Interface-resolving simulation of droplet impact on liquid film of the same fluids using the phase-field method

M. Bagheri, H. Marschall, Technical University of Darmstadt, Computational Multiphase Flows
M. Wörner, Karlsruhe Institute of Technology (KIT), Institute of Catalysis Research and Technology

Motivation and Overall Goal

Motivation

- Gaining further insight into the droplet impact process on thin liquid wall film with application to fuel combustion and exhaust gas aftertreatment:
  - Understanding how to *minimize* the formation of secondary fuel droplets that prompts release of lubricating oil inside the combustion chamber which can trigger pre-ignition
  - Acquiring knowledge to *maximize* the formation of secondary urea/water droplets in the exhaust system to advantageously reduce the wall film in the exhaust pipe

Overall goal

- Development of a *predictive* diffuse-interface approach for multi-phase flows of miscible and immiscible multi-component fluids in an unified modelling framework

Phase-field Method

- The interface has a small but finite thickness [1,3]
- Based on models of fluid free energy [1,3]

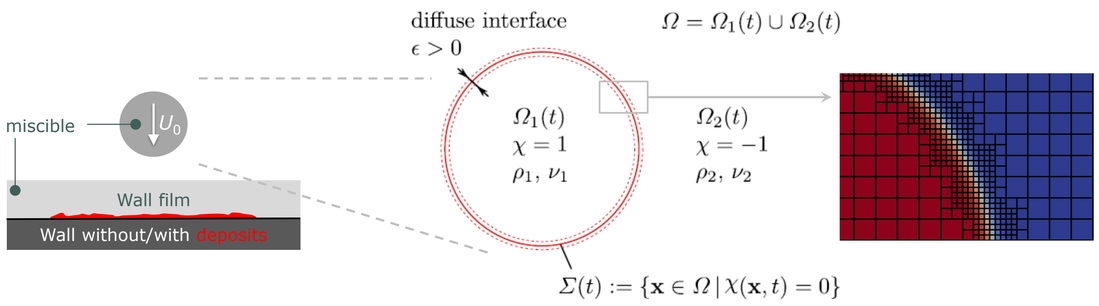


Fig. 1: Representation of the simulation setup for examining the drop-wall film interaction with miscible fluids (left) and the diffusive drop interface in the phase field method (middle & right).

- Continuum thermodynamic diffuse interface model
  - Local phase-field χ [–] $(-1 \le \chi \le 1)$
  - Order parameters (volume averaged)
    $\bar{c} = \alpha_1 - \alpha_2 = \bar{\chi}, \ (-1 \le \bar{c} \le 1)$
  - Capillary width ε [m]
  - Mobility κ [m³s/kg]
- Cahn-Hilliard Navier-Stokes equations (alternatively Allen-Cahn)
  - Chemical potential Φ [J/m³]
  - Interfacial tension σ [N/m]
  - Mixing energy density λ [J/m]

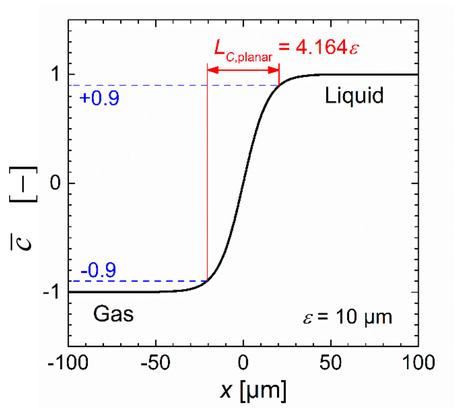


Fig. 2: Profile of the order parameter for a flat interface in equilibrium.

$$\partial_t \bar{c} + \nabla\cdot(\bar{c}\,\mathbf{u}) = \kappa\nabla^2\Phi, \quad \nabla\cdot\mathbf{u} = 0,$$
$$\partial_t(\bar{\rho}\,\mathbf{u}) + \nabla\cdot(\bar{\rho}\,\mathbf{u}\otimes\mathbf{u}) = \nabla\tilde{p} + \nabla\cdot\langle\tau\rangle + \bar{\rho}\,\mathbf{g} + \langle\mathbf{f}_c\rangle.$$

