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Implementation of a Phase Field Method in OpenFOAM® for Simulation of Spreading Droplet & Verification by Test Problems

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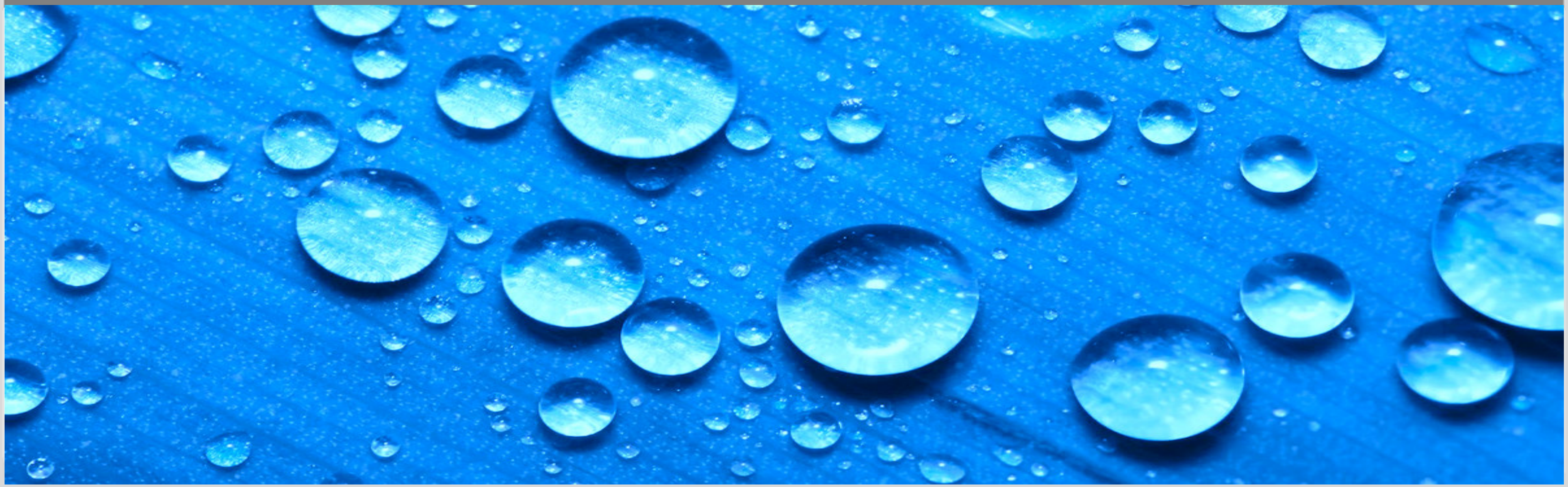
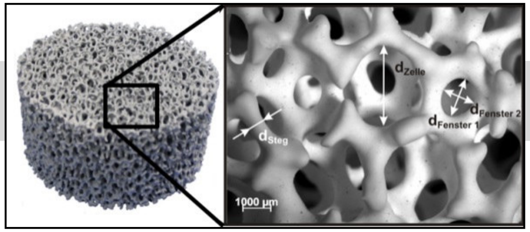


Outline

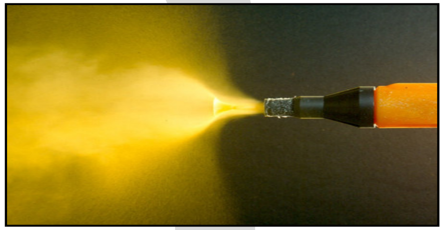
- Motivation
  - Wetting and moving contact lines
  - Why phase field method
- Numerical method
  - Non-dimensional governing equations
  - Implementation of phase field method in OpenFOAM®
- Verification
  - Diffusion term in Cahn-Hilliard equation
  - Surface tension term (drop deformation)
  - Spreading of droplet on flat surface
- Conclusions and outlook

