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POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY

Thermal Hydraulics & Energy System
THE System Lab

Mesoscopic Numerical Study of Cryogenic Bubble Generation and Liquid-Vapor Interface Movement in Microgravity

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Contents

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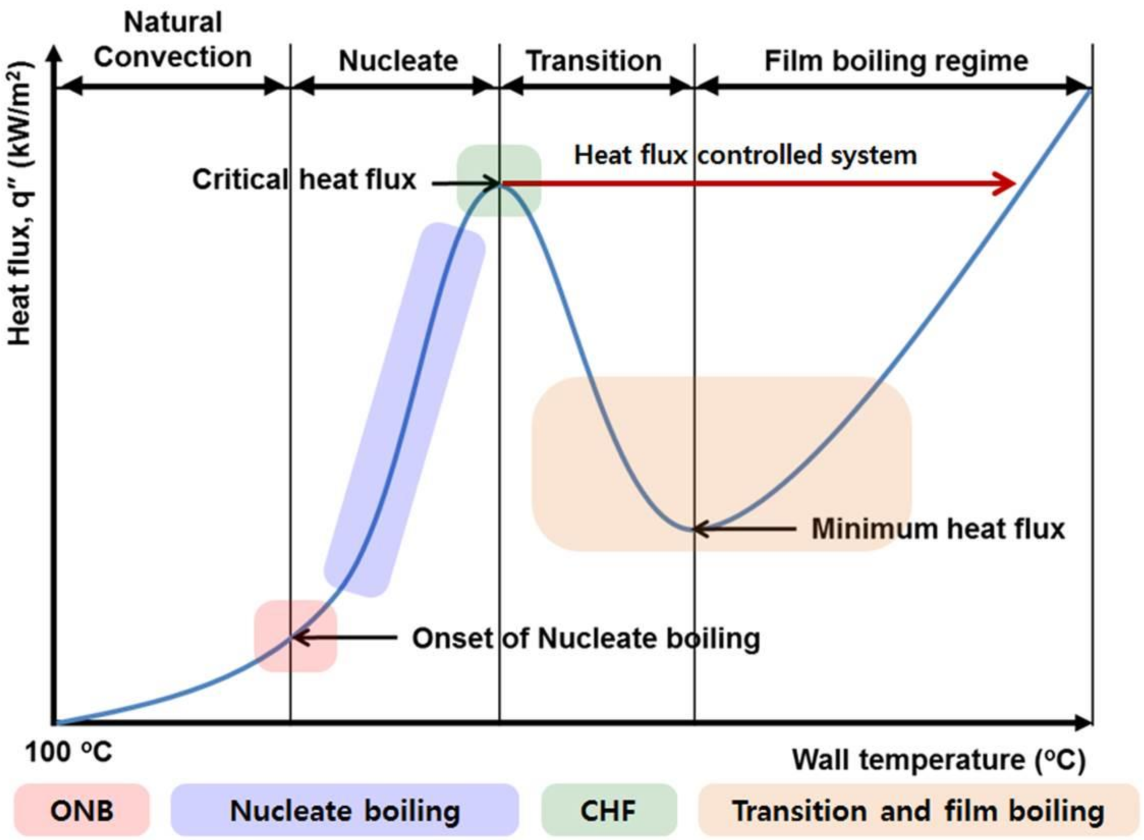
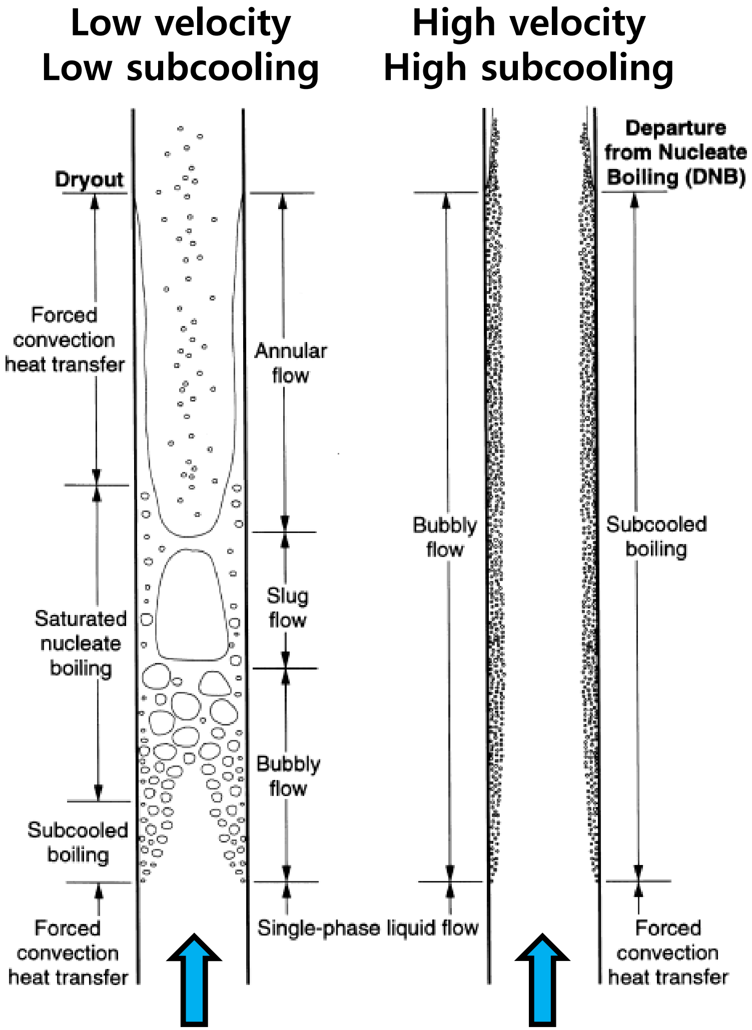
CHAPTER

