Wetting effects on the dynamics of droplets and bubbles at surfaces

Yifan Han[1], Kerstin Eckert[1,2], Gerd Mutschke[1]

1 Helmholtz-Zentrum Dresden-Rossendorf, Institute of Fluid Dynamics, Dresden, Germany
2 Technical University of Dresden, Institute of Process Engineering and Environmental Technology, Dresden, Germany

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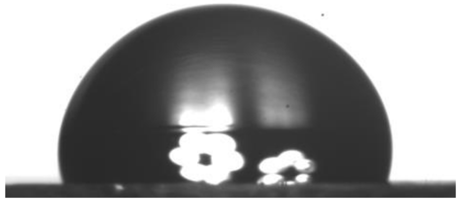
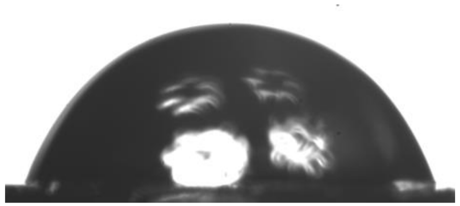
1. Wetting

Wetting describes how a liquid spreads on or adheres to a solid surface.

Static contact angle (θ_s)



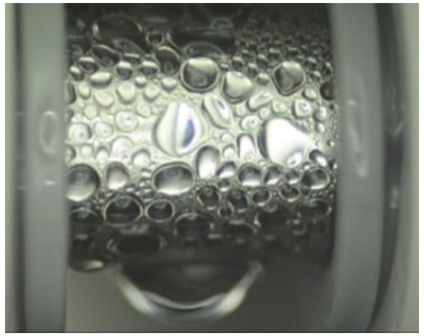
Hydrophobic
$\theta_s > 90°$



Hydrophilic
$\theta_s < 90°$

Applications:

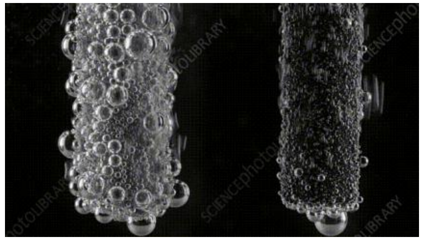
- **Droplets**



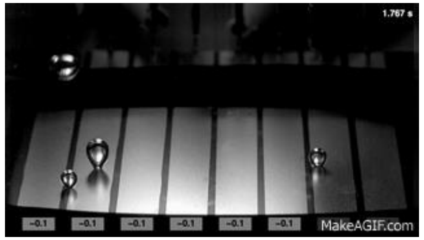
Cooling

Coating

- **Bubbles**

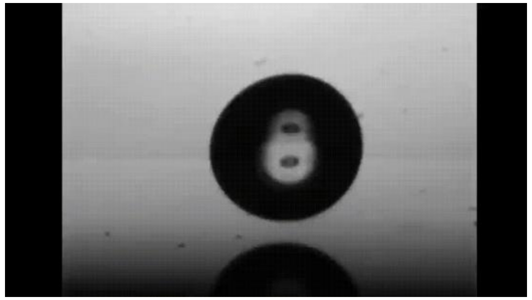


Water Electrolysis

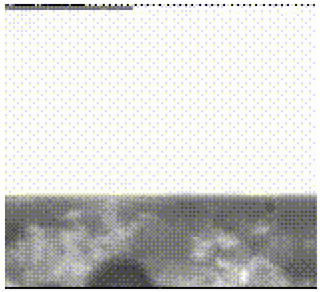


Boiling

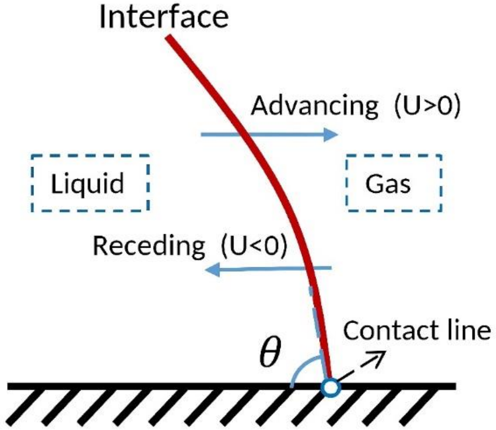
2. Dynamic wetting



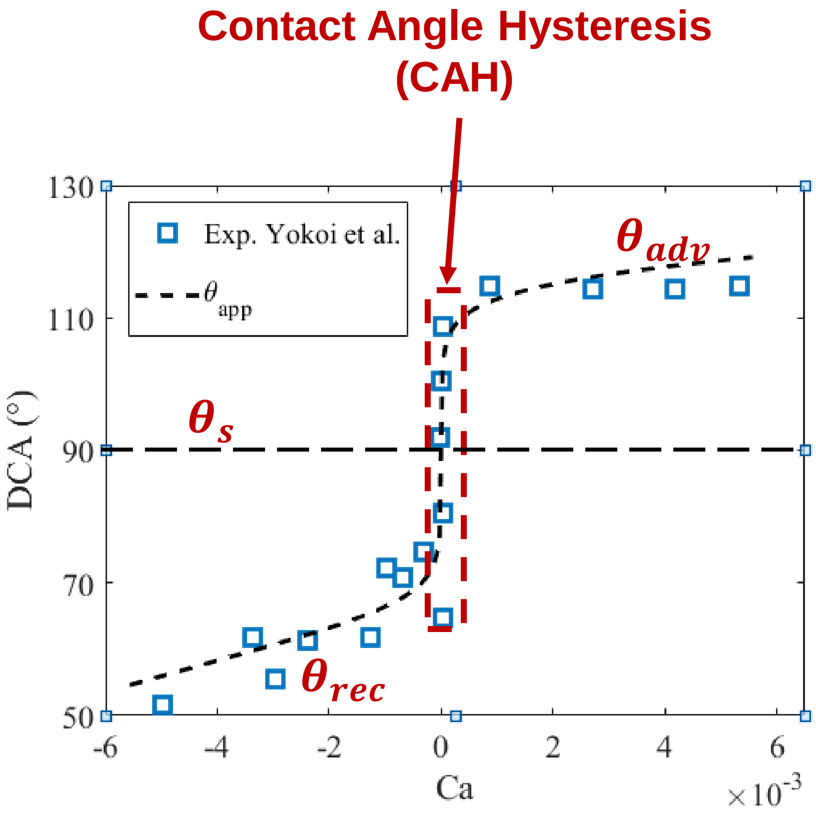
Droplet impact



Bubble growth



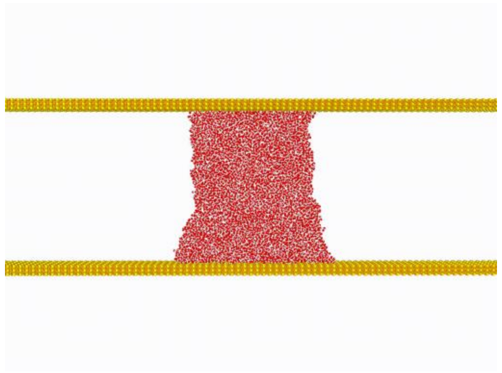
Sketch of contact line



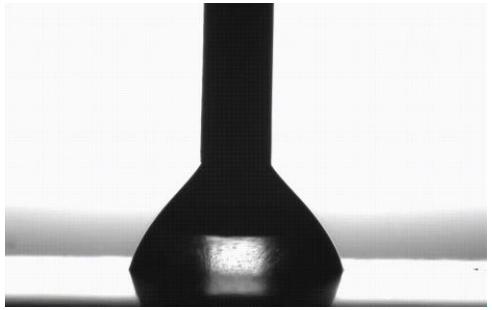
Contact angle VS Capillary number (contact velocity)

$$Ca = \mu U_{CL}/\gamma$$

Microscopic



Macroscopic



[1] Yokoi et al. Physics of Fluids, 2009, 21(7).
[2] Li et al. Colloids and Surfaces A: Physicochemical and Engineering Aspects 673 (2023): 131879.

3. Literature Review

- **Level-Set Method:**
  Interface normal projection
  Spelt. 2005 JCP, Yokoi et al. 2009 POF, Zhang et al. 2020 JCP.

- **Phase-Field Method**
  Surface-energy formulation
  Ding et al. 2007 PRE, Yue et al. 2010 JFM, Yue et al. 2011 POF.

→ **Continuous interface**

- **Volume of Fluid Method**
  Height function
  Afkhami et al. 2009 JCP, (Interfacial cell center velocity)
  Dupont & Legendre 2010 JCP, (Interpolation velocity at f=0.5)
  Fullana et al. 2025. (Time derivative of the contact line)

→ **Sharp interface**

4. Droplet spreading on a surface

Axisymetric setup

Volume of Fluid method

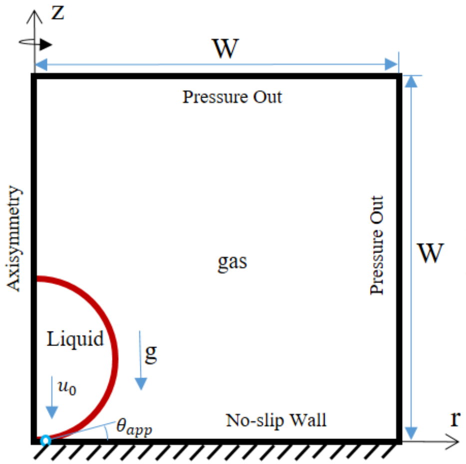
$$\rho = (1-f)\rho_g + f\rho_l, \quad \mu = (1-f)\mu_g + f\mu_l.$$

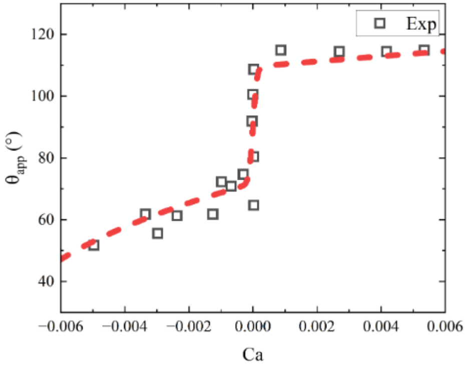
Piecewise linear interface construction (PLIC) method.

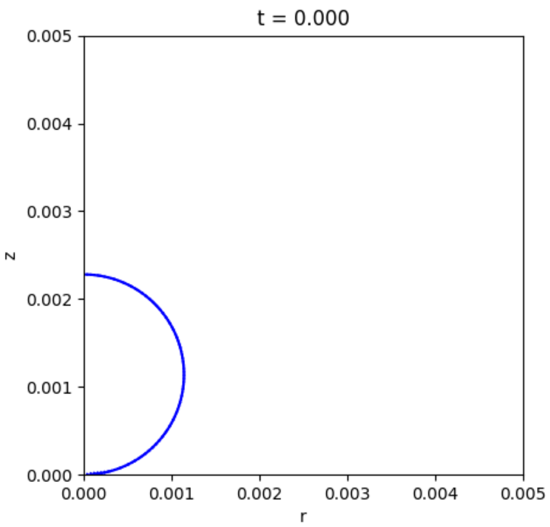
Flow fields & interface motion

$$\nabla \cdot \vec{u} = 0,$$

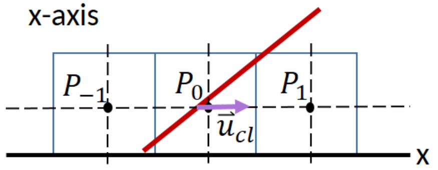
$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = -\frac{1}{\rho}\nabla p + \frac{1}{\rho}\nabla \cdot \{\mu[\nabla \vec{u} + (\nabla \vec{u})^T]\} + \vec{g} + \gamma \kappa \vec{n} \delta_\Sigma,$$







Contact line velocity



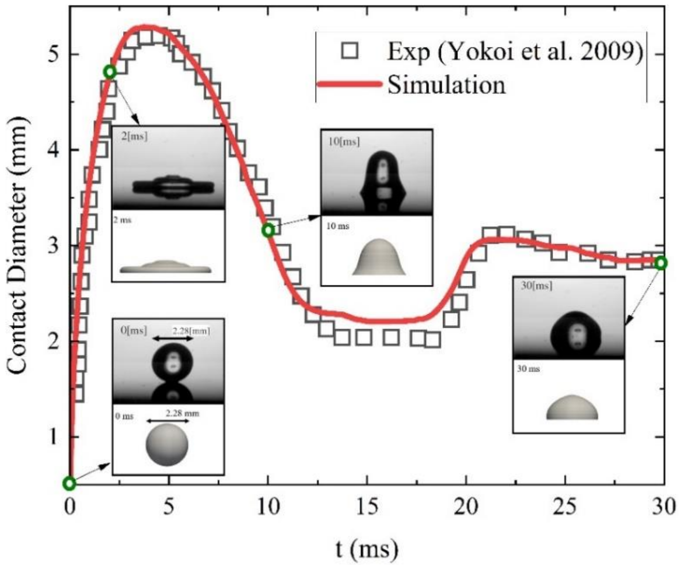
Linear Interpolation

Weber number We=31.7

Initial radius: R = 1.14 mm

Initial velocity: V = 1.0 m/s

$\theta_s(°)$	$\theta_a(°)$	$\theta_r(°)$	$\xi_a(\mathrm{Pa\cdot s})$	$\xi_r(\mathrm{Pa\cdot s})$	C	ϵ
90	109.5	72	0.002	0.002	2×10^4	1.0×10^7



[1] Yokoi et al. Physics of Fluids, 2009, 21(7).

