Development of Phase Field Methods with OpenFOAM® and its Application to Dynamic Wetting Processes

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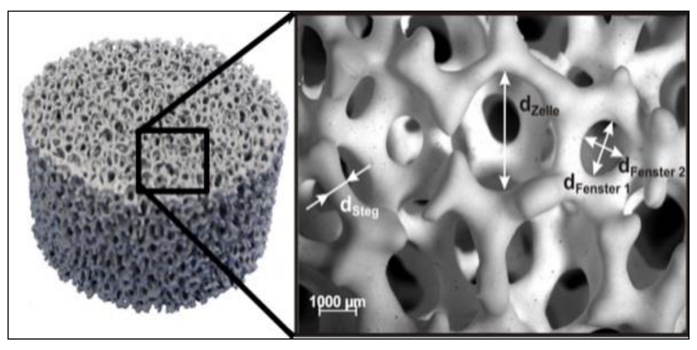
1. Motivation

- **Wetting process in chemical reactor of foam structure**
- ➢ Mathematical consistent modeling of moving contact lines on irregular solid surface
- → Resolve stress singularity at no-slip wall

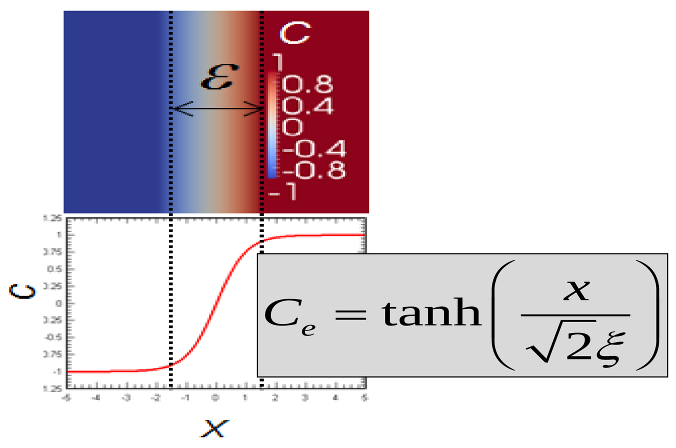


2. Phase Field Methods

- **Cahn-Hilliard (CH) or Allen-Cahn (AC) equation for phase field advection**

CH: $\frac{\partial C}{\partial t}+(\mathbf{u}\cdot\nabla)C=\kappa\nabla^2(\frac{\lambda}{\varepsilon^2}C(C-1)(C+1)-\lambda\nabla^2 C)$ AC: $\frac{\partial C}{\partial t}+(\mathbf{u}\cdot\nabla)C=-\frac{\gamma}{\varepsilon^2}C(C-1)(C+1)+\gamma\nabla^2 C$

- ➢ *C*: phase field;1 for liquid and -1 for gas; it varies continuously over the diffuse interface
- CH or AC is coupled with momentum equ. through surface tension, linear momentum, viscous stress and buoyancy terms

