A Phase Field Method for Numerical Simulation of Wetting and Spreading Processes with OpenFOAM®

X. Cai, M. Wörner, O. Deutschmann

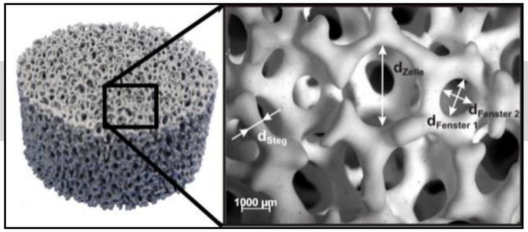
Jahrestreffen der Fachgruppen Computational Fluid Dynamics, Mischvorgänge und Rheologie, 24. – 25. Feb. 2014, Würzburg

Multiphase Flow Group, Institute of Catalysis Research and Technology (IKFT)

Outline

- Motivation
  - Wetting/spreading in industrial applications
  - 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

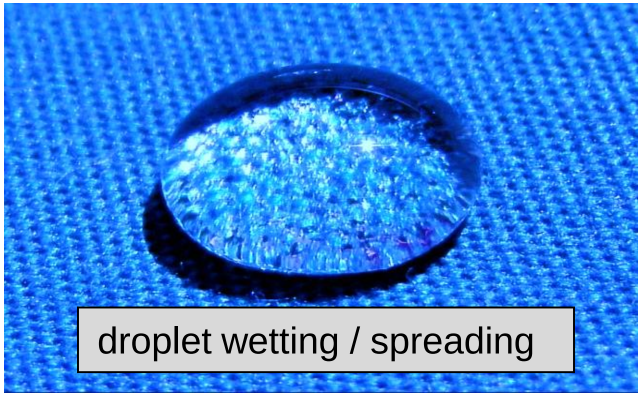
Motivation



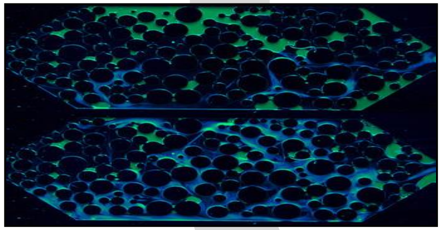
solid sponge chemical reactor

insecticides spray

coating



droplet wetting / spreading

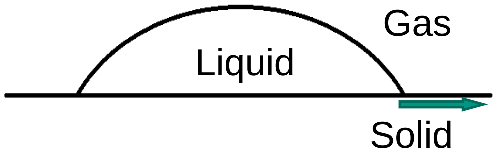


oil recovery from porous structure

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

- This paradox can be resolved by:

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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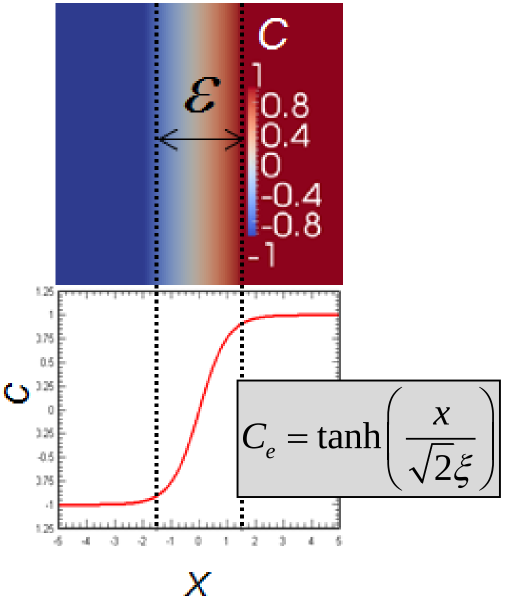
Phase Field Method

- Order parameter (*C*) as phase indicator
  - *C* = 1 for liquid, *C* = -1 for gas
- *C* varies continuously following a *tahn* func.
  - Diffuse interface with a finite thickness
  - Built on physical sense
  - **Sufficient mesh resolution for interface**



$$C_e = \tanh\left(\frac{x}{\sqrt{2}\xi}\right)$$

- Dimensionless Cahn-Hilliard equation

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

$$\Phi = C^3 - C - Cn^2\nabla^2 C \qquad Cn = \frac{\xi}{L}, \qquad Pe_\kappa = \frac{2\sqrt{2}LU\xi}{3\kappa\sigma}$$

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

- *Cn*: interface thickness *Pe*$_\kappa$: ratio of convection to diffusion
  - They are model parameters → **Identification of suitable ranges**

Dimensionless 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

Buoyancy

- Mixture density & viscosity:

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

- Dimensionless Groups:

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

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

Implementation in OpenFOAM®

Open∇FOAM

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

In a single time step

1. Calculate chemical potential
2. Solve C-H eq. for order parameter
3. Calculate surface tension, buoyancy & mixture ρ, μ
4. Solve N-S eqs. for velocity

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Validation of Diffusion Term in C-H Equation

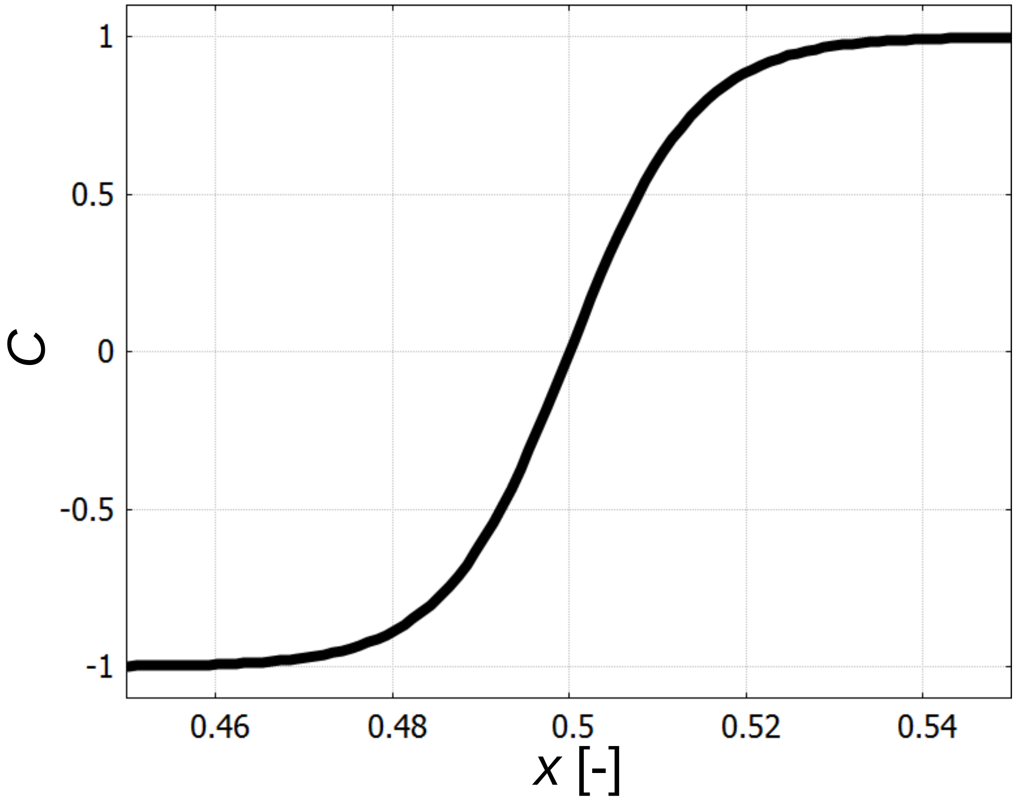
- Diffusion term is formulated from chemical potential gradient

$$\frac{\partial C}{\partial t} = \nabla^2\left(C^3 - C - Cn^2\nabla^2 C\right)$$

→ 4th order derivative in total

- Compare 1D simulation results against following analytical solution:

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



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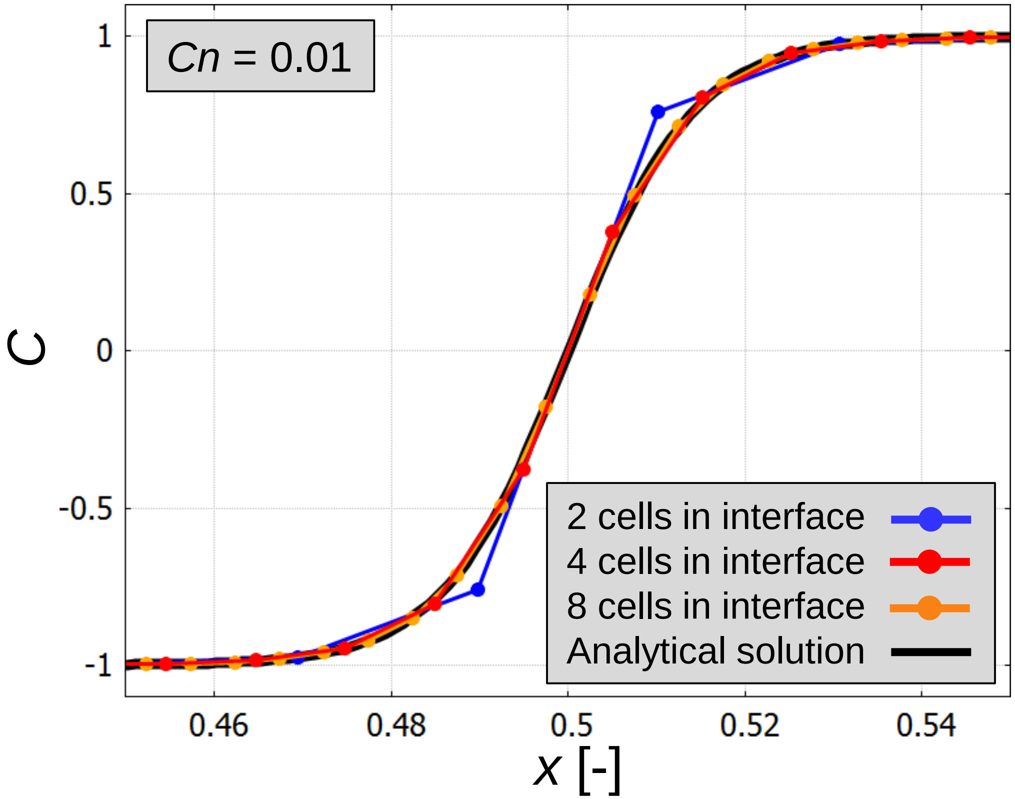
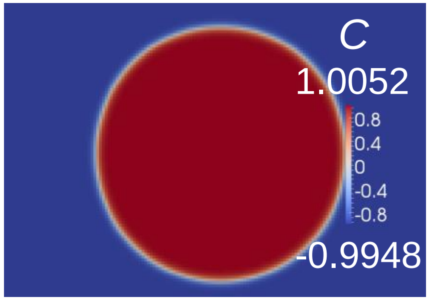
- Interface thickness must be resolved by at least 4 mesh cells to obtain accurate result



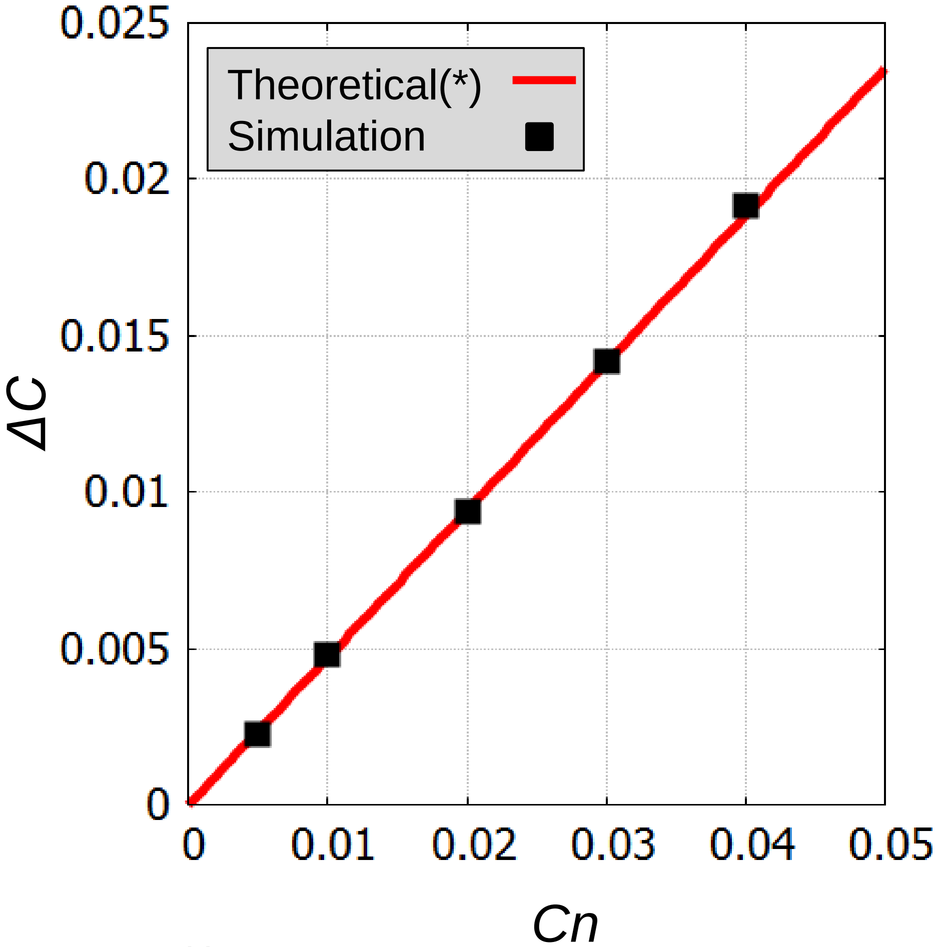
Influence of model parameter: Cahn (*Cn*) No.

