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# 1 **Analysis and prediction of the gas-liquid interfacial area for** 2 **droplets impact on solid surfaces**

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## 13 **Highlights**

- 14 • The interfacial areas of droplets during impact on solid surfaces are analysed.
- 15 • A new correlation for predicting the maximum gas-liquid interfacial area is proposed.
- 16 • The dynamic contact angle with local grid refinement is implemented in the CFD model.
- 17 • The impact of droplets on both hydrophobic and hydrophilic surfaces are studied.
- 18 • The inner flow field of droplets during impact onto a solid surface is described.

19

## 20 **Abstract**

21 A better understanding of the variation of the gas-liquid interfacial area during droplets impact on  
22 solid surfaces in detail is extremely important for process intensification since this can lead to a much-  
23 increased efficiency of the heat and mass transfer. At present, experimental observation is the most  
24 popular method to investigate the droplet behaviours during the impact of the droplet. However, it is  
25 difficult to measure the interfacial areas and observe the transient inner flow field in the droplet. The  
26 CFD with VOF model is a powerful and efficient tool for investigating the visual dynamic behaviours,  
27 interfacial areas and the detailed inner flow field of droplets. Therefore, effective and efficient CFD

28 models are established to investigate the droplet impact onto solid surfaces through using the VOF  
29 model with dynamic contact angle and local grid refinement techniques. The CFD predictions of the  
30 dynamic behaviours of the droplets are in reasonable agreement with experimental data over a wide  
31 range of surface and liquid properties. The simulation results showed that the gas-liquid interfacial area  
32 decreases slightly at the kinematic stage, then increases at the spreading stage, and reaches its maximum  
33 at the end of the spreading stage. The hydrophilic surface promotes the increase of gas-liquid interfacial  
34 area through releasing the liquid-solid interface energy, while the hydrophobic surface promotes the  
35 increase of the gas-liquid interfacial area by promoting droplet breakup. Finally, the energy conversion  
36 of the droplet impact on the solid surface is analysed, and a new correlation for predicting the maximum  
37 gas-liquid interfacial area of the droplet is proposed.

## 38 **Keywords**

39 Drop impact; Interfacial area; Dynamic contact angle; Dynamic local grid refinement; Process  
40 intensification

41

## 42 **1. Introduction**

43 Droplet impact onto solid surfaces is a popular phenomenon in many industrial processes, including  
44 rapid spray cooling of hot surfaces [1-3], spray and jet reactors [4, 5], fuel injection and combustion [6,  
45 7], metal soldering and additive manufacturing [8, 9], etc. In these applications, the interphase heat and  
46 mass transfer occur through the corresponding phase interface; therefore, increasing the interfacial area  
47 is an effective way to enhance the interphase heat and mass transfer. In the process of a droplet normal  
48 impact on a solid surface, the increase of gas-liquid interfacial area is mainly realized by two modes: (i)  
49 Extend the surface of a droplet by the large deformation of the droplet. This is because the surface area  
50 of a sphere is the smallest for the same volume liquid, as it changes from a sphere to another shape, the  
51 interface area increases; (ii) Extend the surface of a droplet by droplet breakup. The specific surface area  
52 of a spherical droplet is  $6/D$ , where  $D$  is the diameter of the droplet, therefore, a big droplet breakup into  
53 small droplets can increase the specific surface area of the droplet. Accurate prediction and control of  
54 the interfacial area of droplets are crucial for optimizing the relevant industrial processes. At present,

55 the impact behaviour of droplets on solid surfaces has been extensively studied, as discussed in several  
56 reviews [10-13]. Among the investigations, the spreading dynamics and the splashing dynamics of  
57 droplets are two important aspects. For the spreading of droplets, many efforts have been made to  
58 understand the changes in droplet diameter and predict the maximum spreading diameter of droplets. A  
59 series of experiments have been designed for observing and measuring the dynamic behaviours of  
60 droplets with different substrates [14-16]. However, very few studies have focused on the change in the  
61 area of the gas-liquid interface when the droplet impacts on a solid surface, mainly because it is difficult  
62 to measure accurately.

63 As a supplement to the experimental techniques, CFD technology has the potential to obtain more  
64 detailed information on the behaviour of droplets. Different numerical schemes have been developed to  
65 track or capture the gas-liquid interface, such as level set methods, volume of fluid (VOF) methods,  
66 front tracking methods, and phase-field methods, etc. Since the VOF model is naturally volume-  
67 conserved, it has been popular for investigating the droplet impact dynamics [17-26]. When simulating  
68 a droplet hitting a surface, the proper treatment of the moving three-phase (gas-liquid-solid) contact line  
69 is very important for improving the simulation accuracy, and it is usually modelled by imposing a  
70 contact angle. Since we are interested in the macroscopic motion of droplets, it is efficient to resolve  
71 only this part of the flow through embedding an apparent contact angle model [27, 28]. The simplest  
72 apparent dynamic contact angle model is the advancing–receding contact angle model, where the fixed  
73 static advancing or receding contact angle is set to a boundary condition when the contact line spreads  
74 or recoils [29, 30]. Further, several empirical formulas of the apparent dynamic contact angle as a  
75 function of the contact line velocity and the prescribed static or dynamic contact angle have been  
76 proposed [24, 31-34]. Among them, the Kistler model [32] is easy to be implement and it has shown the  
77 ability to reproduce the experimental results accurately. In addition, Malgarinos et al. [35] implemented  
78 a wetting force model [36] in VOF simulations, which can overcome the need of a pre-defined dynamic  
79 contact angle law for the cases of low Weber number impacts. In order to accurately predict the  
80 movement of the three-phase contact line and obtain a high-resolution gas-liquid interface, these regions  
81 need very fine grids. However, it is very expensive to use a uniform fine grid considering the required  
82 calculation time and computational resource. Thus, adaptive grid refinement technologies should be

83 used. Theodorakakos and Bergeles [37] proposed a multi-level dynamic local grid refinement method,  
84 which refines the cells that within a prescribed distance from the interface, and Malgarinos et al. [35,  
85 38] proposed and tested a new wetting force model and an interface sharpening scheme using the  
86 dynamic local refined grid. Also, Jian et al. [39] numerically investigated the droplet splashing  
87 mechanism when it impacts on a solid substrate by using a dynamic local grid refinement method.  
88 However, these researches are only performed in 2D simulations, which cannot capture the non-  
89 axisymmetrical fierce crash of droplets. Recently, Cimpeanu and Papageorgiou [40] investigated 3D  
90 high-speed droplets impact onto solid surfaces at arbitrary angles using VOF model with dynamic local  
91 grid refinement. This method allows detailed study of droplet morphology ranging from tens to hundreds  
92 of microns, which proves the power of the modelling method used. Similarly, accurately reproduce the  
93 dynamic behaviour of the droplet and track the change of the interface area through CFD simulations  
94 could be a good way to study the change of the interface area when a droplet impacts on a solid surface.

95 In addition to CFD simulations, it is more efficient to use a mathematical model to predict the  
96 maximum gas-liquid interfacial area of a droplet when it impacts on a solid surface. At present, it is  
97 estimated mainly by approximating the shape of the droplet at maximum spread. Different shape  
98 approximations have been proposed, such as cylindrical disk [14, 41-45], spherical cap [46], ring-like  
99 shape [47], harmonic average of a spherical cap and a cylindrical disk [48], rim-lamella shape [49], etc.  
100 The prediction accuracy of these models depends on the similarity between the approximate shape and  
101 the real shape [49]. In addition to the shape approximation methods, the maximum gas-liquid interfacial  
102 area can be obtained through energy conservation analysis. The accuracy of this method depends on the  
103 calculation of each energy component during droplet impact, especially the prediction of the energy  
104 dissipation. It is worth mentioning that both of the two methods require the maximum spread factor of  
105 the droplet, and different correlations have been established for predicting the maximum spread factor  
106 based on different approaches, including momentum conservation [50], scaling analysis [51, 52] and  
107 energetic analysis [14, 41-45, 48, 49, 53].

108 This paper focuses on the analysis and prediction of the gas-liquid interfacial area for droplets  
109 impacting on solid surfaces through CFD simulation and energetic analysis. The structure of this paper  
110 is organised as follows: Section 2 describes the CFD modelling method of droplet hits a solid surface.

111 Both the 2D axisymmetric and 3D CFD models using the VOF method with the dynamic contact angle  
 112 model and the local grid refinement techniques have been built to accurately capture the gas-liquid  
 113 interface and the moving contact line. In Section 3, the spread factor, interfacial area and inner flow  
 114 field of droplets in different impinging regimes with different liquid properties and surface properties  
 115 are analysed and discussed. Then, in Section 4, a correlation for predicting the maximum gas-liquid  
 116 interfacial area of a droplet is proposed based on the energetic analysis. Finally, conclusions are  
 117 presented in Section 5.

## 118 2. CFD simulation

### 119 2.1. The governing equations

120 In order to track the interface accurately, the VOF model proposed by Hirt and Nichols [54] is used.  
 121 Both the gas and liquid phases are assumed to be incompressible, then the conservation equations for  
 122 mass and momentum and the transport equation for the volume fraction are as follows:

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

$$\frac{\partial}{\partial t}(\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \nabla \cdot \left[ \mu \left( \nabla \vec{u} + \nabla \vec{u}^T \right) \right] + \rho \vec{g} + f_{vol} \quad (2)$$

$$\frac{\partial \alpha_L}{\partial t} + \vec{u} \cdot \nabla \alpha_L = 0 \quad (3)$$

123 where  $\vec{g}$  is the gravitational acceleration,  $f_{vol}$  is the source term considering the effect of surface tension.

124 The fluid properties are the volume-averaged values, as follows:

$$\rho = \alpha_L \rho_L + (1 - \alpha_L) \rho_G \quad (4)$$

$$\mu = \alpha_L \mu_L + (1 - \alpha_L) \mu_G \quad (5)$$

125 Brackbill et al. [55] used the CSF model to convert the surface tension into the body force, and it is  
 126 expressed as:

$$f_{vol} = \sigma_{GL} \kappa \nabla \alpha_L \frac{1}{2} \frac{\rho}{(\rho_L + \rho_G)} \quad (6)$$

127 where  $\sigma_{GL}$  is the surface tension coefficient,  $\kappa$  is the surface curvature, and it is defined in terms of the  
 128 divergence of the unit normal:

$$\kappa = -\nabla \cdot \vec{n}, \quad \vec{n} = \frac{\nabla \alpha_L}{|\nabla \alpha_L|} \quad (7)$$

129 where  $\nabla \alpha_L$  is the gradient of the volume fraction of liquid.

130 The surface normal at the wall-adjacent cell is expressed as:

$$\vec{n} = n_w \cos \theta_d + t_w \sin \theta_d \quad (8)$$

131 where  $n_w$  and  $t_w$  are the unit vectors normal and tangential to the wall, respectively, and  $\theta_d$  is the contact  
132 angle at the wall.

133 The Kistler's dynamic contact angle model [32] and the wetting force model (WFM) [35] were  
134 employed for specifying the contact angle at the wall  $\theta_d$ . For the Kistler's model, the apparent dynamic  
135 contact angle is given as a function of the capillary number and the inverse of Hoffman's function:

$$\theta_d = f_H(Ca + f_H^{-1}(\theta_e)) \quad (9)$$

136 where  $f_H^{-1}$  is the inverse function of Hoffman's function:

$$f_H(x) = \arccos \left\{ 1 - 2 \tanh \left[ 5.16 \left( \frac{x}{1 + 1.31x^{0.99}} \right)^{0.706} \right] \right\} \quad (10)$$

137 where  $x = Ca + f_H^{-1}(\theta_e)$ , and  $Ca = \mu_L u_{cl} / \sigma_{GL}$ . Most surfaces are not smooth and are subject to the effect  
138 of contact angle hysteresis, thus the equilibrium contact angle  $\theta_e$  is replaced by either the quasi-static  
139 advancing contact angle  $\theta_{adv}$  or the quasi-static receding contact angle  $\theta_{rec}$  based on the sign of the  
140 contact line velocity vector [23].

