Reproducing the rich physics of drop impingement experiments on hydrophobic surfaces by phase field simulations

Jahrestreffen der ProcessNet-Fachgruppen Computational Fluid Dynamics und Gasreinigung, Bamberg, 10. – 11. März 2020

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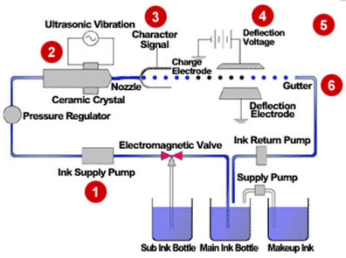
Overview

- Introduction
  - Applications
  - Motivation and goals
  - Definitions
- Numerical approach
  - phaseFieldFoam
  - Problem definition
  - Results
  - Summary

Applications

- Ink Printers
  - The global market size: more than **$25.5 billion** by 2026
- Spray coating
  - The global market size : expected to reach **$15.10 billion** by 2026
- Anti-icing coating
  - The global market size: estimated to reach **$304 million** by 2026



Pic Source: Wikipedia

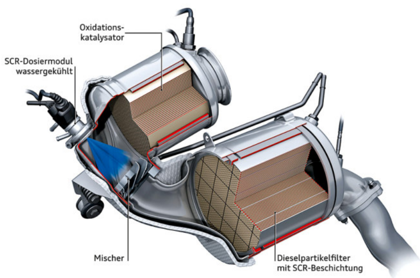
Motivation and goals

- Diesel exhaust gas after treatment
  - **Selective catalytic reduction (SCR):** converting nitrogen oxides (NO_x) with the help of ammonia (NH_3) to harmless nitrogen and water

$$2\,NH_3 + NO + NO_2 \rightarrow 2\,N_2 + 3\,H_2O$$

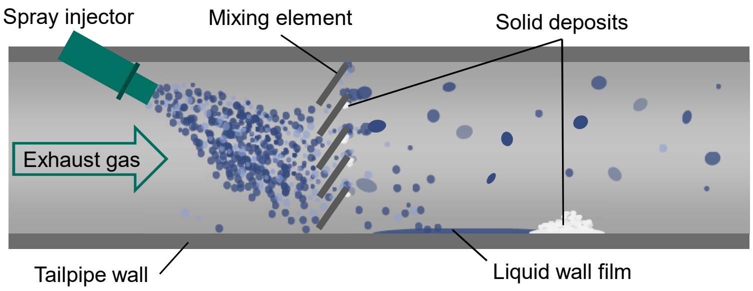
  - Ammonia is provided by spray injection of urea-water-solution (AdBlue®)

$$(NH_2)_2CO\ (l) \Rightarrow NH_3\ (g) + HNCO\ (g)$$
$$HNCO\ (g) + H_2O\ (g) \Rightarrow NH_3\ (g) + CO_2\ (g)$$



Motivation and goals

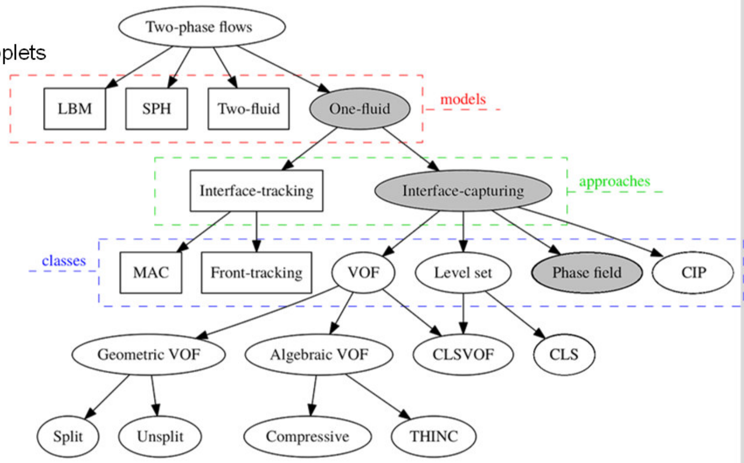
- Challenges in NH_3 treatment
  - Solid deposit formation by incomplete drop evaporation



- Our goal: **Avoiding film formation**
- Our approach: Numerical study of drop impact by phase field method simulations

Why phase field method?

