Extension of local front reconstruction method with controlled coalescence model

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Extension of local front reconstruction method with controlled coalescence model

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The physics of droplet collisions involves a wide range of length scales. This poses a challenge to accurately simulate such flows with standard fixed grid methods due to their inability to resolve all relevant scales with an affordable number of computational grid cells. A solution is to couple a fixed grid method with subgrid models that account for microscale effects. In this paper, we improved and extended the Local Front Reconstruction Method (LFRM) with a film drainage model of Zang and Law [Phys. Fluids **23**, 042102 (2011)]. The new framework is first validated by (near) head-on collision of two equal tetradecane droplets using experimental film drainage times. When the experimental film drainage times are used, the LFRM method is better in predicting the droplet collisions, especially at high velocity in comparison with other fixed grid methods (i.e., the front tracking method and the coupled level set and volume of fluid method). When the film drainage model is invoked, the method shows a good qualitative match with experiments, but a quantitative correspondence of the predicted film drainage time with the experimental drainage time is not obtained indicating that further development of film drainage model is required. However, it can be safely concluded that the LFRM coupled with film drainage models is much better in predicting the collision dynamics than the traditional methods. *Published by AIP Publishing.*
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I. INTRODUCTION

Droplet-laden flows play an important role in many industrial applications and natural processes,¹ like atomization of fuel in combustion engines, spray drying of concentrated milk to produce milk products, liquid-liquid extraction, growth of rain droplets in a cloud, and pollution tracking. The interaction between droplets has a major influence on the dynamics of such flows because of the coalescence and break-up that may occur upon collision.

For certain gas-liquid combinations, these interactions vary based on various parameters expressed in terms of the non-dimensional numbers, Weber number We and offset parameter B . As shown in Fig. 1, the Weber number characterizes the importance of the inertial forces compared to the surface tension forces, and the offset parameter B characterizes the obliqueness of the collision. For example, $B = 0$ represents a head-on collision. The variation of the collision outcomes with these non-dimensional numbers is summarized through collision regime maps. For example, the regime map for the collision of two equal-sized hydrocarbon droplets in 1 atm air is shown in Fig. 2. At high Weber numbers,

the collision is inertia dominated and collision outcomes vary significantly with the offset distance resulting in reflexive separation (IV), coalescence (III), stretching separation (V), and bouncing (II) with increasing offset distance. The reflexive separation is characterized by the formation of a torus shaped droplet, and the reflexive action of the surface tension forces from this torus shape causes separation of the droplet into daughter droplets. In stretching separation, due to the high offset distance, only a portion of the droplets will come in contact. The remaining portions of the drops will tend to flow in the direction of their initial trajectory and consequently stretch the region of interaction, generating daughter droplets.

On the contrary, at low Weber numbers, the collision dynamics of droplets is highly influenced by the drainage of the thin gas film separating the two colliding droplets.² The droplets will bounce (II) if the film is not drained during the collision event or coalesce (III) if the gas film ruptures. The rupture is attributed to the van der Waals surface forces which become dominant at nanometer scale.

In this work, we intend to accurately predict coalescence and break-up using a multiscale modeling approach. Because of the large differences in length scales (mm for droplets and nm for film thickness), it is impossible to resolve all these length scales with an affordable number of computational grid

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FIG. 1. Nomenclature of a general binary collision, where We is the Weber number, B the impact parameter, V_0 the droplet velocity, R_0 the droplet radius, b the offset distance, ρ_l the discrete phase density, and σ the surface tension coefficient. Reproduced with permission from M. Kwakkel, W.-P. Breugem, and B. J. Boersma, "Extension of a CLSVOF method for droplet-laden flows with a coalescence/breakup model," *J. Comput. Phys.* **253**, 166–188 (2013). Copyright 2013 Elsevier.

cells. To ensure that all essential physics are included in the model, the under resolved final stage of the film drainage is accounted for by a sub-grid model. Previously, a few studies have been performed using a similar combination of different fixed grid methods and sub-grid models.^{2,4}

The fixed grid methods for modeling multiphase flows can be divided into two main types: front capturing and front tracking techniques.⁵ In front capturing methods, the interface is implicitly represented by a colour function. Common front capturing methods are the Volume of Fluid (VOF),⁶ and Level Set (LS)⁷ and Coupled Level Set and Volume of Fluid (CLSVOF)⁸ methods. In these methods, droplets generally coalesce automatically when they share a computational cell. This unphysical numerical coalescence can be avoided for the simulation of symmetric binary droplet collision in VOF, by prescribing a volume-fraction boundary condition on the collision plane using ghost cells.² When the boundary condition imposes a zero volume fraction, the droplets will bounce, whereas a symmetry boundary condition will result in coalescence. Another more general approach to avoid numerical

FIG. 2. Schematic of regime map for the collision of two equal sized hydrocarbon droplets in 1 atm air. Reproduced with permission from P. Zhang and C. K. Law, "An analysis of head-on droplet collision with large deformation in gaseous medium," *Phys. Fluids* **23**, 042102 (2011). Copyright 2011 AIP Publishing.

coalescence in VOF is to use a unique colour function for each droplet.^{4,9} A big disadvantage of front capturing methods is that a very fine grid resolution is required for accurate surface tension calculation especially when the droplets undergo complex topological changes.⁴

Front tracking methods are inherently better at surface tension calculation at coarse grid resolution because these methods directly track the interfaces.^{10,11} However, the traditional front tracking method does not allow for coalescence of dispersed elements. To incorporate coalescence, additional routines to merge unstructured meshes are required.¹² This merging of the meshes is complicated because the logical information regarding the marker connectivity should be updated. To avoid the complexity with respect to the merging of droplets, we adopt a front tracking method without connectivity, the Local Front Reconstruction Method (LFRM).¹⁰

Besides the removal of the connectivity, LFRM uses information from the original marker elements to reconstruct the interface in a mass conservative manner. Because the interface is reconstructed independently in each interfacial cell, the method is highly parallelizable. However, this cell-oriented reconstruction leads to numerical coalescence (similar to front capturing methods).¹⁰ To prevent this, the information about marker elements and marker points is stored for each droplet separately.

The complete description of the coalescence process is given in terms of collision frequency and coalescence efficiency.¹³ The flow field around the droplets dictates the collision frequency. Because the flow field is completely resolved by LFRM, a model for the collision frequency is not required. However, a subgrid model for coalescence efficiency is required because this depends on the rupture of the film between the droplets, which is not resolved. These subgrid models can be broadly classified as empirical models and physical models. The empirical models are tuned to fit certain experimental data and are not universal. The physical models make use of information of droplet interaction available from LFRM and, thus, are better suited for the mesoscale framework used in this study.