141 The contact line velocity is calculated from the actual velocity at cells:

$$\vec{u}_{cl} = (u_{cell} \cdot n_t) \frac{n_t}{|n_t|} \quad (11)$$

142 The contact line direction is calculated by:

$$sign = \vec{u}_{cl} \cdot \vec{n} \quad (12)$$

143 If *sign* is positive, then the contact line is receding. If *sign* is negative, the contact line is advancing.

## 144 2.2. Dynamic local grid refinement

145 Level-set method is a popular interface-tracking method for simulating two-phase flows with  
146 topologically complex interfaces [56], and the distance from the gas-liquid interface predicted by the  
147 level-set method can be used as the criteria to refine the grids near the interface. The level-set function  
148 (LSF)  $\varphi$  is defined as a signed distance to the interface, and the  $\varphi$  evolution can be given by:

$$\frac{\partial \varphi}{\partial t} + \nabla \cdot (\vec{u} \varphi) = 0 \quad (13)$$

149 where the interface is the zero-level set, and  $\varphi(x, t)$  can be expressed as:

$$\varphi(x, t) = \begin{cases} +|d| & \text{if } x \in \text{the primary phase} \\ 0 & \text{if } x \in \text{the interface} \\ -|d| & \text{if } x \in \text{the secondary phase} \end{cases} \quad (14)$$

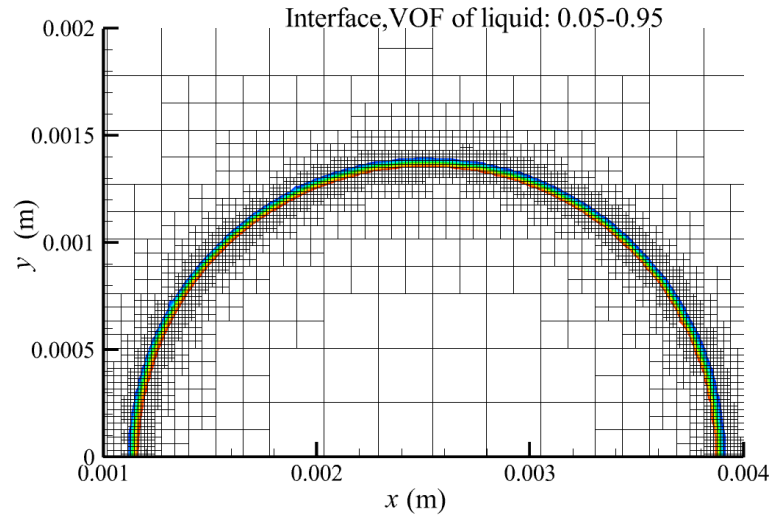
150 where  $d$  is the distance from the interface.

151 In order to increase the calculation efficiency, the dynamic grid refinement region is restricted to a  
 152 certain region that is close to the gas-liquid interface. For the 2D axisymmetric domain, the refinement  
 153 region is within  $0.2D_0$  to the interface, namely  $-0.2D_0 \leq \varphi \leq 0.2D_0$ ; for the 3D domain, the refinement  
 154 region is within  $0.1D_0$  to the interface, namely  $-0.1D_0 \leq \varphi \leq 0.1D_0$ . The level of refinement for a region  
 155 depends on its distance to the interface, and the different refinement regions are marked using the level-  
 156 set function  $\varphi$ . For example, the refined 2D axisymmetric domain is expressed as follows:

$$Level = \begin{cases} 4 & \text{if } |\varphi| \leq \frac{0.2D_0}{8} \\ 3 & \text{if } \frac{0.2D_0}{8} < |\varphi| \leq \frac{0.2D_0}{4} \\ 2 & \text{if } \frac{0.2D_0}{4} < |\varphi| \leq \frac{0.2D_0}{2} \\ 1 & \text{if } \frac{0.2D_0}{2} < |\varphi| \leq 0.2D_0 \\ 0 & \text{if others} \end{cases} \quad (15)$$

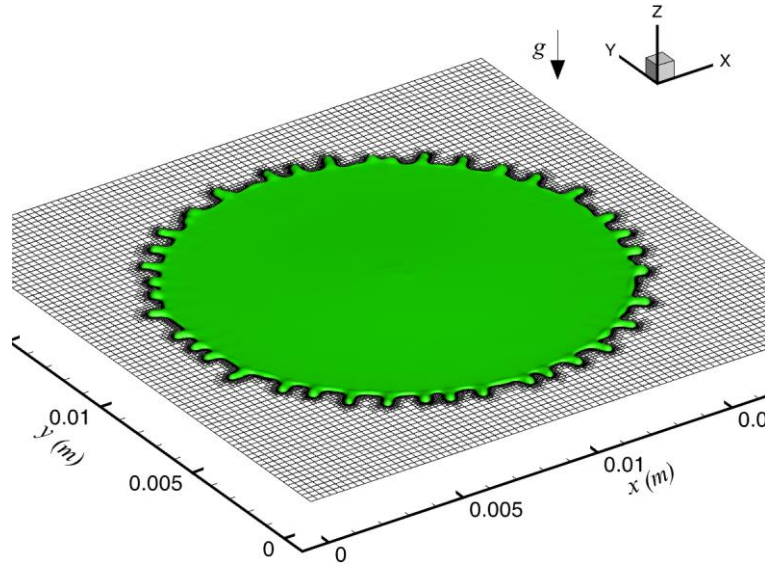
157 where,  $D_0$  is the initial droplet diameter. Refined grids are produced by the method of hanging node  
 158 adaption. If the current level of the cell is lower than expected level, then the cell in the 2D domain is  
 159 split into 4 cells or the cell in the 3D domain is split into 8 cells. Conversely, if the current level is larger  
 160 than the expected level, then this grid is made coarser.

161 The  $60 \times 60$  and  $80 \times 80 \times 80$  identical coarse-level quadrilateral cells were mapped in 2D  
 162 axisymmetric and 3D domains, respectively. Then, the local multi-level grid refinement around the  
 163 interface was applied, as shown in Fig. 1.



164  
165

(a)



166  
167

(b)

168 **Fig. 1.** Geometry, boundary conditions and grid with the dynamic local grid refinement technique. (a)  
169 eZoom of the 4-level of local grid refinement and the interface details of the 2D model, and (b) the 4-  
170 level of the local refinement grid for the 3D model (only 3-levels shown).

171

172 For a 2D domain, it is found that the differences in the temporal evolutions of the spreading ratio  
173 between the 4-level and 5-level refined grid is less than 2% which means that the 4-level refinement can  
174 achieve a grid independent solution. Using this technique, the number of the cells can be reduced by  
175 100 times compared with a uniform refined grid using the same grid resolution in the whole  
176 computational domain. In addition, the minimum cell size around the interface is about 15  $\mu\text{m}$  which  
177 means there are more than 400 nodes on the 2D circumference of the initial droplet. For a 3D domain,

178 a 4-level refined grid can achieve a grid independent solution for the different cases. The minimum cell  
179 size around the interface is about 15  $\mu\text{m}$ , and more than 120,000 nodes are employed on the sphere of  
180 the initial droplet with a diameter of 3.0 mm. In addition, the number of the dynamic local refined cells  
181 varies from 0.8 to 8.0 million, whereas the number of cells is 2,097 million for the whole-domain with  
182 a uniform 4-level refined grid. In this study, for the purpose of saving computing time, this new local  
183 refined grid is only created every 20 time steps.

### 184 2.3. *Boundary conditions and numerical schemes*

185 For the droplet normal impact onto a dry solid surface, the axisymmetric pattern was simulated in  
186 the 2D axisymmetric computational domain for the purpose of saving grids, and the non-axisymmetric  
187 pattern was simulated in the 3D computational domain. In this study, the ranges of the initial velocity  
188 and diameter of the droplets are 0.85 - 4.1  $\text{ms}^{-1}$  and 2.28 - 3.17 mm, respectively. Further, the maximum  
189 spread diameter is less than 6 times that of the initial diameter. Thus, the computational domains are set  
190 to be 15 mm  $\times$  15 mm for the 2D axisymmetric model and 20 mm  $\times$  20 mm  $\times$  20 mm for the 3D model.  
191 The initial condition in the computational domain is a spherical droplet with a uniform velocity where  
192 the initial distance from the centre of the droplet to the wall is equal to its diameter. For the 2D model,  
193 one of the vertical boundaries is set to be the axisymmetric boundary. For the 3D model, the droplet is  
194 located at the middle of the  $x$ - $y$  plane. The wall is a no slip stationary boundary and the wall adhesion is  
195 specified by dynamic contact angle model. The other lines or faces in the computational domain are set  
196 to be the pressure-outlet boundary, and the static pressure is specific as 0 Pa.

197 The PISO algorithm was used to solve the transient pressure and velocity coupling, the body force  
198 weighted discretization was used for the pressure equation, and a second-order upwind scheme was  
199 adopted for the momentum equations. The Geo-Reconstruct scheme was employed for tracking the gas-  
200 liquid interface. Both the level-set functions and the transient schemes were solved using the first-order  
201 upwind scheme, and all the nonlinear equations were linearized and solved using the algebraic multigrid  
202 method [57]. The volume fraction was calculated using the explicit scheme, and the time steps of 0.05  
203  $\mu\text{s}$ , 0.2  $\mu\text{s}$ , 0.5  $\mu\text{s}$  and 2.0  $\mu\text{s}$  have been chosen to test the time step independence, and 0.5  $\mu\text{s}$  was  
204 regarded as the suitable time step size considering both the accuracy and the computational speed. The

205 criterion of convergence is that the residuals of all equations are less than  $10^{-4}$ . The gas-liquid interfacial  
 206 area  $A_{GL}$  was calculated through integrating the gas-liquid interfacial area in each gas-liquid boundary  
 207 cell. In order to eliminate the error at the liquid-solid interface,  $\alpha_L = 0.1$  was regarded as the gas-liquid  
 208 interface.

## 209 2.4. Case descriptions

210 Eight representative cases [14-16, 22-24] were selected for performing the simulations. The  
 211 selected experimental cases have detailed experimental conditions, including liquid properties, surface  
 212 properties and contact angle parameters, as well as clear figures and quantitative results. In addition, in  
 213 order to verify the adaptability of the established CFD model, the selected parameters of experimental  
 214 conditions cover a wide range. The important parameters of these cases are presented in Table 1, and  
 215 the fluid properties of the employed liquid and gas phases are listed in Table 2. In Table 1,  $u_0$  is the initial  
 216 velocity of the droplet,  $D_0$  is the initial diameter of the droplet,  $\theta_{adv}$  and  $\theta_{rec}$  are the quasi-static advancing  
 217 and receding contact angles, respectively. If they were not given in literature, they were assumed equal  
 218 to the static contact angle.  $We$  is the Weber number, which was calculated by  $We = \rho u_0^2 D_0 / \sigma$ .  $Re$  is the  
 219 Reynolds number, which was calculated by  $Re = u_0 D_0 \rho / \mu$ .  $Oh$  is the Ohnesorge number, which represents  
 220 a dimensionless number that relates the viscous forces to the inertial and surface tension forces,  $Oh =$   
 221  $\mu / \sqrt{\rho \sigma D_0} = \sqrt{We} / Re$ .

222

223 **Table 1** Parameters employed in the simulation cases.

No.	Liquid/Wall	$u_0$ (m/s)	$D_0$ (mm)	$\theta_{adv}$ (°)	$\theta_{rec}$ (°)	$We$	$Re$	$Oh$	Ref.
Case 1	Water/Wax	1.18	2.75	105	95	52.3	3,238.5	0.00223	Rioboo [15]
Case 2	Water/Wax	0.85	2.70	97	97	26.7	2,290.4	0.00225	Mao [14]
Case 3	Water/Silicon	1.0	2.28	114	64	31.2	2,275.4	0.00245	Yokoi [24]
Case 4	Water/Glass	1.17	2.7	10	6	50.5	3152.7	0.00225	Šikalo [16]
Case 5	Glycerin/Wax	4.1	2.45	97	90	797.5	105.6	0.26732	Šikalo [23]
Case 6	Glycerin/Wax	1.41	2.45	97	90	94.3	36.3	0.26732	Šikalo [23]
Case 7	Water/Wax	3.6	3.17	105	95	561.7	11,389.2	0.00208	Rioboo [15]
Case 8	Tin/Steel	3.0	2.7	140	140	322.3	29,504.1	0.00061	Bussmann [22]

224

225

226

227

228 **Table 2** Properties of the liquids and gas that were used in the simulations.

Liquid/Gas	$\sigma$ (N m <sup>-1</sup> )	$\mu$ (mPa.s)	$\rho$ (kg m <sup>-3</sup> )	$Ca$ at $u_{cl}=1$ m s <sup>-1</sup>
Water	0.073	1.0	998	0.0137
Glycerin	0.063	116	1220	1.841
molten tin	0.530	1.93	7030	0.0036
Air	-	0.0179	1.225	-

229

230 Upon considering all the simulated cases, the contact angle is within the range of 6° - 140°, the  
 231 Weber number is within the range of 26.7 - 797.5, and the Reynolds number is within the range of 36.3  
 232 - 29,504.1. Specifically, Case 1 - 3 are concerned with the water droplet impact on hydrophobic surfaces.  
 233 Case 4 is about the impact of a water droplet on a hydrophilic surface. Case 5 and 6 refer to the glycerin  
 234 droplet impact on hydrophobic surfaces, where the glycerin has a higher viscosity than water, and  
 235 therefore this results in a bigger value of the Ohnesorge number  $Oh$  and the capillary number  $Ca$ . In  
 236 addition, Case 7 and 8 are about the water and molten tin droplets impact on hydrophobic surfaces with  
 237 high  $Re$  numbers, which result in non-axisymmetric patterns, therefore they were simulated using 3D  
 238 models.