Motivation

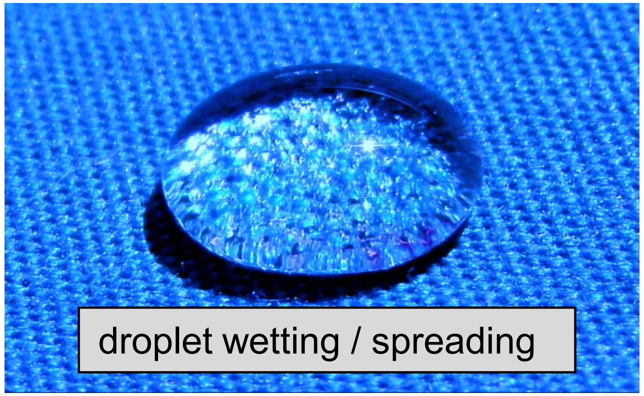


solid sponge chemical reactor

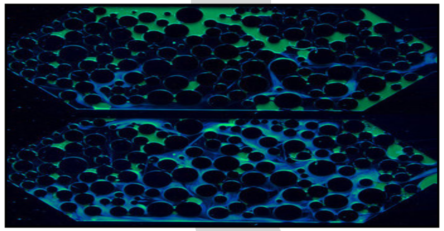
insecticides spray



coating



droplet wetting / spreading

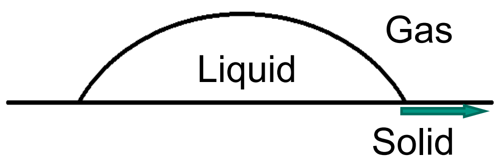


oil recovery from porous structure

lubrication

ink-jet printing

Focus & Difficulty of Numerical Modeling



Paradox btw. motion of contact line & no-slip BC

$$\frac{\partial F}{\partial t} + \cancel{(\mathbf{u}\cdot\nabla)F} = 0$$

F: phase indicator function

- The paradox is resolved differently in:

Sharp interface method

- e.g. VOF, Level-set method
- via Navier-slip BC

$$u_W = L_s \left.\frac{\partial u}{\partial n}\right|_W$$

- L_s is slip length → difficult to choose in physical sense!

Diffuse interface method

- e.g. Phase Field Method
- via diffusion term

$$\frac{\partial C}{\partial t} + (\mathbf{u}\cdot\nabla)C = \kappa\nabla^2\phi$$

- *C* is order parameter
- *Φ* is chemical potential

$$\Phi = \beta(C^3 - C) - \alpha\nabla^2 C$$

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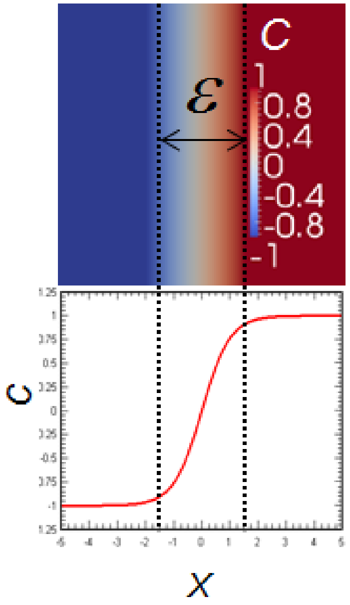
Phase Field Method (PFM)

- Order parameter (C) as phase indicator
  - C = 1 for liquid, C = -1 for gas
- Across interface, C varies continuously

$$C_e = \tanh\left(\frac{x}{\sqrt{2}\xi}\right) \quad \text{where} \quad \xi = \sqrt{\frac{\alpha}{\beta}}$$

  - Equilibrium interface thickness (ε) as distance btw. C = -0.9 to C = 0.9 $\rightarrow \varepsilon = 4.164\xi$



- Evolution governed by Cahn-Hilliard equation:

$$\frac{\partial C}{\partial t} + (\mathbf{u}\cdot\nabla)C = \frac{1}{Pe_\kappa}\nabla^2\Phi \qquad \Phi = C^3 - C - Cn^2\nabla^2 C$$

$$Cn = \frac{\xi}{L}, \quad Pe_\kappa = \frac{2\sqrt{2}LU\xi}{3\kappa\sigma}$$

L, U :	reference length & velocity
κ :	mobility parameter
σ :	surface tension coefficient
ξ :	mean-field thickness

- $Cn \rightarrow$ interface thickness $Pe_\kappa \rightarrow$ ratio of convection to diffusion
  - They are model parameters $\rightarrow$ suitable ranges need to be identified

Equation for Two-phase Flow

- Cahn-Hilliard equation is coupled with momentum equation:

$$\rho(C)Re\left(\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right)=-\nabla p+\mu(C)\nabla^2\mathbf{u}-\frac{1}{Ca\cdot Cn}C\nabla\Phi(C)-\frac{1}{2}\frac{Eo}{Ca}(C+1)\mathbf{e}_z$$

Surface tension | Gravity

- Mixture density & viscosity:

$$\rho(C)=\frac{1}{2}\left((C+1)-\frac{\rho_B}{\rho_A}(C-1)\right)\quad \mu(C)=\frac{1}{2}\left((C+1)-\frac{\mu_B}{\mu_A}(C-1)\right)$$