There are two classes of physical models:¹³ energy models and film drainage models. The energy models¹⁴ are based on the notion that during collisions due to turbulent agitation, the molecular attraction force between the colliding interface has less impact than the forces resulting from the turbulent motion of the fluid on the coalescence efficiency, and thus, colliding droplets are more likely to become merged immediately without liquid film thinning. For such cases, the Weber number will be high and it is safe to assume that the film drainage time amounts to zero.⁴ These cases can be directly resolved by fixed grid methods as shown by numerous studies.^{4,9,15,16}

With the film drainage models, variation of the film thickness versus time can be calculated, and thus, these models provide an estimate of the total film drainage time between contact and coalescence.^{3,17} The calculated film drainage time can be used as an input by fixed grid methods to allow/restrict coalescence of droplets, which is especially crucial for collisions in low Weber number regimes [i.e., regimes (I)–(III) in Fig. 2]. A similar approach was chosen by Kwakkel *et al.*⁴ to simulate

binary droplet collisions with the CLSVOF method. We choose a recent model of Zhang and Law³ from this class of film drainage models. This model is able to predict the coalescence-bouncing-coalescence transition for hydrocarbons and the bouncing-coalescence transition for water.³

In this paper, we discuss the improvement and extension of the local front reconstruction method with a film drainage model. In Sec. II, the numerical method is presented with focus on the details of the improvements. Section III contains the details of the coalescence module with the film drainage model and the details of the break-up module. In Sec. IV, the improved LFRM is verified and validated with standard tests. Next, the results of simulations of the (near) head-on collision of two equal tetradecane droplets in different collision regimes are discussed. The framework is first validated with simulations using the experimental film drainage time. Next, the sensitivity of the simulation results due to the film drainage model and the grid resolution are discussed. Finally, a summary of the main conclusions of the present study is provided in Sec. V.

II. METHODOLOGY

A. Governing equations

In this study, both fluids are assumed to be incompressible, immiscible, and Newtonian. Furthermore, a one-fluid formulation is used for both phases, taking into account the surface tension by a source term $\mathbf{F}_\sigma$. Thus, the resulting governing equations are as follows:

$$\nabla \cdot \mathbf{u} = 0, \quad (1)$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \nabla \cdot (\mathbf{u}\mathbf{u}) = -\nabla p + \rho \mathbf{g} - \nabla \cdot \boldsymbol{\tau} + \mathbf{F}_\sigma, \quad (2)$$

where ρ is mass density, $\mathbf{u}$ is fluid velocity, t is time, p is pressure, $\mathbf{g}$ is gravitational acceleration, and $\boldsymbol{\tau}$ is fluid stress tensor.

B. Numerical method

The interface is represented by an unstructured mesh of triangular markers, which are formed by the connection of the Lagrangian points situated at the corners of these markers. The markers enable advection of the interface and surface tension calculation. $\mathbf{F}_\sigma$ is calculated on the Eulerian grid using the hybrid method of Shin *et al.*,¹⁸ which combines the advantage of accurate curvature calculation (similar to the pull force model¹¹ in front tracking methods) and the proper balance of pressure and surface tension force at the discrete level (similar to the continuum surface model¹⁹ in front capturing methods).

Subsequently, the governing equations are solved by a fractional step method²⁰ to obtain the flow field at the next time step. The method consists of two steps: In the first step, a projection of velocity $\mathbf{u}^n$ is calculated using information from the previous time step

$$\mathbf{u}^{n*} = \mathbf{u}^n + \frac{\Delta t}{\rho^n} [-\rho \nabla \cdot (\mathbf{u}\mathbf{u}) - \nabla p + \rho \mathbf{g} - \nabla \cdot \boldsymbol{\tau} + \mathbf{F}_\sigma]^n. \quad (3)$$

This equation is spatially discretized on a staggered grid using a finite volume approach. The convective term is discretized with a second order flux-delimited Barton scheme,²¹

whereas the diffusion term is discretized with a second order central scheme. If the time step restriction due to the diffusion terms is too stringent, it can be relaxed by treating a part of the diffusion terms implicitly. After the projected velocities are calculated, the velocity field is corrected in the pressure correction step. In this step, the pressure is corrected such that resulting velocity field satisfies the continuity equation,

$$\nabla \cdot \left[\frac{\Delta t}{\rho^n} \nabla (\delta p) \right] = \nabla \cdot \mathbf{u}^n, \quad (4)$$

where $\delta p = p^{n+1} - p^n$ is the pressure correction. This pressure Poisson equation is solved using a robust and efficient parallel Block-Incomplete Cholesky Conjugate Gradient (B-ICCG) solver.

Once the flow field is solved, the interface is advected: i.e., the Lagrangian points are moved using locally interpolated fluid velocities. The fluid velocities are interpolated from the Eulerian grid points to Lagrangian points using cubic spline interpolation, whereas the marker points are moved using a 4th order Runge-Kutta scheme.¹¹

Due to the advection of Lagrangian points, the mesh quality decreases, causing the need for a reconstruction procedure,¹⁰ which is detailed in Sec. II C. Finally, the physical properties are updated using local phase fractions in each cell. From the calculated phase fractions, the average mass density and viscosity are calculated in each grid cell by algebraic and harmonic averaging, respectively. The local phase fraction can be calculated by geometric analysis using the position of the interface.¹¹ This method is exact and computationally more efficient than solving the Poisson equation used in the original LFRM method.¹¹

C. Local front reconstruction method

The overall LFRM reconstruction procedure consists of four simple steps as shown in Fig. 3:

1. **Localization**—The interface of the discrete phase is cut by a reconstruction grid (similar to the Eulerian grid but not necessarily coinciding with it) such that each part of the interface lies completely inside one cell.
2. **Edge line reconstruction**—The edge line corresponding to the cut interface is traced out on relevant faces of the cell, and a new edge line (containing only two edge points and a fitting point) is reconstructed in an area conserving manner. However, in Fig. 3, an ideal situation is depicted, where each face contains exactly two edge points with not more than one point on each edge. For the cases where there is more than one edge point, a marker points reduction algorithm²² is used to reduce the number of points to less than or equal to one.
3. **Centroid calculation**—Using edge points and fitting points of all the faces, a centroid is calculated. An intermediate interface is formed by connecting the centroid with intermediate edge lines.
4. **Volume fitting**—Finally, the centroid is moved in the normal direction of the intermediate interface such that original volume of the dispersed phase is conserved in the given cell.

The above described procedure deals with an ordinary case without interface merging. When complex topological

FIG. 3. Schematic of the reconstruction procedure for LFRM: (a) localization of the interface, (b) edge line reconstruction, (c) centroid calculation, and (d) volume fitting. Reproduced with permission from S. Shin, I. Yoon, and D. Juric, “The local front reconstruction method for direct simulation of two- and three-dimensional multiphase flows,” *J. Comput. Phys.* **230**, 6605–6646 (2011). Copyright 2011 Elsevier.

changes involving coalescence and break-up occur, there are more than two edge points on a cell face (even after marker points reduction), and consequently, an additional procedure termed tetra-marching is used.¹⁰ This procedure facilitates the merging/break-up of the interface in a continuous manner such that the reconstructed interface is a closed surface without holes.

In the original LFRM method, the information about the position of three vertices of each marker is stored separately: i.e., a vertex shared among different markers is stored repeatedly in different data structures corresponding to different markers. To decrease memory usage and increase robustness, the marker location is stored in linked-list data structures. Furthermore, this also enables implementation of a mesh smoothing procedure. The smoothing procedure of Kuprat *et al.*,²³ which results in an enhanced mesh quality for the front tracking method,²⁴ is also implemented in our LFRM.

