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

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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

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

  \[
  2 \text{NH}_3 + \text{NO} + \text{NO}_2 \rightarrow 2 \text{N}_2 + 3 \text{H}_2\text{O}
  \]

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

- \((\text{NH}_2\text{CO}) \rightarrow \text{NH}_3\text{(g) + HNCO (g)}\)
- \(\text{HNCO (g) + H}_2\text{O (g) \rightarrow NH}_3\text{(g) + CO}_2\text{(g)}\)
Motivation and goals

- Challenges in NH₃ 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

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**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

![VOF vs phase field](image1)

**Definitions**

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

- **Surface wettability**
  - Hydrophilic $\theta < 90$
  - Hydrophobic $90 < \theta < 130$
  - superHydrophobic $\theta > 130$

![Surface wettability](image2)

- **Dimensionless parameters**

$$We = \frac{\rho V^2 d}{\sigma}, Re = \frac{\rho V d}{\mu}$$
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phaseFieldFoam

- Governing Equations
  - Cahn-Hilliard equation
  \[ \partial_t C + \nabla \cdot (C \mathbf{u}) = M \nabla^2 \phi_{\text{in}} \]
  - Chemical potential
  \[ \phi_{\text{in}} = \lambda \epsilon e^{-\lambda (C^3 - C)} - \lambda \nabla^2 C \]
  - Continuity equation
  \[ \nabla \cdot \mathbf{u} = 0 \]
  - Navier-Stokes
  \[ \partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \left[ \mu \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right] + \rho \mathbf{g} + \mathbf{f}_\sigma \]
  - Surface tension
  \[ \mathbf{f}_\sigma = -\phi_{\text{in}} \nabla C \]
  - Thermophysical properties
  \[ \rho = \frac{1+C}{2} \rho_l + \frac{1-C}{2} \rho_v \]
  \[ \mu = \frac{1+C}{2} \mu_l + \frac{1-C}{2} \mu_v \]
Determining the phase field parameters $\varepsilon$, $\lambda$, $M$

- Cahn number
  - $L_{\text{ref}} = \text{characteristic macroscopic length scale (e.g. drop diameter)}$
  - $Cn = \varepsilon / L_{\text{ref}} = \mathcal{O}(10^{-2})$ → $Cn = 0.01$

- Mixing energy parameter
- Mobility parameter
  - Proportionality factor $\chi$ [m s/kg]
  - $\lambda = 3\varepsilon \sigma / \sqrt{8}$
  - $M = \chi \varepsilon^2$
  - $\chi = \mathcal{O}(10^{-1} - 10^0)$ → $\chi = 1$

Boundary condition

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


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Code development and support

- Dr. Holger Marschall (TU Darmstadt)
- Dr. Martin Wörner (KIT)
- ...

Implementation in OpenFOAM

- Open source computational fluid mechanics (CFD) C++ toolbox
- foam-extend-4.0

Validation


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Problem Definition

- Grid Generation
  - BlockMesh
  - Axisymmetric, uniform grid
  - Domain size (3d, x 3d,)

- Boundary Conditions
  - equilibrium contact angle: \( \theta_i = [100--170] \)
  - No slip for velocity

- Material Properties: water droplet

- Discretization:
  - Temporal scheme: Crank-Nicolson / Euler
  - Divergence scheme: Gamma

Results

- Compare numerical result with experimental data

- Spreading ratio
  \[ \beta = \frac{d}{d_o} \]

\[ \beta \] vs. \( t \) [ms]

\[ \beta_{\max} \]

\[ d_o = 2\text{mm}, \theta_i = 161^\circ, e = 7 \]

\[ 0 \text{ms}, 2.0 \text{ms}, 3.6 \text{ms}, 7.2 \text{ms}, 11.0 \text{ms}, 2 \text{mm} \]

Results

- Initial drop velocity effect on spreading time
  \[ u_0 \quad t_{\beta_{\max}} \]

- Initial drop velocity effect on spreading time
  \[ u_0 \quad t_{\text{ct}} \quad ? \]

No obvious trend

\[ d_0 = 2.3 \text{mm}, \theta_0 = 120^\circ \]

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Results

- Effect of initial velocity and diameter on contact time
  \[ t_{\text{ct}} = 0.91 \sqrt{\rho_1 d_0^2 / \sigma} \]
Results

Air entrapment regime

A: No bubble air

B: bubble stick to surface

C: floating bubble air

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Results

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

C: floating bubble air


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!