- Dimensionless parameters:

$$Re=\frac{\rho_A LU}{\mu_A},\quad Ca=\frac{2\sqrt{2}\mu_A U}{3\sigma},\quad Eo=\frac{(\rho_A-\rho_B)gL^2}{\sigma}$$

g: gravitational acceleration; ρ_A: droplet density; ρ_B: ambient fluid density; μ_A: droplet viscosity;

Implementation in OpenFOAM®

- *icoDyMFoam* as starting point
  - Incompressible, laminar, Newtonian
  - Transient, allow for mesh adaptation
- Cahn-Hilliard (C-H) equation added as scalar transport equation
  - Implicit convection
  - Explicit diffusion, 4th order derivative
- Surface tension & gravity added into momentum equation as
  - Explicit source terms
- Numerical schemes in following simulations
  - Convection: central differencing
  - Time integration: backward

From time-step *n* to *n*+1

1. Update chemical potential (Φ) field
   - using order parameter (C) field at time-step n
2. Calculate C field at time-step n+1
   - solving C-H equation
   - with Φ field from above
   - and velocity (U) field at time-step n
3. Get surface tension, gravity & mixture ρ, μ
   - using C field at time-step n+1
4. Obtain U field at time-step n+1
   - solving N-S equation with PISO algorithm

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Validation of Diffusion Term in C-H Equation

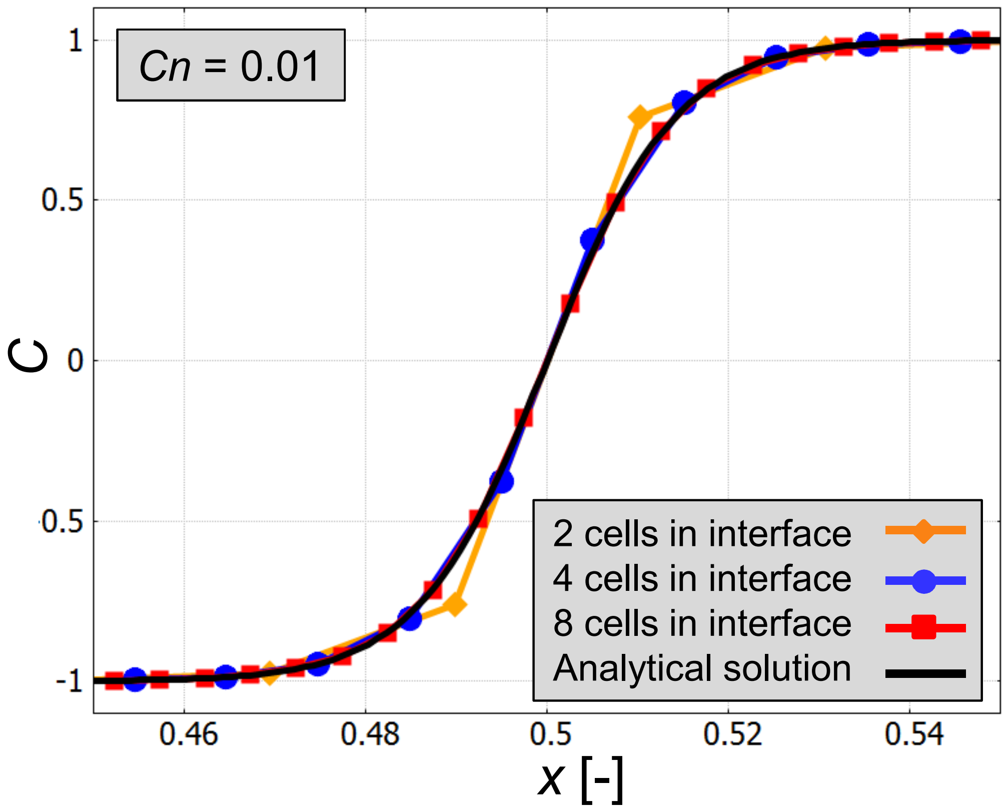
- Diffusion term is formulated from chemical potential gradient

$$\frac{\partial C}{\partial t} = \nabla^2 \Phi \quad \Phi = C^3 - C - Cn^2 \nabla^2 C$$ → 4^{th} order derivative in total

- Compare 1D simulation results against following analytical solution:

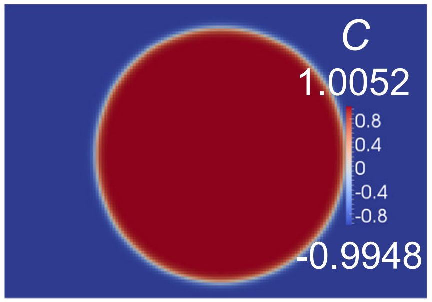
$$C = \tanh\left(\frac{x}{\sqrt{2}Cn}\right)$$