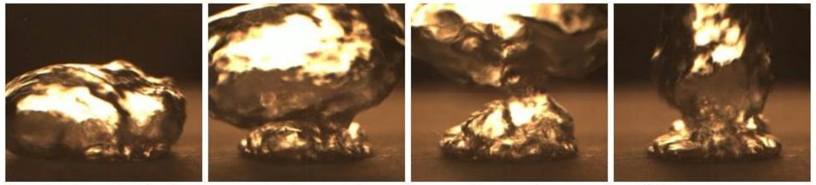
I Introduction

Boiling Curve






High speed visualization of film boiling


High speed visualization of nucleate boiling

[1] Mudawar, I., & Bowers, M. B. International Journal of Heat and Mass Transfer (1999).

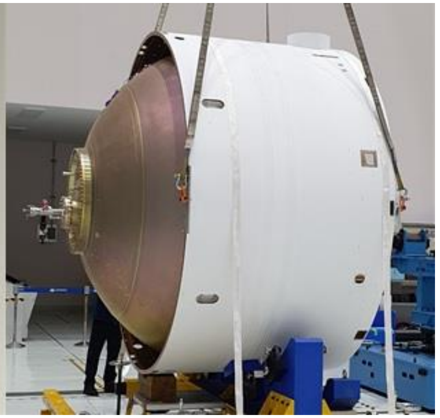
Space Exploration

KER / LOX
NURI

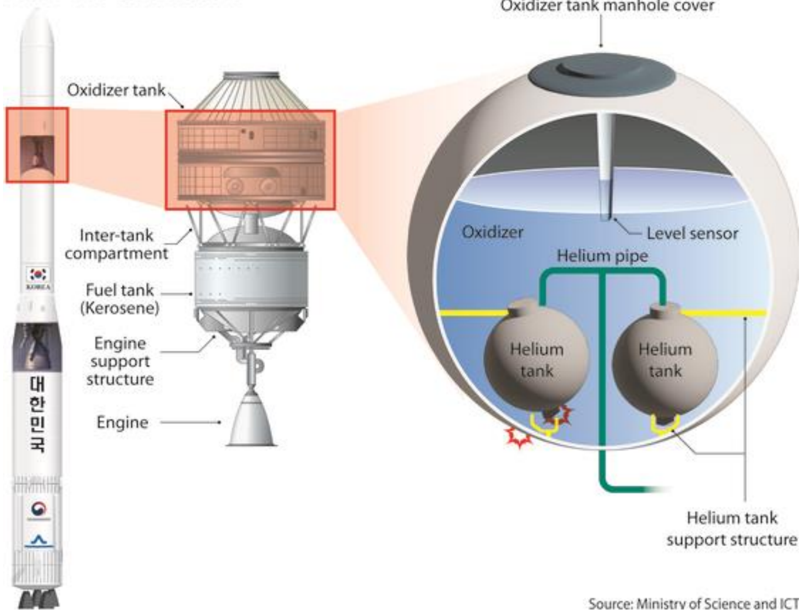
LCH4/ LOX
Zhuque-2

LH2/LOX
H3, Japan

- Launch vehicle with **cryogenic propellants**
  - Liquid oxygen (90 K), liquid methane (120 K), liquid hydrogen (20 K)
- Cryogenic propellants with extreme thermophysical property
  - Extremely low temperature (T < 100 K)
  - Gas vs fluid density = 1000 vs 1 kg/m^3
- Extreme propellants with Extreme structures
  - Compared like flying beer bottle
- **Upper stage with cryogenic propellants!**



Nuri-ho structure



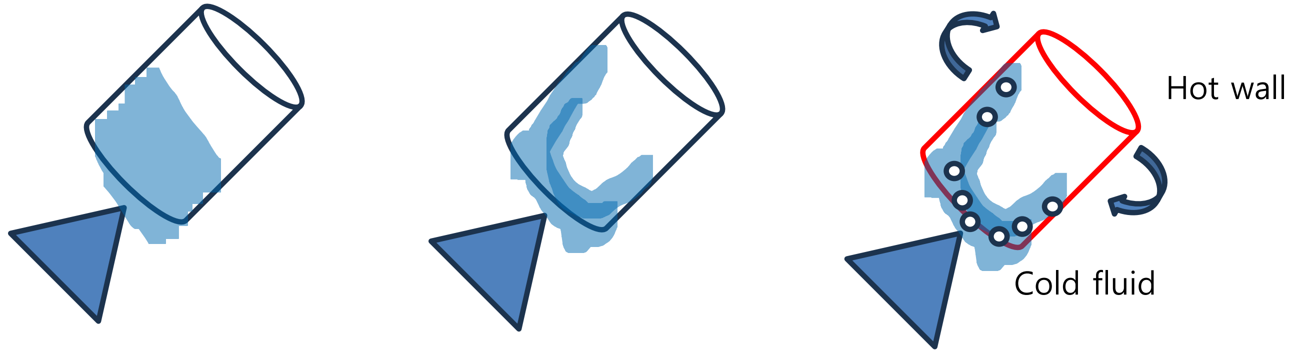
Space Exploration

- Restart Failure of Atlas-Centaur 4 (1964)
- KSLV-II NURI 1st Launch failure (3rd stage)

- What happens to fluid in microgravity??
  – **subcooled liquid in microgravity**

- What happens to cryogenic propellants in microgravity **when the wall is hot?**
  – **saturated (or boiling) liquid in microgravity**