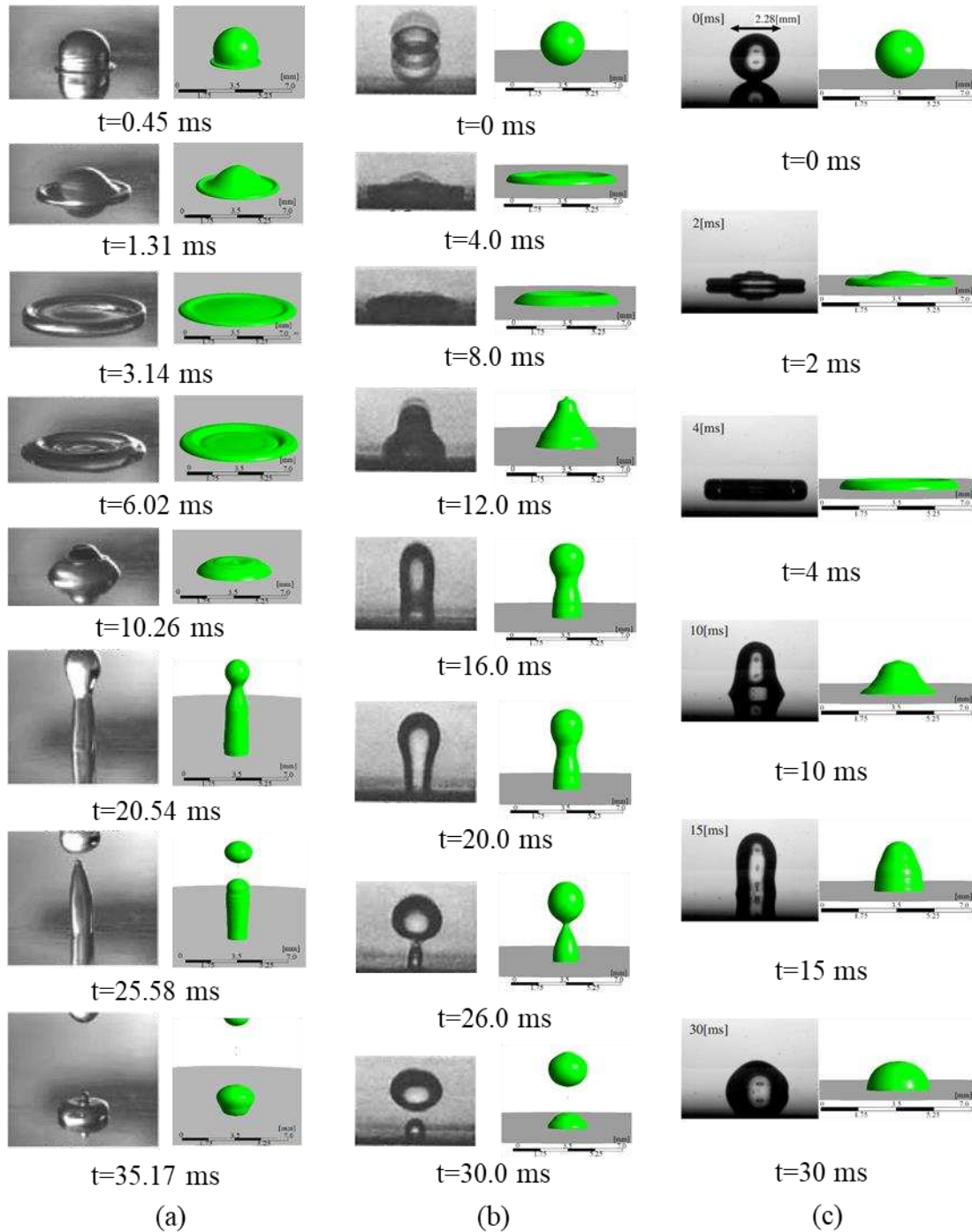
### 239 **3. Simulation results and discussion**

#### 240 *3.1. The impact of water droplets on hydrophobic surface*

##### 241 *3.1.1. The droplet dynamics and 2D axisymmetric model validation*

242 Water droplets impacting hydrophobic surfaces is a typical process in many applications [58-60].  
 243 Accurately reproducing the dynamic impact process through CFD simulation is very important for  
 244 analysing their detailed behaviours. Comparisons of the simulation and the experimental results of Cases  
 245 1-3 are shown in Fig. 2. It shows that the simulated spatial-temporal evolutions of the spread, recoil,  
 246 rebound and breakup behaviours are in good agreement with the experimental results [14, 15, 24]. The  
 247 time evolution of the impact process can be divided into four stages: the kinematic, spreading, relaxation  
 248 and wetting/equilibrium stages. At the kinematic stage, the droplet is like a truncated sphere, and no  
 249 lamella forms and spreads. With the increase of time, the droplet begins to spread, and it is governed by

250 inertia. At the same time, the surface tension and viscosity combine to damp the droplet spreading, and  
251 a rim of the spreading lamella appears at the edge of the spreading droplet film. At the end of the  
252 spreading stage, the droplet reaches its maximum spreading. Then, the gas-liquid-solid contact line of  
253 the droplet begins to recede, and this is called the relaxation stage, where the surface tension minimizes  
254 the gas-liquid interface of the droplet. Take Case 1 as an example, during the relaxation stage, the droplet  
255 goes from a pancake shape (at  $t = 6.02$  ms,  $t^* = 2.58$ ) to a truncated sphere on the hydrophobic surface  
256 (at  $t = 10.26$  ms,  $t^* = 4.40$ ), as shown in Fig. 2 (a). Then, depending on different kinetic energies  
257 contained, there are different movement regimes. If the droplet contains sufficient kinetic energy, then  
258 part of the droplet can bounce back from the solid surface as shown in Fig. 2 (a) and (b). Otherwise it  
259 sticks to the surface and reaches equilibrium after several oscillations, as shown in Fig. 2 (c).

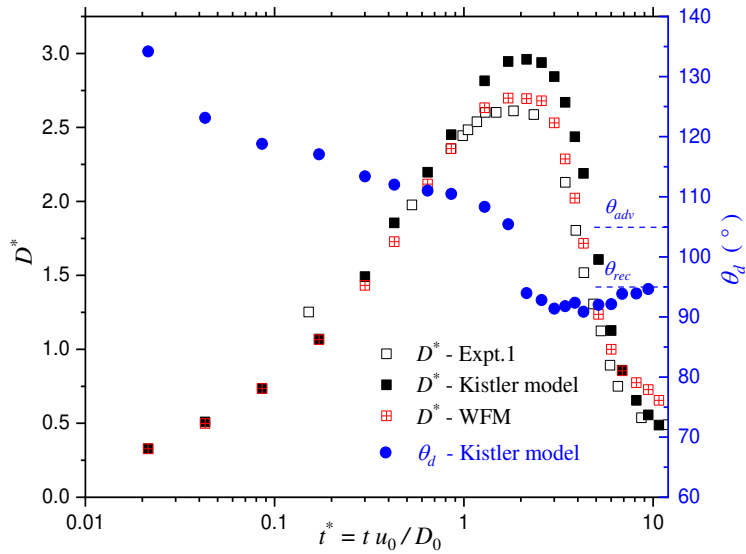


260

261 **Fig. 2.** Experimental and CFD simulation results of the dynamic droplets during the spreading, recoiling  
 262 and bouncing regimes: (a) Case 1, based on Rioboo et al. [15], (b) Case 2, based on Mao et al. [14], and  
 263 (c) Case 3, based on Yokoi et al. [24].  
 264

265 The spread factor  $D^*$  is defined as  $D/D_0$ , where  $D$  is the diameter of the liquid-solid contact  
 266 interface, and  $D_0$  is the initial droplet diameter. For a further validation of the 2D axisymmetric model,  
 267 the time evolution of the spread factor  $D^*$  in Case 1 is presented in Fig. 3. The development stages of  
 268  $D^*$  matched well with the experimental measurements [15] when employing the Kistler model [32] or

269 the wetting force model (WFM) [36]. The simulated maximum spread factor  $D_m^*$  is 2.96 with the Kistler  
 270 model and 2.69 with the WFM method, and the experimental result is 2.62. The difference between the  
 271 simulated maximum spread factor  $D_m^*$  and the experimental measured  $D_m^*$  is within 13%, which  
 272 indicates that the 2D axisymmetric CFD model is acceptable for investigating the detailed behaviour of  
 273 the droplet impact. Since the Kistler model is more robust for simulating the impact at different  
 274 conditions, it was used to produce the CFD results in this paper. In addition, the time evolution of the  
 275 dynamic contact angle when employing the Kistler model is plotted in Fig. 3, and the values of the  
 276 experimental measured advancing contact angle  $\theta_{adv}$  and receding contact angle  $\theta_{rec}$  are also marked in  
 277 the figure. An interaction between the fluid viscosity, the surface tension, the inertia and the substrate  
 278 leads to the real-time dynamic contact angle  $\theta_d$  being a function of the velocity of the contact line  $u_{cl}$ ,  
 279 which is very important for reproducing the dynamic impact process in the simulation [61].

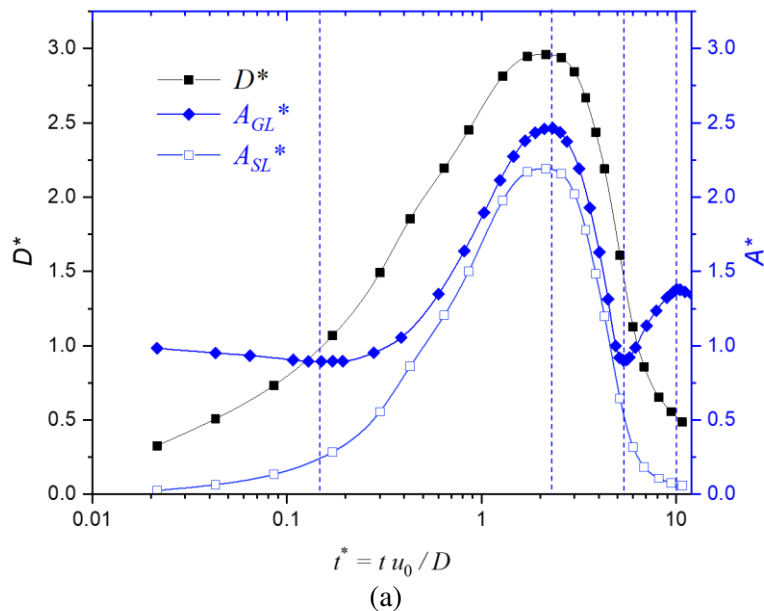


280  
 281 **Fig. 3.** Time evolutions of the spread factor of a water droplet and the dynamic contact angle in Case 1  
 282 using both the Kistler model [32] and the wetting force model (WFM) [36] for the hydrophobic surface.  
 283

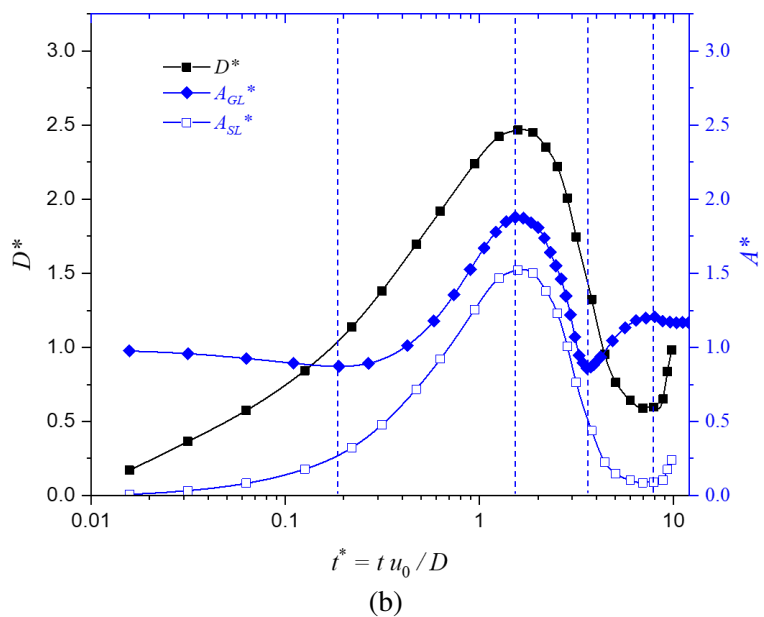
### 284 3.1.2. Variations of the interfacial areas