III. EXTENSION WITH COALESCENCE AND BREAK-UP MODULE

Without special precautions, the coalescence of the droplets in LFRM occurs automatically when they share a reconstruction cell. To prevent numerical coalescence, the data structure of each droplet is stored with a unique identifier. Thus, during the interface reconstruction of a particular droplet, it does not feel the presence of other droplets even if two droplets share reconstruction cells. However, this prevents coalescence completely. To simulate coalescence between two droplets at a desired time, their data structures have to be merged and the merged droplet has to be given a unique

identifier, which is handled by the coalescence module. Similarly, each daughter droplet is given a unique identifier when formed after break-up of a droplet, which is handled by the break-up module.

A. Coalescence module

1. Film drainage model

To ensure two-way coupling between the LFRM and the film drainage model, we follow a similar approach as Kwakkel *et al.*⁴ In this approach, the external flow around the droplets is resolved by the fixed grid method and provides the necessary input data for the film drainage model, e.g., the initial interaction velocity and orientation of colliding droplets and the

FIG. 4. Geometrical parameters for the droplet collision model of Zhang and Law.³ Reproduced with permission from M. Kwakkel, W.-P. Breugem, and B. J. Boersma, “Extension of a CLSVOF method for droplet-laden flows with a coalescence/breakup model,” *J. Comput. Phys.* **253**, 166–188 (2013). Copyright 2013 Elsevier.

FIG. 5. Variation of film thickness $\tilde{h}$ with time $\tilde{t}$ at various initial Weber numbers. (a) Transition from coalescence regime (I) to bouncing regime (II). (b) Transition from bouncing regime (II) to coalescence regime (III).

contact time between colliding droplets. The other way round, the internal flow in the drainage film is approximated by the film drainage model and provides an input to LFRM, i.e., the collision outcome and film drainage time. When the droplets come very close to each other within the same Eulerian cell, the pressure in the unresolved film is represented by the nearest pressure nodes located inside the droplets. This is in accordance with the physical expectation that for a nearly flat film

the pressure inside the film is of the same order of magnitude as the pressure inside the droplets close to the interface.⁴

As mentioned before, the film drainage model of Zhang and Law³ is chosen for this study. The model is limited to head-on collisions of two equal sized droplets in a gaseous environment. It is applicable for collisions corresponding to low/medium Weber numbers because in these cases the extent of droplet deformation is comparable to the original radius of the droplet and the droplet shape is close to a truncated sphere with a flattened cap.³ The model takes into consideration the most essential physics of a binary droplet collision: the deformation of the droplets, viscous dissipation of kinetic energy through internal droplet motion, the dynamics and rarefied nature of the gaseous film in between the droplets, and the van der Waals forces during the last stage of drainage.

The model consists of a nonlinear system of ordinary differential equations (ODE) which determine the evolution of four variables: the radius of the truncated sphere $R(t)$, the radius of the flattened disk $a(t)$, the perpendicular distance from the center of the sphere to the flattened disk $b(t)$, and the thickness of the entrapped film between the flattened disks $h(t)$. The system of ODEs is non-dimensionalized using the impact velocity V_0 and radius R_0 prior to collision. The non-dimensional equations are as follows:

$$\tilde{a}\tilde{a}' + \tilde{b}\tilde{b}' = \tilde{R}\tilde{R}', \quad (5)$$

Algorithm 1. Coalescence module.

```

1: for all droplets pairs do
2:   Calculate the domain (bounding box) for both droplets in terms of grid
   cell units
3:   Determine if the domain of the two droplets overlap
4:   for cells in overlap domain do
5:     Determine if the droplets are in "contact"
6:     if the droplets are in "contact" then
7:       if the droplets pair is not in the collision list then
8:         Add the droplets pair to the collision list
9:         Calculate the film drainage time ( $t_{\text{drainage}}$ )
10:        Store the coalescence time ( $t_{\text{coalescence}} = t_{\text{contact}} + t_{\text{drainage}}$ )
11:      else
12:        if current time ( $t$ )  $\geq$  coalescence time ( $t_{\text{coalescence}}$ ) then
13:          Droplets are merged and removed from the collision list
14:        else
15:          Remove droplets pair from the collision list

```

FIG. 6. Steps of the flagging algorithm in the break-up module: (a) initiation of flagging in a random interface cell, (b) flagging of the neighbouring interface cells, (c) recursive calling of the flagging function in the already flagged cells, (d) after completion of flagging of first element, initiation of flagging of second element, (e) completion of flagging of all interface cells, and (f) unique identifier given to each element based on the assigned flag.

where $\sim$ represents the corresponding non-dimensional variable and the superscript $'$ represents the derivative with respect to the non-dimensional time $\tilde{t}$,

$$\tilde{a}' = - \left(\frac{\tilde{R} + \tilde{b}}{2\tilde{a}} \right) \tilde{b}', \quad (6)$$

$$\tilde{R}' = - \left(\frac{\tilde{R} - \tilde{b}}{2\tilde{R}} \right) \tilde{b}', \quad (7)$$

$$\tilde{b}'' = \frac{2(2\tilde{R} - \tilde{b})}{(\tilde{R} + \tilde{b})} \tilde{G}'' - \frac{3}{2\tilde{R}} (\tilde{b}')^2, \quad (8)$$

Algorithm 2. Break-up module.

```

1: for all droplets do
2:   Reset  $N_t$  and  $N_f$  to 0
3:   Reset level to 1
4:   Reset all  $flag_c$  to 0
5:   Calculate the total cell count  $N_t$  (total cells containing interface)
6:   while flagged cell count  $N_f \neq$  cellcount  $N_t$  do
7:     Select a random cell  $c_r$  containing interface and  $flag_c = 0$ 
8:     function RECURSION cell  $c_r$ 
9:       Set  $flag_c = level$ 
10:       $N_f = N_f + 1$ 
11:      for all neighbour cells  $c_n$  containing interface do
12:        if  $flag_c = 0$  then
13:          RECURSION(cell  $c_n$ )
14:      if flagged cell count  $N_f \neq$  cellcount  $N_t$  then
15:         $level = level + 1$ 
16:      Prepare clusters of cells with same  $flag_c$ 
17:      Assign an unique droplet number to each cluster

```

TABLE I. Errors in pressure jump and magnitude of parasitic currents for different Laplace numbers.

La	$E(\Delta p)$	Ca
12	1.46×10^{-4}	2.05×10^{-5}
120	8.38×10^{-6}	1.27×10^{-5}
1 200	3.53×10^{-5}	1.65×10^{-5}
12 000	4.24×10^{-3}	1.53×10^{-5}

TABLE II. Literature values for the magnitude of parasitic currents.

Literature	La	Ca
de Sousa <i>et al.</i> ²⁷	250	$O(10^{-4})$
Singh and Shyy ²⁸	250–12 000	$O(10^{-4})$
Dijkhuizen <i>et al.</i> ¹¹	1–10 000	$O(10^{-5})$
Current work	120–12 000	$O(10^{-5})$

FIG. 7. Evolution of the interface in a 3D vortical field.