Stable pressure | Stable pressure | Violent pressure increase



regular propellant In acceleration gravity
Acc >= 1g

regular propellant In microgravity
Acc < 1g

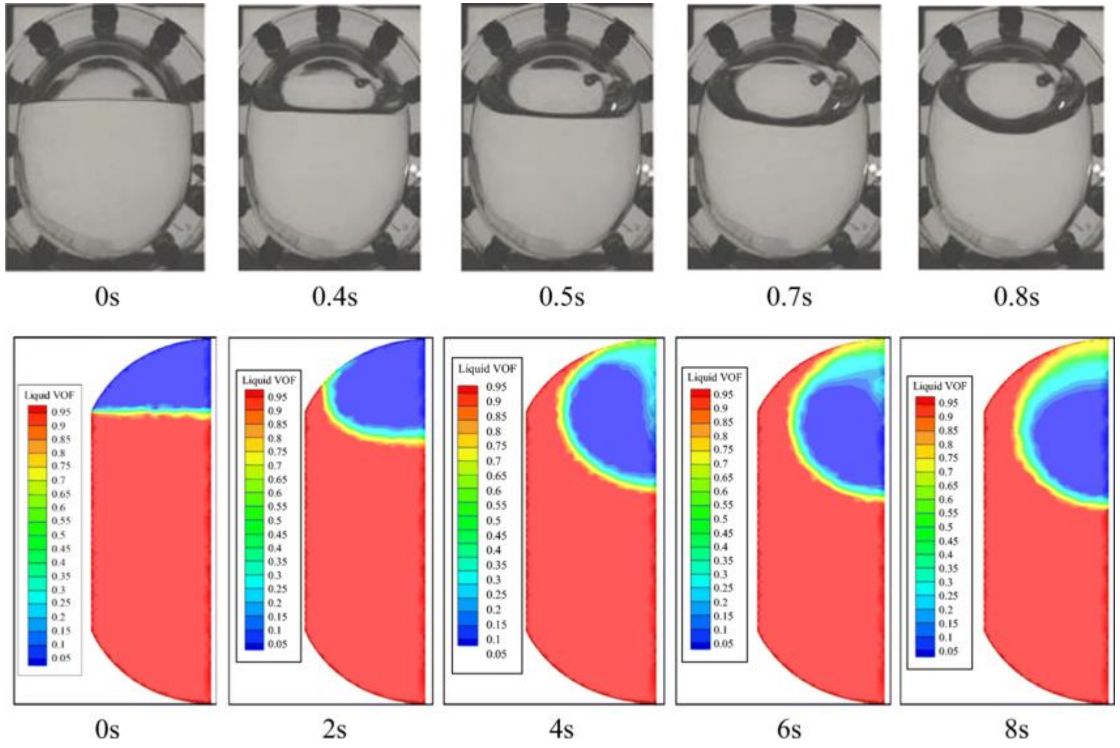
Cryogenic propellant In microgravity
Acc < 1g

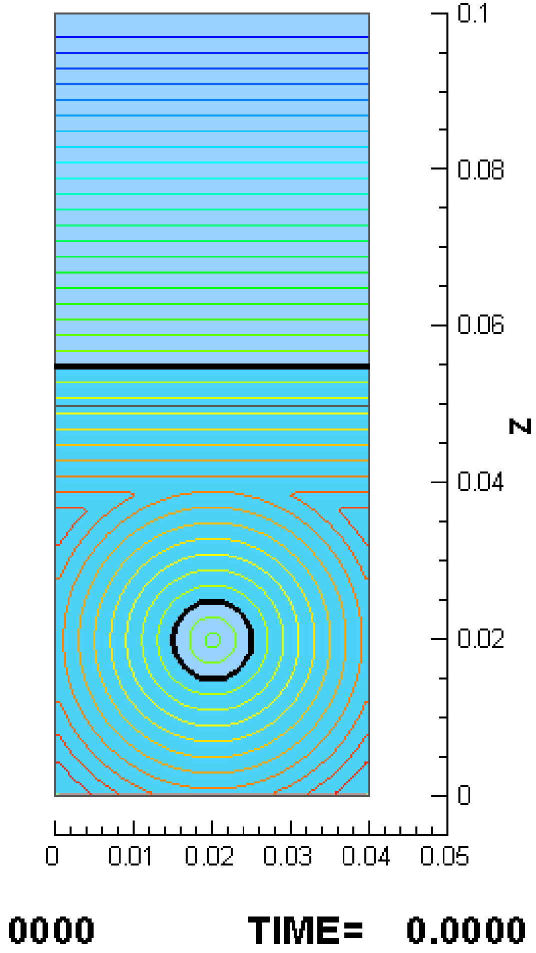
KSLV-II (NURI), 2021

Atlas-Centaur, 1964

Research Trend for Space Exploration

- Microgravity experiments
  - Drop tower… &
- Compared with CFD
  - Two-Fluid model
  - VOF(Volume of Fluid) method