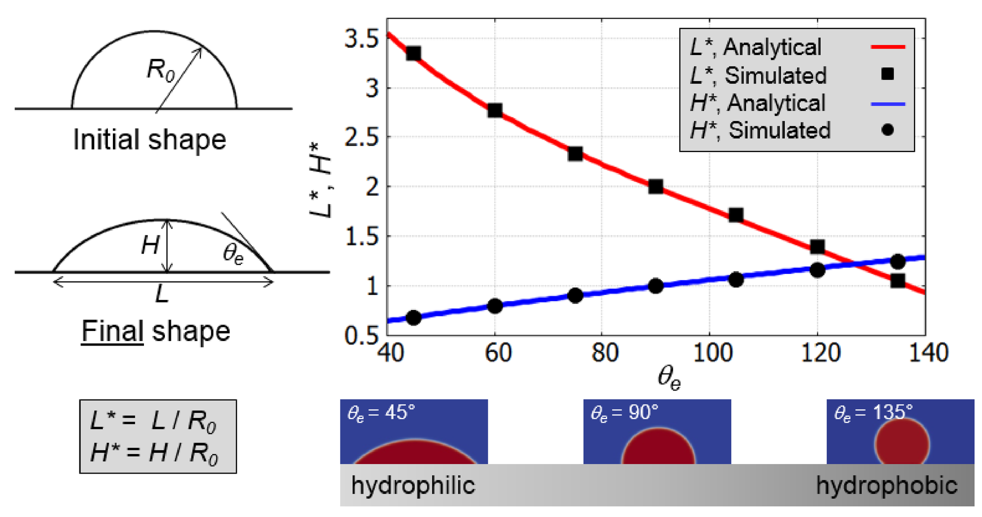


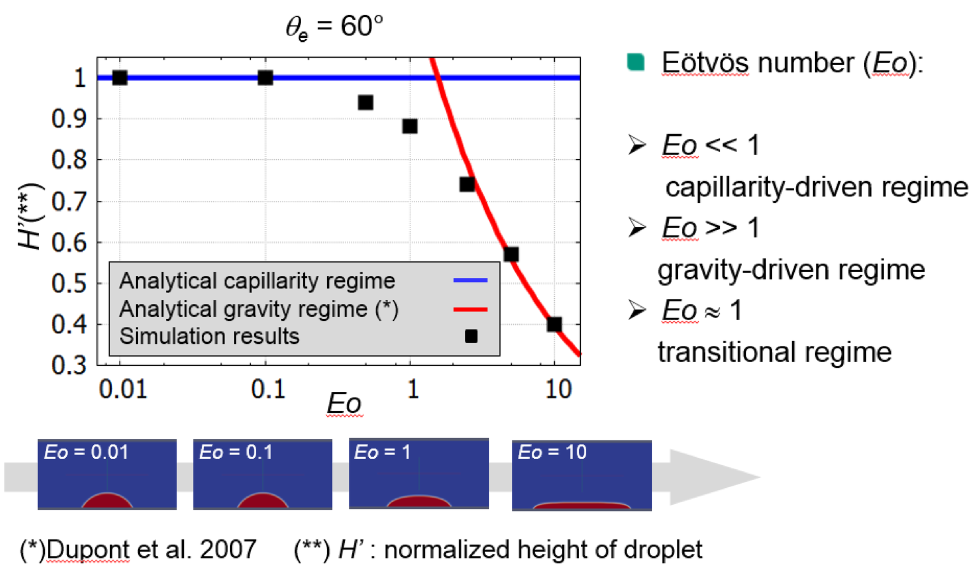
3. Development and Implementation

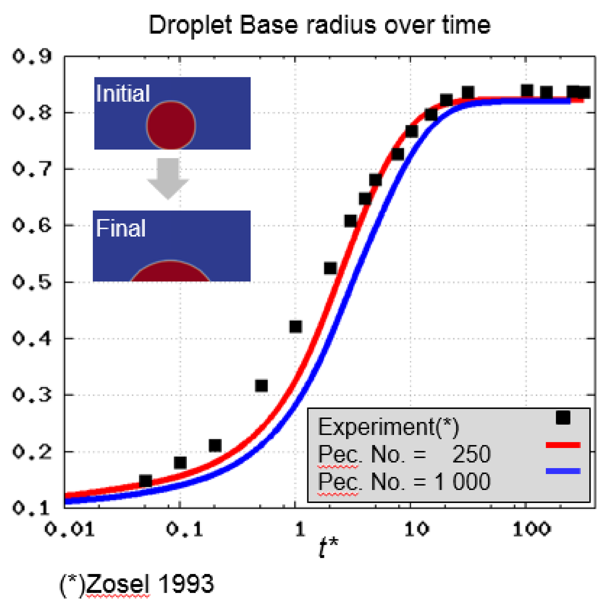
- ➢ Platform: OpenFOAM® (an open source CFD software package); *interDyMFoam* as starting point
- ➢ In Cahn-Hilliard, the mobility (4th order derivative) is for now treated in segregated manner with time-step sub-cycling
- ➢ In Allen-Cahn, Lagrange multiplier implemented to enforce phase volume conservation property
- ➢ In momentum equation, relative density flux term due to diffusion of components (central to volume conservation)
- ➢ Surface tension term is implemented as surface tension energy density