- Interface thickness must be resolved by at least 4 mesh cells to obtain accurate result



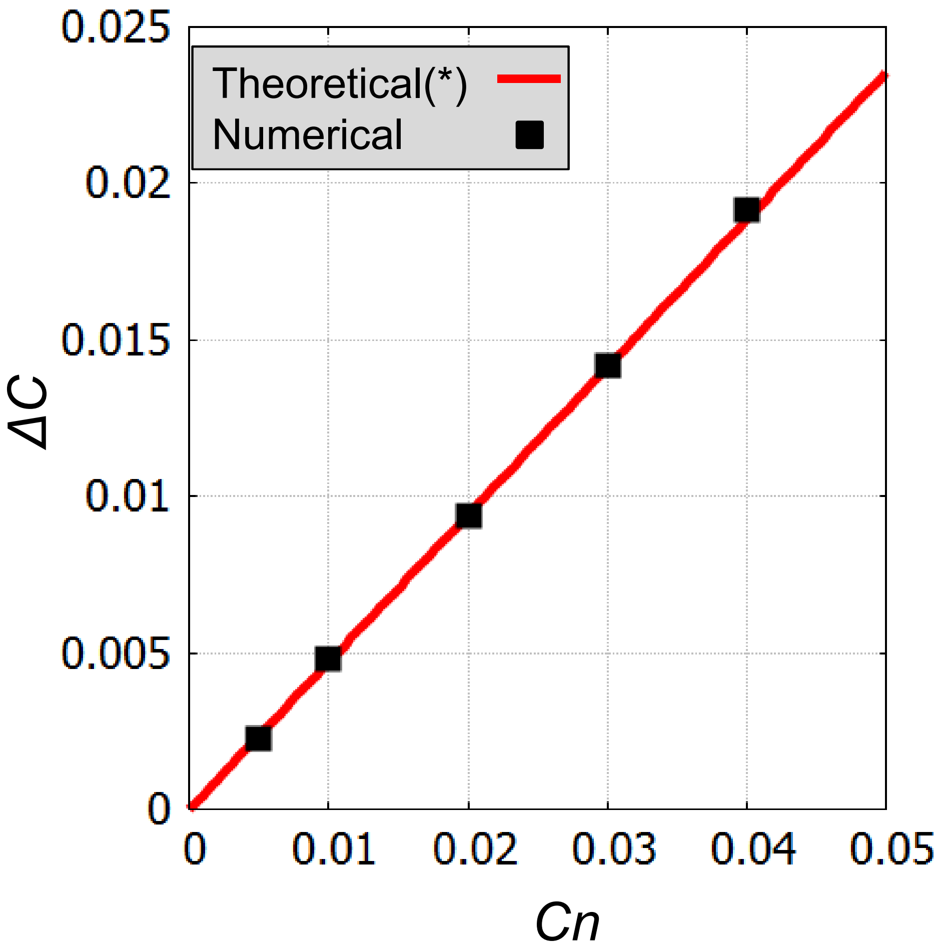
Influence of model parameter (*Cn*)

- "out-of-physical-bounds" in order parameter (*C*) in 2D domain



Shift in limits ΔC = 0.0052

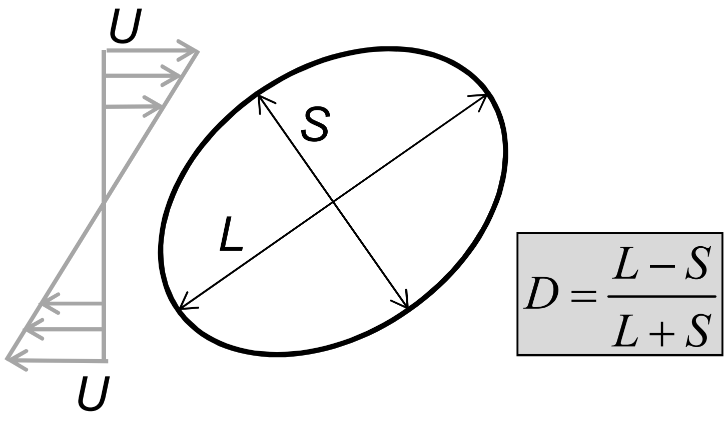
- Theoretical analysis(*) gave linear relation btw. ΔC and *Cn*
- *Cn* $\rightarrow$ interface thickness
- Compromise btw. accuracy and computational cost $\rightarrow$ $Cn = 0.01$
- Suitable value for $Pe_\kappa = 1000$ (see paper)