Apparent contact angle

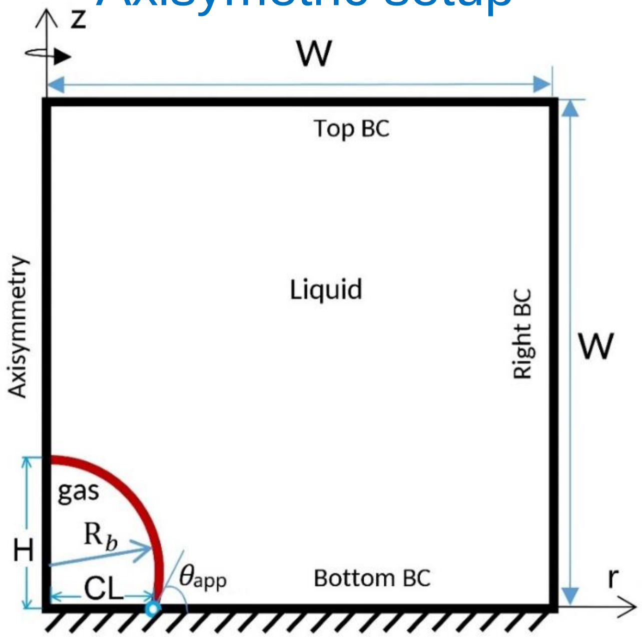
$$\theta_{local} = \arccos\left\{\cos\theta_s - \frac{\xi Ca}{\mu} - \frac{C_{pin}\tanh(C*Ca)}{\gamma}\right\}$$ **Microscopic**

$$\theta_{app}^3 = \theta_{local}^3 + 9Ca\ln(\epsilon)$$ **Macroscopic**

[2] Dwivedi et al. Physical Review Fluids, 2022, 7(3): 034002.

5. Bubble growth in oversaturated liquids

Axisymetric setup



[1] Gennari et al. Chemical Engineering Science 259 (2022): 117791.

Flow fields & interface motion

$$\nabla\cdot\vec{u} = \dot{m}\left(\frac{1}{\rho_g}-\frac{1}{\rho_l}\right)\delta_\Sigma,$$

$$\frac{\partial\vec{u}}{\partial t}+\vec{u}\cdot\nabla\vec{u} = -\frac{1}{\rho}\nabla p+\frac{1}{\rho}\nabla\cdot\{\mu[\nabla\vec{u}+(\nabla\vec{u})^T]\}+\frac{\vec{f}_\gamma}{\rho}+\vec{g},$$

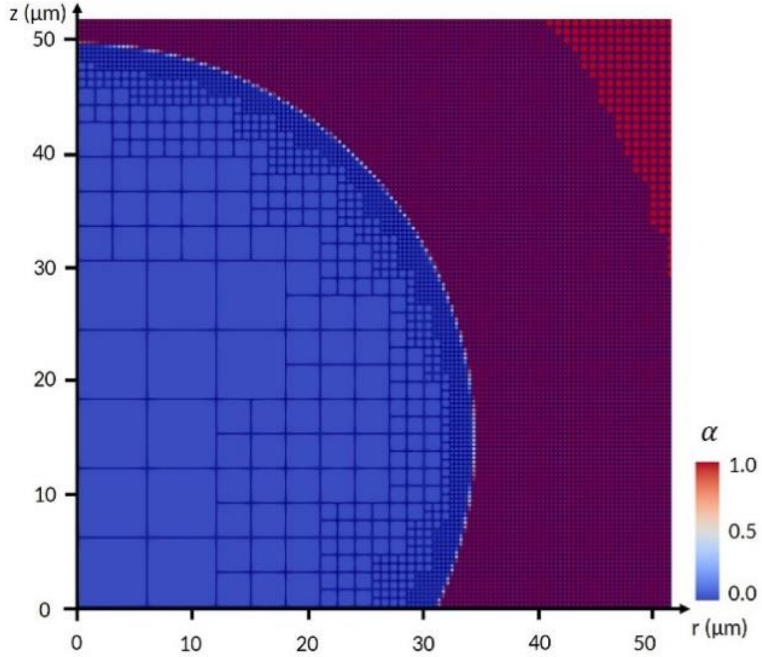
Species transport & mass flux

$$\frac{\partial\alpha}{\partial t}+\nabla\cdot(\alpha\vec{u}) = -\frac{\dot{m}}{\rho_l}\delta_\Sigma,$$

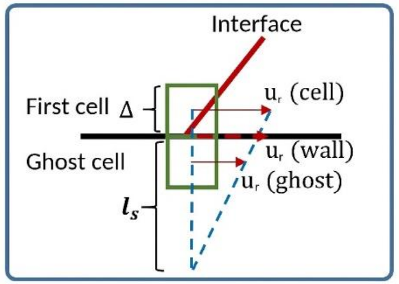
$$\frac{\partial c}{\partial t}+\vec{u}\cdot\nabla c = \nabla\cdot(D\nabla c)-\frac{\dot{m}}{M_a}\delta_\Sigma,$$

$$\dot{m} = \frac{M_g D}{1-\rho_g/\rho}\frac{\partial c}{\partial\vec{n}_\Sigma},$$

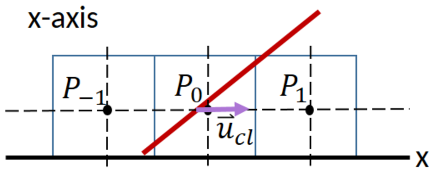
Adaptive Mesh Refinement



Navier-slip BC



Contact line velocity



Linear Interpolation

Apparent contact angle

$$\theta_{local} = \arccos\left\{\cos\theta_s - \frac{\xi Ca}{\mu} - \frac{C_{pin}\tanh(C*Ca)}{\gamma}\right\}$$ **Microscopic**

$$\theta_{app}^3 = \theta_{local}^3 + 9Ca\ln(\epsilon)$$ **Macroscopic**

[2] Dwivedi et al. Physical Review Fluids, 2022, 7(3): 034002.

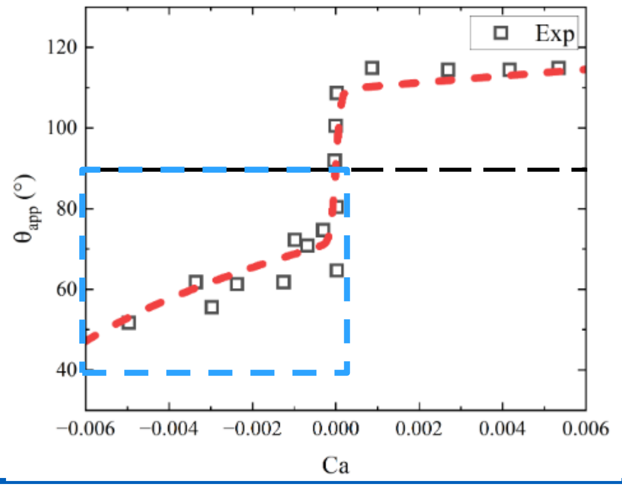
DRESDEN concept HZDR

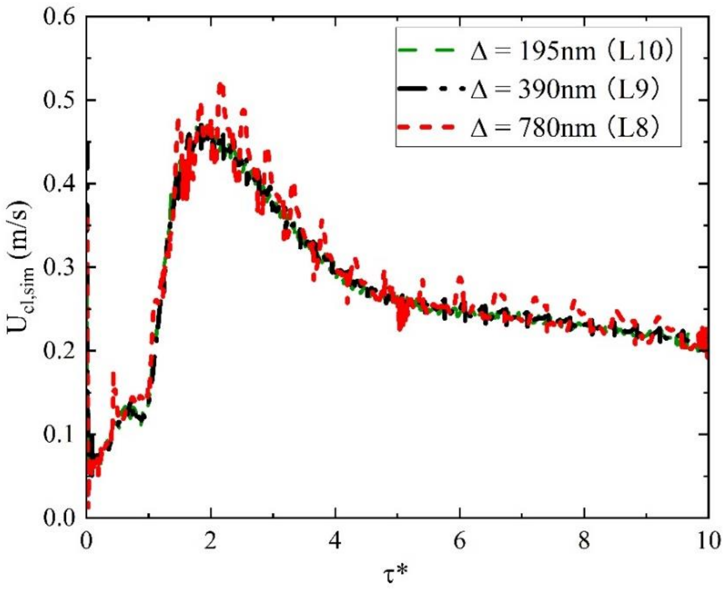
5. Bubble growth in oversaturated liquids

Validation

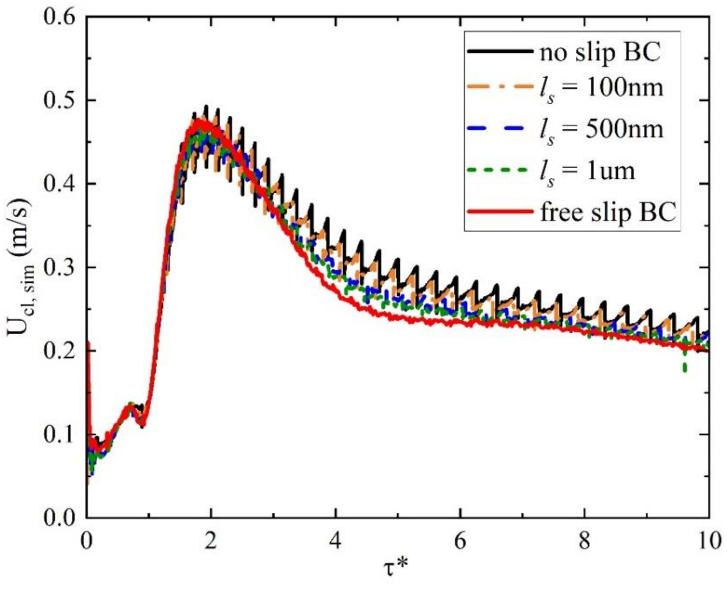
Initial setup:

- Oxygen bubble in oversaturated water;
- Bubble radius from 10 to 100 um;
- Initial contact angle: 90°;
- Oversaturation ratio: $\zeta = \frac{c_b - c_s}{c_s}$=7;
- Dynamic wetting curve:





Mesh size



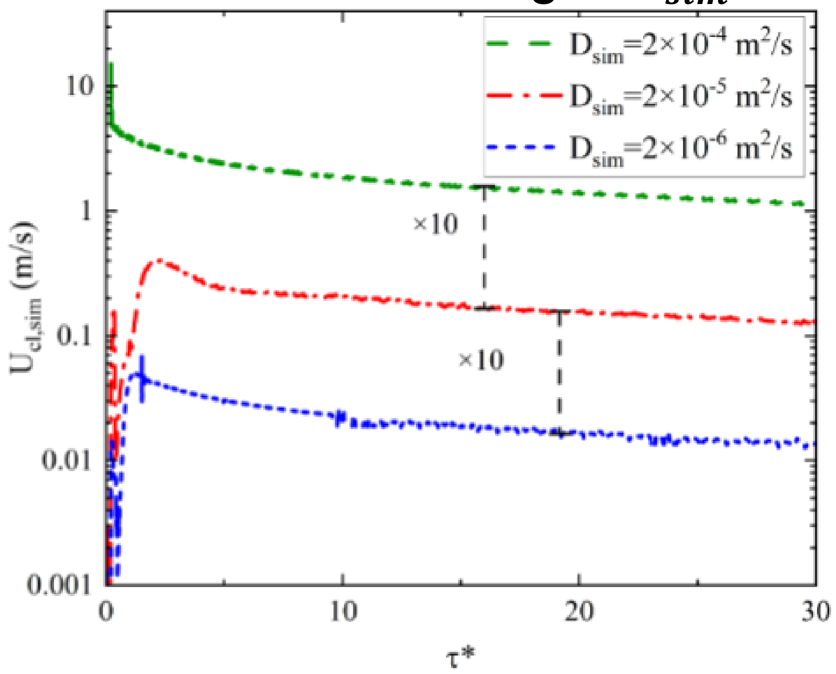
Navier slip BC

5. Bubble growth in oversaturated liquids

Issue of slow growth rates

	Boiling	Oversaturation Growth
Mass transfer rate	$10^{-3} \sim 10^{-1}\ \mathrm{kg/m^2 \cdot s}$	$10^{-7} \sim 10^{-3}\ \mathrm{kg/m^2 \cdot s}$
Timescale	Milliseconds to seconds	Seconds to Minutes
Dominant force	**Inertia force**	**Surface tension force**