285 The interfacial areas are crucial parameters for affecting the interface heat and mass transfer. In  
 286 order to analyse and compare the variations of the gas-liquid interfacial area and the solid-liquid  
 287 interfacial area in different impact regimes, two interfacial area factors were proposed. (i) The gas-liquid  
 288 interfacial area factor  $A_{GL}^*$  is defined as  $A_{GL}^* = A_{GL}/A_{GL0}$ , where  $A_{GL}$  is the real-time gas-liquid interfacial  
 289 area and  $A_{GL0}$  is the initial gas-liquid interfacial area of the spherical droplet; (ii) The solid-liquid

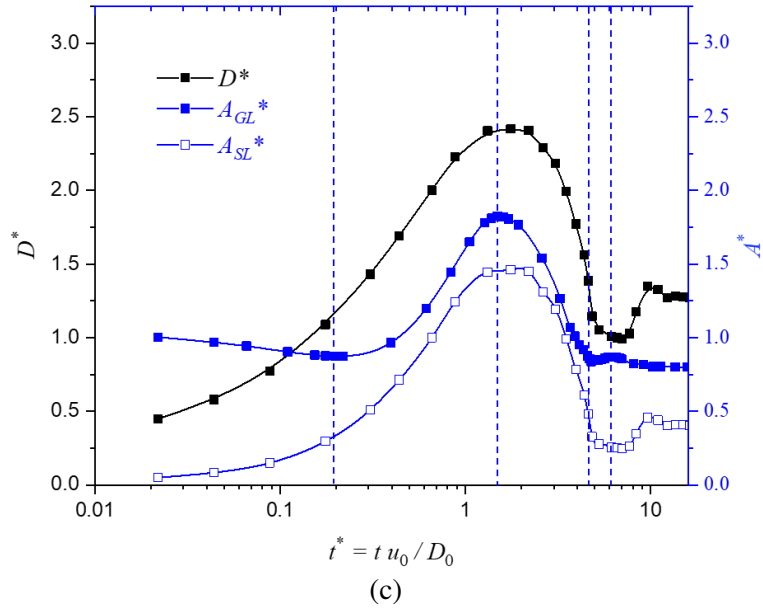
290 interfacial area factor  $A_{SL}^*$  is defined as  $A_{SL}^* = A_{SL}/A_{GL0}$ , where  $A_{SL}$  is the real-time solid-liquid interfacial  
 291 area. Variations of  $A_{GL}^*$ ,  $A_{SL}^*$  and the spread factor  $D^*$  of the droplets in Case 1–3 are presented in Fig.  
 292 4.



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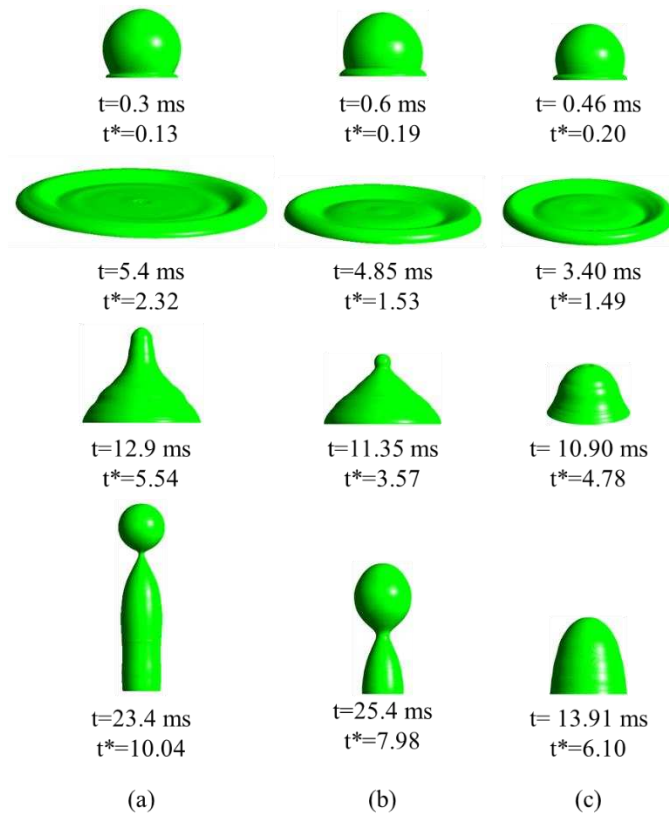


**Fig. 4.** Variation of the spread factor and gas-liquid interfacial area factor: (a) Case 1, based on Rioboo et al. [15], (b) Case 2, based on Mao et al. [14], and (c) Case 3, based on Yokoi et al. [24].

As shown in Fig. 4,  $A_{GL}^*$  can be divided into five stages by four changing points according to the variation of its value. Accordingly, the morphologies of the droplets at the four  $A_{GL}^*$  changing points are shown in Fig. 5. From observing Fig. 4 and Fig. 5, at the kinematic stage,  $A_{GL}^*$  slightly decreases due to the droplet changing from a sphere to a truncated sphere and part of the gas-liquid interface being replaced by the solid-liquid interface  $A_{SL}$ . Then, at the spreading stage, the gas-liquid interfacial area increases with the shape of the droplet changing from the truncated sphere to the lamella, and the increase of the gas-liquid interfacial area keeps pace with the increasing of the droplet diameter. At the end of the spreading stage, the  $D^*$ ,  $A_{GL}^*$  and  $A_{SL}^*$  almost reach their maximum value at the same time, and the  $A_{GLm}^*$  (maximum  $A_{GL}^*$ ) of Cases 1-3 are 2.47, 1.88 and 1.82, respectively. Then, the gas-liquid-solid contact line begin to recede under the action of surface tension, and the regained kinetic energy makes the droplet rebound. During the rebound process,  $A_{GL}^*$  first decreases to its minimum value, then it increases with the longitudinal stretch of the droplet. When  $A_{GL}^*$  decreases to its minimum value, the droplet is similar to a conical shape as shown in Fig. 5. Before it reaches its minimum value, the surface tension acts as a driving force for the drop rebound, while with the increase of  $A_{GL}^*$ , it becomes a resistance for the droplet prolonging. If the droplet has a tall rebound, then the surface tension can shrink the prolonged liquid column and squeeze out a small droplet at the top of the liquid column, as shown in Fig. 5 (a) and (b). Before the droplet separate from the liquid column, the gas-liquid interfacial area

321 reaches its second extremum. Then, the gas-liquid interfacial area decreases and oscillates before the  
 322 droplet reaches a balanced state. Looking at the whole process, it can be found that  $D^*$  and  $A_{GL}^*$  have  
 323 different variation trends, which means the variation of the gas-liquid interfacial area  $A_{GL}$  cannot be  
 324 simply represented by the variation of the droplet diameter. Comparing Fig. 4 (a) and (b), it can be found  
 325 that with a higher impact velocity,  $A_m^*$  becomes bigger, which is one of the ways for process  
 326 intensification.

327

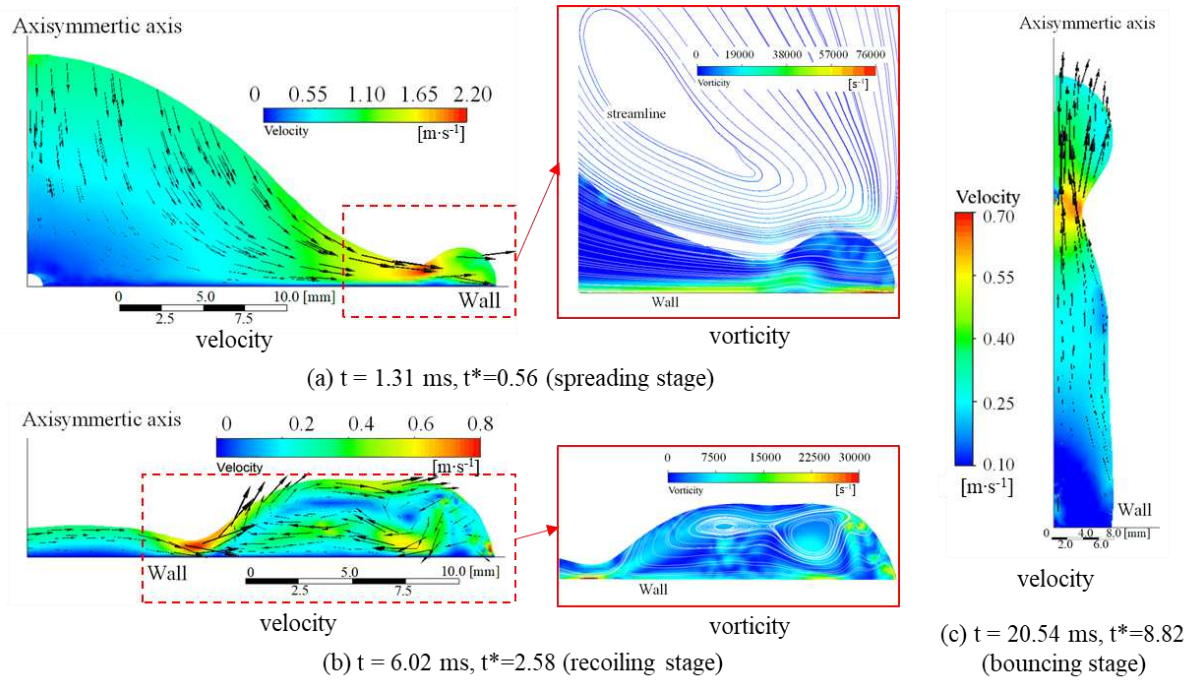


328

329 **Fig. 5.** Morphologies of the droplets at the  $A_{GL}^*$  changing points shown in Fig. 4: (a) Case 1, (b) Case  
 330 2, and (c) Case 3.

331

332 3.1.3. Inner flow field of the droplet during impact

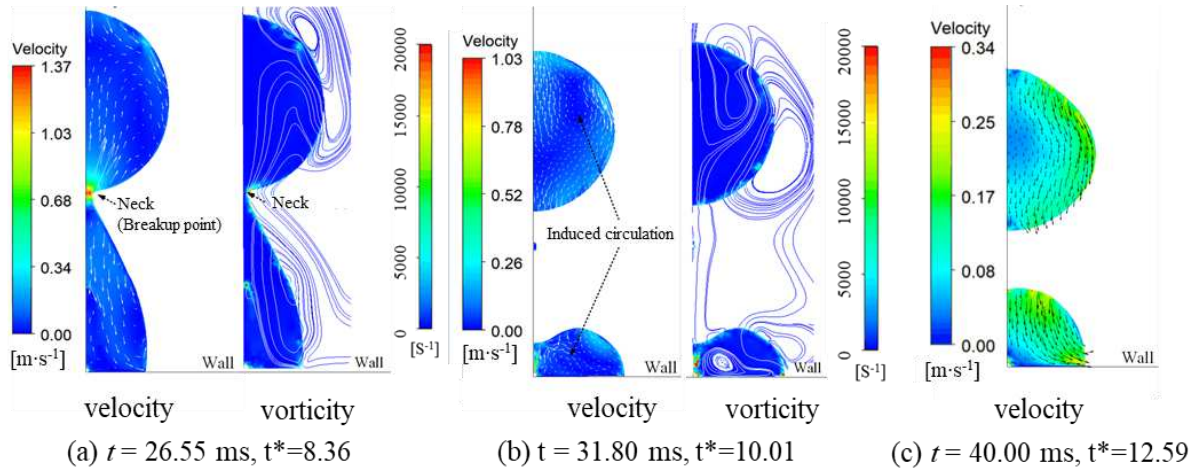


333  
 334 **Fig. 6.** The velocity vector and the vorticity distribution of the droplet during spreading, recoiling and  
 335 bouncing regimes in Case 1.