- Interface-capturing vs Interface-tracking
  - Topological changes
    - Breakup/coalescence of bubbles/droplets
    - Liquid film formation
  - Computational cost
  - Accuracy
  - 3D complex Geo

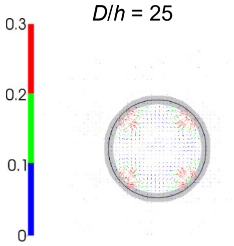


F. Jamshidi, H. Heimel, M. Hasert, X. Cai, O. Deutschmann, H. Marschall, M. Wörner, *Comp. Phys. Commun.* **236** (2019) 72–85

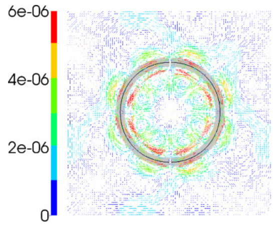
Why phase field method?

- VOF vs phase field
  - Dominance of surface tension forces at small scales
    - Numerical artifact of "spurious currents"
  - Wetting behavior
    - Conflict between contact line motion and no-slip boundary condition

InterFoam: VOF
D/*h* = 25



phaseFieldFoam
D/*h* = 50



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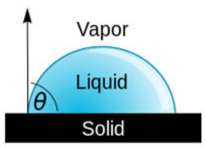
Definitions

- Drop impact outcomes on dry solid surface
  - Deposition
  - Rebounding
  - Splash

- Surface wetteability
  - Hydrophilic $\theta_e < 90$
  - Hydrophobic $90 < \theta_e < 130$
  - superHydrophobic $\theta_e > 130$



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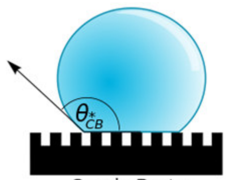
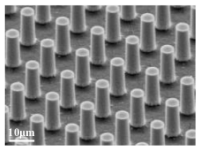


Cassie-Baxter

Nano Structure



- Dimensionless parametes $We = \frac{\rho_L V_0^2 d_0}{\sigma}, \mathrm{Re} = \frac{\rho_L V_0 d_0}{\mu_L}$

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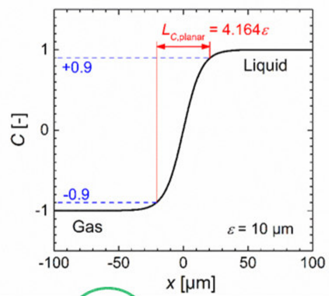
phaseFieldFoam

- Governing Equations
  - Cahn-Hilliard equation $$\partial_t C + \nabla\cdot(C\,\mathbf{u}) = M\nabla^2\phi_{\mathrm{m}}$$
  - Chemical potential $$\phi_{\mathrm{m}} = \lambda\varepsilon^{-2}(C^3 - C) - \lambda\nabla^2 C$$
  - Continuity equation $$\nabla\cdot\mathbf{u} = 0$$
  - Navier-Stokes $$\partial_t(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) = -\nabla p + \nabla\cdot\left[\mu\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}\right)\right] + \rho\mathbf{g} + \mathbf{f}_\sigma$$
  - Surface tension $$\mathbf{f}_\sigma = -\phi_{\mathrm{m}}\nabla C$$
  - Thermophysical properties $$\rho = \frac{1+C}{2}\rho_{\mathrm{L}} + \frac{1-C}{2}\rho_{\mathrm{G}}$$ $$\mu = \frac{1+C}{2}\mu_{\mathrm{L}} + \frac{1-C}{2}\mu_{\mathrm{G}}$$

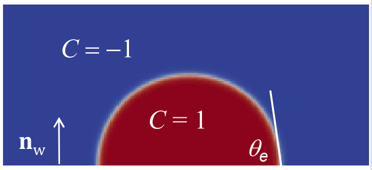


phaseFieldFoam

- Determining the phase field parameters ε, λ, M
  - Cahn number — $Cn = \varepsilon / L_{ref} = \mathcal{O}(10^{-2})$ → $Cn = 0.01$
    - L_{ref} = characteristic macroscopic length scale (e.g. drop diameter)
  - Mixing energy parameter — $\lambda = 3\varepsilon\sigma / \sqrt{8}$
  - Mobility parameter — $M = \chi \varepsilon^2$
    - Proportionality factor χ [m·s/kg] — $\chi = \mathcal{O}(10^{-1} - 10^{1})$ → $\chi = 1$