Use an enlarged D_{sim}

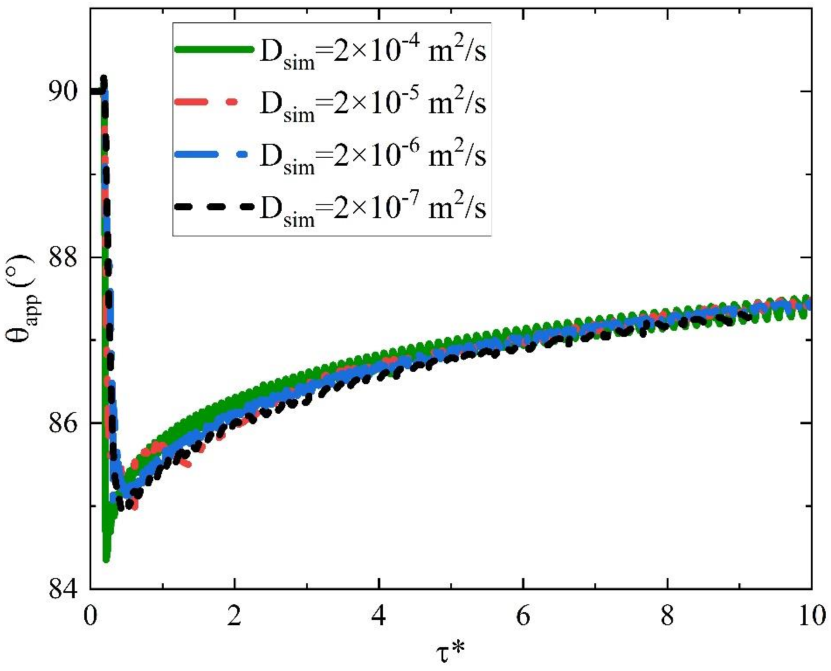


$$\mathrm{We} = \frac{\rho_l U_{cl,sim}^2 R_0}{\gamma} < 1$$

Dynamic wetting → Rescaling contact velocity

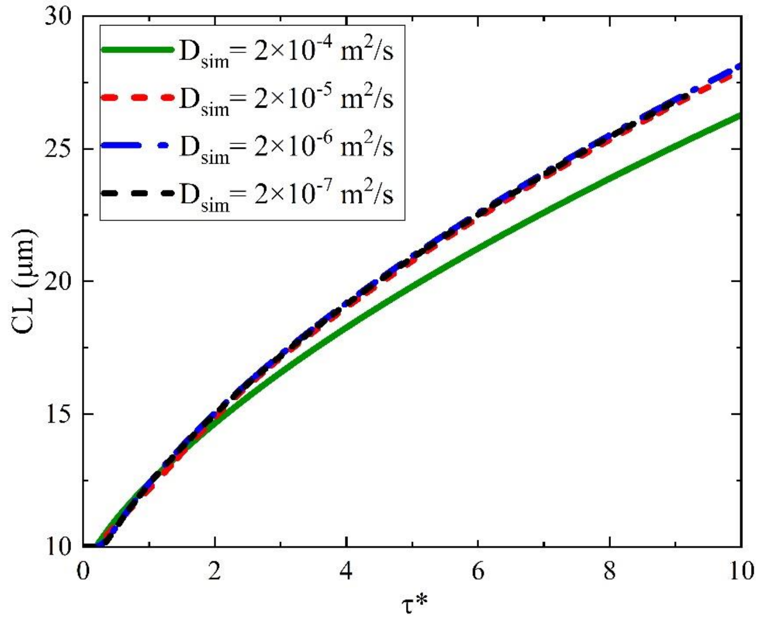
$$U_{cl,res} = U_{cl,sim} \cdot \frac{D}{D_{sim}}$$

$$t = t_{sim} \cdot \frac{D_{sim}}{D}$$

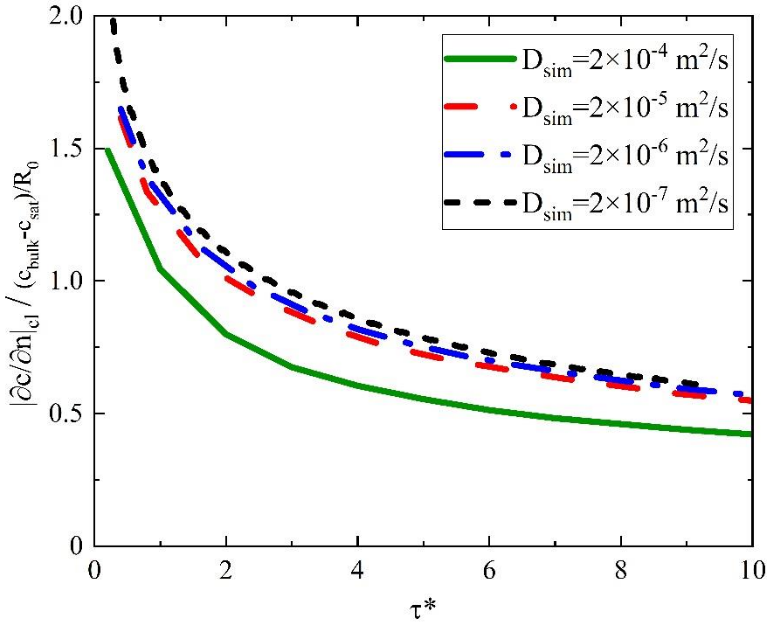


5. Bubble growth in oversaturated liquids

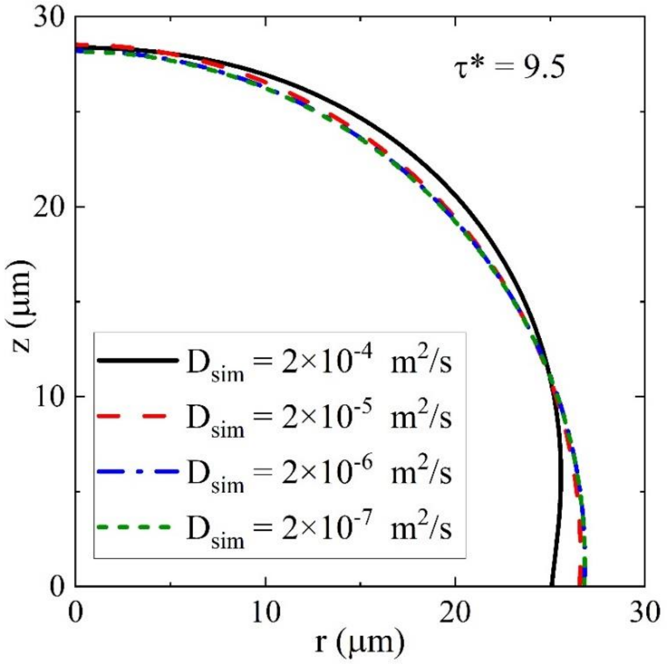
Issue of slow growth rates



Contact Line



Concentration gradient

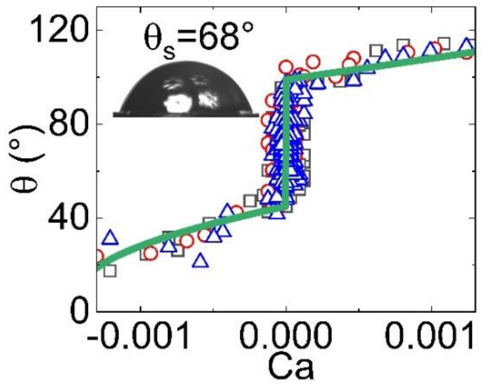


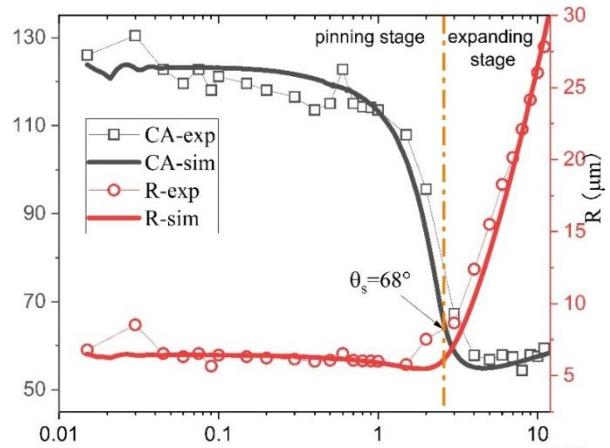
Bubble shapes

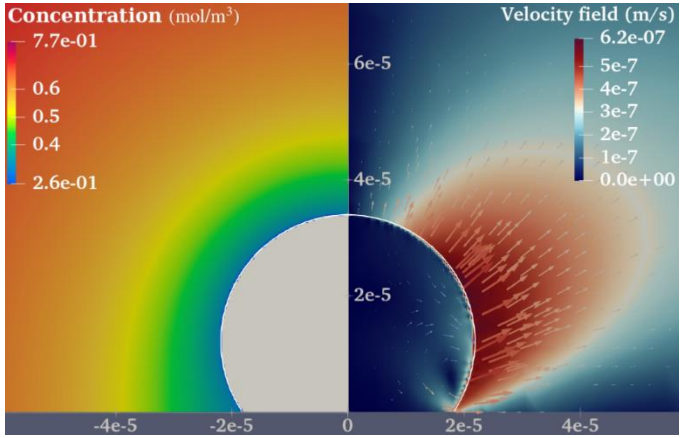
5. Bubble growth in oversaturated liquids

Validation with experimental results of single air bubble growth on two surfaces

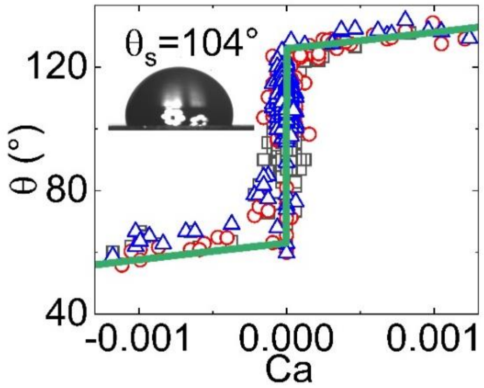
Hydrophilic surface

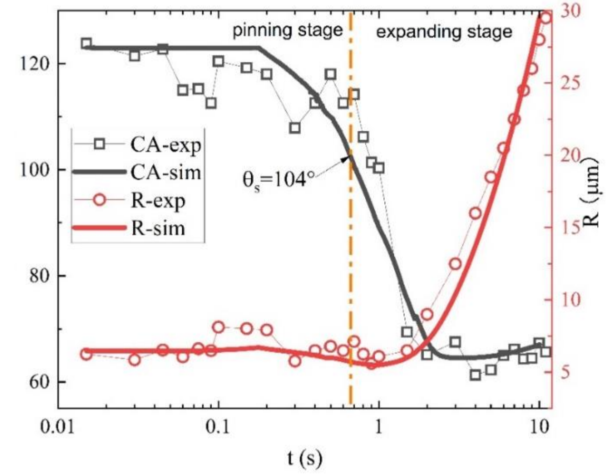


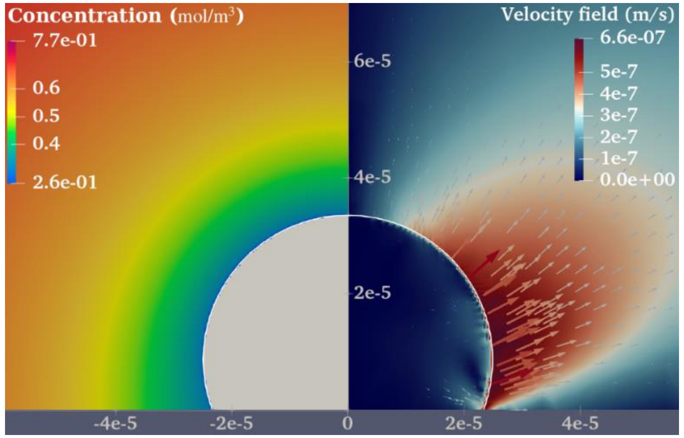




Hydrophobic surface



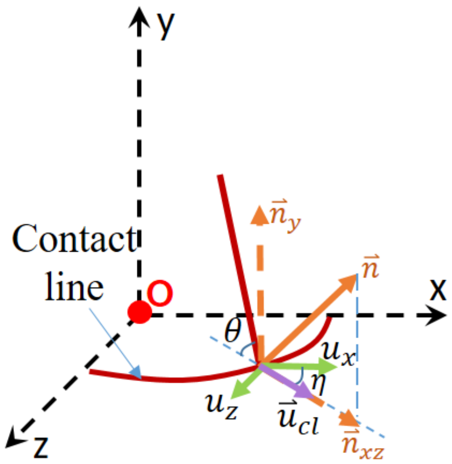




[1] Li et al. Colloids and Surfaces A: Physicochemical and Engineering Aspects 673 (2023): 131879.
[2] Han et al. Int. J. Multiph. Flow, 2025, accepted.