336 Parameters of the droplet inner flow field, such as the velocity vector, the vorticity distribution and  
 337 the thickness of the boundary layer, significantly affect the calculation of viscous dissipation in the  
 338 droplet [41-43, 45, 48] and the interfacial heat and mass transfer [62]. However, these parameters are  
 339 very difficult to be measured by experimental methods, therefore they are analysed through using the  
 340 accurately reproduced results from CFD simulation. Fig. 6 shows the velocity and vorticity vertical  
 341 cross-section diagrams of the droplet in Case 1 at the spreading, recoiling and bouncing regimes. At  $t =$   
 342  $1.31 \text{ ms}$  ( $t^* = 0.56$ ), the droplet is in the spreading stage, as shown in Fig. 6 (a). Under the action of  
 343 inertial force, the sphere is stretched into a pie disk shape, and the larger liquid surface is exposed to the  
 344 gas phase. In addition, a small bubble can be observed under its centre, and a detailed explanation about  
 345 this phenomenon can be seen in the literature [11]. The leading edge of the rim is unstable soon after  
 346 impact, and a hemispherical ring is formed due to the solid surface being hydrophobic. The maximum  
 347 velocity is located at the ring groove (in 3D view) between the truncated sphere and the hemispherical  
 348 ring. As shown in the vorticity contour diagram of Fig. 6 (a), during the spreading stage, there is a thin  
 349 layer with a high vorticity in the near-wall region, where the viscous dissipation mainly occurred. In this  
 350 stage, there are two reasons for enhancing the interfacial heat and/or mass transfer: (i) due to the

351 existence of the high vorticity region, the thermal resistance of the liquid-solid interface can be  
352 significantly reduced by the strong convective heat transfer; (ii) the dramatically increased gas-liquid  
353 and liquid-solid interfaces are favourable for the interfacial heat and/or mass transfer. At  $t = 6.02$  ms ( $t^*$   
354  $= 2.58$ ), the droplet is at the beginning of the (receding) relaxation stage, as shown in Fig. 6 (b). The  
355 liquid at the outer edge of the disk is in a recoiling motion under the action of the surface tension, while  
356 the liquid near the axisymmetric axis is still in a spreading motion. Thus, there are induced vortices  
357 inside the spreading lamella, as shown in Fig. 6 (b), and these vortices generate viscous dissipation. The  
358 small vortices near the gas-liquid interface can enhance the surface renewal, thus enhancing the  
359 interfacial heat and/or mass transfer, and the large vortices in the droplet facilitate the internal convective  
360 heat and/or mass transfer. At  $t = 20.54$  ms ( $t^* = 8.82$ ), the droplet is at the bouncing stage, as shown in  
361 Fig. 6 (c). The inertia overcomes the gravity and makes the droplet rebound from the wall. Under the  
362 action of surface tension, the inherent instability of the liquid column leads to the appearance of thin  
363 necks, where the velocity is maximum, and the liquid column may break into two or more small droplets.  
364 The breakup stage is investigated by the results obtained in Case 2.

365 In the rebound and breakup stages, the velocity vectors and vorticity distribution of the liquid phase  
366 of Case 2 are plotted in Fig. 7. At the beginning of the breakup, as shown in Fig. 7(a), a neck is found  
367 connecting the two spheres. The liquid in both the upper and lower spheres moves away from the neck,  
368 and this leads to the breakup at the narrow neck. In Fig. 7(b), these two spheres are completely broken,  
369 and the induced vortices appear inside both the two small droplets. The lower one adheres to the wall,  
370 whereas the upper one flies away. After several milliseconds, the induced vortices disappear and the  
371 upper droplet begins to fall down, as shown in Fig. 7(c). In this stage, the surface tension plays a  
372 dominant role in the droplet breakup and vortex generation.



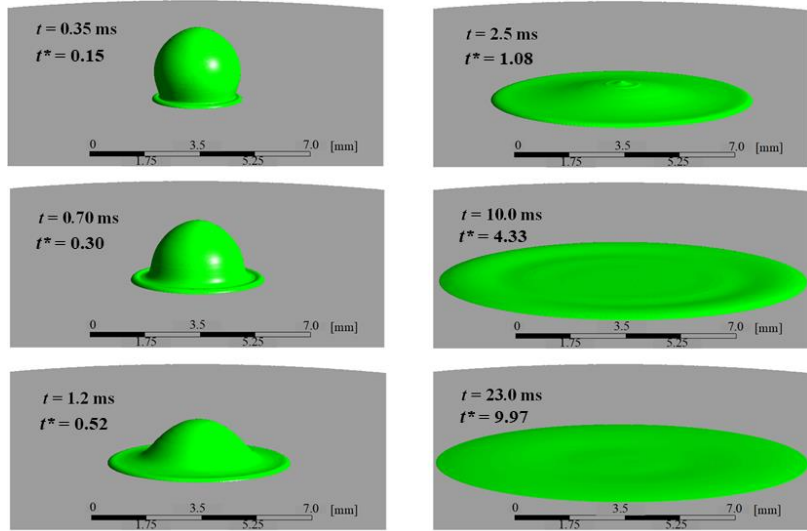
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374 **Fig. 7.** The velocity, vorticity and streamlines of the droplet during the breakup regime of Case 2.

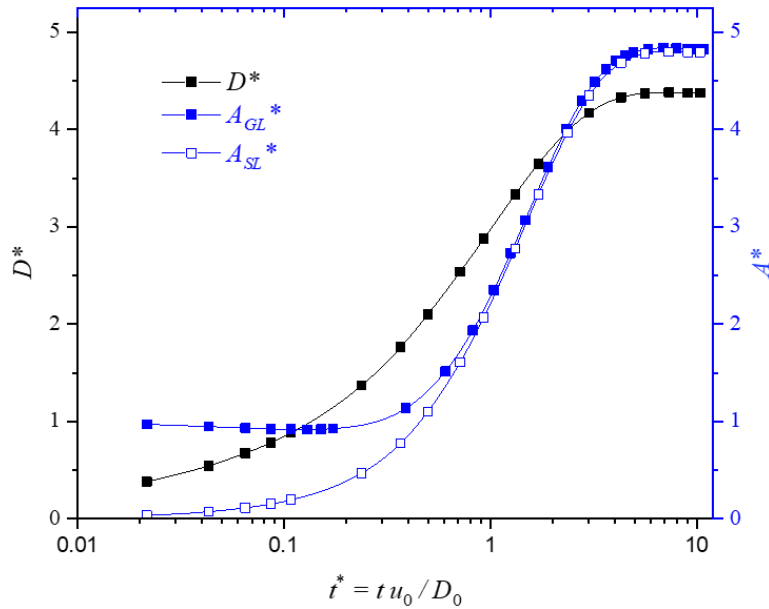
375 **3.2. The impact of water droplet on hydrophilic surface**

376

377 Case 4 is used for analysing the droplet dynamics and the variation of the interfacial areas when a  
 378 droplet impacts on a hydrophilic surface. The measured  $\theta_{adv}$  and  $\theta_{rec}$  are  $10^\circ$  and  $6^\circ$  respectively [16],  
 379 and the characteristic time  $t_c$  is equal to 2.31 ms. The time evolution of the droplet morphology is shown  
 380 in Fig. 8(a), and the spread factor  $D^*$ , the gas-liquid interfacial area factor  $A_{GL}^*$  and the solid-liquid  
 381 interfacial area factor  $A_{SL}^*$  of the water droplet during the impact are shown in Fig. 8(b). During the  
 382 kinematic stage, the shape of the droplet changes from a sphere to a disk; the solid-liquid interfacial area  
 383 keeps increasing while the gas-liquid interfacial area keeps slightly decreasing. Then, at the spreading  
 384 stage, both the gas-liquid interfacial area and the solid-liquid interfacial area increases rapidly. There is  
 385 no obvious recoil stage for the hydrophilic surface. Finally, the droplet enters an equilibrium state, and  
 386 the  $A_{GL}^*$  and  $A_{SL}^*$  are almost identical, which means that the liquid is almost shaped like a flat film.  
 387 With the diameter of the droplet increasing by 4.4 times, the gas-liquid interfacial area increases by  
 388 about 4.8 times. For the hydrophilic surface, the ratio of the increased area to the increased diameter is  
 389 much larger than that of the hydrophobic surface at the similar initial condition, as shown in Case 1 by  
 390 Fig. 4(a). This is because the solid-liquid adhesive force is a driving force for increasing the gas-liquid  
 interfacial area for the hydrophilic surface.



(a)



(b)

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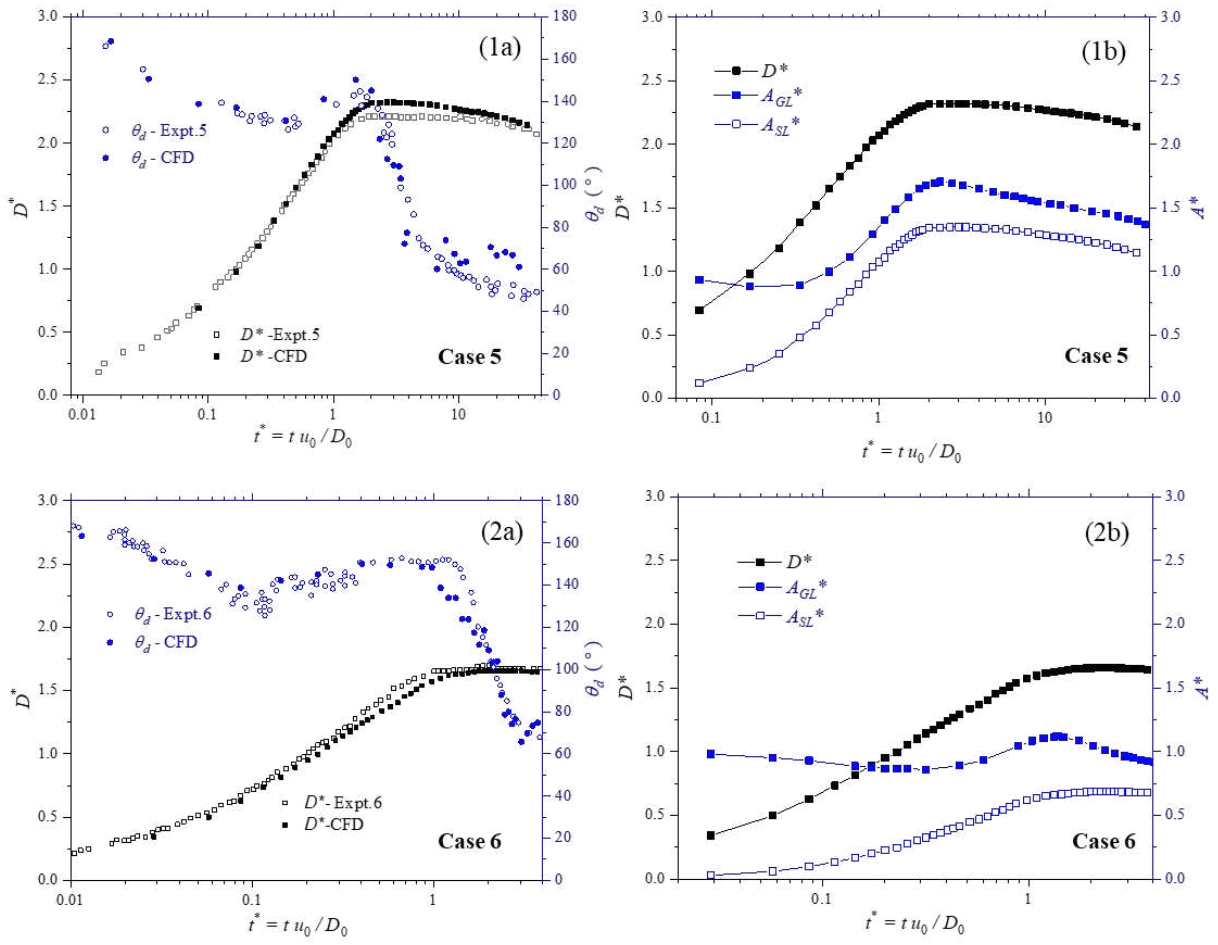
395 **Fig. 8.** (a) The time evolution of the droplet impact on a hydrophilic surface in Case 4, and (b) The time  
396 evolution of the spread factor  $D^*$ , the gas-liquid interfacial area factor  $A_{GL}^*$  and the solid-liquid  
397 interfacial area factor  $A_{SL}^*$  of the water droplet in Case 4.

398

### 399 3.3. The impact of a high viscous droplet on hydrophobic surface

400 The viscosity of the liquid phase is a crucial parameter for influencing the droplet impact dynamics  
401 and the variation of the gas-liquid interface. The impact of glycerin droplet on wax surface was  
402 investigated. Glycerin has a much higher viscosity (116 mPa.s) than water. The initial velocity was set  
403 to  $u_0 = 4.1$  m/s and 1.41 m/s. The detailed parameters are listed in Table 1 as Cases 5 and 6. Both the  
404 simulation and the experimental results of the time evolution of the spread factor  $D^*$  and the dynamic

405 contact angle  $\theta_d$  of Cases 5 and 6 are shown in Fig. 9(1a) and (2a). It can be seen that  $D^*$  and  $\theta_d$  match  
 406 well with the experiments [23], which means that the CFD model can reproduce the high viscosity  
 407 droplet impact process accurately. Compared with the water droplet, the high viscosity liquid droplet  
 408 has a bigger change of the dynamic contact angle  $\theta_d$  during the impact. Taking Case 5 as an example, as  
 409 shown in Fig. 9(1a), during the kinematic and spreading stages,  $\theta_d$  is about  $140^\circ$ . When the droplet goes  
 410 into the receding stage,  $\theta_d$  decreases quickly to around  $60^\circ$ . This is because the high viscosity glycerin  
 411 has a large viscous force, making the contact angle hysteresis more obvious than water.