- Boundary condition

$$\mathbf{n}_w \cdot \nabla C = \frac{1 - C^2}{\sqrt{2}\varepsilon} \cos\theta_e$$



D. Jacqmin, *J. Comput. Phys.* **155** (1999) 96–127
J. Kim, *Commun. Comput. Phys.* **12** (2012) 613–661

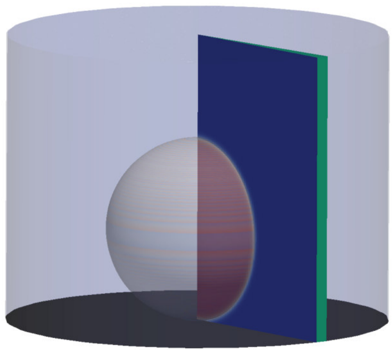
phaseFieldFoam

- Code development and support
  - Dr. Holger Marschall (TU Darmstadt)
  - Dr. Martin Wörner (KIT)
  - …
- Implementation in Open∇FOAM
  - Open source computational fluid mechanics (CFD) **C++** toolbox
  - foam-extend-4.0
- Validation

X. Cai, H. Marschall, M. Wörner, O. Deutschmann, *Chem. Eng. Technol.* **38** (2015) 1985–1992
X. Cai, M. Wörner, H. Marschall, O. Deutschmann, *Catalysis Today* **273** (2016) 151–160
X. Cai, M. Wörner, H. Marschall, O. Deutschmann, *Emission Control Science and Technology* **3** (2017) 289–301

Problem Definition

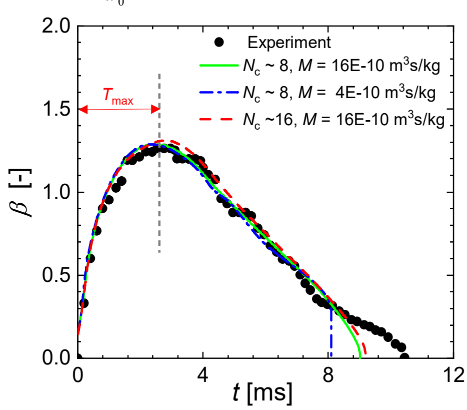
- Grid Generation
  - BlockMesh
  - Axisy symmetric , uniform grid
  - Domain size ($3d_0/2$ x $3d_0$)



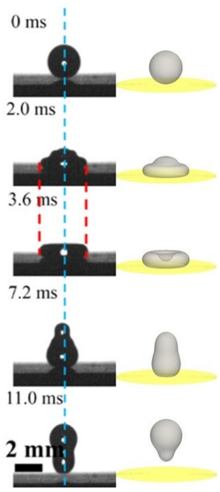
- Boundary Conditions
  - equiliburium contact angle: $\theta_e = [100-170]$
  - No slip for velocity
- Material Properties: water droplet
- Descritizetion :
  - **Temporal scheme**: Crank-Nicolson / Euler
  - **Divergence scheme** : Gamma

Results

- Compare numerical result with experimental data
  - Spreading ratio $\beta = \frac{d}{d_0}$



$d_0 = 2mm, \theta_0 = 161, We = 7$

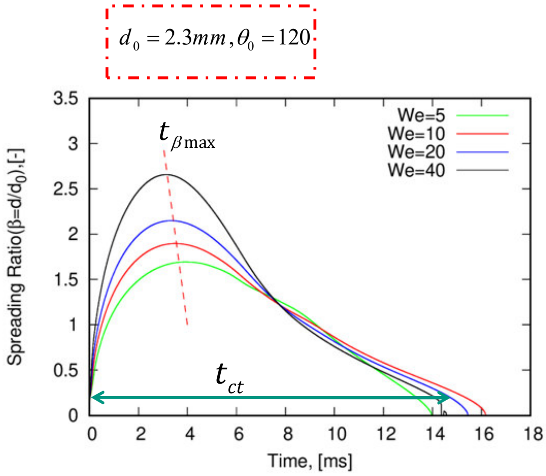


Shen, Y., Tao, J., Wang, G., Zhu, C., Chen, H., Jin, M., Xie, Y., *Journal of Physical Chemistry C* 122.13 (2018): 7312-7320