6. 3D Dynamic wetting

Methodology



Velocity projection

$$\eta = \tan^{-1}\left(\frac{n_z}{n_x}\right)$$

$$\vec{u}_{cl} = (u_x \cos\eta + u_z \sin\eta)\vec{e}_\eta$$

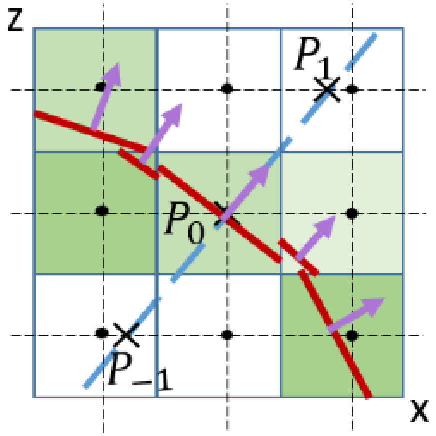
If $\vec{u}_{cl} \cdot \vec{n}_{xz} > 0$, advancing
If $\vec{u}_{cl} \cdot \vec{n}_{xz} < 0$, receding

$$\theta = \theta(\vec{u}_{cl})$$

Geometrical interface interpolation

The contact angle need to be set at each point. $u_{cl,i} \rightarrow \theta_i$

xz-plane

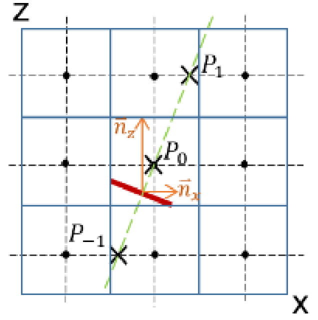


[1] Han et al. 2025, in preparation.

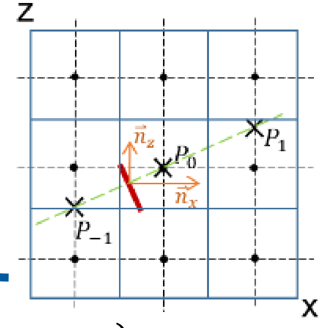
Algorithm of contact line velocity interpolation

1. Identify all the interfacial cells at the first grid layer。
2. Compute the interface normal vector of $\boldsymbol{n}$ each cell.
3. Compare the absolute values of $\boldsymbol{n_x}$ and $\boldsymbol{n_z}$.
4. Compute the gradient of f in the normal direction. $\frac{\partial f}{\partial n} \approx \frac{f(P_1) - f(P_{-1})}{\overline{P_1 P_{-1}}}$
5. Perform a linear interpolation of x and z velocity components.

if $|n_x| < |n_z|$



if $|n_x| \geq |n_z|$

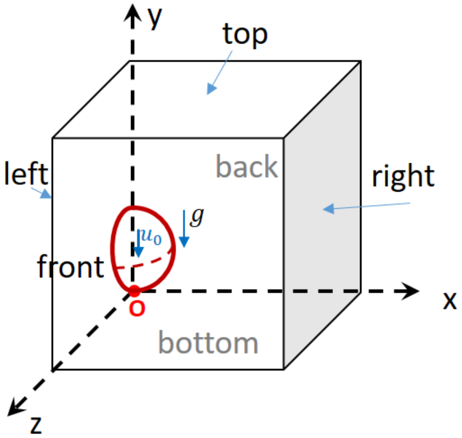


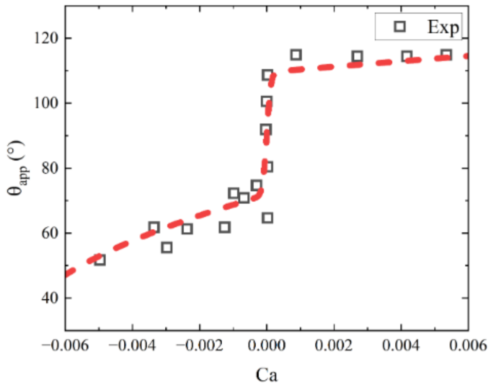
$$u_{x/z,interp} = u_{x/z}(P_0) + \frac{u_{x/z}(P_0) - u_{x/z}(P_{adj})}{f_{P_0} - f_{P_{adj}}}(f_{0.5} - f_{P_0})$$

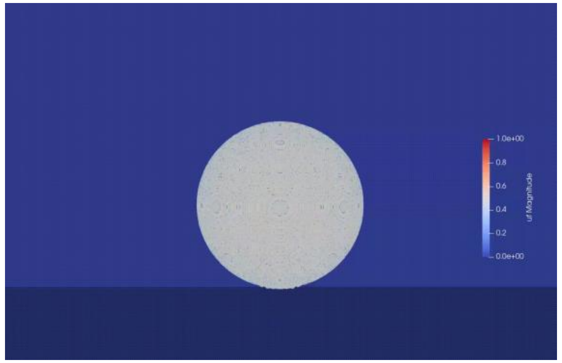
DRESDEN concept HZDR

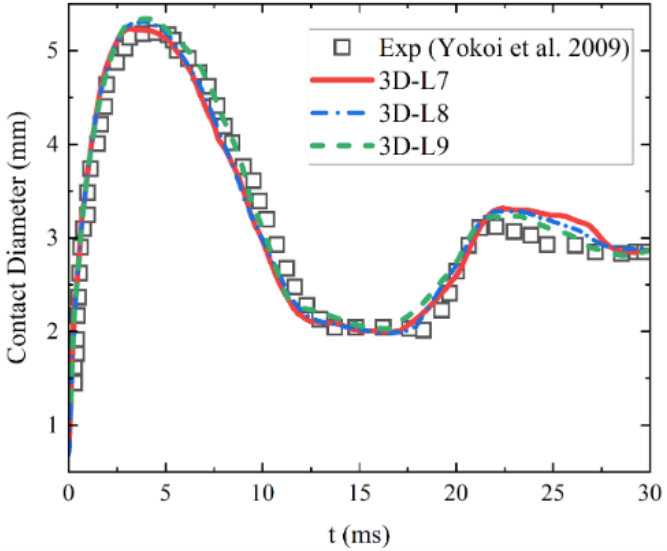
6. 3D Dynamic wetting

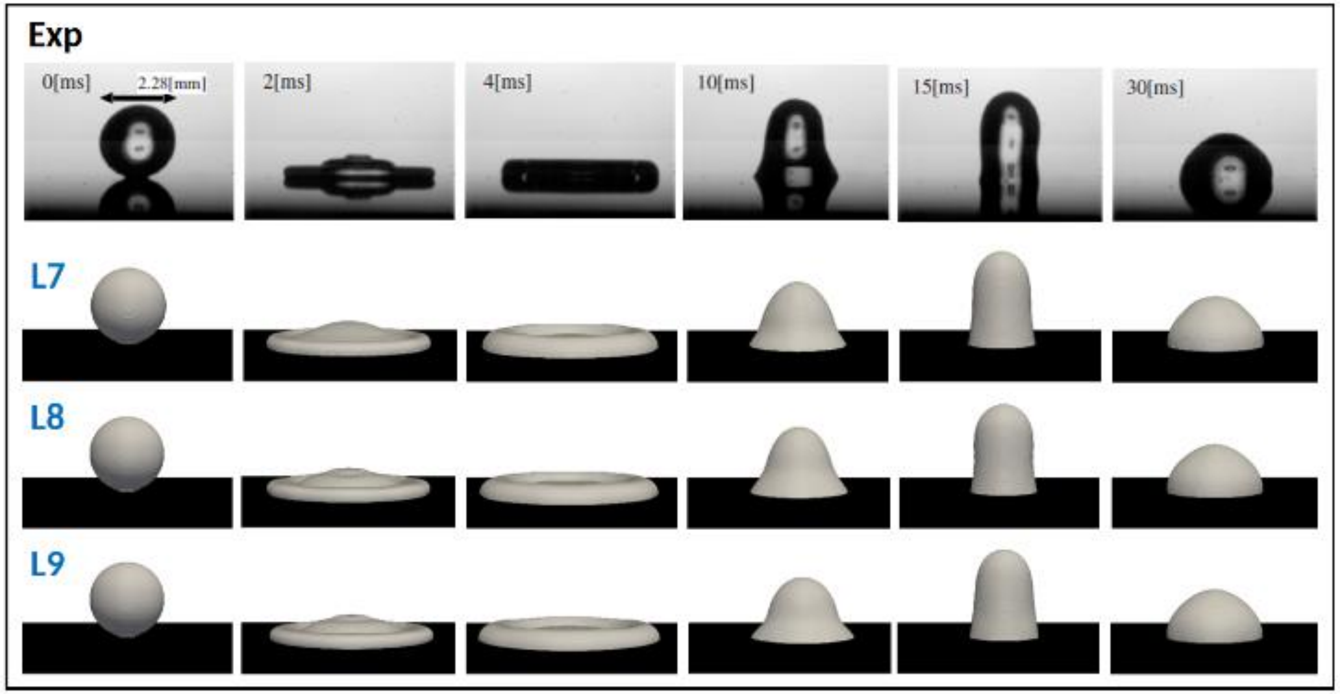
Case 1: A spreading droplet on a solid surface (low Weber number)











Weber number We=31.7

Initial radius: R = 1.14 mm

Initial velocity: V = 1.0 m/s

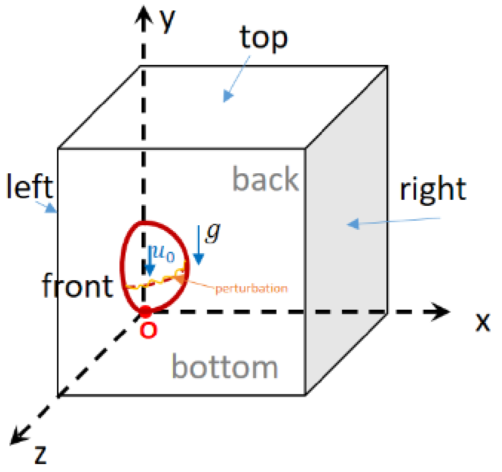
Bottom: no-slip BCs & dynamic wetting model

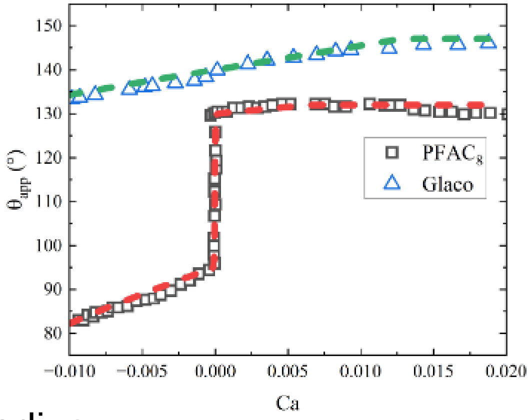
$\theta_s(°)$	$\theta_a(°)$	$\theta_r(°)$	$\xi_a(\mathrm{Pa\cdot s})$	$\xi_r(\mathrm{Pa\cdot s})$	C	ϵ
90	109.5	72	0.002	0.002	2×10^4	1.0×10^7

[1] Yokoi et al. Physics of Fluids, 2009, 21(7).

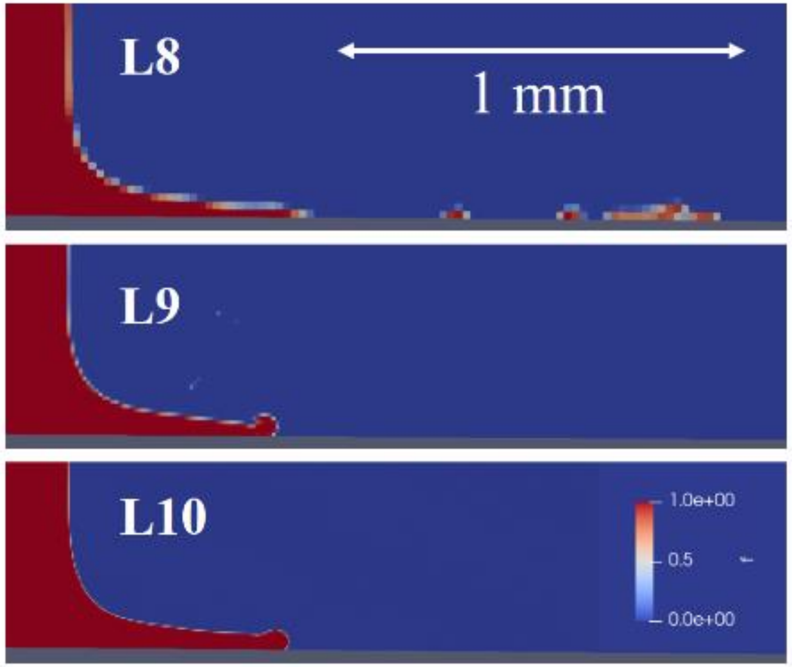
6. 3D Dynamic wetting

Case 2: A splashing droplet on hydrophilic surfaces (high Weber number)