- “out-of-physical-bound” in order parameter (*C*) in 2D domain



Shift in limit $\Delta C = 0.0052$

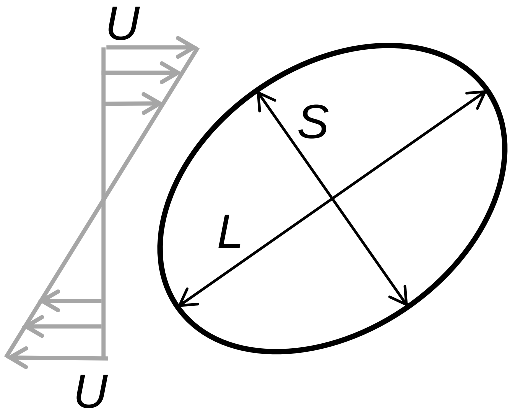
- Theoretical analysis(*) gives linear relation btw. ΔC and *Cn*
- Simulation results agree
- *Cn* → interface thickness
- Compromise btw. accuracy and computational cost → $Cn = 0.01$
- Suitable value for $Pe_\kappa = 1000$(**)



(*) Yue et al. 2007
(**) Cai et al. 2013

Validation of Surface Tension Term

- Surface tension force is formulated in a potential form

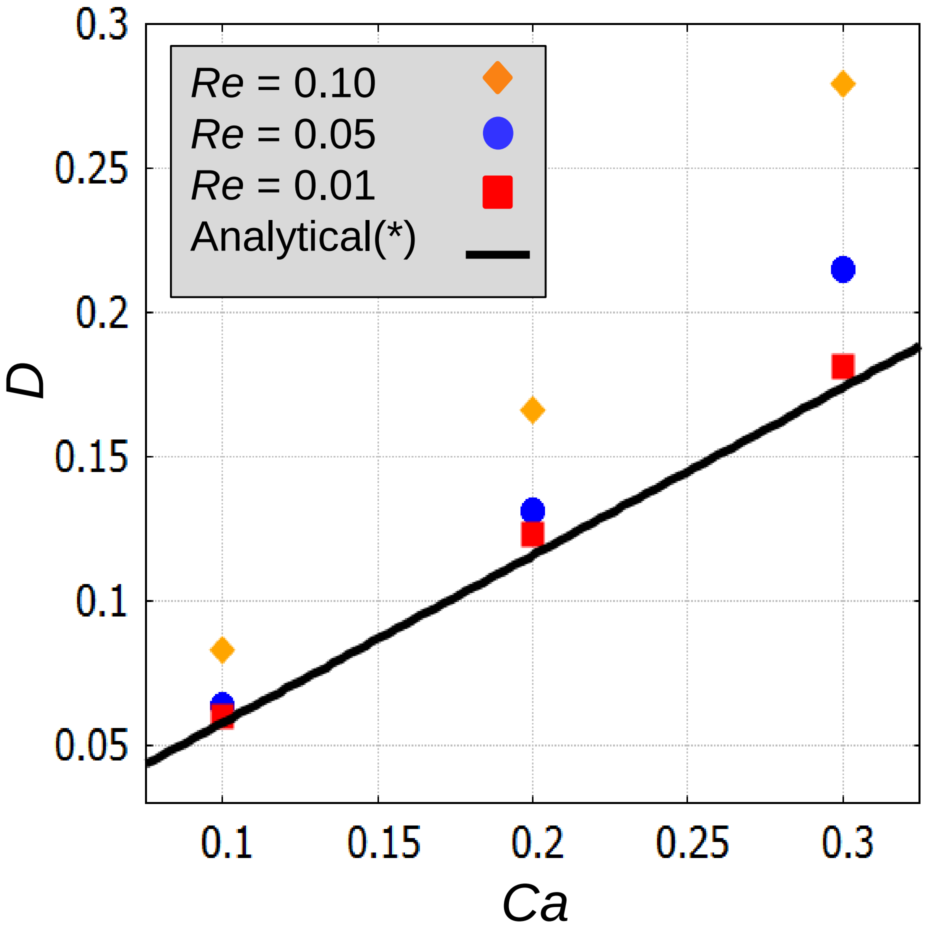


$$D = \frac{L - S}{L + S}$$

Drop deformation in shear flow

- Analytical solution(*) relates deformation parameter (*D*) to Capillary no. (*Ca*)