FIG. 8. Grace diagram²⁶ indicating the bubble rise simulations done in this study. From Clift *et al.*, *Bubbles, Drops and Particles*. Copyright 1978 Academic Press. Reproduced with permission from Academic Press.

where the superscript '' represents the second derivative with respect to the non-dimensional time $\tilde{t}$,

$$\tilde{h}' = -\frac{4Re_l\tilde{h}^3}{9\lambda\tilde{a}^4} \left(\tilde{G}'' + \tilde{A}_H \frac{\tilde{a}^2}{\tilde{h}^3} \right) \Delta(Kn) - 2\tilde{\kappa}\tilde{h}, \quad (9)$$

where $Re_l = 2\rho_l R_0 V_0 / \mu_l$ is the droplet Reynolds number, $\lambda = \mu_g / \mu_l$ is the gas to liquid viscosity ratio, $\tilde{A}_H = A_H / 8\pi\rho_l V_0^2 R_0^3$ is the non-dimensional Hamaker constant, $\Delta(Kn)$ is a non-dimensional function³ of the Knudsen number $Kn = \lambda_g / h$ with λ_g the mean free path of gas molecules, $\tilde{\kappa} = \tilde{a}' / \tilde{a}$ is the radial strain rate of the disk-shaped interface, and $\tilde{G}$ is the

non-dimensional distance between the center of mass C_m and the flattened disk in Fig. 4.

In Eqs. (8) and (9), $\tilde{G}''$ is given by

$$\tilde{G}'' = -\frac{36}{Re_l^3} \frac{\tilde{\Phi}_l}{\tilde{b}'} \frac{(2\tilde{R} - \tilde{b})}{(\tilde{R} + \tilde{b})} - \frac{24}{We} \frac{\tilde{R}'}{\tilde{b}'} (2\tilde{R} - \tilde{b}), \quad (10)$$

where $We = 8\rho_l V_0^2 R_0 / \sigma$ is the Weber number and $\tilde{\Phi}_l$ is the viscous dissipation rate inside the droplet. The viscous dissipation rate is given by

$$\begin{aligned} \tilde{\Phi}_l = & \left(\frac{21}{48} \tilde{R} \tilde{\eta}^2 - \frac{1}{24} \tilde{R}^2 \tilde{\eta}^3 + \frac{21}{96} \tilde{\eta} \right) e^{-2\tilde{\eta}(\tilde{R} + \tilde{b})} \\ & + \frac{1}{48} (\tilde{R}^2 - \tilde{b}^2)^2 \tilde{\eta}^5 + \frac{1}{24} (\tilde{R}^2 - \tilde{b}^2) \tilde{b} \tilde{\eta}^4 \\ & + \frac{1}{48} (23\tilde{R}^2 - 21\tilde{b}^2) \tilde{\eta}^3 + \frac{21}{48} \tilde{b} \tilde{\eta}^2 - \frac{21}{96} \tilde{\eta}, \end{aligned} \quad (11)$$

where $\tilde{\eta} = 1.503 (Re_l |\tilde{\kappa}| / 2)^{1/2}$.

Equations (5)–(9) are integrated in time using the ODE solver of the GNU Scientific Library (GSL) with the following initial conditions:

$$\tilde{h}(0) = \tilde{h}_d \exp(-\delta \tilde{h}_d^{3/2} / \lambda), \quad (12)$$

$$\tilde{a}(0) = [\tilde{h}(0)]^{1/2}, \quad (13)$$

$$\tilde{b}(0) = [1 - \tilde{a}^2(0)]^{1/2}, \quad (14)$$

$$\tilde{b}'(0) = -1, \quad (15)$$

$$\tilde{R}(0) = 1, \quad (16)$$

where $\tilde{h}_d = (3Ca/2)^{1/2}$ is the film thickness at the initial contact of the droplets with $Ca = \mu_g V_0 / \sigma$ the capillary number, and δ is an empirical coefficient. This empirical coefficient influences the initial film thickness and is given by $\delta = (10\mu_l / \sigma)^{-1.6}$.³ For tetradecane droplets in air, δ turns out to be 1.42. However, the collision outcome is sensitive to this empirical constant and to obtain an exact match with the experimentally observed collision outcome, and $\delta = 1.837$ was used in Ref. 4. Using $\delta = 1.837$, the evolution of film thickness $\tilde{h}$ in time $\tilde{t}$ for collisions of tetradecane droplets in air at various initial Weber numbers is shown in Fig. 5. It can be seen that the transition from coalescence to bouncing occurs at $We = 2.3$, whereas the transition from bouncing to coalescence occurs

TABLE III. Comparison of simulated Reynolds number Re_C to the experimental results Re_G obtained from the Grace diagram.²⁶

Case	BubbleRegime	M	Eo	Re_G	Re_C
A	Spherical	1.26×10^{-3}	1.0	1.7	1.7
B	Ellipsoidal	9.71×10^{-4}	1.0×10^1	2.2×10^1	2.3×10^1
C	Skirted	9.71×10^{-1}	9.71×10^1	2.0×10^1	1.8×10^1
D	Intermediate spherical cap + wobbling	9.71×10^{-12}	9.71	2.6×10^3	2.8×10^3
E	Wobbling	1.0×10^{-12}	1.94	2.0×10^3	2.2×10^3
F	Dimpled ellipsoidal cap	1.0×10^3	9.71×10^1	1.5	1.6
G	Intermediate skirted + ellipsoidal	9.71×10^{-4}	3.88×10^1	6.0×10^1	5.8×10^1
H	Intermediate ellipsoidal + wobbling	9.71×10^{-8}	1.0×10^1	2.6×10^2	2.9×10^2

FIG. 9. Snapshots of bubble shapes for the bubble regimes indicated in Table III.

at $We = 12.3$. These agree with the experimentally observed regime boundaries.²⁵

2. Numerical implementation

After the droplets are advected, each droplet pair is checked for collision. If the droplets are in “contact” (i.e., when they share a common reconstruction cell), they are added to the collision list and the film drainage time is calculated using the film drainage model. The exact instant of “contact” is expected to be of less importance, as the film drains very fast initially compared to the later stage of drainage.⁴ Using the calculated drainage time, the time of coalescence of droplets (if the prediction is coalescence) is estimated by $t_{coalescence} = t_{contact} + t_{drainage}$. If the prediction is bouncing, then the coalescence time is taken as infinity. Thus, a collision is initiated by storing the coalescence time for a colliding droplet pair. For the droplet pair in the collision list, the droplets are merged at the estimated coalescence time if they are still in “contact.” All these steps are handled by the coalescence module explained in Algorithm 1.

Since the mesh information of each droplet is stored with a unique identifier, the coalescence module combines the data structures of two droplets and assigns the identifier of any one of these droplets. The other identifier is added to the free identifier list, which can be used if new droplets are created in the future. After the data structures have been merged, the physical merging of the interface meshes is performed by LFRM.

B. Break-up module

The break-up of a droplet into daughter droplets can be caused by the interaction of the flow with a droplet or by the coalescence events between droplets [for example, regimes (IV) and (V) in Fig. 2]. In the current study, no physical break-up model is implemented and the break-up of the droplet is numerical in nature based on the size of the reconstruction grid. It is expected that numerical break-up will not have a critical impact on the collision dynamics,⁴ as the neck formation prior to break-up is very fast (compared to the film drainage process).