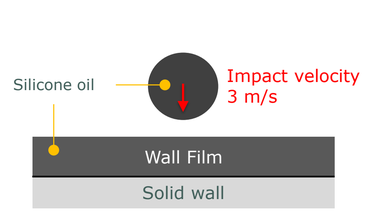
$$\Phi(\bar{c}) = \tfrac{\lambda}{\epsilon^2}\Psi'(\bar{c}) - \lambda\nabla^2\bar{c} \ \text{ with } \Psi(\bar{c}) = \tfrac{1}{4}\left(\bar{c}^{\,2}-1\right)^2, \Psi' = \bar{c}^{\,3} - \bar{c}; \ \langle\mathbf{f}_c\rangle = -\bar{c}\nabla\Phi,$$

$$\langle\boldsymbol{\tau}\rangle = -\langle\mu\rangle\left(\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathsf{T}}\right) \text{ with } \langle\mu\rangle = \tfrac{1-\bar{c}}{2}\bar{\mu}^1 + \tfrac{1+\bar{c}}{2}\bar{\mu}^2; \ \bar{\rho} = \tfrac{1-\bar{c}}{2}\bar{\rho}^1 + \tfrac{1+\bar{c}}{2}\bar{\rho}^2.$$

- Implemented in OpenFOAM (new top level solver phaseFieldFoam, PFF)
- Dynamic adaptive techniques of high performance computing
- Interface relaxation model for high dynamics:
  - **Equilibrium Planar**: Standard formulation where diffuse mixing energy is considered to be equal to the interfacial energy, assuming a planar interface at equilibrium.
    $$\lambda = \frac{3}{\sqrt{8}}\sigma\,\epsilon$$
  - **Relaxation**: Novel formulation where the interfacial energy is non-constant, see [3], and the interface has its own local relaxation dynamics.
    $$\lambda = \frac{3}{\sqrt{8}}\sigma\,\epsilon\frac{|\nabla\bar{c}|^2}{\frac{|\nabla\bar{c}|^2}{2} + \frac{\psi(\bar{c})}{\epsilon^2}}$$

Preliminary Results

- **Research Questions:**
  1. To what extent (quantitatively) can the crown diameter and opening angle in the case of a drop impact on wall films of identical fluids be brought into agreement with experimental results?
  2. Which methodological extensions are necessary?
- **Test Case Description**



Fluid	Silicone Oil	Computational Settings	
Kinematic viscosity	5 cSt = $5{\cdot}10^{-6}$ m²/s	Diffuse Interface Model	Cahn-Hilliard
Interfacial tension	17.7 mN/m	Domain Configuration	Axisymmetric
Density	920 kg/m³	Adaptive Mesh Refinement	Yes
Droplet diameter	1.5 mm	Cahn number	0.005
Drop impact velocity	3 m/s	Domain Size $\left[Cn = \frac{\epsilon}{D_0}\right]^*$	$[L_x = 9D_0 \,\&\, L_z = 4.5D_0]$
Film thickness	0.5 mm		