(*) Yue et al. 2007

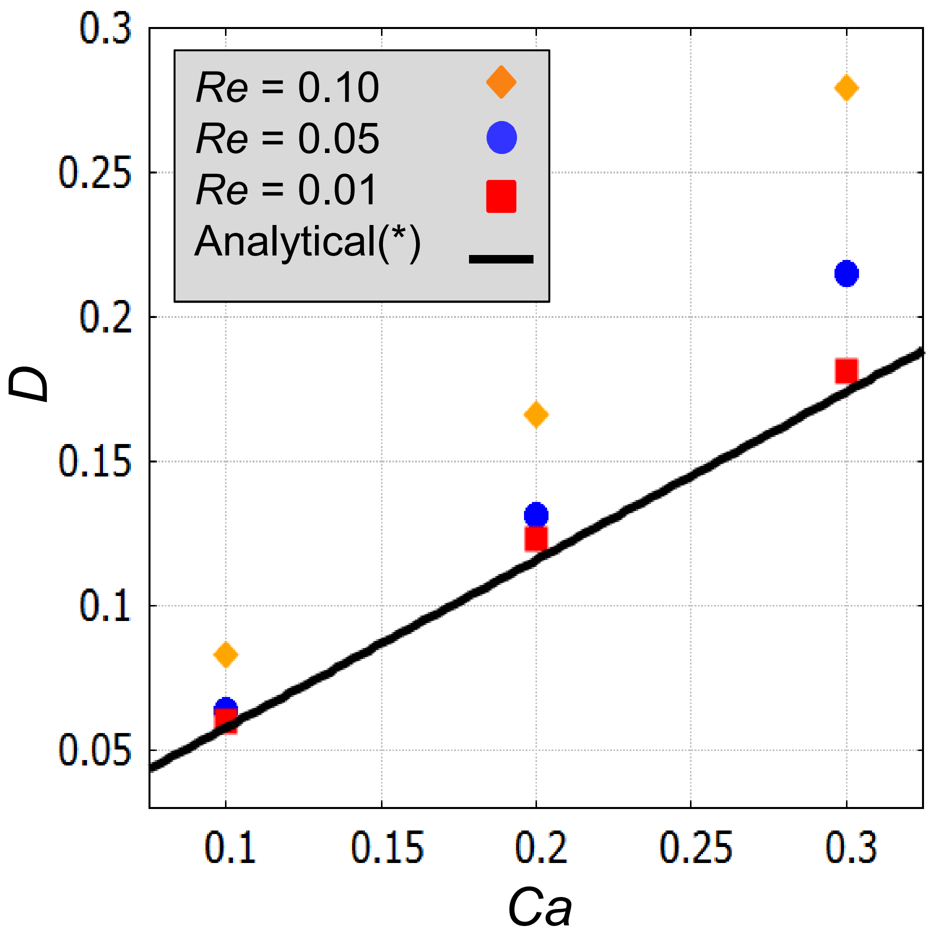
Validation of Surface Tension Term

- Surface tension force is formulated in a potential form



Drop deformation in shear flow

- Analytical solution(*) relates deformation parameter (*D*) to Capillary no. (*Ca*)
  - ➢ Assumptions: same *μ*, *ρ* and <u>creeping</u> unbounded flow



(*) Taylor 1934

Capillarity-driven Droplet Spreading / Dewetting

- Young's equation:

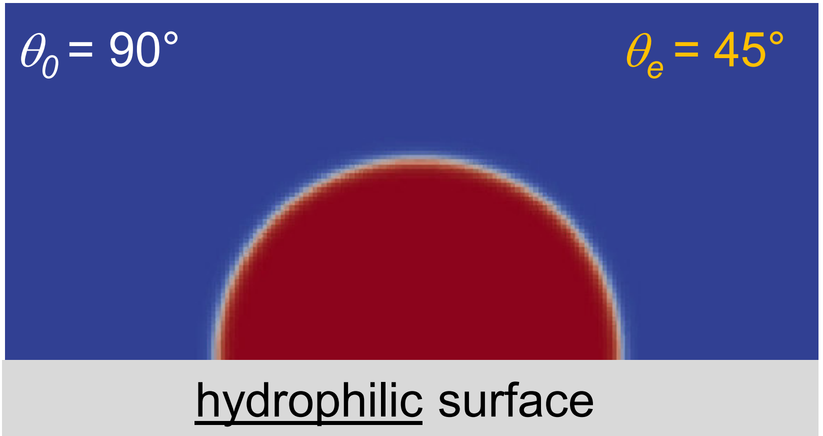
$$\cos(\theta_e) = \frac{\gamma_{SG} - \gamma_{SL}}{\gamma_{LG}}$$