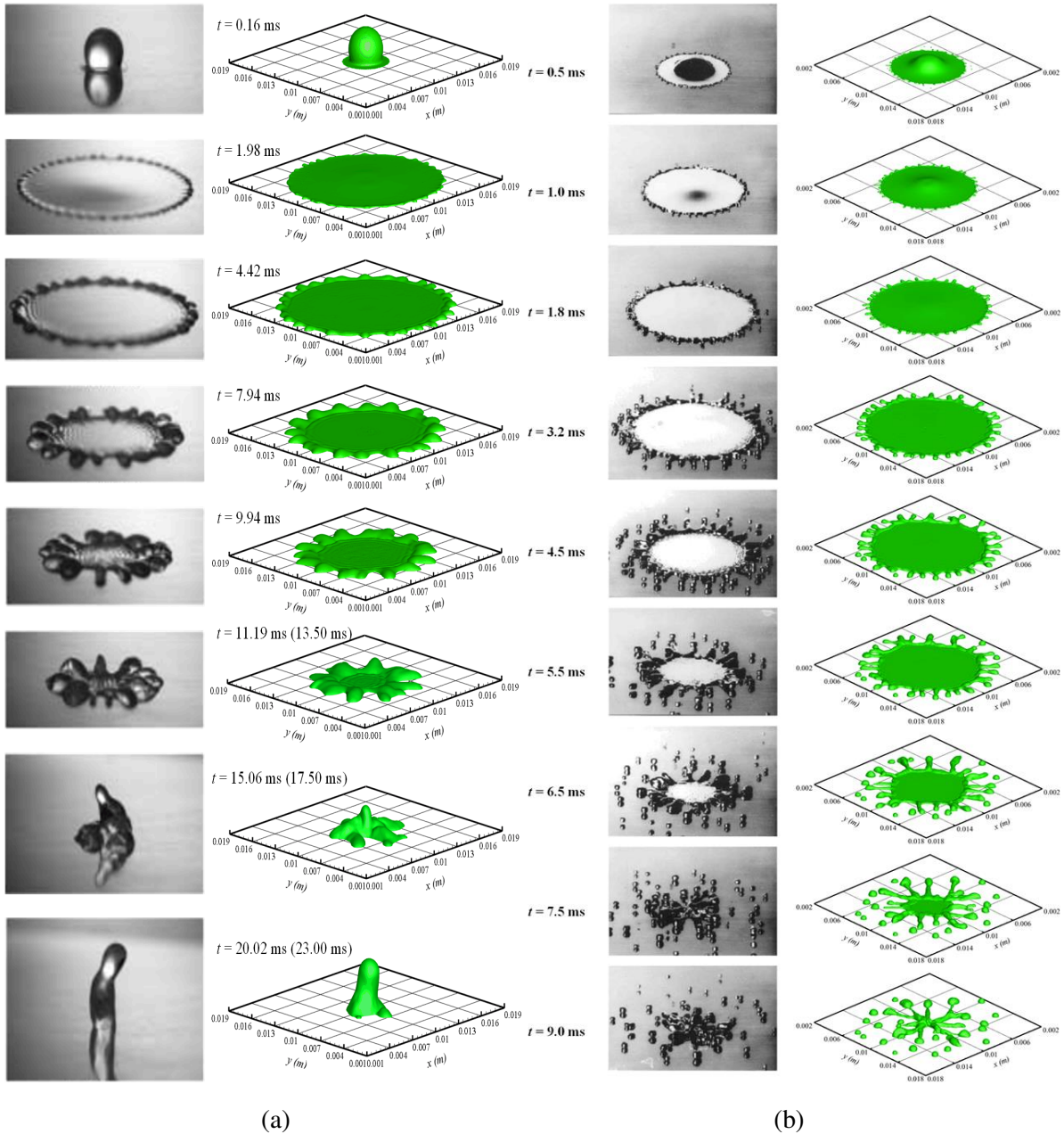
412  
 413 **Fig. 9.** Variations of spread factor  $D^*$ , the dynamic contact angle  $\theta_d$ , and the interfacial area factors  $A_{GL}^*$   
 414 and  $A_{SL}^*$  in Cases 5 and 6.  
 415

416 The variations of  $A_{GL}^*$  and  $A_{SL}^*$  in Case 5 and Case 6 are analysed based on the simulation results,  
 417 as shown in Fig. 9(1b) and (2b). After impact and before reaching the equilibrium state, the droplet  
 418 oscillation is much weaker compared to water. For Case 5, as shown in Fig. 9(1b), with a high impact  
 419 velocity 4.1 m/s, the maximum gas-liquid interfacial area factor  $A_{GLm}^*$  is 1.71. For Case 6, with the  
 420 impact velocity at 1.41 m/s,  $A_{GLm}^*$  is 1.12, which means that the gas-liquid interfacial area only increased

421 slightly. For high viscosity liquids, although the impact velocity and static contact angle are both large  
422 enough, the viscous dissipation absorbs a large amount of kinetic energy, making the bounding and  
423 breakup behaviours difficult to occur. The results show that the normal impact is not a good way to  
424 increase the interface area of high viscosity liquid, while due to the obvious contact angle hysteresis,  
425 oblique impact may be a better way to stretch the droplet and increase the area of the interface.

### 426 3.4. *The impact of a droplet on hydrophobic surface at a high speed*

427 At a high impact velocity, perturbations can be observed on the rim, which can result in fingering  
428 or splashing [15, 22]. These behaviours are asymmetrical; therefore, they can only be simulated by the  
429 3D models. Cases 7 and 8 are used to investigate the fingering and splashing, respectively, and both the  
430 experimental results and the simulation results are shown in Fig. 10. In Case 7, the impact velocity of  
431 the water droplet is  $3.6 \text{ m s}^{-1}$ , the static  $\theta_{adv}$  and  $\theta_{rec}$  of the water droplets on the hydrophobic wax surface  
432 are  $105^\circ$  and  $95^\circ$ , respectively, and the characteristic time  $t_c$  is equal to 0.88 ms. The flow appearance  
433 of the water droplet is shown in Fig. 10(a). During the whole impact process, no splash occurs, but the  
434 minimum film thickness is less than  $50 \text{ }\mu\text{m}$ . Therefore, the 4-level dynamic refined grid, which makes  
435 the minimum cell size  $15 \text{ }\mu\text{m}$  (1/200 of droplet diameter), is necessary for accurately simulating the 3D  
436 fingering impact process. As a result, a good agreement in the appearances between the numerical results  
437 and the experimental photographs was achieved. Several fingers appear soon after impact, and then both  
438 the size and number of the fingers gradually increase until the rim reaches its maximum spreading. The  
439 experimental and numerical  $D_m^*$  are 5.03 and 5.16, respectively. After the maximum spreading ( $t = 3.80$   
440 ms,  $t_m^* = 4.32$ ), the surface tension force pulls the fingers back with coalescence, and eventually makes  
441 the rim recoil and bounce. It is worth noting that there is a time lag for the simulation results after 10  
442 ms, which might be due to the effect of the roughness on the dynamic contact angle. However, the  
443 simulation results were still more accurate than the previous simulation results as shown in Ref. [63],  
444 where the non-physical splashing occurred along the circumference of the droplet after the maximum  
445 spreading.



446

447

448 **Fig. 10.** The simulation and experimental results for droplet impact at the fingering and splashing regime:  
 449 (a) Case 7, based on Rioboo et al. [15], and (b) Case 8, based on Bussmann et al. [22].

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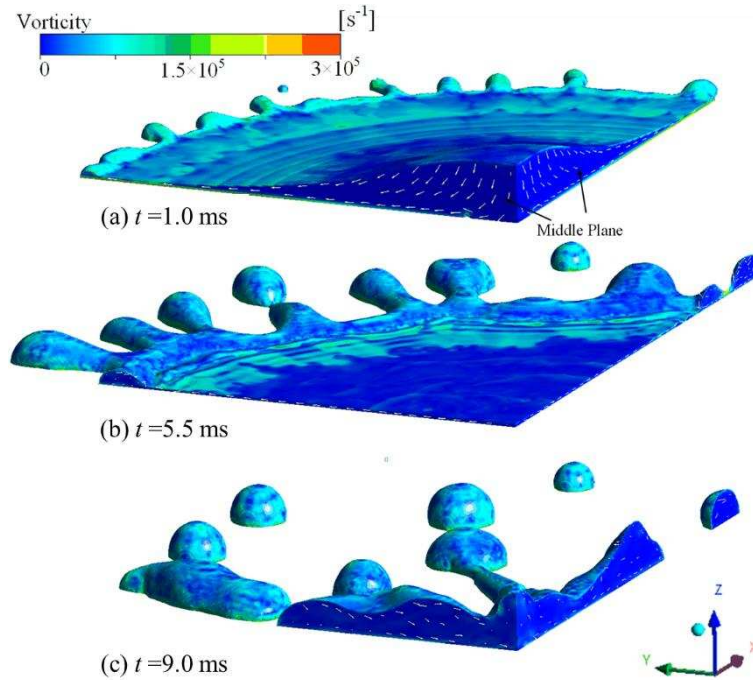
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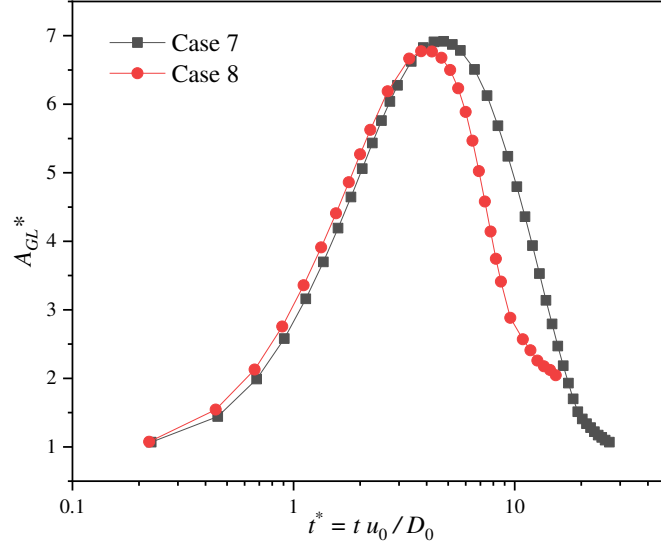
The flow appearance of the molten tin droplet in Case 8 is shown in Fig. 10(b), where the molten tin droplet has an initial velocity of  $3.0 \text{ m s}^{-1}$ , the characteristic time  $t_c$  is  $0.90 \text{ ms}$ , and the droplet reaches the maximum spread diameter at about  $t = 3.2 \text{ ms}$ . The 3D velocity vectors and vorticity distributions in the liquid phase of Case 8 are plotted in Fig. 11. At  $t = 1.0 \text{ ms}$ , the droplet is at the spreading stage as shown in Fig. 11 (a). Due to the instability and a higher velocity of the rim, the vorticity at the outer region is higher than that in the central region of the droplet during the spreading stage. At  $t = 5.5 \text{ ms}$ , the rim begins to splash and recoil as shown in Fig. 11 (b). Then the central liquid film recoils faster

458 than the fingers, which leads to the pinching off of the secondary droplets. Because of their low speed,  
 459 these satellite droplets tend to stay where they were cut off. At  $t = 9.0$  ms, there is a big snowflake  
 460 droplet in the central region of the computational domain, which drags the surrounding satellite droplets  
 461 together to form a new core as shown in Fig. 10(b) and Fig. 11 (c).



462  
 463 **Fig. 11.** The 3D velocity vectors and vorticity distributions in liquid phase during the fingering and  
 464 splashing regimes in Case 8.

465 The variations of the gas-liquid interfacial area index  $A_{GL}^*$  of Cases 7 and 8 are shown in Fig. 12.  
 466 The  $A_{GL}^*$  curves are similar for the two cases during the spreading stage. The  $A_{GL}^*$  sharply increases,  
 467 which means that the gas-liquid interfacial area is greatly increased due to the high-speed impact. Then,  
 468 only one peak appears on each curve during the observing period. This is because the fingering or  
 469 splashing consumes a large amount of energy, which damps the oscillation. During the receding stage,  
 470 the  $A_{GL}^*$  of Case 8 goes down faster than that of Case 7 due to the bigger surface tension and droplet  
 471 splash. Finally, the  $A_{GL}^*$  in Case 8 is bigger than that in Case 7 due to the generation of many satellite  
 472 droplets. It is difficult to form a thin film with a large surface area after droplet impact on hydrophobic  
 473 surfaces; therefore, promoting droplet breakup is a good choice for enhancing the gas-liquid interfacial  
 474 area.



475  
476 **Fig. 12.** The variations of the  $A_{GL}^*$  in Cases 7 and 8.

477

#### 478 **4. Energetic analysis of the maximum gas-liquid interfacial area**

##### 479 *4.1. Derivation of the correlation*

480 As has been observed from the CFD simulation results, during the impact of droplet on solid surface,  
481 the droplet has the biggest gas-liquid interfacial area almost at the end of the spreading stage. According  
482 to the law of conservation of energy, the change of the total surface energy  $\Delta E_s$  during the spreading  
483 stage of the impact process can be expressed as follows:

$$\Delta E_s = E_k + E_p - W \quad (16)$$

484 where  $E_k$  is the initial kinetic energy of the droplet,  $E_p$  is the released potential energy, and  $W$  is the  
485 energy dissipation.