4. Validation (using Cahn-Hilliard)

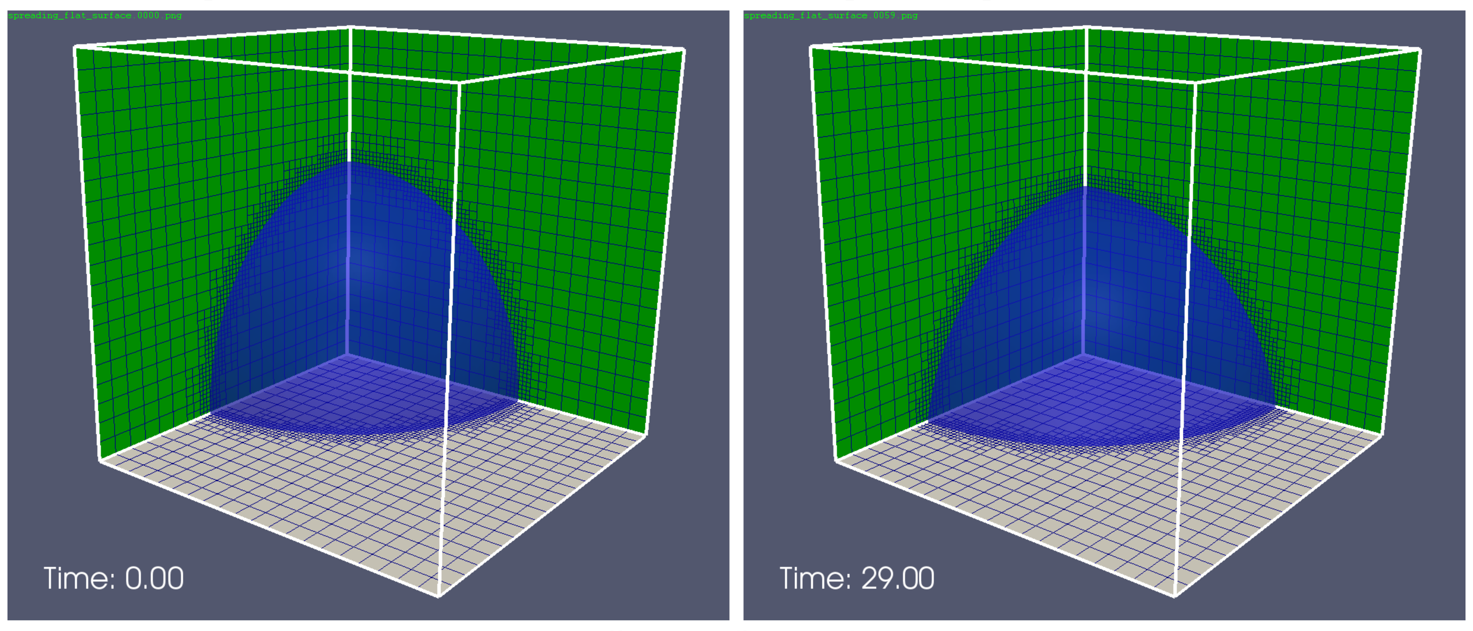
- **2D Static mesh simulation**



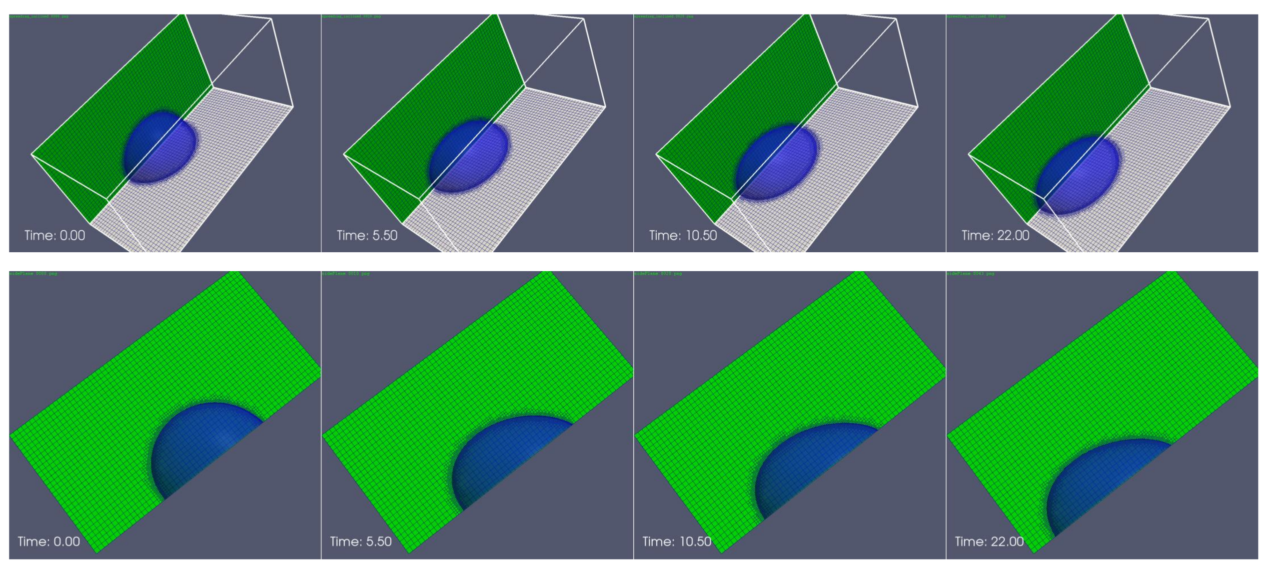




- **3D Adaptive Mesh Refinement (AMR) simulation interface region (refinement level = 2)**



Spreading on flat surface



Spreading and sliding on 45° inclined surface

5. Outlook

- ➢ Compensation scheme for wall energy relaxation model
- ➢ Block-coupled solution approach to phase field transport in Cahn-Hilliard equation
- ➢ Chemically and geometrically heterogeneous surface
- ➢ Pinning effect of droplet on inclined surface
- ➢ Representative complex sponge structure

❑ We acknowledge funding by Helmholtz Energy Alliance "Energy-efficient chemical multiphase processes"