Another candidate for the cryogenic boiling simulation
→ Lattice Boltzmann Method (LBM)

Numerical Simulation on Interface Evolution and Pressurization Behaviors in Cryogenic Propellant Tank on Orbit
Umemura, Yutaka, et al. "Numerical Modeling of Boiling Flow in a Cryogenic Propulsion System." 51st AIAA/SAE/ASEE Joint Propulsion Conference. 2015.
https://webpark1362.sakura.ne.jp/researches/
From Prof. T. Himeno at the University of Tokyo .

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CHAPTER

II Lattice Boltzmann Method

1. Lattice Boltzmann Method

1. Perturbation

$$f = f_i^{eq} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} + \cdots, (\epsilon = Kn)$$

$$f^{neq} = f - f^{eq}$$

2. Taylor Expansion

$$\mathcal{O}(\epsilon): \left(\partial_t^{(1)} + c_{i\alpha}\partial_\alpha^{(1)}\right) f_i^{eq} = -\frac{1}{\tau} f_i^{(1)}$$

$$\mathcal{O}(\epsilon^2): \partial_t^{(2)} f_i^{eq} + \left(\partial_t^{(1)} + c_{i\alpha}\partial_\alpha^{(1)}\right)\left(1 - \frac{\Delta t}{2\tau}\right) f_i^{(1)} = -\frac{1}{\tau} f_i^{(2)}$$

Chapman-Enskog Analysis

Kinetic theory → **Continuum mechanics**

Boltzmann equation

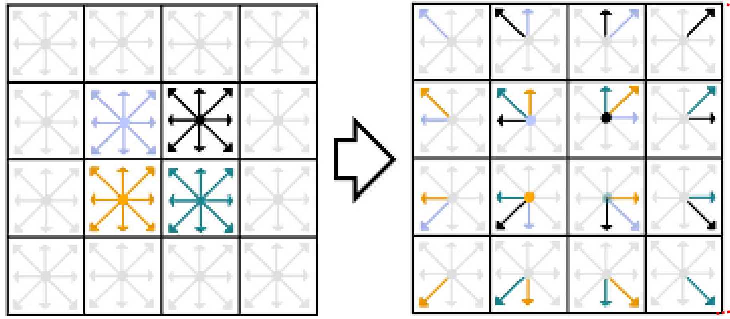
$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t}\right)\frac{dt}{dt} + \left(\frac{\partial f}{\partial x_\beta}\right)\frac{dx_\beta}{dt} + \left(\frac{\partial f}{\partial \xi_\beta}\right)\frac{d\xi_\beta}{dt} = \boldsymbol{\Omega}(\boldsymbol{f}),$$

$f(\boldsymbol{x}, \boldsymbol{\xi}, t)$: *Distribution function*

Discretization

Lattice Boltzmann equation

$$f_i(\boldsymbol{x} + \boldsymbol{c_i}\Delta t, t + \Delta t) - f_i(\boldsymbol{x}, t) = -\frac{\Delta t}{\tau}\left(f_i(\boldsymbol{x}, t) - f_i^{eq}(\boldsymbol{x}, t)\right)$$