486 The change of the total surface energy  $\Delta E_s$  is composed of three parts, as follows:

$$\Delta E_s = \sigma_{GL}\Delta A_{GL} + \sigma_{SL}\Delta A_{SL} + \sigma_{SG}\Delta A_{SG} \quad (17)$$

487 where  $\sigma_{GL}$  is the interfacial energy between the gas and the liquid phase, that is, the surface tension  
488 coefficient of the liquid;  $\sigma_{SL}$  is the interfacial energy between the solid surface and the liquid phase;  $\sigma_{SG}$   
489 is the interfacial energy between the solid surface and the gas phase.  $\Delta A_{GL}$ ,  $\Delta A_{SL}$  and  $\Delta A_{SG}$  are the  
490 change of the gas-liquid interfacial area, the change of the solid-liquid interfacial area and the change  
491 of the solid-gas interfacial area, respectively.

492 During a droplet impact on a solid surface, the increase of the solid-liquid interfacial area is equal

493 to the decrease of the solid-gas interfacial area, that is  $\Delta A_{SL} = -\Delta A_{SG}$ , therefore,  $\Delta E_s$  can be expressed  
 494 as follows:

$$\Delta E_s = \sigma_{GL}\Delta A_{GL} - (\sigma_{SG} - \sigma_{SL})\Delta A_{SL} \quad (18)$$

495 According to the Young equation [64, 65], the relationship between  $\sigma_{SG}$ ,  $\sigma_{SL}$  and  $\sigma_{GL}$  can be  
 496 expressed as follows:

$$\sigma_{SG} - \sigma_{SL} = \sigma_{GL}\cos\theta_Y \quad (19)$$

497 where  $\theta_Y$  is the theoretical Young's contact angle, which represents solely the energetic effect of the  
 498 surfaces [49].

499 Substituting Eq. (19) into Eq. (18),  $\Delta E_s$  can be expressed as follows:

$$\Delta E_s = \sigma_{GL}(\Delta A_{GL} - \Delta A_{SL}\cos\theta_Y) \quad (20)$$

500 In order to investigate the variation of the gas-liquid interfacial area, combining Eq.(16) and Eq.  
 501 (20),  $\Delta A_{GL}$  can be expressed as follows:

$$\Delta A_{GL} = \frac{E_k + E_P - W}{\sigma_{GL}} + \Delta A_{SL}\cos\theta_Y \quad (21)$$

502 In order to resolve the value of  $\Delta A_{GL}$ , the parameters on the right-hand side of Eq. (21) are  
 503 calculated as follows:

504 (i) The initial kinetic energy  $E_k$  is calculated by

$$E_k = 0.5\rho\frac{\pi D_0^3}{6}u_0^2 \quad (22)$$

505 (ii) During the spreading process, the released protential energy  $E_P$  is

$$E_P = \rho\frac{\pi D_0^3}{6}g\Delta H \quad (23)$$

506 where  $\Delta H$  is the decreased value of the centre of mass of the droplet. At the maximum spreading state,  
 507 the thickness of the droplet can be calculated by equating the volume of the spherical droplet with  
 508 diameter  $D_0$  to that of a cylinder with height  $h_m$  and diameter  $D_m$  [42], then

$$h_m = \frac{2D_0^3}{3D_m^2} \quad (24)$$

509 The height of the centre of mass of the droplet can be assumed to be  $0.5 h_m$ , therefore

$$\Delta H = H_0 - \frac{D_0^3}{3D_m^2} \quad (25)$$

510 where  $H_0$  is the initial height of centre of mass of the droplet, and Eq. (23) can be expressed as:

$$\Delta E_p = \rho \frac{\pi D_0^3}{6} g \left( H_0 - \frac{D_0^3}{3D_m^2} \right) \quad (26)$$

511 (iii) The  $\Delta A_{SL}$  is the change of the solid-liquid interfacial area; before impacting, it is zero; after  
 512 impacting, the solid-liquid contact area is assumed as a circular cross section; therefore, it is calculated  
 513 through:

$$\Delta A_{SL} = \frac{\pi D_m^2}{4} \quad (27)$$

514 (iv) According to the recent research [45, 49], the dissipation work  $W$  is composed of three parts:  
 515  $W = W_{vis} + W_{sp} + W_{cl}$ , where  $W_{vis}$  is the viscous dissipation within the boundary layer,  $W_{sp}$  is the  
 516 spontaneous dissipation associated with the “interfacial relaxation”, and  $W_{cl}$  is the contact line  
 517 dissipation due to the moving three-phase contact line.

518 The viscous dissipation  $W_{vis}$  can be calculated as follows [41]:

$$W_{vis} = \int_0^{t_m} \int_{\Omega} \Phi d\Omega dt \approx \Phi \Omega t_m \quad (28)$$

519 where  $\Phi$  is the viscous dissipation function,  $\Omega$  is the volume where the dissipation occurs, and  $t_m$  is the  
 520 elapsed time for a droplet to reach its maximum spread from the beginning of the impact. Chandra and  
 521 Avedisian [41] suggested that the viscous dissipation function can be estimated by using

$$\Phi \approx \mu \left( \frac{U_c}{L_c} \right)^2 \quad (29)$$

522 where  $U_c$  and  $L_c$  denote the characteristic velocity and the characteristic length, respectively. Initially,  
 523 Chandra and Avedisian [41] took the droplet initial velocity  $u_0$  as  $U_c$ , the droplet height at the maximum  
 524 spread  $h_m$  as  $L_c$ , and the cylindrical disk volume  $\pi D_m^2 h_m / 4$  as  $\Omega$ . Later, Pasandideh-Fard et al. [42]  
 525 modified the parameters by assuming the viscous dissipation occurs in a boundary layer with thickness  
 526  $\delta = 2D_0 / \sqrt{Re}$ , therefore they took  $L_c = \delta$ , and  $\Omega = \pi D_m^2 \delta / 4$ . Mao et al. [14] and Park et al. [46]  
 527 pointed out that the boundary-layer thicknesses for low- and high- viscosity liquids need to be  
 528 considered separately. For low viscosity liquids,  $\delta < h_m$ , it is reasonable to take  $L_c = \delta$  and  $\Omega =$

529  $\pi D_m^2 \delta / 4$ . For high viscosity liquids,  $\delta > h_m$ , it is more reasonable to take  $L_c = h_m$  and  $\Omega = \pi D_m^2 h_m / 4$   
530 due to the viscous dissipation occurring within the whole droplet. Yonemoto and Kunugi [48] believed  
531 that the shear stress occurs in the liquid film that spreads along the solid surface, therefore they took the  
532 radial liquid velocity along the solid surface  $u_R$  as  $U_c$ , and they estimated that  $u_R = 3u_0/8$ . From the  
533 CFD simulation results, as shown in Fig. 6 (a), for the low-viscosity fluid, the shear stress mainly exists  
534 in a thin liquid film near the wall. Therefore, we consider that it is reasonable to adopt the radial velocity  
535  $u_R$  as the characteristic velocity. However,  $u_R$  is not a constant along the radial direction, and it changes  
536 over time in the spread stage, making it difficult to predict its value. In the vicinity of the centre of the  
537 droplet,  $u_R$  is smaller than the initial impact velocity  $u_0$ , but at the outer edge of the droplet,  $u_R$  is larger  
538 than  $u_0$ . Therefore, it is reasonable to assume that the average radial velocity of the droplet is equal to  
539 the initial velocity, that is,  $u_R = u_0$ . Based on this assumption, the  $t_m$  can be estimated by  $t_m =$   
540  $D_m/2u_R = D_m/2u_0$ , which is the same as the  $t_m$  adopted by Yonemoto and Kunugi [48], Huang and  
541 Chen [45] and Wang et al. [49]. According to the above analysis, the parameters in this paper are defined  
542 as follows:  $L_c = \delta$ ,  $U_c = u_0$ ,  $\Omega = \pi D_m^2 \delta / 4$ ,  $t_m = D_m/2u_0$ , where  $\delta = 2D_0/\sqrt{Re}$ . Therefore, the  
543 viscous dissipation is as follows:

$$W_{vis} = \frac{\pi \rho u_0^2 D_m^3}{16 \sqrt{Re}} \quad (30)$$

544 In addition, the spontaneous dissipation is as follows [45, 49]:

$$W_{sp} = \alpha \frac{\pi \rho u_c^2 D_m^3}{16 \sqrt{Re_c}} \quad (31)$$

545 where  $u_c$  is the critical velocity and  $Re_c$  is the associated critical Reynolds number,  $Re_c = \rho D_0 u_c / \mu$ .  $\alpha$   
546 is the coefficient to denote the portion of the whole spontaneous dissipation. For  $u_0 < u_c$ ,  $\alpha = 1$ ; for  
547  $u_0 \geq u_c$ ,  $\alpha = u_c / u_0$ . The  $u_c$  can be estimated through [45]:

$$u_c = \left\{ \frac{4\sigma_{GL}}{(\rho\mu D_0)^{0.5} \beta_{sph}} \left[ \frac{4}{\beta_{sph}^2} - 2(1 - \cos \theta_{D_m}) + \cos \theta_{D_m} \sin^2 \theta_{D_m} \right] \right\}^{2/3} \quad (32)$$

548 where  $\beta_{sph} = \left( 4 / (2 - 3\cos \theta_{D_m} \sin^2 \theta_{D_m} - 2\cos^3 \theta_{D_m}) \right)^{1/3}$ ,  $\theta_{D_m}$  is the apparent contact angle at the  
549 maximum spread. Because  $\theta_{D_m}$  is difficult to measure and the  $\theta_{D_m}$  is very close to the advancing contact

550 angle  $\theta_{adv}$  for many surfaces as shown in [49],  $\theta_{D_m}$  is assumed to equal to  $\theta_{adv}$  in this paper.

551 During the spreading process, the contact line dissipation caused by the friction force at the contact  
 552 line can be calculated through [49]:

$$W_{cl} = \frac{\pi D_m^2}{4} \sigma_{GL} (\cos \theta_Y - \cos \theta_{adv}) \quad (33)$$

553 Therefore, summing up Eqs. (30), (31) and (33),  $W$  can be expressed as:

$$W = \frac{\pi \rho u_0^2 D_m^3}{16 \sqrt{Re}} + \alpha \frac{\pi \rho u_c^2 D_m^3}{16 \sqrt{Re_c}} + \frac{\pi D_m^2}{4} \sigma_{GL} (\cos \theta_Y - \cos \theta_{adv}) \quad (34)$$

554 Then, substitute Eqs. (22), (26), (27) and (34) into Eq. (21), and introduce the maximum spread  
 555 factor  $D_m^*$ , which is defined as  $D_m^* = D_m/D_0$ ,  $\Delta A_{GL}$  can be expressed as:

$$\Delta A_{GL} = \frac{\rho \frac{\pi D_0^3}{6} \left( 0.5u_0^2 + g \left( H_0 - \frac{D_0}{3D_m^{*2}} \right) \right) - \frac{\pi \rho u_0^2 D_0^3 D_m^{*3}}{16 \sqrt{Re}} - \alpha \frac{\pi \rho u_c^2 D_0^3 D_m^{*3}}{16 \sqrt{Re_c}}}{\sigma_{GL}} + \frac{\pi D_0^2 D_m^{*2}}{4} \cos \theta_{adv} \quad (35)$$

556 The dimensionless maximum gas-liquid interfacial area is defined as  $A_{GLm}^* = A_{GLm}/A_{GL0} = 1 +$   
 557  $\Delta A_{GL}/A_{GL0}$ , where  $A_{GL0} = \pi D_0^2$ ,  $A_{GLm}$  is the maximum gas-liquid interfacial area. Therefore,  $A_{GLm}^*$  can  
 558 be expressed as:

$$A_{GLm}^* = 1 + \frac{\rho D_0 \left( 0.5u_0^2 + g \left( H_0 - \frac{D_0}{3D_m^{*2}} \right) \right) - \frac{\rho u_0^2 D_0 D_m^{*3}}{16 \sqrt{Re}} - \alpha \frac{\rho u_c^2 D_0 D_m^{*3}}{16 \sqrt{Re_c}}}{\sigma_{GL}} + \frac{D_m^{*2}}{4} \cos \theta_{adv} \quad (36)$$