Results

- Initial drop velocity effect on spreading time
  U_0 ↑ $t_{\beta \max}$ ↓
- Initial drop velocity effect on spreading time
  U_0 ↑ t_{ct} ?

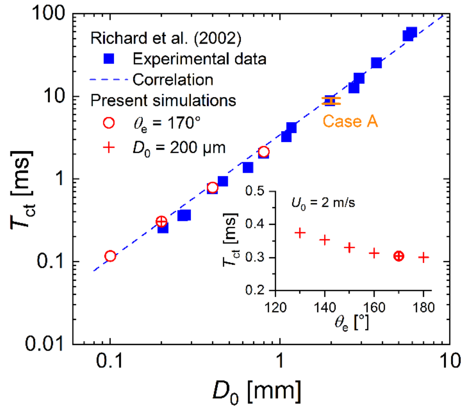
No obvious trend

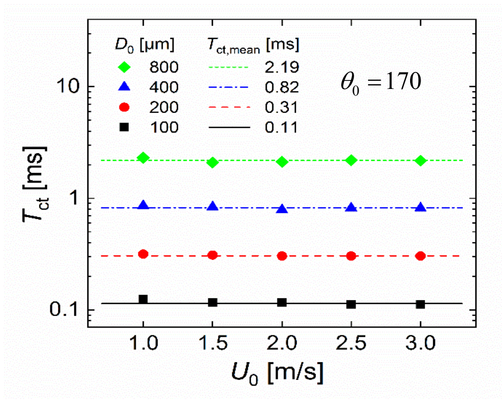


D. Richard, C. Clanet, D. Quéré, Contact time of a bouncing drop, Nature, 417 (2002) 811

Results

- Effect of initial velocity and diameter on contact time $t_{ct} = 0.91\sqrt{\rho_L d_0^3 / \sigma}$