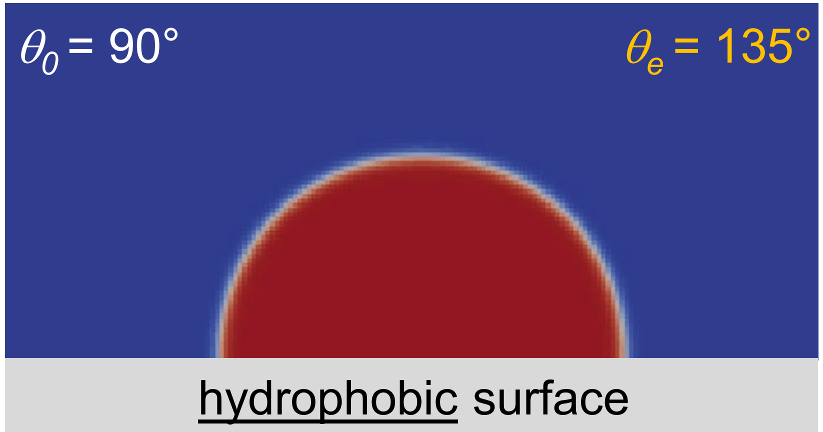
  - θ_e: equilibrium contact angle
  - Surface wettability

- In PFM, θ_e is specified via Neumann BC for order parameter:

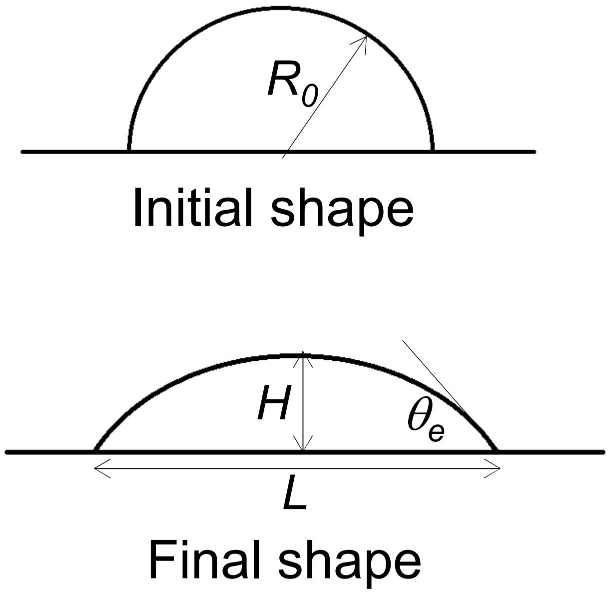
$$\hat{\mathbf{n}}_s \cdot \nabla C = -\frac{\sqrt{2}\cos\theta_e}{2Cn}(C^2 - 1)$$