*D_0: Droplet diameter

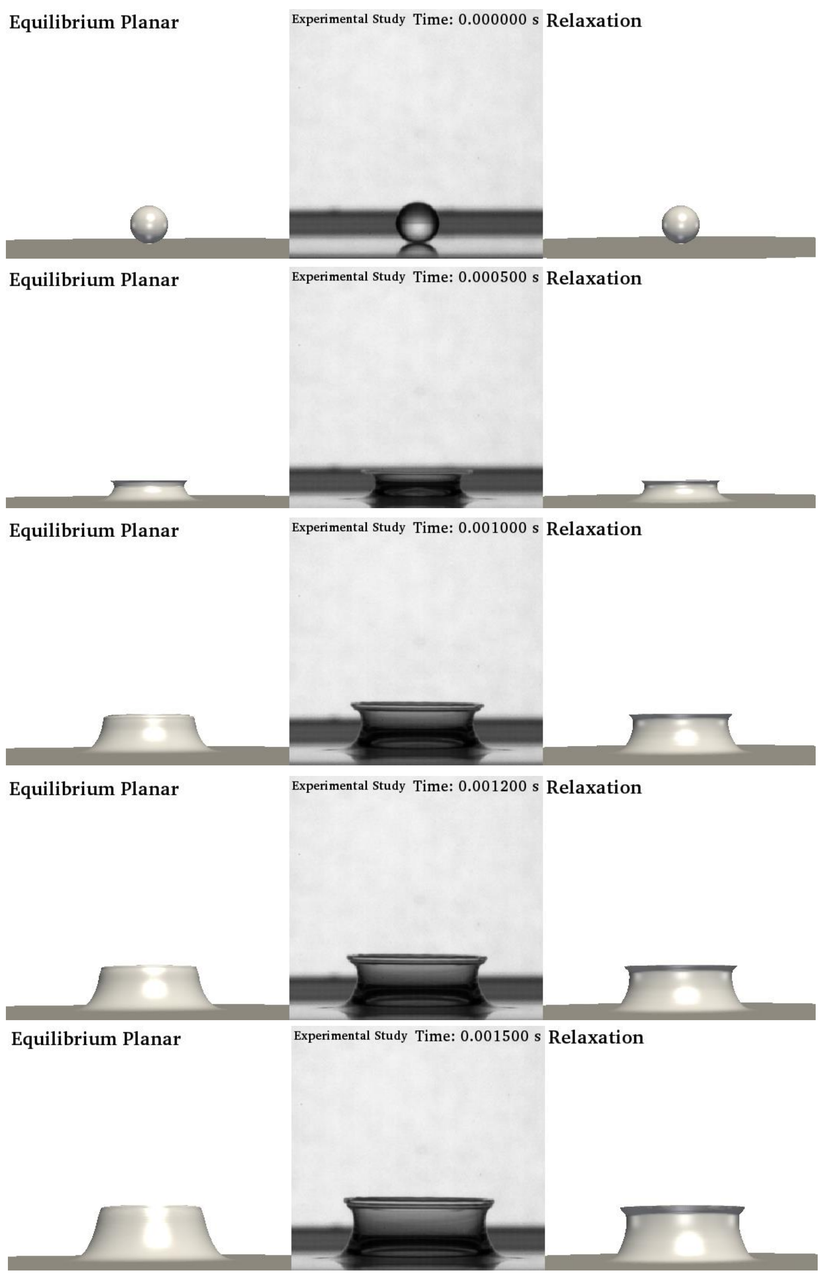


Fig. 3: Comparison of the standard equilibrium mixing energy model (left) and the novel relaxation mixing energy model (right) with the experimental study (middle). Experiments have been performed by B. Stumpf from Technical University of Darmstadt, Department of Fluid Mechanics and Aerodynamics.

Highlights & Outlook

- Interface relaxation model is essential for correct prediction of the dynamics of the corona as visualized by the experimental studies
- Very low artificial / parasitic currents [2]
- Extension of the solver for M phases and N components as well as for miscible and immiscible systems
- Further validation of the method based on experimental studies

References

[1] Jacqmin, D., 1999. Calculation of two-phase Navier–Stokes flows using phase-field modeling. *Journal of Computational Physics*, *155*(1), pp.96-127.

[2] Jamshidi, F., Heimel, H., Hasert, M., Cai, X., Deutschmann, O., Marschall, H. and Wörner, M., 2019. On suitability of phase-field and algebraic volume-of-fluid OpenFOAM® solvers for gas–liquid microfluidic applications. Computer Physics Communications, 236, pp.72-85.

[3] Yue, P., Feng, J.J., Liu, C. and Shen, J., 2004. A diffuse-interface method for simulating two-phase flows of complex fluids. *Journal of Fluid Mechanics*, *515*, pp.293-317.

SFB/Transregio 150
Turbulente, chemisch reagierende Mehrphasenströmungen in Wandnähe

TECHNISCHE UNIVERSITÄT DARMSTADT

Karlsruhe Institute of Technology