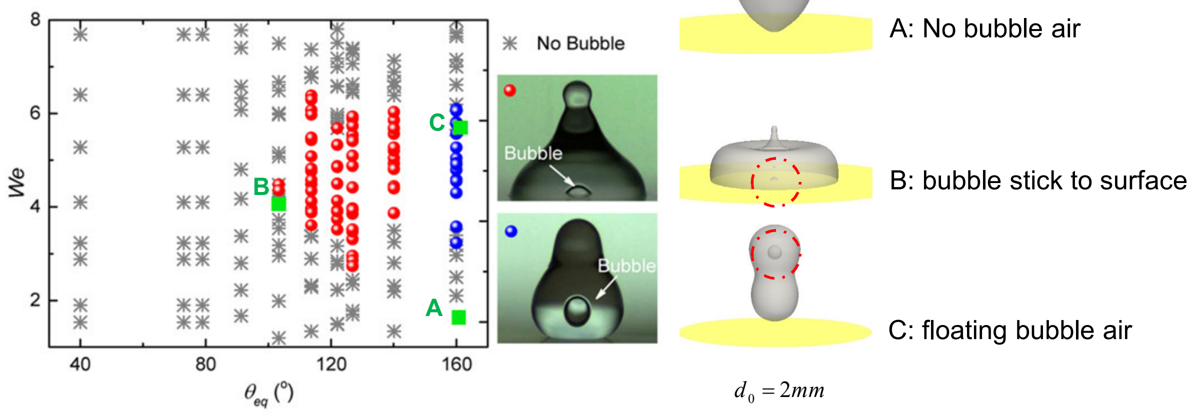




D. Richard, C. Clanet, D. Quéré, Contact time of a bouncing drop, Nature, 417 (2002) 811

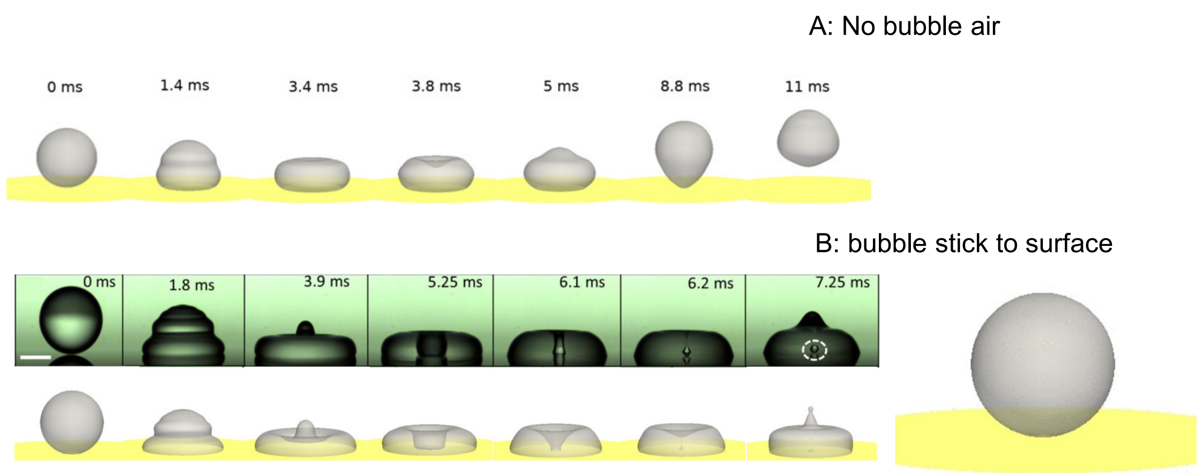
Results

- Air entrapment regime



L. Chen, L. Li, Z.-D. Li, K. Zhang, Langmuir, 33 (2017) 7225-7230

Results

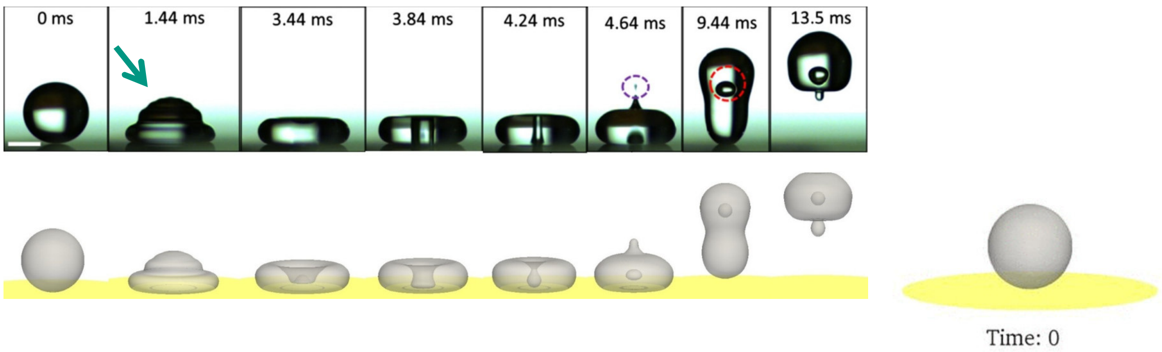


Lin, S., Zhao, B., Zou, S., Guo, J., Wei, Z., Chen, L., *Journal of colloid and interface science* 516 (2018): 86-97

Results

- Capillary wave (t=1.44 ms)
- Small drop ejection (t=4.64 ms)
- Air entrapment (t=9.44 ms)

C: floating bubble air



Lin, S., Zhao, B., Zou, S., Guo, J., Wei, Z., Chen, L., *Journal of colloid and interface science* 516 (2018): 86-97

Summary

- Achievements and current limitations
  - Method can well describe wetting phenomena ✓
  - Method can handle real density and viscosity ratios ✓
  - appropriate value for mobility is found ✓
  - Keep *C* bounded (implement and must test!)
  - Consider heat transfer (implement and validation is going on!)

Thanks for your attention!