- If $\theta_0 \neq \theta_e$, droplet begins to move with $\theta \to \theta_e$

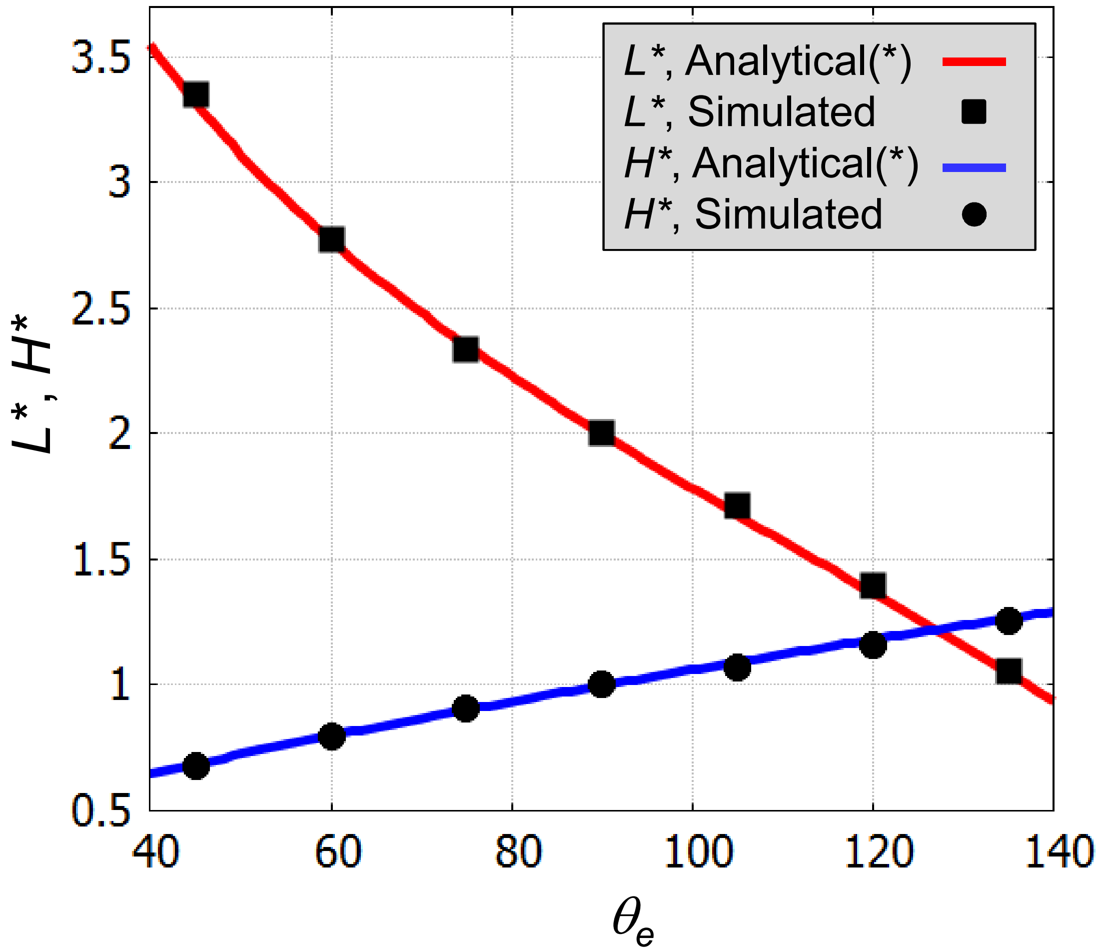




Capillarity-driven Droplet Spreading / Dewetting

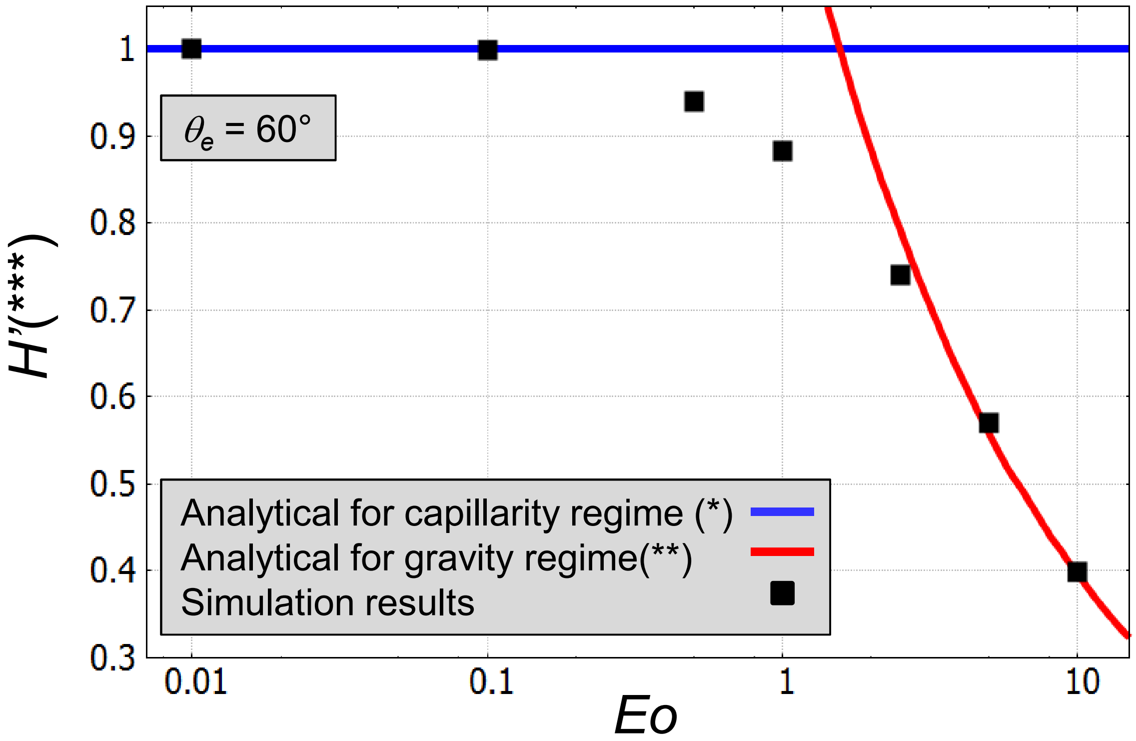


$L^* = L / R_0$
$H^* = H / R_0$



(*) Chen et al. 2009

Capillarity- / Gravity-driven Spreading

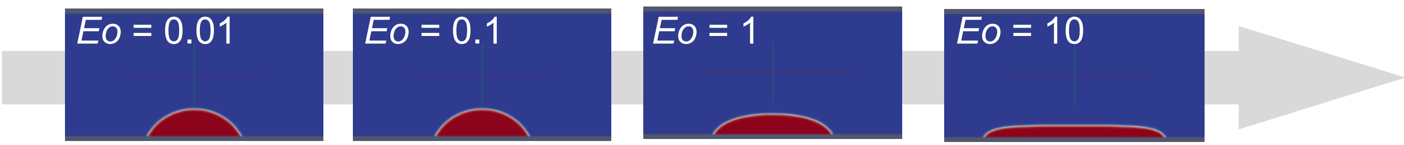


- Eötvös number (*Eo*): gravity / capillarity

➢ *Eo* << 1
  capillarity-driven regime

➢ *Eo* >> 1
  gravity-driven regime

➢ *Eo* ≈ 1
  transitional regime



(*)Chen et al. 2009 (**)Dupont et al. 2007 (***) $H' = H/H_0$, H_0: analytical height of capillarity spreading

Conclusions and outlook

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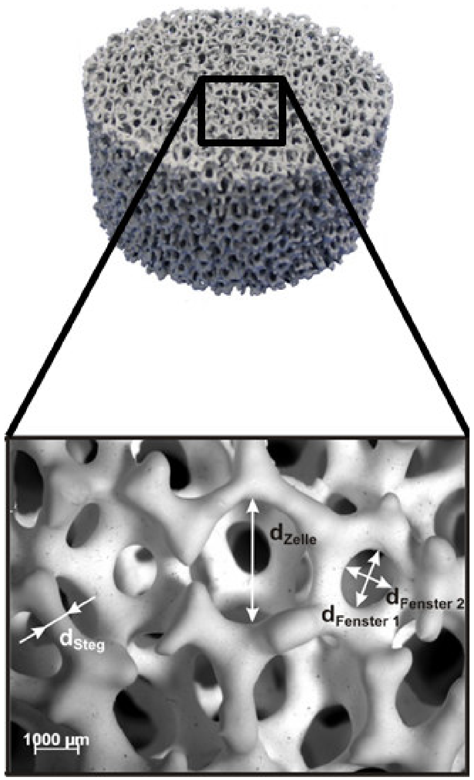
- Phase field method has been implemented in OpenFOAM®