	R_0 (mm)	u_0 (m/s)	We
PFAC8	1.224	2.34	187
Glaco	1.356	2.09	167



t = 0.3 ms

Initial perturbation of droplet radius

$$R_{0,p} = R_0 \left[1 + A_p \cos(2\pi N x) \cos(2\pi N z)\right]$$

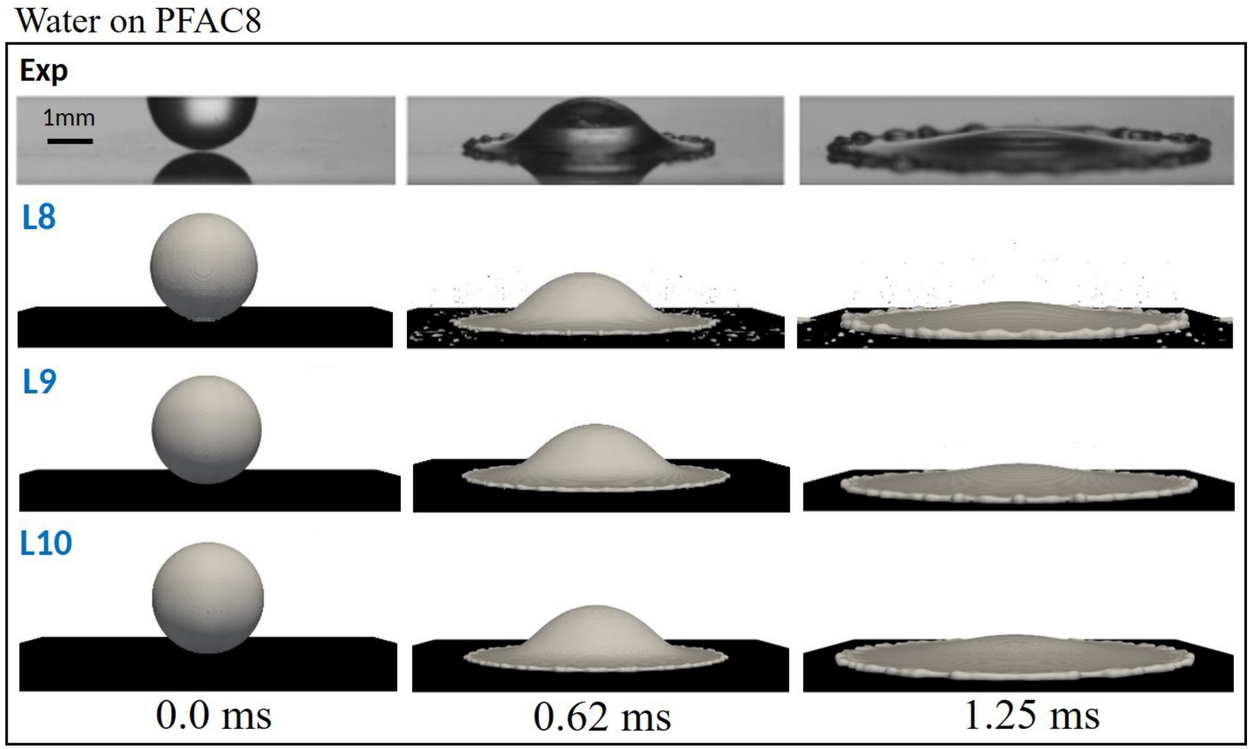
Bottom: no-slip BCs & dynamic wetting model

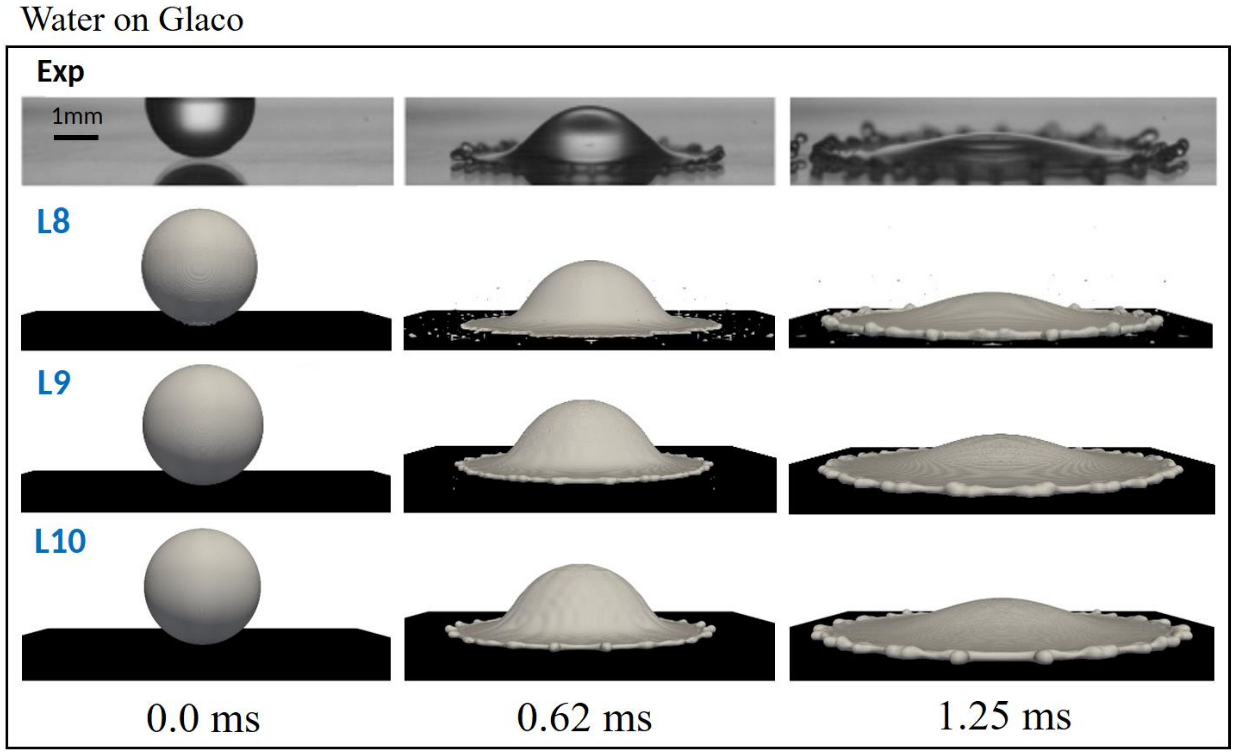
	$\theta_s(°)$	$\theta_a(°)$	$\theta_r(°)$	$\xi_a(\mathrm{Pa \cdot s})$	$\xi_r(\mathrm{Pa \cdot s})$	C	ϵ
PFAC8	120	130	95	0.0001	0.01	2×10^4	1.0×10^4
Glaco	140	147	133	0.0025	0.0025	1	1.0×10^4

[1] Quetzeri-Santiago et al. Physical review letters, 2019, 122(22): 228001

6. 3D Dynamic wetting

Case 2: A splashing droplet on hydrophilic surfaces (high Weber number)