➢ Assumptions: same μ, ρ and creeping unbounded flow



(*) Taylor 1934

Capillarity-driven Droplet Spreading / Dewetting

- Young’s equation:

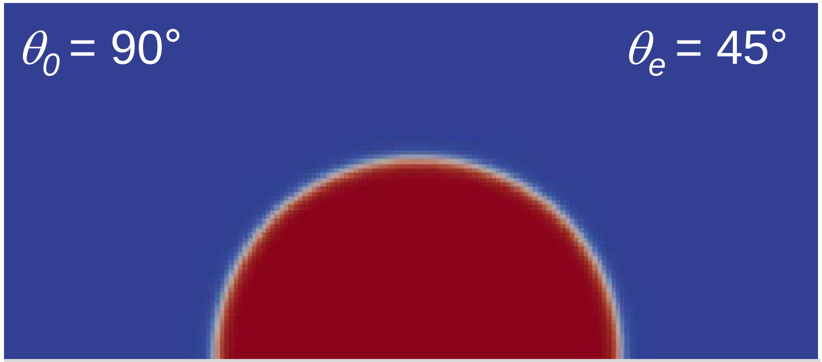
$$\cos(\theta_e) = \frac{\gamma_{SG} - \gamma_{SL}}{\gamma_{LG}}$$

  - θ_e: equilibrium contact angle
  - Surface wettability

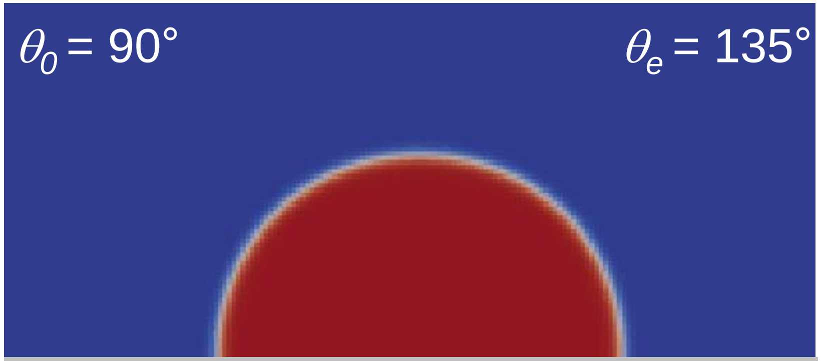
- θ_e is specified via Neumann BC for order parameter:

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

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

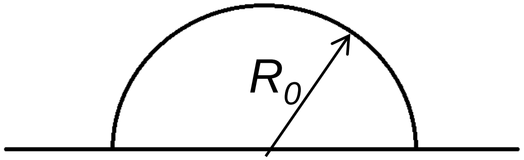


hydrophilic surface

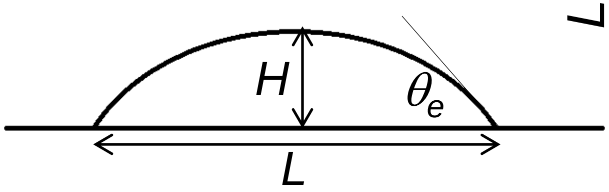


hydrophobic surface

Capillarity-driven Droplet Spreading / Dewetting

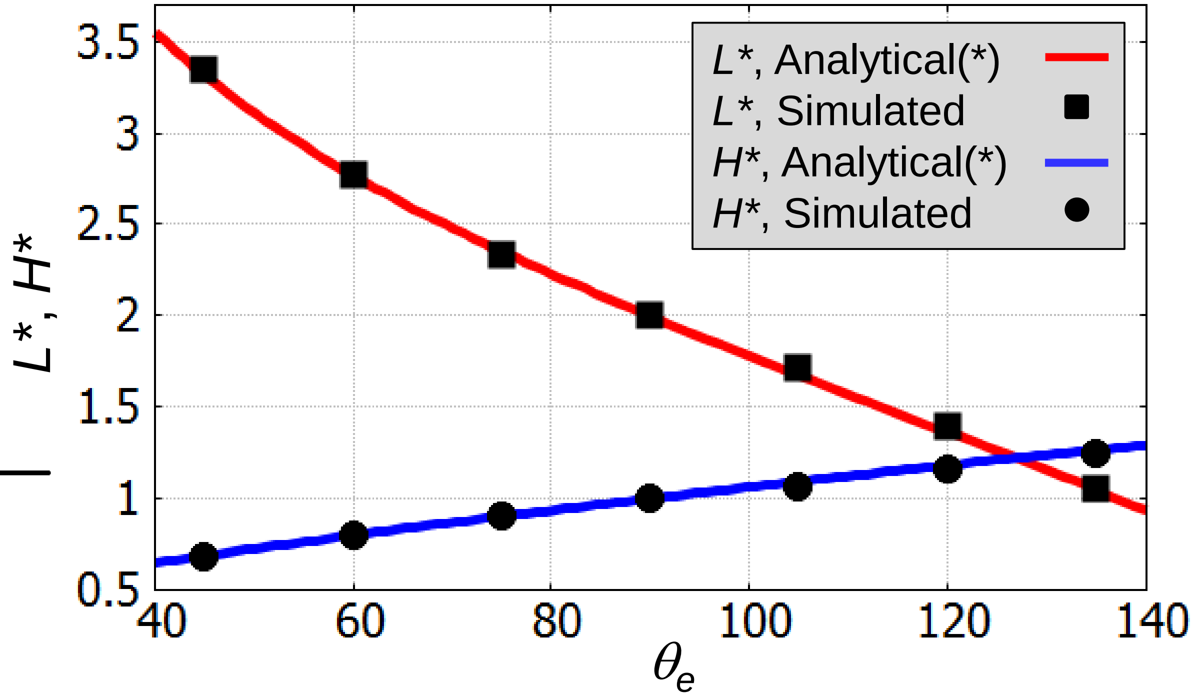


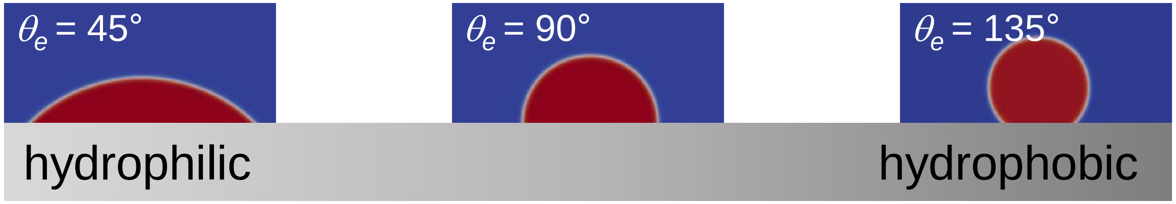
Initial shape



Final shape