Upon break-up, the physical separation of the interface meshes is performed by LFRM, but the mesh information of all the daughter droplets would be stored with the identifier of the parent droplet if no precautions were taken. This could cause numerical coalescence between droplets if they collide subsequently. Thus, it is important to separate the data structure of the daughter droplets and assign each daughter droplet a unique identifier to avoid numerical coalescence. The break-up module is used to find the disjoint droplets that are subsequently assigned a new “droplet-number.” This is achieved by using a recursive flagging algorithm; see Fig. 6. The details of the break-up module are provided in Algorithm 2.

IV. RESULTS AND DISCUSSION

As a first step, we verify the implementation of LFRM using two standard tests. These tests are (1) the stationary bubble test to verify implementation of the surface tension model and (2) the standard advection test to verify the implementation of the interface advection and reconstruction procedure. Subsequently, the current implementation is validated by comparing computed shapes and velocities of gas bubbles rising in quiescent viscous liquids with experimental data summarized in the Grace diagram.²⁶ In Sec. IV C, the simulation results of binary droplet collisions using the extended LFRM method are compared to experiments and other simulation results. The evolution of energy during these simulations is discussed to obtain further insight into the observed results. The section ends with a discussion about the influence of the film drainage model and grid size on the simulated collision dynamics.

A. Verification

1. Stationary bubble test

In this test, the simulation of a 3D spherical bubble is carried out in zero gravity. The exact pressure jump across the interface for such a bubble (with radius R) is calculated from the Young-Laplace equation,

$$\Delta p_{exact} = \sigma \kappa = \frac{2\sigma}{R}. \quad (17)$$

In an ideal case, the curvature will be uniform across the whole bubble and the surface tension force will exactly balance the pressure gradient across the interface resulting in a zero velocity field. However, the error in the curvature calculation and/or the mismatch of the pressure gradient and surface tension forces at the discrete level will give rise to unphysical fluid motions, termed parasitic currents. Thus, the accuracy of the surface tension calculation is quantified in terms of the error in the calculated pressure jump with respect to the analytical pressure jump and of the magnitude of the parasitic currents.

The magnitude of the parasitic currents is expressed in terms of the capillary number $Ca = (\mu_1 u_{\max})/\sigma$. The error in the pressure jump, Δp , can be calculated as

$$E(\Delta p) = \frac{|\Delta p - \Delta p_{exact}|}{\Delta p_{exact}}, \quad (18)$$

The pressure jump is calculated using the average pressures in the bubble and in the fluid. The simulations are carried out for different Laplace numbers $La = \rho \sigma D/\mu^2$. The grid size is selected such that there are 20 grid cells across the bubble diameter similar to de Sousa *et al.*²⁷ and Dijkhuizen *et al.*¹¹ The simulations are run for time $t = T_\mu$, where $T_\mu = \rho D^2/\mu$ is the viscous dissipation timescale, whereas the interface is

reconstructed every 100 time steps. The calculated errors in Δp and Ca are summarized in Table I. Table II shows that the parasitic currents are comparable to the results obtained using the 3D front tracking class of methods available in the literature.

2. Standard advection test

In this test, an initially spherical interface is stretched by a 3D rotational flow field.¹⁰ This velocity field is given by

$$\mathbf{u}(\mathbf{x}, t) = \begin{bmatrix} 2 \sin^2(\pi x) \sin(2\pi y) \sin(2\pi z) \cos(\pi \frac{t}{T}) \\ -\sin^2(\pi y) \sin(2\pi x) \sin(2\pi z) \cos(\pi \frac{t}{T}) \\ -\sin^2(\pi z) \sin(2\pi y) \sin(2\pi x) \cos(\pi \frac{t}{T}) \end{bmatrix}, \quad (19)$$

where T is the period of velocity variation. A sphere of radius 0.15 is placed at (0.35, 0.35, 0.35) in a unit domain and a period T of 3 s is chosen. The sphere will deform in time from $t = 0$ to $T/2$ and will ideally return to the original position and shape in time from $t = T/2$ to T . But in practice, a deviation in geometry and volume will develop on the final state of the sphere in comparison to the original state. These errors can be quantified in terms of mass error, E_m , and geometrical error, E_g , as follows:

$$E_m = \frac{|\sum_{i,j,k} \phi_{i,j,k}^{initial} - \sum_{i,j,k} \phi_{i,j,k}^{final}|}{\sum_{i,j,k} \phi_{i,j,k}^{initial}}, \quad (20)$$

FIG. 10. Merging collision sequence in regime (I). LFRM results from the present study, CLSVOF from Ref. 4, and FT and experimental results from Ref. 25. Conditions: tetradecane in 1 atm air, $R_0 = 107.2 \mu\text{m}$, $We = 2.3$, and $B = 0$. The film drainage time observed in experiments is $t_d = 0.270$ ms. The time sequence for the LFRM results is the same as for the experimental results.

FIG. 13. Near head-on separating collision sequence in regime (IV). LFRM results from the present study, CLSVOF from Ref. 4, and experimental results from Ref. 31. Conditions: tetradecane in 1 atm nitrogen, $R_0 = 168 \mu\text{m}$, $We = 62.2$, and $B = 0.06$. The film drainage time is assumed to be zero.

$$E_g = \frac{\sum_{i,j,k} |\phi_{i,j,k}^{\text{initial}} - \phi_{i,j,k}^{\text{final}}|}{\sum_{i,j,k} \phi_{i,j,k}^{\text{initial}}}, \quad (21)$$

where $\phi_{i,j,k}$ is the phase fraction in cell (i, j, k).

The grid size is taken to be 30 cells across the diameter such that the sheared drop does not fragment during stretching. The evolution of interface shape is shown in Fig. 7. The geometrical and mass errors calculated at $t = T$ are 9.87×10^{-5} and 4.11×10^{-5} , respectively.

(a)

(b)

FIG. 14. Energy budget and VDR evolution for the droplet collision in regime (I), Fig. 10.

B. Validation

A spherical gas bubble released in a liquid will attain a terminal velocity and a characteristic shape (after a small time interval from its release) based on the physical properties of gas and liquid and on the bubble diameter. Grace condensed a large body of experimental data into the “Grace diagram,”²⁶ which enables the prediction of shape and terminal rise velocity, Reynolds number (Re) using the dimensionless size, Eötvös number (Eu), and the dimensionless fluid properties, Morton number (M). These non-dimensional numbers are defined as:

- Reynolds number $Re = \frac{\rho_l u d_b}{\mu_l}$ describes the importance of inertial forces with respect to viscous forces.
- Eötvös number $Eu = \frac{g d_b^2 (\rho_l - \rho_g)}{\sigma}$ describes the importance of gravitational forces with respect to surface tension forces.
- Morton number $M = \frac{g \mu_l^4 (\rho_l - \rho_g)}{\rho_l^2 \sigma^3}$ describes the influence of liquid properties on the behaviour of a rising bubble.

where d_b is the sphere equivalent bubble diameter, u is rise velocity, and g is the gravitational acceleration.