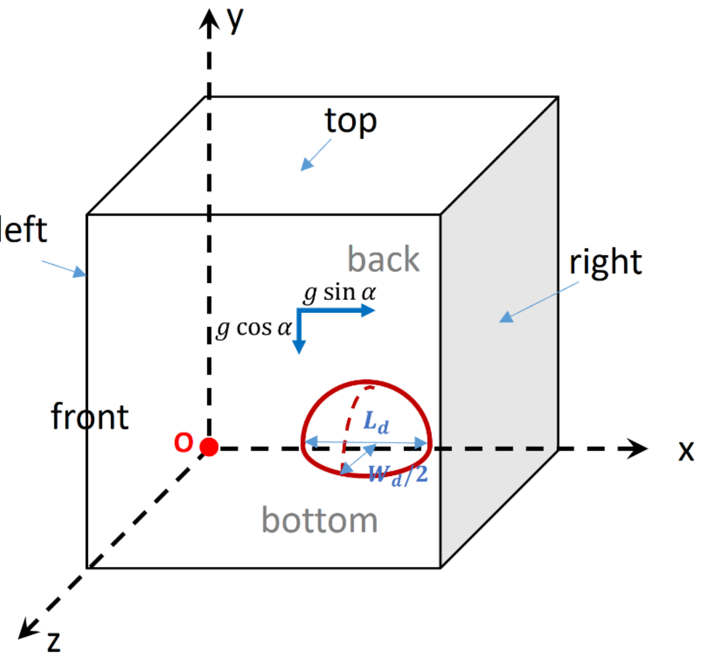




[1] Quetzeri-Santiago et al. Physical review letters, 2019, 122(22): 228001

6. 3D Dynamic wetting

Case 3: A sliding droplet on inclined surfaces

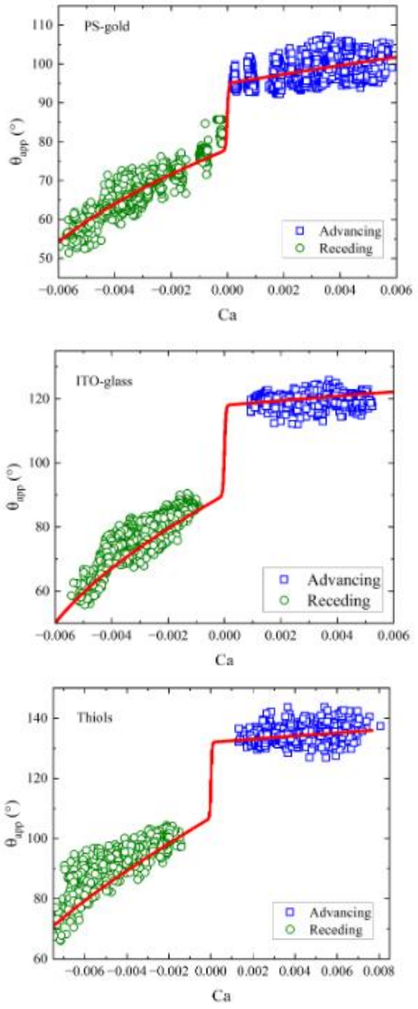


Initial radius 2.5 mm
Static contact angle
Inclined angle: α=25-70°

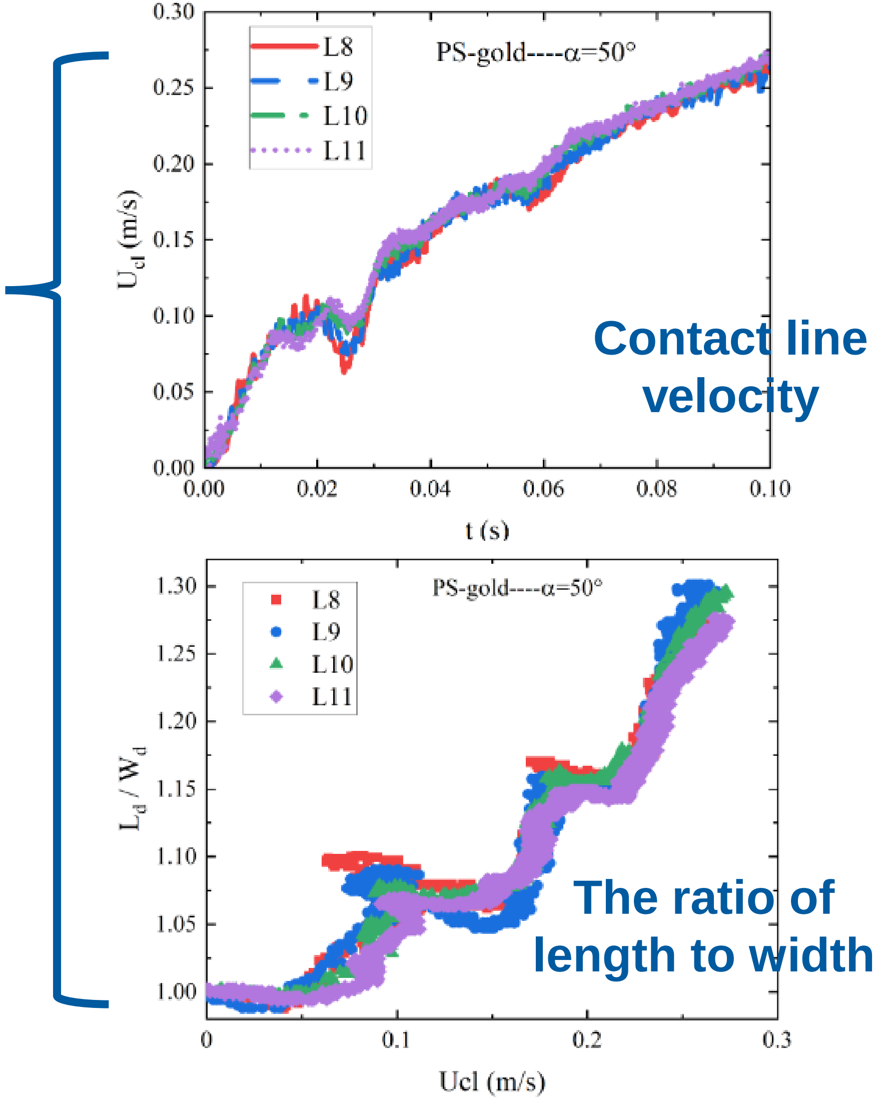
PS-gold

ITO-glass

Thiols



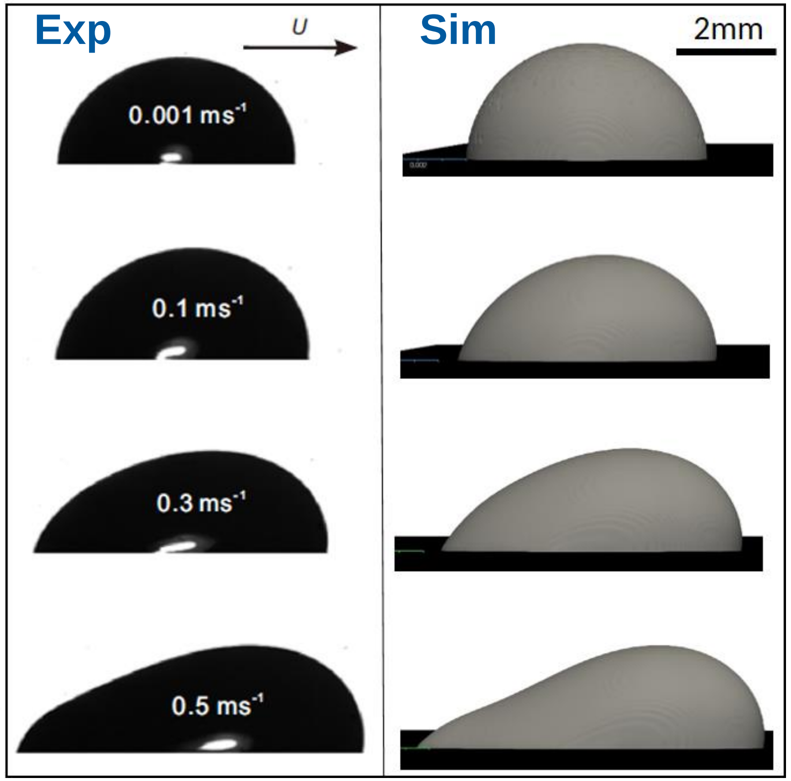
Resolution tests



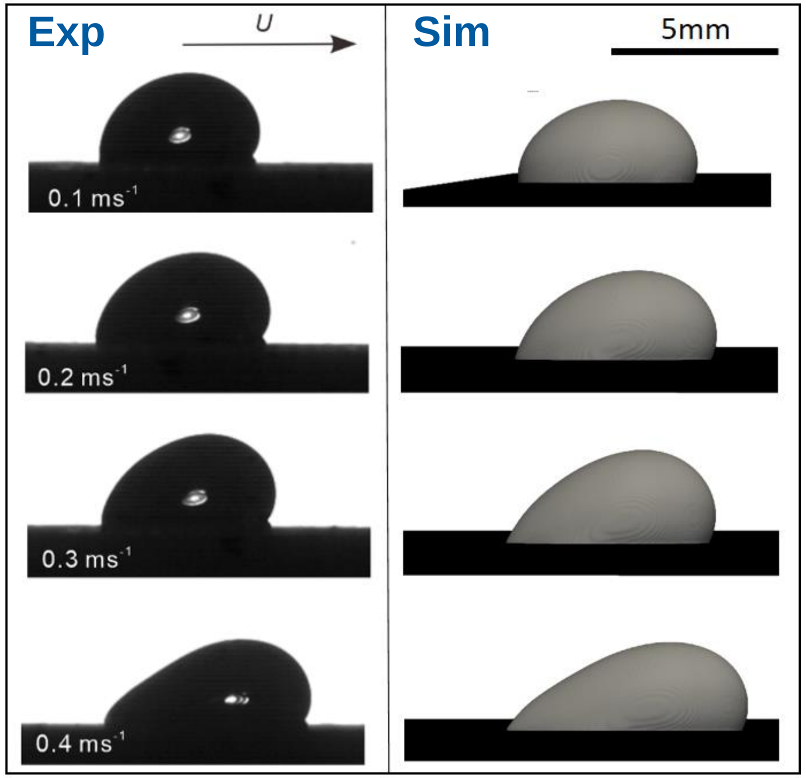
[1] Li et al. Nature communications, 2023, 14(1): 4571.

6. 3D Dynamic wetting

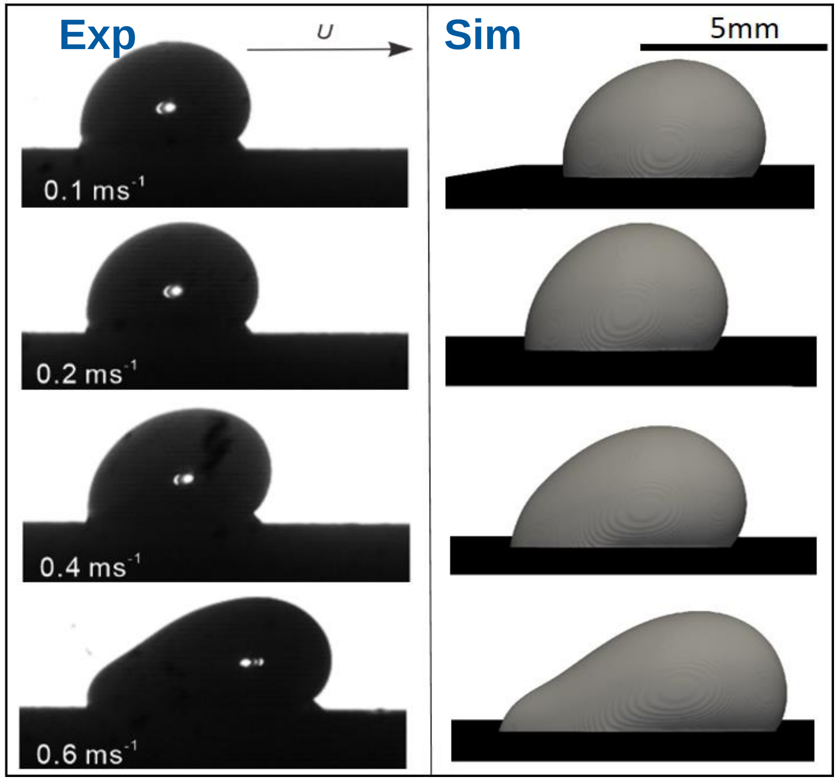
Case 3: A sliding droplet on inclined surfaces



PS-gold



ITO-glass

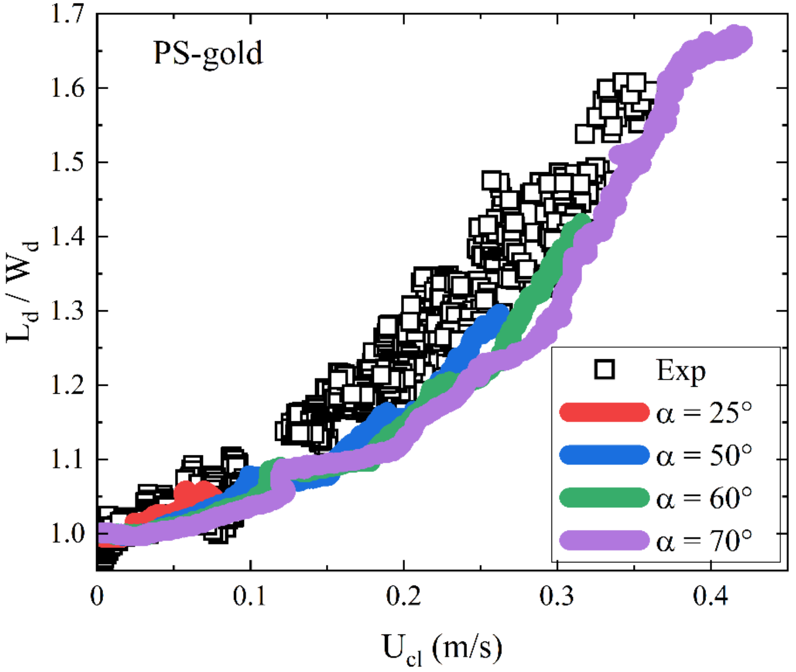


Thiols

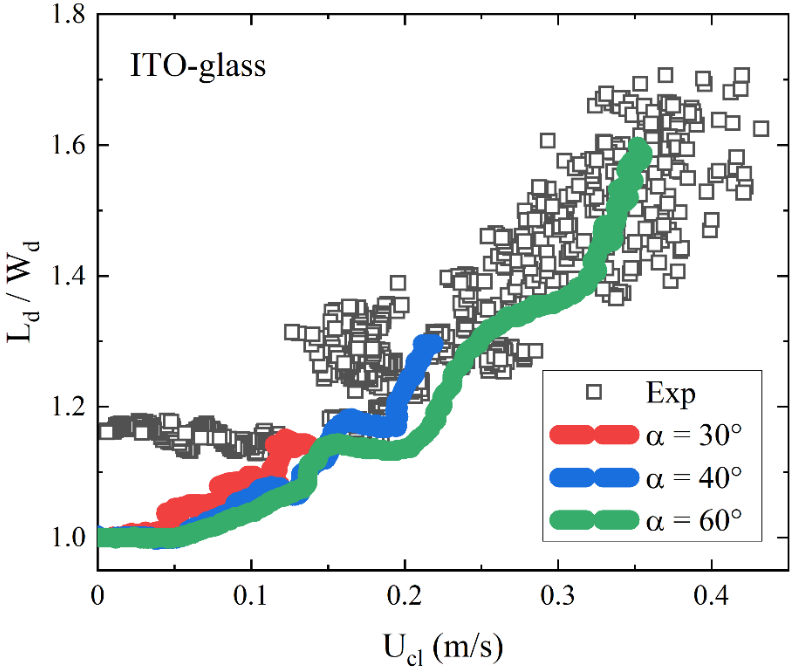
[1] Li et al. Nature communications, 2023, 14(1): 4571.

6. 3D Dynamic wetting

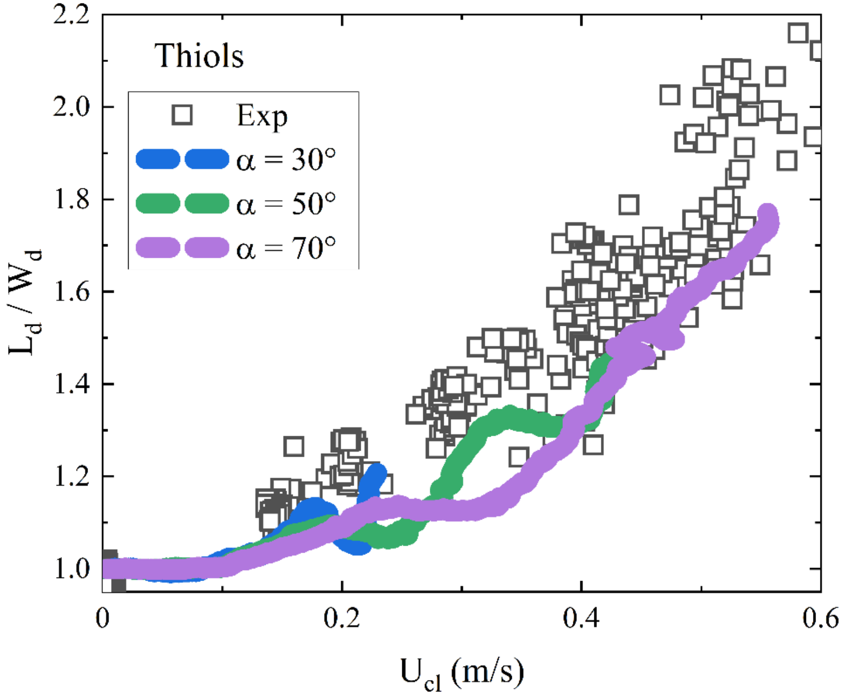
Case 3: A sliding droplet on inclined surfaces



PS-gold



ITO-glass



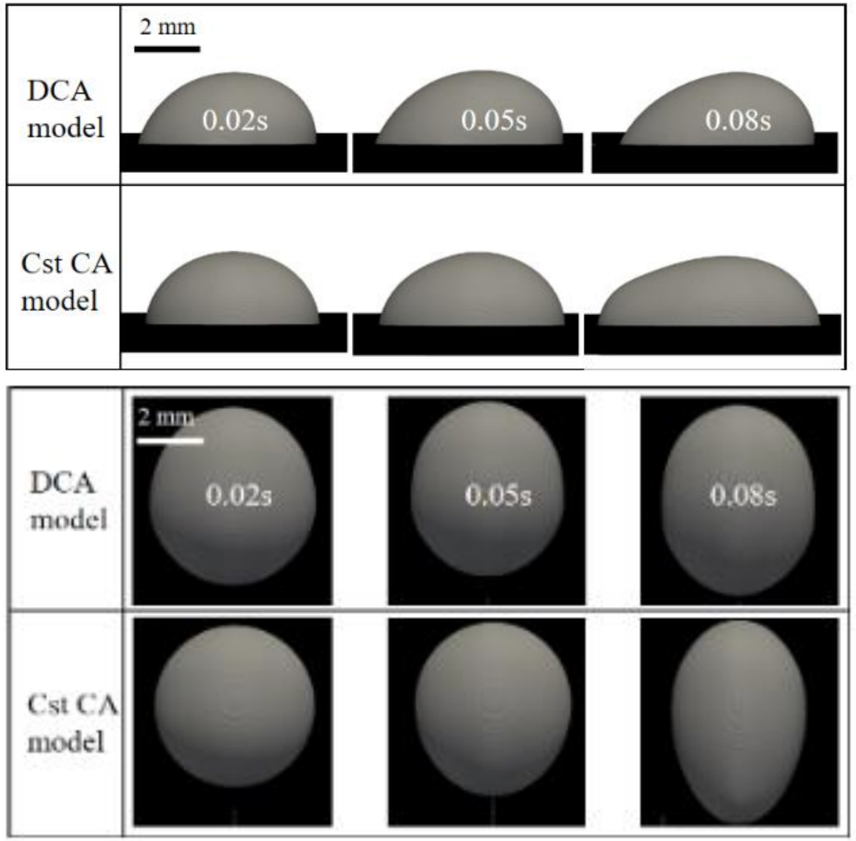
Thiols

[1] Li et al. Nature communications, 2023, 14(1): 4571.