four cells at timestep *t* after collision

four cells at timestep *t+1* after streaming

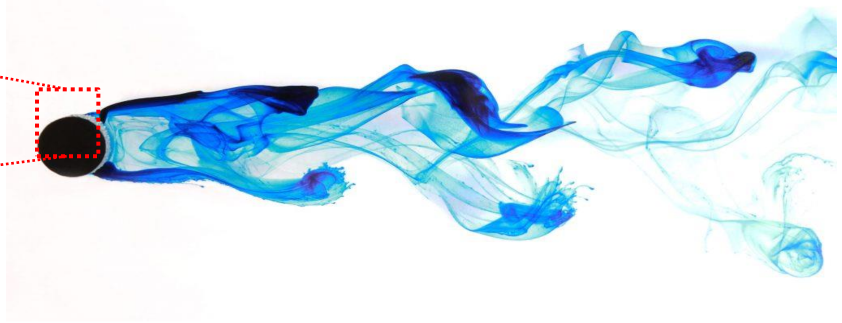
Navier-Stokes equation

$$\partial_t \rho + \partial_\gamma(\rho u_\gamma) = 0$$

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha p + \partial_\beta[\eta(\partial_\alpha u_\beta + \partial_\beta u_\alpha)]$$

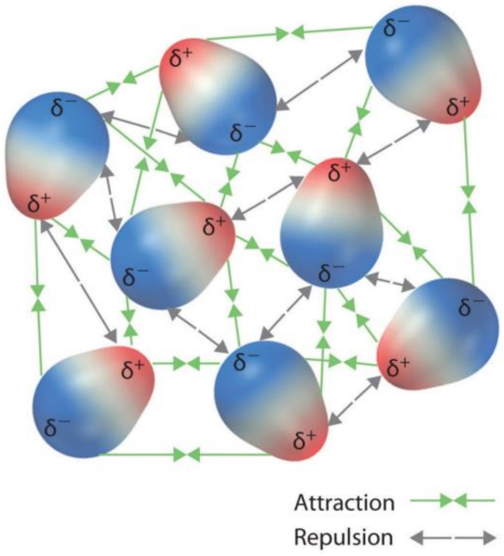
$$\sum_i f_i = \sum_i f_i^{eq} = \rho \qquad \sum_i c_i f_i = \sum_i c_i f_i^{eq} = \rho \boldsymbol{u}$$

$$P = \rho c_s^2, \qquad \eta = \rho c_s^2\left(\tau - \frac{\Delta t}{2}\right), \qquad \eta_B = \frac{2}{3}\eta$$



2. Interaction force & Forcing scheme

Phase segregation between different phases can emerge **automatically** as a result of **particle interaction**



$$F_{interface} = \kappa\rho\nabla\Delta\rho \qquad \boldsymbol{P}_{FE} = \left(p_{EOS} - \kappa\rho\nabla^2\rho - \frac{\kappa}{2}|\nabla\rho|^2\right)\boldsymbol{I} + \kappa\nabla\rho\nabla\rho$$

Shan-Chen discretized interaction force : $F^{SC}(x) = -\psi(x)G\sum_i w_i\psi(x + c_i\Delta t)c_i\Delta t$

Pressure tensor term with Shan-Chen interaction force :

$$\boldsymbol{P}_{SC} = \left(p_b + \frac{c_s^2 G}{2}\psi^2 + \frac{c_s^4 G}{4}(\nabla\psi)^2 + \frac{c_s^4 G}{2}\psi\Delta\psi\right)\boldsymbol{I} - \frac{c_s^4 G}{2}\nabla\psi\nabla\psi$$

Equation of state

LBE with Guo force term

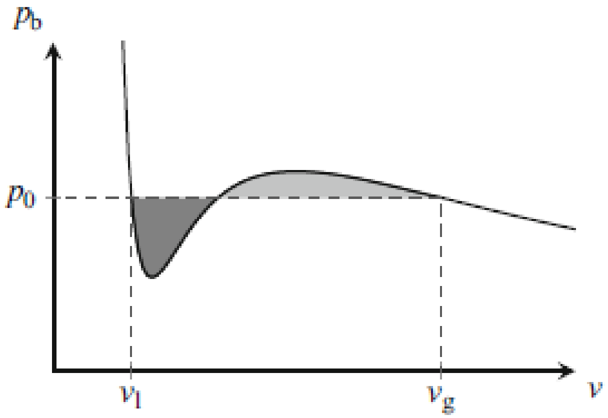
$$f_i(\boldsymbol{x} + \boldsymbol{c_i}\Delta t, t + \Delta t) - f_i(\boldsymbol{x}, t) = -\frac{\Delta t}{\tau}\left(f_i(\boldsymbol{x}, t) - f_i^{eq}(\boldsymbol{x}, t)\right) + \left(1 - \frac{\Delta t}{2\tau}\right)F_i\Delta t$$