We simulate 8 different regimes similar to van Sint Annaland *et al.*²⁹ as shown in Fig. 8. The simulations are carried out with 20 cells across the bubble diameter, whereas the

domain size is selected to amount 5 times the bubble diameter in all coordinate directions. The bubble is initially placed at (0.50, 0.50, 0.67) of the domain. A window shifting principle is applied to keep the bubble at approximately the same position from the system boundaries.³⁰ The comparison of the calculated Reynolds numbers and those obtained from the Grace diagram is given in Table III, whereas snapshots of the bubble shape are given in Fig. 9. From the figure and the table, it can be concluded that the computed shapes and velocities compare well with the results obtained from the Grace diagram.²⁶

C. Binary droplet collisions

1. Validation using experimental film drainage times

In the case of (near) head-on collisions between equal sized hydrocarbon droplets, four regimes of collision outcome are observed with increasing We . As seen in Fig. 2, these regimes are (I) Coalescence with minor deformation, (II) Bouncing, (III) Coalescence with major deformation, and (IV) Coalescence with separation resulting in the production of daughter droplets. To validate the modified LFRM method, a case of binary droplet collision from each of these regimes is simulated and compared with experiments^{25,31} and other simulation methods.^{4,25}

The grid cell size is selected such that 12 grid cells are taken across the droplet radius (R_0) (similar to the grid size

FIG. 15. Energy budget and VDR evolution for the droplet collision in regime (II), Fig. 11.

used in Ref. 4 for CLSVOF and Ref. 25 for FT). The computational domain has dimensions $8R_0 \times 10R_0 \times 8R_0$ with the largest dimension in the direction of the initial velocity of the droplets. Free slip boundary conditions are used on all domain boundaries. The initial distance between the droplet centers is taken as $2.8R_0$. Each droplet is initialised with a uniform velocity field, V_0 , but in the opposite direction. For each case, the Weber number and impact parameter (Fig. 1) are provided as input parameters. The film drainage time is provided by experimental observations.²⁵

The collisions in regime (I) result in a coalescence of the droplets. A collision of tetradecane droplets in 1 atm air, $R_0 = 107.2 \mu\text{m}$, $V_0 = 0.305 \text{ m/s}$, $We = 2.3$, and $B = 0$ is shown in Fig. 10. The obtained result from LFRM matches well with the results from the Coupled Level Set Volume of Fluid method,⁴ the Front Tracking method,²⁵ and experimental data.²⁵ In this regime, the coalescence occurs around the time of maximum deformation ($t = 0.391 \text{ ms}$). After the coalescence, the cusp at the merged interface is quickly flattened ($t = 0.420 \text{ ms}$). This phenomenon is nicely captured by all the numerical simulations.

A collision of tetradecane droplets in 1 atm air, $R_0 = 167.6 \mu\text{m}$, $We = 9.33$, and $B = 0$ is shown in Fig. 11. The bouncing in regime (II) obtained by LFRM agrees well with experimental data²⁵ and other simulation results with FT²⁵ and CLSVOF.⁴

Contrary to the coalescence of regime (I), the coalescence of regime (III) results in substantial deformation before merging ($t = 0.366 \text{ ms}$). A collision of tetradecane droplets in 1 atm air, $R_0 = 169.7 \mu\text{m}$, $We = 13.63$, and $B = 0$ is shown in Fig. 12. In this regime, the droplet is flattened to a disk shape, while the center of the rear face is still heading forward resulting in a dimpled shape between 0.370 and 0.500 ms. Although this is not very clear in the experimental results,²⁵ it is captured by all the numerical simulations.

The near head-on collisions in regime (IV) result in the separation of the droplets after merging as the kinetic energy is sufficient to overcome the surface energy. Because of the high We , a film drainage time of zero is used. The collision of tetradecane droplets in 1 atm nitrogen, $R_0 = 168 \mu\text{m}$, $We = 62.2$, and $B = 0.06$ is shown in Fig. 13. The different colours of the droplets indicate that each droplet has a different droplet number and a separate data structure.

The results obtained using LFRM show a better match with the experimental results³¹ compared to the CLSVOF method.⁴ In Fig. 13, a premature separation is seen for CLSVOF ($t = 1.952 \text{ ms}$). The origin of this premature separation is the less accurate curvature estimation in strongly deformed regions⁴ (between 0.062 ms and 0.850 ms), which influences the surface tension force, and (over time) the droplet shape. Thus, the results indicate a more accurate surface

FIG. 16. Energy budget and VDR evolution for the droplet collision in regime (III), Fig. 12.

FIG. 17. Energy budget and VDR evolution for the droplet collision in regime (VI), Fig. 13.

tension calculation for the same grid size for LFRM. This is expected because in the hybrid surface tension model used in this study, the curvature is calculated directly from the unstructured mesh. Thus, the curvature calculation is more accurate in LFRM than in CLSVOF, especially on coarse grids. In addition, the size of the satellite droplet ($t = 2.89$ ms) resembles the experimental data better compared to the CLSVOF results.

2. Evolution of energy

In this section, the evolution of the different contributions to the energy for different collision cases presented in Sec. IV C 1 is analyzed. Since the energy conservation equation is not solved in the simulation, the contributions to the energy are evaluated through the velocity fields and the droplet surface geometry. The total energy consists of kinetic and surface energy before collision and in addition to this dissipated energy after collision. These are evaluated as follows:

- Surface energy: It is calculated for each bubble as

$$E_s = \sigma A_b, \quad (22)$$

where σ is surface tension coefficient and A_b is surface area of the droplet.

- Kinetic energy: It is calculated by summing kinetic energies over all grid cells. Kinetic energy in a given cell is given by

$$E_k = \sum_{i,j,k} E_{k,i,j,k} = \sum_{i,j,k} \frac{1}{2} (mv^2)_{i,j,k}. \quad (23)$$

- Dissipated energy: The dissipation function ϕ measures the local volumetric viscous dissipation rate and is calculated by

$$\phi = \mu \left[2 \left(\frac{\partial u_i}{\partial i} \right)^2 + \left(\frac{\partial u_i}{\partial j} + \frac{\partial u_j}{\partial i} \right)^2 \right], \quad (24)$$

where μ is the dynamic viscosity and velocity gradients are represented in Einstein notation. The dissipation function is calculated in each cell using second order central finite difference approximations. The volume integral of ϕ gives the viscous dissipation rate (VDR). The time integral of the VDR gives the total amount of dissipated energy,

$$E_\phi = \int_0^t \int_0^V \phi dV dt = \int_0^t VDR dt. \quad (25)$$

TABLE IV. Comparison of calculated drainage time with experimental data.

We	$t_{d,calc}$ (ms)	$t_{d,exp}$ (ms)
2.3	0.340	0.270
13.63	0.416	0.246

The calculated energies in the plots are normalized by the initial total energy, and the VDR is normalized by the maximum VDR value obtained during the course of the collision.

Figure 14 shows the evolution of the contributions to the energy for the collision in regime (I). It can be seen that from the instant of contact, the kinetic energy is converted into dissipated and surface energy. The surface energy is maximum just before the rupture, indicating that the rupture occurs just after the maximum deformation is achieved. The rupture also

leads to a spike in the VDR, because of the perturbation in the local flow field due to the sudden coalescence of the interfaces. The coalesced droplet undergoes oscillations leading to further dissipation losses.