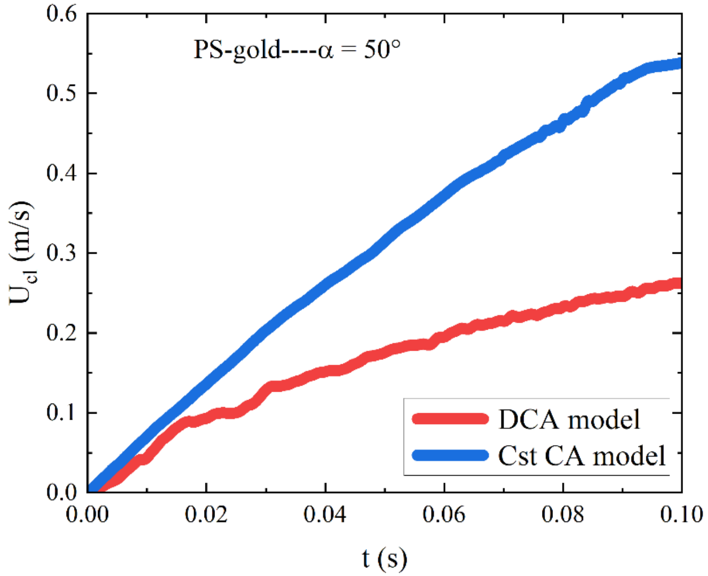
6. 3D Dynamic wetting

Case 3: A sliding water droplet on inclined surfaces

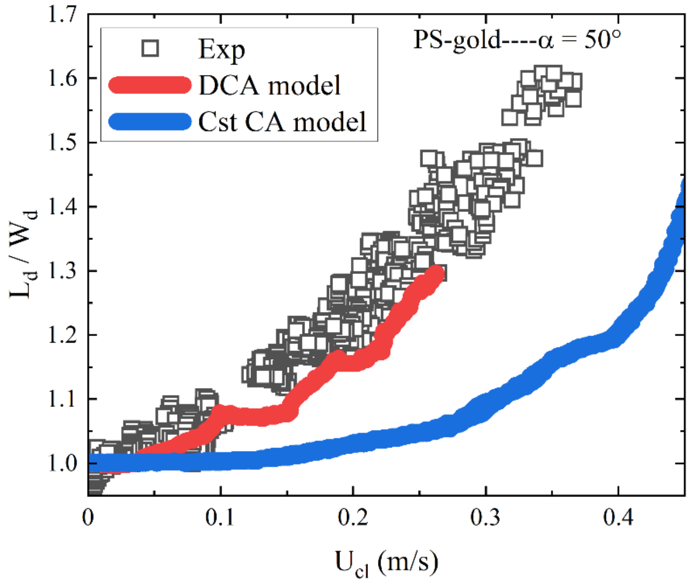
Dynamic vs Static models



Contact line velocity



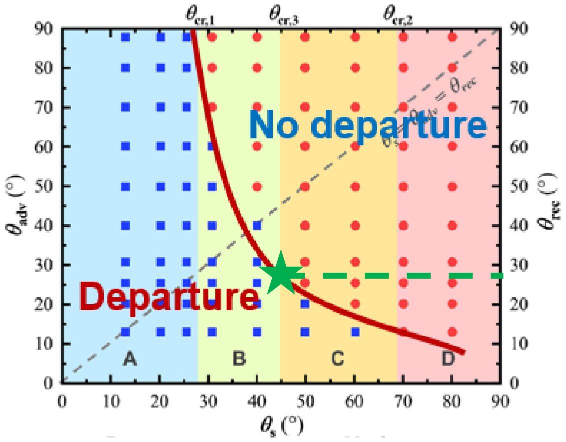
The ratio of length to width



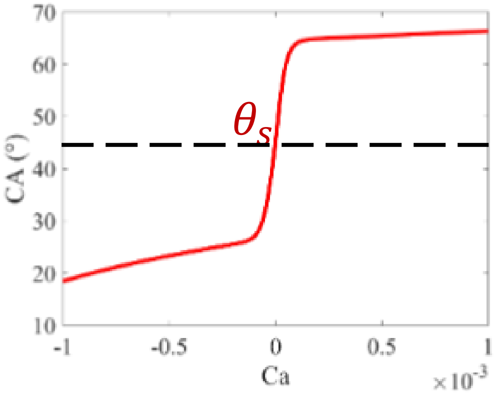
[1] Li et al. Nature communications, 2023, 14(1): 4571.

7. 3D Dynamic wetting

Bubble coalescence on a hydrophilic surface

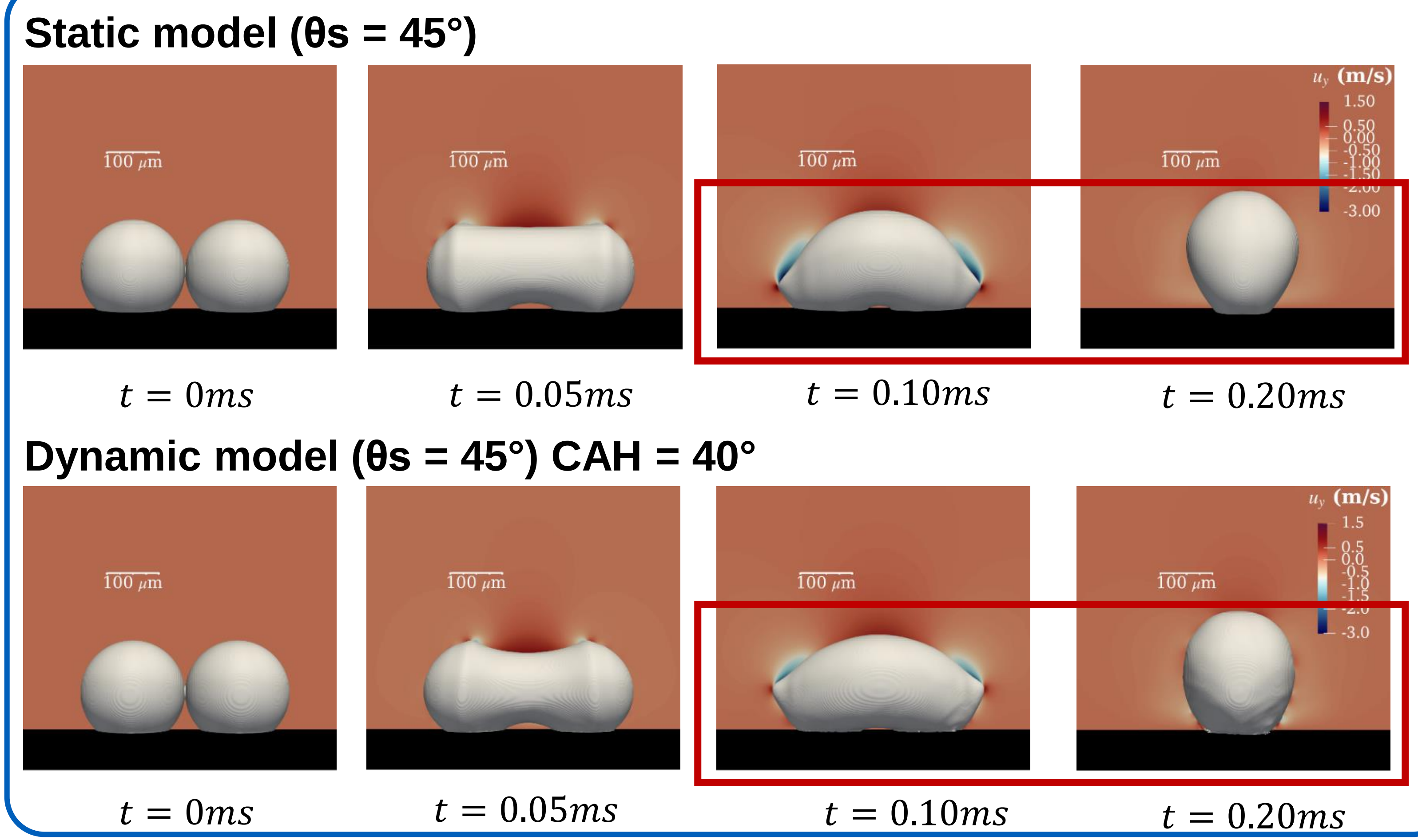


[1] Zhao et al. Langmuir 38.34 (2022): 10558-10567



θs = 45° CAH = 40°

Air-water: R0 = 100 µm

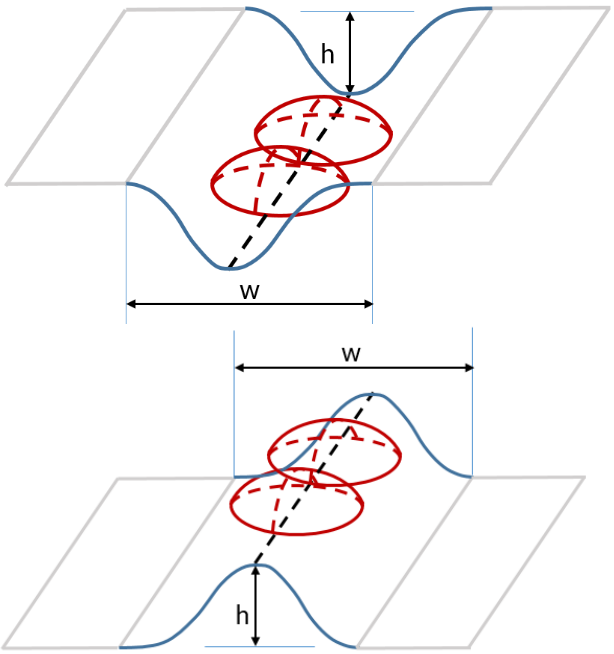


7. Bubble coalescence on structured surfaces

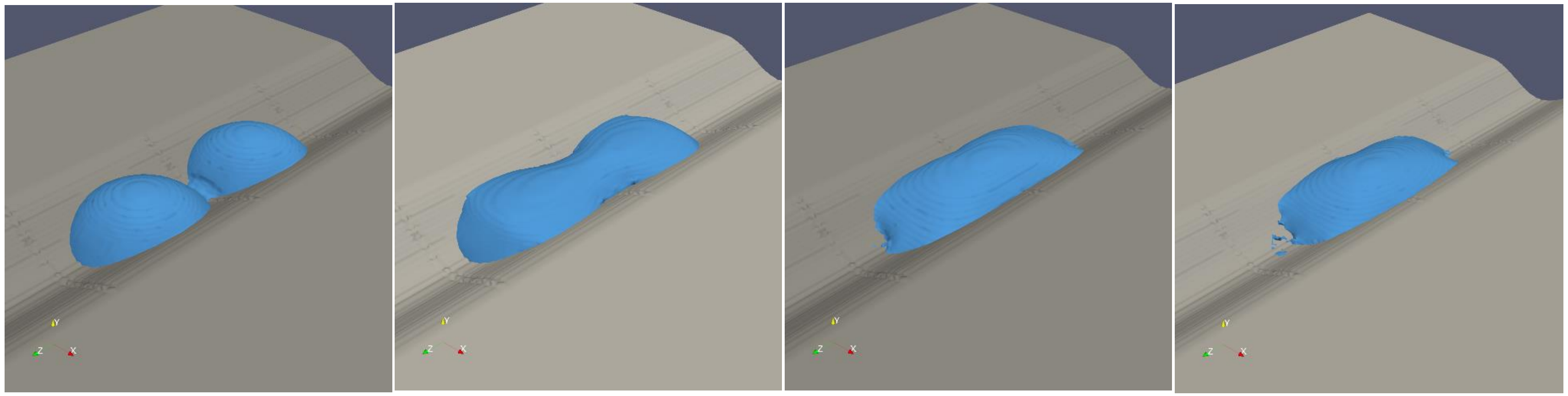
Static contact angle model

[1] Tavares et al. Computer & Fluids (2024)