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

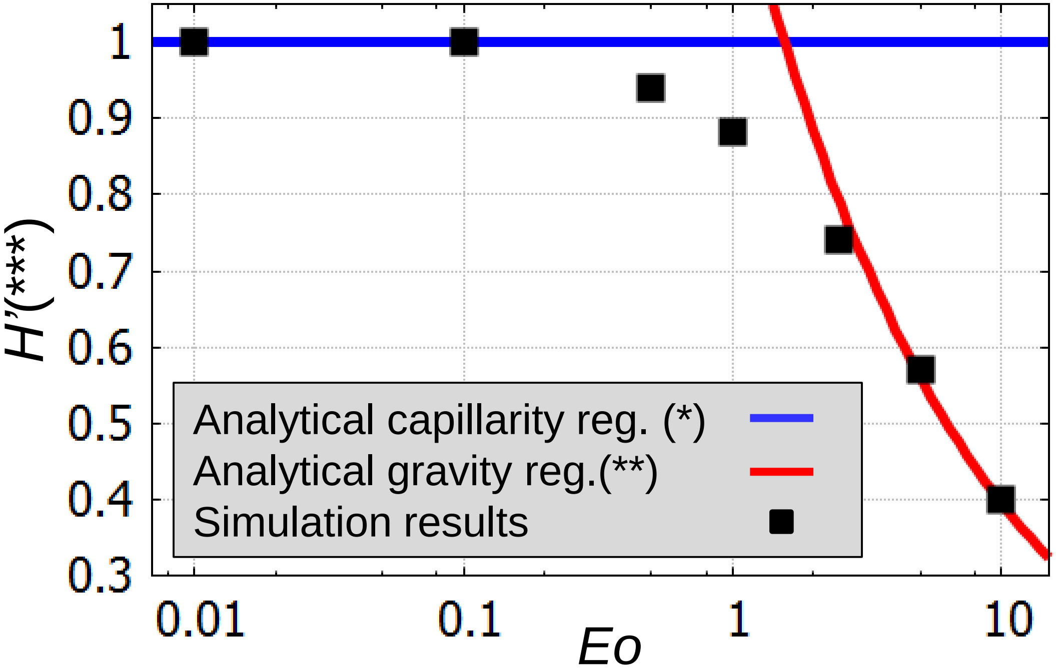




(*) Chen et al. 2009

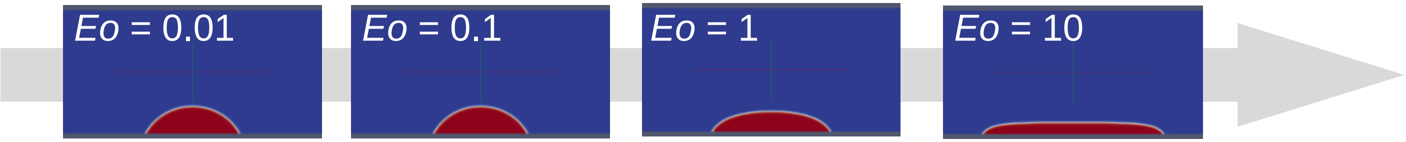
Capillarity- / Gravity-driven Spreading

$\theta_e = 60°$



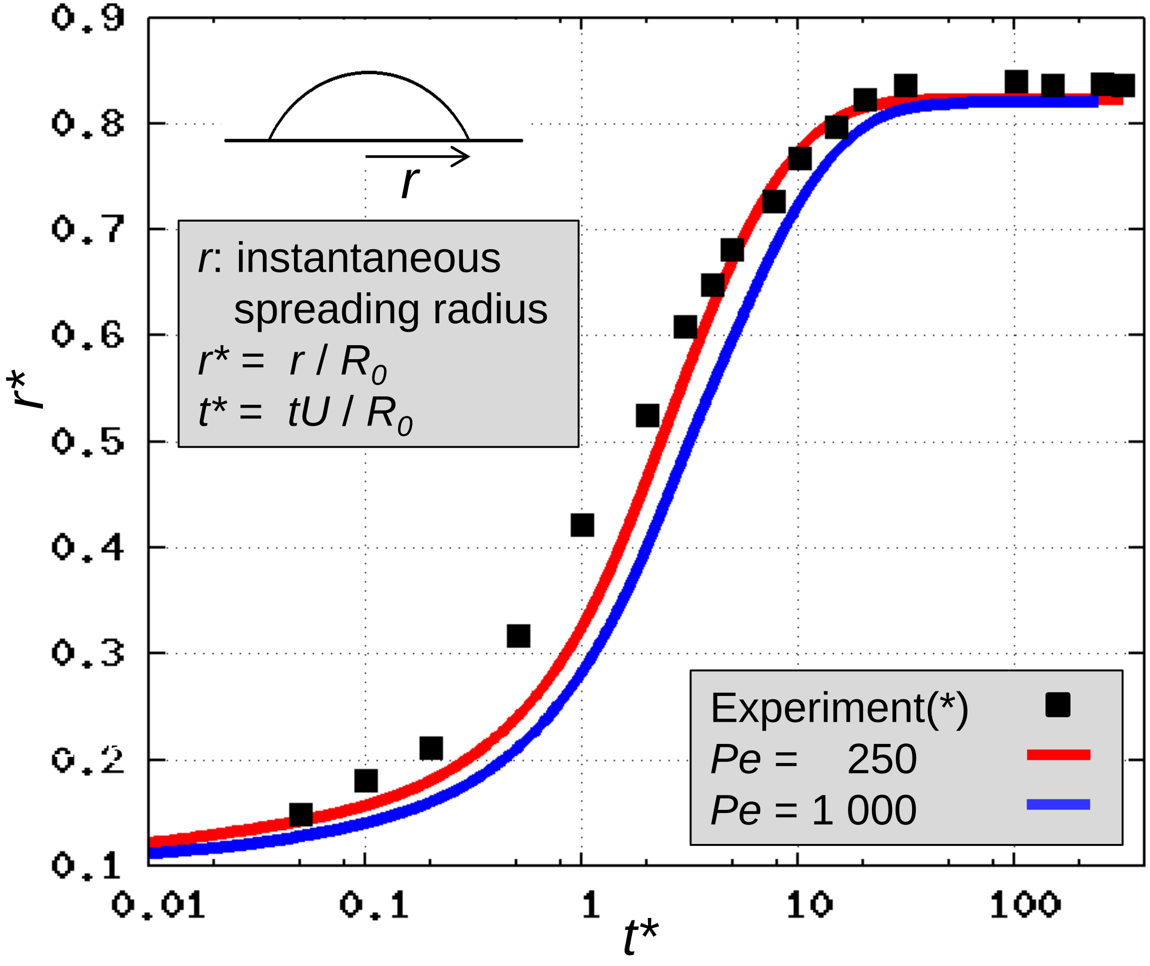
- Eötvös number (*Eo*):

- ➢ *Eo* << 1
  capillarity-driven regime
- ➢ *Eo* >> 1
  gravity-driven regime
- ➢ *Eo* ≈ 1
  transitional regime