## 559 4.2. Results comparison

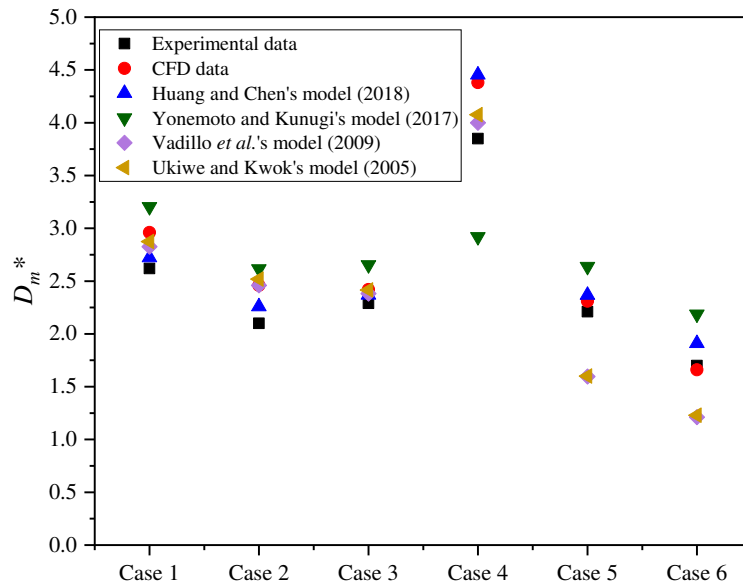
560 The maximum spread factor  $D_m^*$  is a critical factor for calculating the  $A_{GLm}^*$  by Eq. (36). In addition  
 561 to the experimental measurements, a series of models for predicting  $D_m^*$  have been developed based on  
 562 different approaches [14, 41-45, 48-53]. Several widely used or recently established models [43, 48, 53]  
 563 were selected for predicting the  $D_m^*$  in Case 1-6, and the predicted results were compared with the results  
 564 from the experimental measurements and CFD simulations, as shown in Fig. 13. Cases 7 and 8 were not  
 565 used for comparison because of the asymmetry and fragmentation of the droplets. In Cases 1-4, the  
 566 difference of the predicted  $D_m^*$  by the Ukiwe and Kwok model [43] and the experimental data is within  
 567 20%, but  $D_m^*$  is underestimated in Cases 5-6, where a high viscosity liquid was used. The Vadillo et al.  
 568 model [53] gave a slightly better prediction of  $D_m^*$  than the Ukiwe and Kwok model for Cases 1-4, but

569  $D_m^*$  was also underestimated in Cases 5-6. This means the above two models are not suitable for high  
570 viscosity liquids. The Yonemoto and Kunugi model [48] overestimated  $D_m^*$  by about 25% in all the cases  
571 except Case 4, where the  $D_m^*$  was massively underestimated. In the Yonemoto and Kunugi model [48],  
572 the simple averaged contact angle of the static and advancing contact angles are used. Since the  
573 static contact angles were not reported in the references for the experimental data, they were calculated  
574 according to the Tadmor model [66], which might produce some deviations. The Huang and Chen  
575 model [45] gave a better prediction of  $D_m^*$  compared with the other theoretical models except Case 4,  
576 where a hydrophilic surface was used. For Case 4, the predicted  $D_m^*$  by the Huang and Chen model [45]  
577 was about 16% higher than the experimental data, but it was close to the CFD simulation result. The  
578 error is likely a result of the difficulty in accurately measuring the very small contact angle of the  
579 employed hydrophilic surface. Therefore, the model developed by Huang and Chen [45] was  
580 recommended for predicting  $D_m^*$  in this paper, and it is expressed as follows:

$$\frac{3}{4} \left( \frac{We}{\sqrt{Re}} + \frac{We_c}{\sqrt{Re_c}} \right) D_m^{*4} + 3(1 - \cos \theta_{adv}) D_m^{*3} - (We + 12) D_m^* + 8 = 0, u_0 < u_c, \quad (37)$$

$$\frac{3}{4} \left( \frac{We_c}{\sqrt{Re_c}} \frac{Re_c}{Re} + \frac{We}{\sqrt{Re}} \right) D_m^{*4} + 3(1 - \cos \theta_{adv}) D_m^{*3} - (We + 12) D_m^* + 8 = 0, u_0 \geq u_c$$

581 where  $We^* = \rho D_0 u_c^2 / \sigma_{GL}$ ,  $Re_c = \rho D_0 u_c / \mu$  and  $u_c$  is expressed in Eq. (32).



582

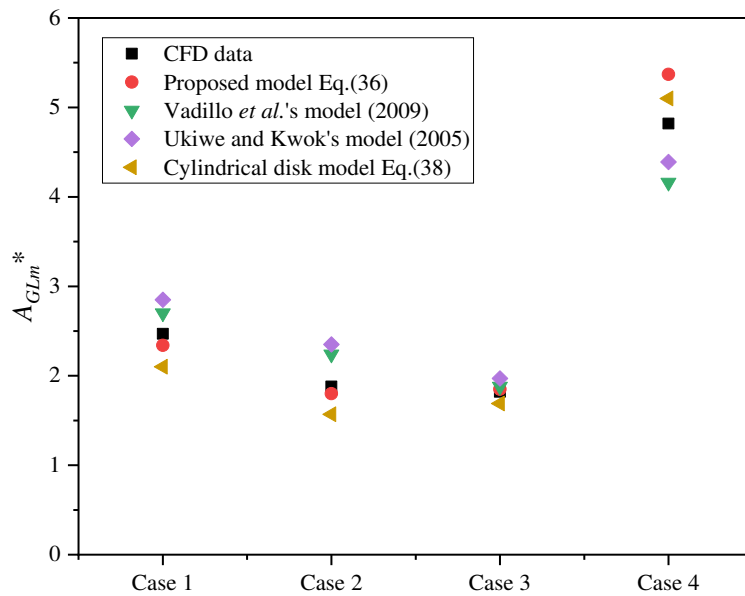
583 **Fig. 13.** Comparison of the  $D_m^*$  predicted by different theoretical models [43, 45, 48, 53] with the  
584 experimental and CFD simulation results for the investigated cases [14-16, 23, 24].

585 At present, the widely used maximum gas-liquid interfacial area model is the cylindrical model

586 [43], which assumes that the droplet spreads into a cylindrical disk with a base diameter  $D_m$  at the  
 587 maximum spread. The gas-liquid interfacial area is the sum of the top surface area and the side area of  
 588 the cylinder, and  $A_{GLm}^*$  is expressed as follows:

$$A_{GLm}^* = \frac{A_{GLm}}{A_{GL0}} = \frac{\frac{\pi D_m^2}{4} + \pi D_m \frac{2D_0^3}{3D_m^2}}{\pi D_0^2} = \frac{D_m^{*2}}{4} + \frac{2}{3D_m^*} \quad (38)$$

589 In addition, similar to Eq. (36), different  $A_{GLm}^*$  models can be derived by using different  
 590 combinations of dissipation works and contact angles. Two models were developed by us based on the  
 591 equations in literatures [43, 53], and the predicted results by these models are shown in Fig. 14. The  $D_m^*$   
 592 used in these models were calculated by Eq. (37). Since there was no available experimental data of the  
 593 gas-liquid interfacial area, the CFD simulation results were used as a reference for comparisons. Since  
 594 most of the models were not applicable to high viscosity droplets, only Cases 1 – 4 were used for  
 595 comparing the prediction results. The predicted results from all these models show a consistent variation  
 596 trend. In addition, the difference between the  $A_{GLm}^*$  predicted by Eq. (36) and from CFD simulations is  
 597 within 12%. The maximum differences between the prediction results based on the models of Vadillo et  
 598 al. [53] and Ukiwe et al. [43] and the simulation results are 20% and 25%, respectively. For the  
 599 cylindrical model Eq. (38), the differences between the predicted  $A_{GLm}^*$  and the CFD simulation results  
 600 are within 16%.



601  
 602 **Fig. 14.** Comparison of the  $A_{GLm}^*$  from the CFD simulation and different models.

### 603 4.3. *Remarks on the maximum gas-liquid interfacial area model*

604 In this paper, a maximum gas-liquid interfacial area correlation is derived from analysing the  
605 energy conversion of the droplet when it impacts on a solid surface, which has shown a good prediction  
606 performance. Compared with the shape approximation methods, the energetic modelling method can  
607 clearly identify the main factors that affect the change of the gas-liquid interfacial area. It can be seen  
608 from the model that increasing the impact velocity, reducing the surface tension of the liquid, and  
609 reducing the gas-liquid advancing contact angle can promote the increase of the gas-liquid interfacial  
610 area. The higher the viscosity of the liquid, the more energy is dissipated during the impact, which  
611 weakens the increase in the gas-liquid interfacial area. In engineering applications, identifying major  
612 and minor factors that affect the change of the interfacial area can provide guidance for optimization.  
613 The accuracy of the model depends largely on the calculation of the dissipative work. Therefore, further  
614 efforts should be made to better describe the effect of dissipation. Also, accurately describing the  
615 evolution of the dynamic contact angle during the droplet impact on the solid surface is a way to improve  
616 the accuracy of the model, which is currently still a topic of ongoing research. In addition,  $D_m^*$  is a  
617 critical parameter for influencing the accuracy of all the interfacial area predictive models. Therefore,  
618 developing high reliability  $D_m^*$  models with a broad adaptive condition is very important for predicting  
619 the gas-liquid interfacial area accurately.

## 620 **5. Conclusions**

621 (i) Both 2D and 3D CFD simulations have been performed to investigate the variation of the  
622 interfacial areas when droplets impact on solid surfaces. In order to obtain the accurate data of interfacial  
623 areas, the VOF model with the dynamic contact angle and the local grid refinement techniques have  
624 been used, and the dynamic behaviours of the droplets have been accurately reproduced. The CFD model  
625 was validated through comparing with the available experimental data from experiments conducted over  
626 a wide range of surface properties and liquid properties.

627 (ii) The simulation results show that the gas-liquid interfacial area slightly decreases at the kinetic  
628 stage, then increases at the spreading stage, and it reaches the maximum at the end of the spreading  
629 stage. A large initial impact velocity leads to a large increase in the gas-liquid interfacial area, while a

630 high viscosity weakens the increase in the interface area due to the increase in dissipation work. For the  
631 droplet impact on a hydrophilic surface, the hydrophilic surface can promote the increase in the gas-  
632 liquid interfacial area by releasing the liquid-solid interface energy. Meanwhile, for the droplet  
633 impacting on a hydrophobic surface, the gas-liquid interfacial area can be enhanced by breaking up the  
634 droplet into small droplets.

635 (iii) By analysing the energy conversion of the droplet impact on a solid surface, a new correlation  
636 for predicting the maximum gas-liquid interfacial area of the droplet has been proposed. The accurate  
637 dissipative work equation is the basis of the accurate prediction of the gas-liquid interface area.  
638 Compared with the CFD simulation results and other models, the new correlation has been shown to be  
639 a good prediction of the performance. In addition, this study leads to a much better understanding of the  
640 behaviour of the interface areas when droplets impact on a solid surface.

641

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647 studies.

648

## 649 **Nomenclature**

$A_{GL}$	gas-liquid interfacial area
$A_{SG}$	solid-gas interfacial area
$A_{SL}$	solid-liquid interfacial area
$A_0$	initial gas-liquid interfacial area of the droplet
$A^*$	gas-liquid interfacial area factor
$D$	the diameter of the liquid-solid contact interface
$D_0$	initial droplet diameter
$D_m$	maximum spread diameter
$D_m^*$	maximum spread factor

$E_k$	the initial kinetic energy
$E_p$	the potential energy
$E_s$	the total surface energy
$f_{vol}$	surface tension source term
$h_m$	height of the droplet at the maximum spread
$k$	the curvature of the interface
$N$	unit normal vector
$p$	pressure
$t^*$	dimensionless time
$t_c$	the characteristic time
$t_m$	time at the end of the spreading stage
$t_m^*$	maximum spreading dimensionless time
$u$	velocity
$u_{cl}$	contact line velocity
$u_0$	initial impact velocity
$W$	the energy loss due to dissipation

*Greek symbols*

$A$	volume fraction
$\theta_{adv}$	advancing contact angle
$\theta_d$	dynamic contact angle
$\theta_{rec}$	receding contact angle
$\varepsilon_L$	liquid holdup
$\mu$	dynamic viscosity
$\nu$	kinematic viscosity
$\rho$	density
$\sigma_{GL}$	surface tension coefficient of liquid
$\sigma_{SG}$	the solid-gas interfacial energy
$\sigma_{SL}$	the solid-liquid interfacial energy
$\varphi$	signed distance to the interface in level-set method
$\Phi$	viscous dissipation function
$\Omega$	the volume where the dissipation occurs
$\delta$	thickness of the boundary layer

*Subscripts*

$G$	gas phase
$L$	liquid phase

<i>Ca</i>	capillary number
<i>Oh</i>	Ohnesorge number
<i>Re</i>	Reynolds number
<i>We</i>	Weber number
<i>WFM</i>	wetting force model

651

652 **References**

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