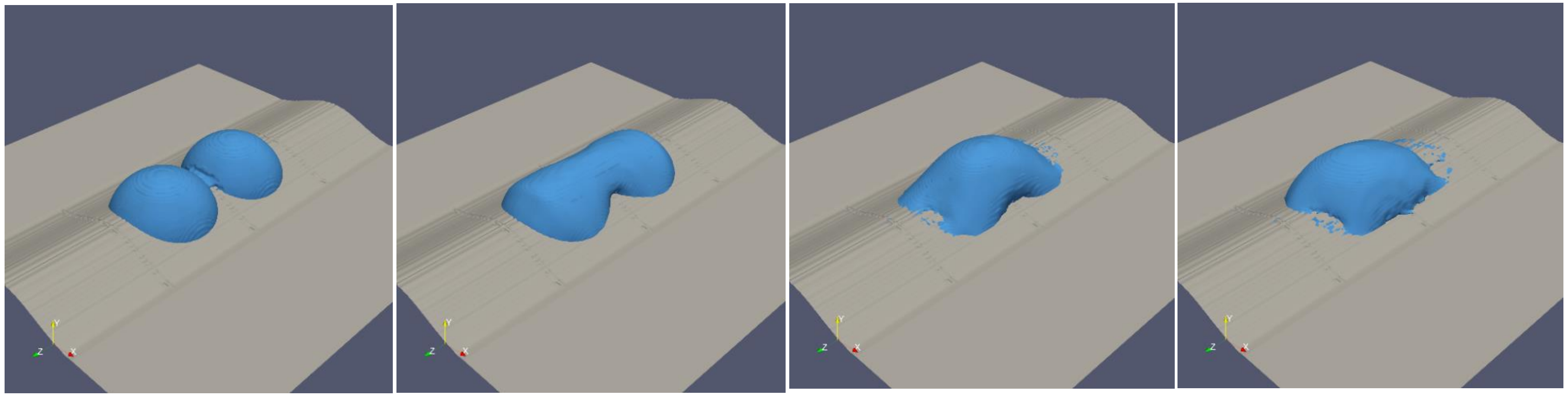
(Embedded Boundary Method)



h=40um, w=200um
R0 = 100 um, CA = 120°



$t = 0ms$ $t = 0.04ms$ $t = 0.1ms$ $t = 0.2ms$

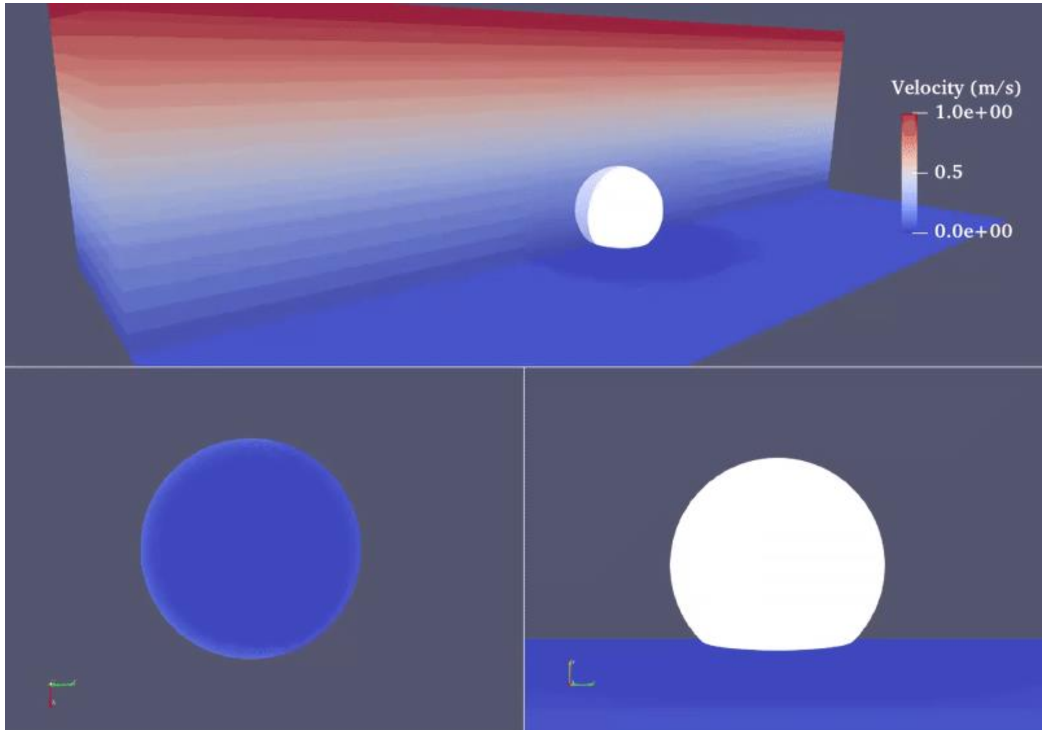


$t = 0ms$ $t = 0.04ms$ $t = 0.1ms$ $t = 0.2ms$

8. Conclusions and Outlook

Conclusions:

- A dynamic wetting model is implemented in 2D and 3D.
- Validated for oversaturation driven bubble growth.
- Validated for droplet spreading, splashing, and sliding.



Outlook:

- Bubble coalescence on different surfaces.
- Bubble detachment.
- Bubbles in shear flow.

Thanks for listening!

Email: yi.han@hzdr.de

Acknowledgment: The project H2Giga-SINEWAVE-Oxysep

AP1. Dimensionless equations

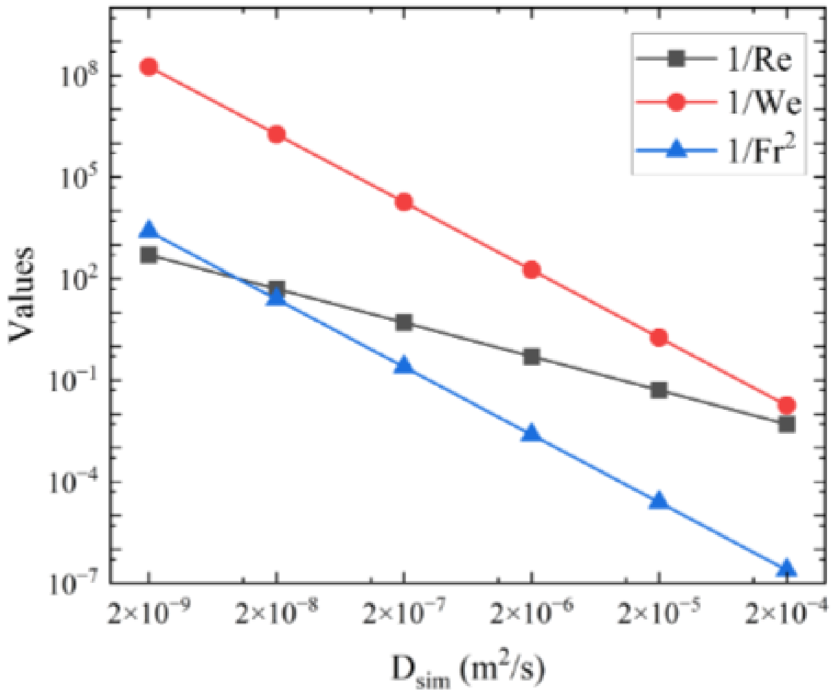
$$\mathrm{Re} = \frac{\rho_l D}{\mu_l}, \qquad \mathrm{We} = \frac{\rho_l D^2}{\gamma R_0}, \qquad \mathrm{Fr} = \frac{D}{\sqrt{g R_0^3}}.$$

$$\nabla^* \cdot \vec{u}^* = \frac{\zeta}{He(1-\rho_g^*/\rho^*)}(1-\rho_g^*)\frac{\partial c^*}{\partial \vec{n}_\Sigma}\delta_\Sigma^*,$$

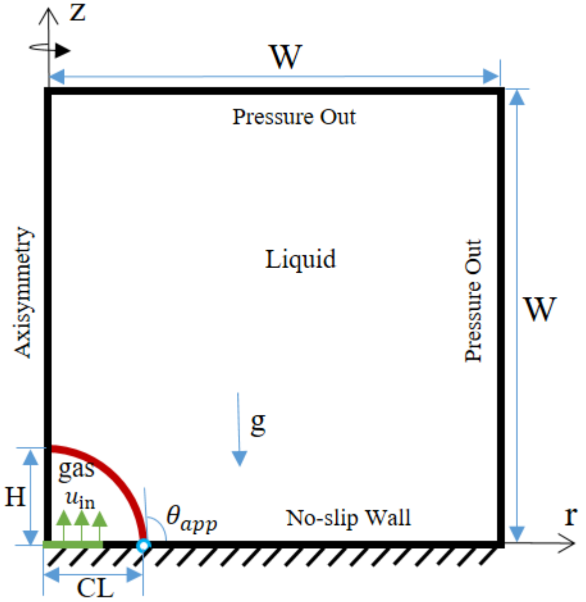
$$\frac{\partial \vec{u}^*}{\partial \tau^*} + \vec{u}^* \cdot \nabla^* \vec{u}^* = -\frac{\nabla^* p^*}{\rho^*} + \frac{1}{\rho^* \mathrm{Re}}\nabla^* \cdot \{\mu^*[\nabla^* \vec{u}^* + (\nabla^* \vec{u}^*)^T]\} + \frac{\kappa^* \vec{n}_\Sigma \delta_\Sigma^*}{\rho^* \mathrm{We}} + \frac{\vec{z}}{\mathrm{Fr}^2 |\vec{z}|},$$

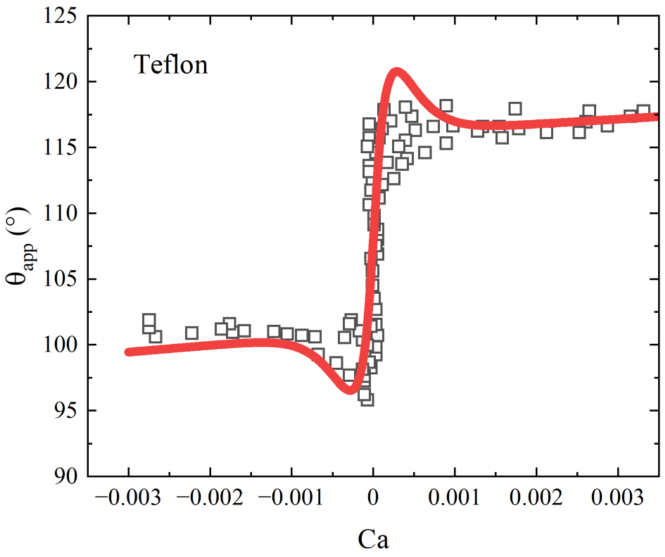
$$\frac{\partial \alpha}{\partial \tau^*} + \nabla^* \cdot (\alpha \vec{u}^*) = -\frac{\zeta}{He(1-\rho_g^*/\rho^*)}\rho_g^* \frac{\partial c^*}{\partial \vec{n}_\Sigma}\delta_\Sigma^*,$$

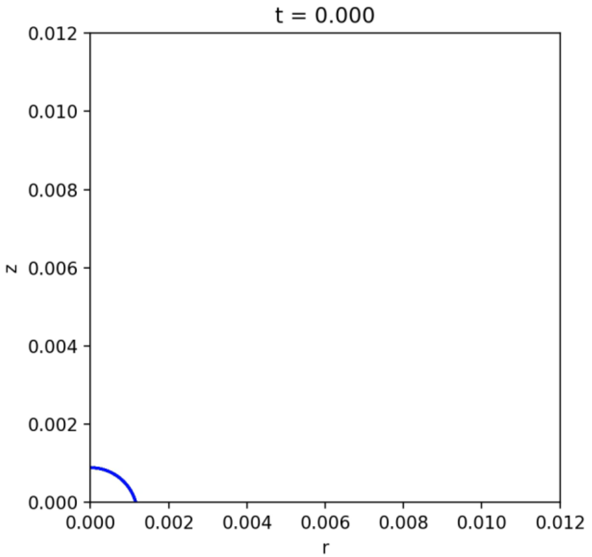
$$\frac{\partial c^*}{\partial \tau^*} + \vec{u}^* \cdot \nabla^* c^* = \nabla^* \cdot (\nabla^* c^*) - \frac{1}{(1-\rho_g^*/\rho^*)}\frac{\partial c^*}{\partial \vec{n}_\Sigma}\delta_\Sigma^*,$$

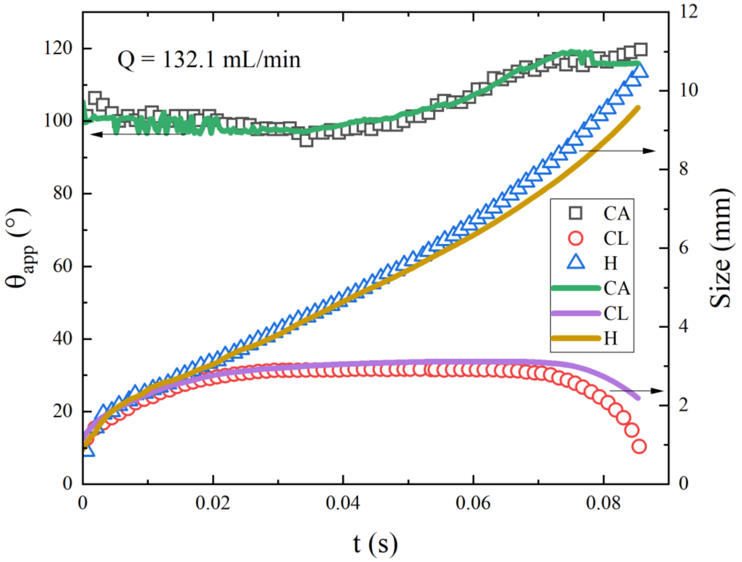


AP2. Bubble departure on solid surface









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https://doi.org/10.1007/s00348-020-2919-7

RESEARCH ARTICLE

Influence of wetting conditions on bubble formation from a submerged orifice

H. Mirsandi[1] · W. J. Smit[1] · G. Kong[1] · M. W. Baltussen[1] · E. A. J. F. Peters[1] · J. A. M. Kuipers[1]

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Dimensional parameters
rho_l = 998
rho_g = 1.25
mu_l = 1.0e-3
mu_g = 1.82e-5
F_sigma = 0.0725
Domain width (W): 12 mm
Gravity: 9.8 m/s^2
R_injec = 0.5 mm