examine it further, we consider case 3 with three equilibrium contact angle variants: (1)  $\theta_e = 20$ , (2)  $\theta_e = 135$  and (3)  $\theta_e = 160$ . The computationally obtained dimensionless wetting diameter, the contact angle and the height of the droplet at r = 0 in



Fig. 5 Computationally obtained dimensionless wetting diameter (a), the contact angle (b) and the height of the droplet at r = 0 (c) with different contact angle models for case 7



Fig. 6 Computationally obtained dimensionless wetting diameter (a), the contact angle (b) and the height of the droplet at r = 0 (c) with different contact angle models for case 3 with  $\theta_e = 20^\circ$  and  $\beta = 1,000$ 

these three variants are presented in Fig. 7. It is clear from Fig. 7 (bottom row) that all contact angle models induce same flow dynamics for non-wetting liquid droplets. However, this is not the case in the wetting and partially wetting liquid droplets. In the wetting droplet case (var 1), each contact angle model induce different flow dynamics, see Fig. 7 (first row). Since  $\theta_e = 20^\circ$  in var 1, recoiling is very unlikely to occur. However, the droplet recoils in the M2 and M3 models. By contrast, the droplet keeps spreading in the M1 model. Further, the obtained contact angle ( $\theta_c$ ) is above 100° and 60° in the M2 and M3 models, respectively, whereas  $\theta_c$  is around 25° in the M1 model. It should be noted that  $\beta = 10$  is used in all variants of Fig. 7. Our experiences show that  $\beta$  has to be increased while decreasing  $\theta_{e}$ . Thus, we perform another computation for the variant 1 with  $\beta = 1,000$ . The obtained numerical results are plotted in Fig. 8. It can be seen that all contact angle models induce almost same flow dynamics for  $\theta_e = 20^\circ$  variant when  $\beta$  is chosen as 1,000. This observation clearly shows that  $\beta$  is very influential on the flow dynamics of the wetting droplets. Thus, the choice of  $\beta$  is more important apart from the choice of contact angle model for the wetting and partially wetting droplets. A small value of  $\beta$  induce different flow dynamics

for different contact angle models. Nevertheless, the flow dynamics of the droplet obtained with the M1 model appears to be more physical (no recoiling observed) even for a small value of slip number.

### 6 Summary

In this paper, effects of dynamic contact angle models on the flow dynamics in sharp interface simulation of impinging liquid droplets on a horizontal surface are investigated. The finite element simulations are performed using the arbitrary Lagrangian–Eulerian approach. Four different contact angle models are considered in this study. To investigate the considered models, the water and glycerin liquid droplets with different impinging velocities and equilibrium contact angle are used. The computationally obtained wetting diameter and the contact angle with different contact angle models are compared with their corresponding experimental results. Based on the numerical studies in the previous sections, we have the following conclusions. The empirical contact angle model proposed by Bracke et al. (1989) is applicable only for droplets with



**Fig. 7** Computationally obtained dimensionless wetting diameter (*first column*), the contact angle (*second column*) and the height of the droplet at r = 0 (*third column*) with different contact angle models for case 3 with  $\theta_e = 20$  (*top row*),  $\theta_e = 135$  (*middle row*) and  $\theta_e = 160$  (*bottom row*)



Fig. 8 Computationally obtained dimensionless wetting diameter (a), the contact angle (b) and the height of the droplet at r = 0 (c) with different contact angle models for case 3 with  $\theta_e = 20^\circ$  and  $\beta = 1,000$ 

small capillary number, say Ca < 0.1. Next, all four considered contact angle models induce almost same flow dynamics in non-wetting droplet simulations, say  $\theta_e >$ 

 $140^{\circ}$ . For the wetting and partially wetting droplets, the flow dynamics obtained with all contact angle models are similar when the slip number is high. Even for a droplet

with  $\theta_e = 15^\circ$ , the recoiling phenomenon is observed in the theoretical (Hocking 1995) and empirical (Jiang and Slattery 1979) models, when the slip number is small. On the contrary, the recoiling is not observed when the equilibrium value is used for the dynamic contact angle. Further, the results obtained with the equilibrium model are in good agreement with experimental observations. Thus, we prefer the equilibrium contact angle model for sharp interface schemes. Also, we stress that irrespective of a contact angle model, the influence of the slip number is high on the flow dynamics of the wetting and partially wetting droplets. Nevertheless, the effects of contact angle models on the flow dynamics are negligible when the slip number is chosen appropriately. In this work, the influence of the slip number on the flow dynamics is not studied in detail, but we observed that the slip number has to be large when the equilibrium contact angle value is small. The appropriate choice of the slip number for computations of impinging droplets will be a subject for future research.

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