(*)Chen et al. 2009 (**)Dupont et al. 2007 (***) *H'* : normalized height of droplet

Capillarity-driven Droplet Spreading Process



r: instantaneous spreading radius

$r^* = r / R_0$

$t^* = tU / R_0$

(*) Zosel 1993

- Smaller *Pe* → smaller Δt

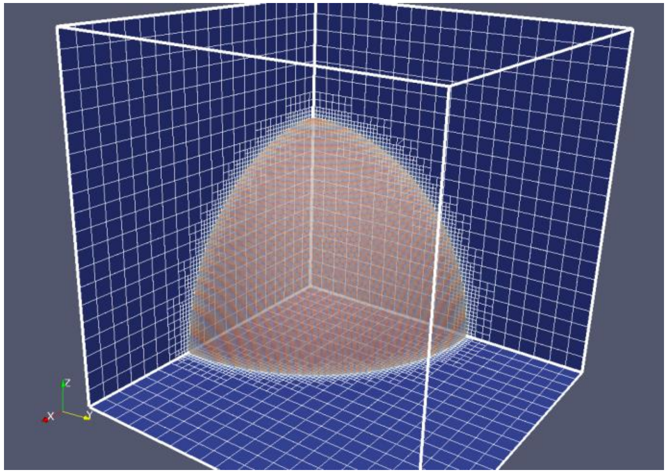
Pe	Max. Δt
1000	$2*10^{-3}$
250	$1*10^{-3}$
100	$1*10^{-4}$

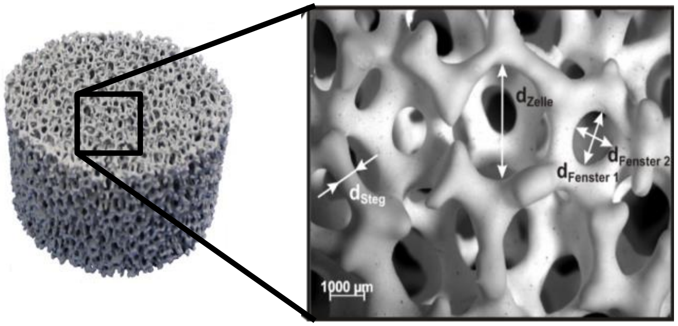
- Strict limitation on Δt from 4th order diffusion

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

Outlook on Next Steps

- Optimization of current numerical scheme
  - Decomposing Cahn-Hilliard eq. into 2 Helmholtz eqs. (Yue et al. 2004)
- 3D adaptive mesh refinement simulation
  - Mesh refinement around interface
- Take into account dynamic contact angle
  - $\theta_d = f(\theta_{e,} Ca_{cl})$
- Application in sponge chemical reactor
  - Wetting process on 3D irregular surface





Conclusions

- Phase field method has been implemented in OpenFOAM®

- The method has been verified in terms of
  - Identification of suitable ranges for model parameters
  - Surface tension force

- The method is capable of
  - predicting spreading/dewetting process
  - reproducing two spreading regimes
  - achieving good agreement with experimental data

Acknowledgement

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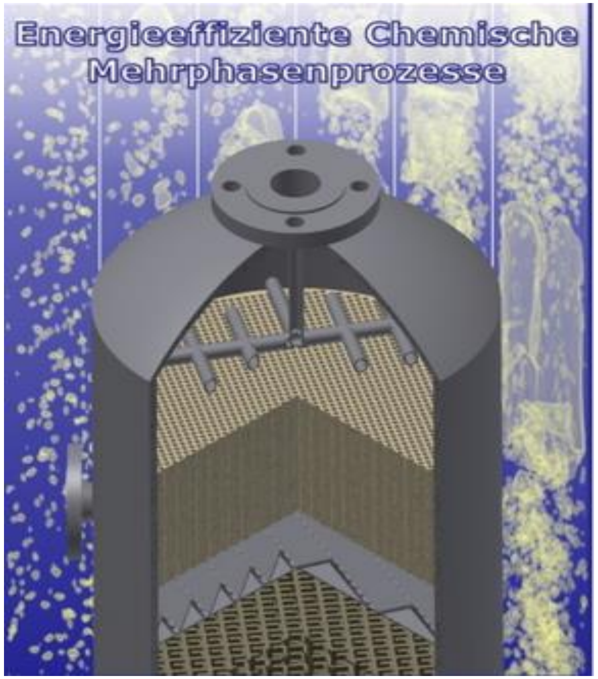

(*) Website: https://www.hzdr.de/db/Cms?pNid=2972

Thank you for your attention!

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