In addition, the figure shows an abrupt reduction of the total energy which corresponds to a similar change in surface energy indicating that the energy reduction is caused by a sudden change in the interfacial area. Similar sharp jumps in total and surface energy are observed for merging sequences in the literature (Refs. 25 and 12), suggesting that the modeled

FIG. 18. Merging collision sequences [in regime (I)] for different drainage times. The far left column corresponds to an immediate (numerical) coalescence, the middle column is to the experimentally observed outcome, and the far right column shows droplet bouncing. Conditions: tetradecane in 1 atm air, $R = 107.2 \mu\text{m}$, $V_0 = 0.305 \text{ m/s}$, $We = 2.3$, and $B = 0$.

process is an approximation of the reality. The actual rupture commences in a small area, leading to an extremely rapid motion of the surrounding film due to high surface tension pull forces. This leads to further rupture and, at times, creation of very small droplets. In the current approach, these rapid small scale processes are entirely ignored. As a consequence, the true dissipation rate at this instant is not computed well. Although the spike is seen, the true spike will be much higher.

However, we observe that both before and after the merger, the total energy is well conserved.

The evolution of the energy contributions in regime (II) is shown in Fig. 15. At maximum deformation, the surface energy is at a maximum and the kinetic energy is at a minimum. After this instant, the surface energy goes back to its initial value, but the kinetic energy is reduced due to viscous dissipation. The evolution of the VDR

FIG. 19. Merging collision sequences [in regime (III)] for different drainage times. The far left column corresponds to an immediate (numerical) coalescence, the middle column is to the experimentally observed outcome, and the far right column shows droplet bouncing. Conditions: tetradecane in 1 atm air, $R_0 = 169.7 \mu\text{m}$, $We = 13.63$, and $B = 0$.

indicates that dissipation increases rapidly at the instant of contact.

The qualitative behaviour of energy evolution in regime (III), Fig. 16, is the same as that in regime (I), Fig. 14. However, as the initial velocity of the droplets is high, the merging occurs faster and dissipation losses are also higher. In addition, a second spike in the VDR is obtained due to the oscillation of the merged droplet.

In regime (IV), Fig. 17, coalescence of the droplets is instantaneous upon contact (i.e., numerical coalescence). Thus, the reduction in the total energy is not as significant as in regimes (I) and (III). The first spike in the VDR is due to merging. After merging, the droplet reaches a state of maximum deformation (torus shape). This results in a reflexive

action which converts surface energy back to kinetic energy and also dissipation energy (second spike in VDR). After the second spike in the kinetic energy, the droplet starts stretching again but in the longitudinal direction leading to a break-up into three droplets. Such separation is called reflexive separation. Unlike merging, there is no significant change in the surface energy of the system upon break-up of the droplet.

3. Effect of film drainage time on collision dynamics

In Sec. IV C 1, simulations of droplet collisions in coalescence regimes (I) and (III) were performed using experimental film drainage times. As explained before, film drainage times can also be calculated using the film drainage model of Zhang and Law.³ Table IV shows that the model is able to predict the

FIG. 20. Merging collision sequences [in regime (III)] for grid resolutions. Conditions: tetradecane in 1 atm air, $R = 169.7 \mu\text{m}$, $V_0 = 0.591 \text{ m/s}$, $We = 13.63$, and $B = 0$.

film drainage time in the correct order of magnitude, but still a deviation is found with respect to the experimental values. To find the effect of the drainage time, the collision of tetradecane droplets in air [cases of regimes (I) and (III)] is simulated with different values of the film drainage time.

The simulation results of regime (I) for different drainage times are presented in Fig. 18. The results from left to right correspond to the drainage time $t_d = 0$ (numerical coalescence), $t_d = 0.235$ ms, $t_d = 0.270$ ms (experimentally observed drainage time), $t_d = 0.340$ ms (predicted by film drainage model for $\delta = 1.8327$), and $t_d > t_c$ (bouncing droplets). When the droplets coalesce before the instant of maximum deformation, the droplets first flatten and then elongate in the direction of initial velocity. In contrast, the flattening is not observed when the coalescence occurs after maximum deformation. The inclusion of the film drainage model will avoid this; however, a lag in the evolution of topology is observed due to the delayed coalescence. Finally, when the film drainage time is larger than the contact time, the droplets bounce.

Similarly, the simulation results of regime (III) for different drainage times are presented in Fig. 19. The results from left to right correspond to drainage time $t_d = 0$ (numerical coalescence), $t_d = 0.200$ ms, $t_d = 0.246$ ms (experimentally observed drainage time), $t_d = 0.416$ ms (predicted by film drainage model for $\delta = 1.8327$), and $t_d > t_c$ (bouncing droplets). It can be seen that an early coalescence will lead to substantial stretching and might end up in break-up. Again, this is not observed in the results obtained by the inclusion of the film drainage model. Similar to the results in regime (I), a lag in the evolution of topology is observed due to the delayed coalescence. Thus, it can be concluded that the prediction of the film drainage time is crucial for an accurate simulation of collision dynamics. Clearly, further theoretical developments of the film drainage model are required.

4. Effect of grid dependency on collision dynamics

The contact timer is initiated when the droplets share a common grid cell, and thus, the moment of coalescence will be influenced by the grid size. This effect is investigated by simulating droplet collision with fixed drainage time but varying grid size. The results are shown in Fig. 20. It can be seen that the rupture of the film is delayed for finer grid size $D/h = 32$, although this small delay does not seem to have a significant influence on the further developments. In addition, it can be seen that the delay is not significant in the case of $D/h = 16$ and $D/h = 24$. This is because the film drainage is faster initially and then tends to be slower in later stages. However, when coupled with the film drainage model, the Weber number (which is calculated at contact of the droplets) will vary with the instance of contact and this will also influence the calculated film drainage time.

V. CONCLUSION

We have implemented a hybrid front tracking method without connectivity, the Local Front Reconstruction Method (LFRM).¹⁰ This method can easily handle complex topological changes like droplet break-up. However, the original method

applies numerical coalescence of droplets. In our implementation, this is prevented by storing the information about marker elements and marker points for each droplet separately. We have incorporated an efficient and exact geometric method to calculate the phase fraction. Also, we have implemented a smoothing procedure to enhance the mesh quality.

A controlled coalescence between droplets is accomplished by merging data structures of two droplets at the prescribed film drainage time after contact is initiated. Similarly, the break-up of a droplet is achieved by splitting the data structure of the droplet. The framework of these coalescence and break-up modules is kept generic such that any film drainage model can be easily incorporated. In this study, we have chosen the film drainage model of Zhang and Law.³

The implementation of LFRM is verified with standard tests, i.e., the stationary bubble test and the standard advection test, and validated with the experimental data obtained from the Grace diagram²⁶ for rising bubbles. The extended LFRM is validated by carrying out simulations of the (near) head-on collision of two equal tetradecane droplets at different Weber numbers corresponding to different collision regimes using the experimental drainage time. The results show a better agreement with experimental data compared to other methods,^{4,25} especially at high impact velocities. It also turned out that if the correct film drainage time is available, then LFRM can simulate droplet collisions with physical realism. The energy evolution during these collisions is calculated to get further insight into the collision dynamics.