- The method has been carefully verified in terms of
  - Identification of suitable ranges for model parameters (Cahn no. & Peclet no.)
  - Surface tension force
- The method is capable of
  - Accurately predicting spreading/dewetting process
  - Successfully reproducing two spreading regimes
- Next steps
  - Compare time evolution of contact angle, height & base radius of droplet against experimental data
  - Non-equilibrium BC: dynamic contact angle depends on contact line speed
  - Dynamic mesh adaptation
  - Simulate wetting process on irregular surface (real sponge geometry in multiphase reactors)



Acknowledgement

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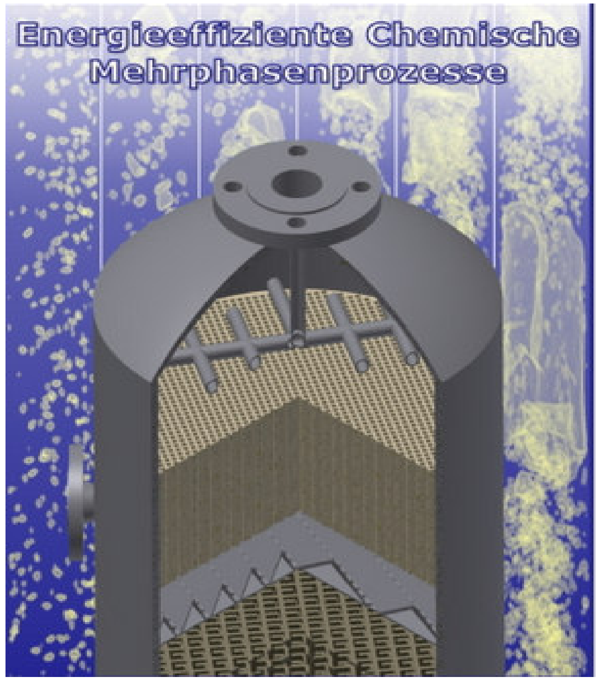
  - Partners:



(*) Website: https://www.hzdr.de/db/Cms?pNid=2972