The influence of the film drainage time on the collision dynamics is studied by carrying out simulations of a specific collision using several film drainage times. The results show the dependency of collision dynamics on film drainage time. The model of Zhang and Law³ gives correct collision outcomes, but quantitative predictions of film drainage time are not accurate enough and show strong dependency on the empirical parameter δ . Therefore, a better subgrid model for the film drainage is required. Finally, the effect of grid dependency on collision dynamics is investigated. The results show that the grid dependent contact instant has only a minor influence on the collision dynamics and that this aspect is less important than the accuracy of the film drainage model. However, the LFRM coupled with film drainage model is much better in predicting the collision dynamics than any traditional method (without a coalescence model).

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¹C. Crowe, M. Sommerfeld, and Y. Tsuji, *Multiphase Flows With Droplets and Particles* (CRC Press, Boca Raton, 1998).

²L. Mason, G. Stevens, and D. Harvie, "Multi-scale volume of fluid modelling of droplet coalescence," in *Ninth International Conference on CFD in the Minerals and Process Industries* (CSIRO, Melbourne, Australia, 2012).

³P. Zhang and C. K. Law, "An analysis of head-on droplet collision with large deformation in gaseous medium," *Phys. Fluids* **23**, 042102 (2011).

- ⁴M. Kwakkel, W.-P. Breugem, and B. J. Boersma, "Extension of a CLSVOF method for droplet-laden flows with a coalescence/breakup model," *J. Comput. Phys.* **253**, 166–188 (2013).
- ⁵G. Tryggvason, R. Scardovelli, and S. Zaleski, *Direct Numerical Simulations of Gas-Liquid Multiphase Flows* (Cambridge University Press, Cambridge, 2011).
- ⁶M. van Sint Annaland, N. Deen, and J. Kuipers, "Numerical simulation of gas bubbles behaviour using a three-dimensional volume of fluid method," *Chem. Eng. Sci.* **60**, 2999–3011 (2005).
- ⁷J. A. Sethian and P. Smereka, "Level set methods for fluid interfaces," *Annu. Rev. Fluid Mech.* **35**, 341–372 (2003).
- ⁸S. van der Pijl, A. Segal, C. Vuik, and P. Wesseling, "A mass-conserving level-set method for modelling of multi-phase flows," *Int. J. Numer. Methods Fluids* **47**, 339–361 (2005).
- ⁹N. Nikolopoulos, K.-S. Nikas, and G. Bergeles, "A numerical investigation of central binary collision of droplets," *Comput. Fluids* **38**, 1191–1202 (2009).
- ¹⁰S. Shin, I. Yoon, and D. Juric, "The local front reconstruction method for direct simulation of two- and three-dimensional multiphase flows," *J. Comput. Phys.* **230**, 6605–6646 (2011).
- ¹¹W. Dijkhuizen, I. Roghair, M. V. S. Annaland, and J. Kuipers, "DNS of gas bubbles behaviour using an improved 3D front tracking model—Model development," *Chem. Eng. Sci.* **65**, 1427–1437 (2010).
- ¹²M. R. Nobari, Y. J. Jan, and G. Tryggvason, "Head-on collision of drops—A numerical investigation," *Phys. Fluids* **8**, 29–42 (1996).
- ¹³Y. Liao and D. Lucas, "A literature review on mechanisms and models for the coalescence process of fluid particles," *Chem. Eng. Sci.* **65**, 2851–2864 (2010).
- ¹⁴W. Howarth, "Coalescence of drops in a turbulent flow field," *Chem. Eng. Sci.* **19**, 33–38 (1964).
- ¹⁵Y. Pan and K. Suga, "Numerical simulation of binary liquid droplet collision," *Phys. Fluids* **17**, 082105 (2005).
- ¹⁶N. Nikolopoulos, A. Theodorakakos, and G. Bergeles, "Off-centre binary collision of droplets: A numerical investigation," *Int. J. Heat Mass Transfer* **52**, 4160–4174 (2009).
- ¹⁷A. Chesters, "The applicability of dynamic-similarity criteria to isothermal, liquid-gas, two-phase flows without mass transfer," *Int. J. Multiphase Flow* **2**, 191–212 (1975).
- ¹⁸S. Shin, S. I. Abdel-Khalik, V. Daru, and D. Juric, "Accurate representation of surface tension using the level contour reconstruction method," *J. Comput. Phys.* **203**, 493–516 (2005).
- ¹⁹J. U. Brackbill, D. B. Kothe, and C. Zemach, "A continuum method for modeling surface tension," *J. Comput. Phys.* **100**, 335–354 (1992).
- ²⁰S. Das, N. G. Deen, and J. A. M. Kuipers, "Immersed boundary method (ibm) based direct numerical simulation of open-cell solid foams: Hydrodynamics," *AIChE J.* **63**, 1152–1173 (2017).
- ²¹J. Centrella and J. R. Wilson, "Planar numerical cosmology. II—The difference equations and numerical tests," *Astrophys. J., Suppl. Ser.* **54**, 229–249 (1984).
- ²²E. Aulisa, S. Manservigi, and R. Scardovelli, "A mixed markers and volume-of-fluid method for the reconstruction and advection of interfaces in two-phase and free-boundary flows," *J. Comput. Phys.* **188**, 611–639 (2003).
- ²³A. Kuprat, A. Khamayseh, D. George, and L. Larkey, "Volume conserving smoothing for piecewise linear curves, surfaces, and triple lines," *J. Comput. Phys.* **172**, 99–118 (2001).
- ²⁴I. Roghair, M. V. S. Annaland, and J. Kuipers, "An improved front-tracking technique for the simulation of mass transfer in dense bubbly flows," *Chem. Eng. Sci.* **152**, 351–369 (2016).
- ²⁵K.-L. Pan, C. K. Law, and B. Zhou, "Experimental and mechanistic description of merging and bouncing in head-on binary droplet collision," *J. Appl. Phys.* **103**, 064901 (2008).
- ²⁶R. Clift, J. Grace, and M. Weber, in *Bubbles, Drops and Particles*, edited by Dover Edition (Academic Press, New York, 1978).
- ²⁷F. de Sousa, N. Mangiavacchi, L. Nonato, A. Castelo, M. Tomé, V. Ferreira, J. Cuminato, and S. McKee, "A front-tracking/front-capturing method for the simulation of 3D multi-fluid flows with free surfaces," *J. Comput. Phys.* **198**, 469–499 (2004).
- ²⁸R. Singh and W. Shyy, "Three-dimensional adaptive Cartesian grid method with conservative interface restructuring and reconstruction," *J. Comput. Phys.* **224**, 150–167 (2007), special Issue Dedicated to Professor Piet Wesseling on the occasion of his retirement from Delft University of Technology.
- ²⁹M. van Sint Annaland, W. Dijkhuizen, N. Deen, and J. Kuipers, "Numerical simulation of behavior of gas bubbles using a 3-D front-tracking method," *AIChE J.* **52**, 99–110 (2005).
- ³⁰M. Baltussen, J. Kuipers, and N. Deen, "A critical comparison of surface tension models for the volume of fluid method," *Chem. Eng. Sci.* **109**, 65–74 (2014).
- ³¹J. Qian and C. Law, "Regimes of coalescence and separation in droplet collision," *J. Fluid Mech.* **331**, 59–80 (1997).