$$F_i = w_i\left(\frac{c_{i\alpha}}{c_s^2} + \frac{(c_{i\alpha}c_{i\beta} - c_s^2\delta_{\alpha\beta})u_\beta}{c_s^4}\right)F_\alpha$$

External force

$$\rho = \sum_i f_i \qquad \rho\boldsymbol{u} = \sum_i c_i f_i + \frac{\boldsymbol{F}}{2}$$

3. Equation of state (EOS)



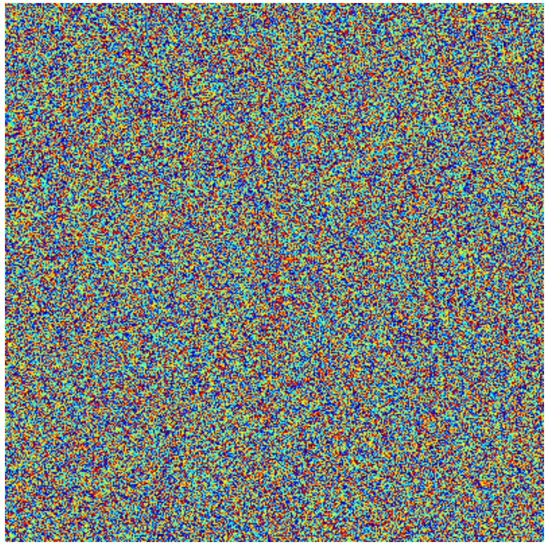


Fig. Phase segregation (Isothermal)

Maxwell area construction rule that allows to obtain phase transition densities :

$$p_0 = c_s^2\rho_g + \frac{c_s^2\Delta t^2 G}{2}\psi^2(\rho_g) = c_s^2\rho_l + \frac{c_s^2\Delta t^2 G}{2}\psi^2(\rho_l)$$

Equation of state (EOS) : Included in the interaction force
→ Enabling phase segregation

$$p_b + \frac{c_s^2 G}{2}\psi^2 = p_{EOS} \rightarrow \psi(\boldsymbol{x}) = \sqrt{\frac{2(p_{\mathrm{EOS}} - \rho c_s^2)}{G c_s^2}}$$

Ex) Peng-Robinson EOS

$$p_{\mathrm{EOS}} = \frac{\rho R T}{1 - b\rho} - \frac{a\varphi(T)\rho^2}{1 + 2b\rho - b^2\rho^2}$$

$$\varphi(T) = \left[1 + \left(0.37464 + 1.54226\omega_{acentric} - 0.26992\omega_{acentric}^2\right)\left(1 - \sqrt{T/T_c}\right)\right]^2$$

$a = 3/49, b = 2/21, R = 1,$ $\omega_{acentric} = 0.022$ (**for oxygen**)

4. Coupling Temperature

Thermodynamic relation of entropy $Tds = c_v dT + T\left(\frac{\partial P}{\partial T}\right)_v dv = c_v dT + T\left(\frac{\partial P}{\partial T}\right)_v d\left(\frac{1}{\rho}\right) = c_v dT - T\frac{1}{\rho^2}\left(\frac{\partial P}{\partial T}\right)_\rho d\rho$

Entropy balance equation $\rho T\frac{ds}{dt} = \nabla\cdot(\lambda\nabla T)$ $\quad \frac{dT}{dt} = \nabla\cdot\left(\frac{\lambda}{\rho c_v}\nabla T\right) + \frac{T}{\rho^2 c_v}\left(\frac{\partial P}{\partial T}\right)_\rho \frac{d\rho}{dt}$

Mass conservation $\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{U}) = 0$

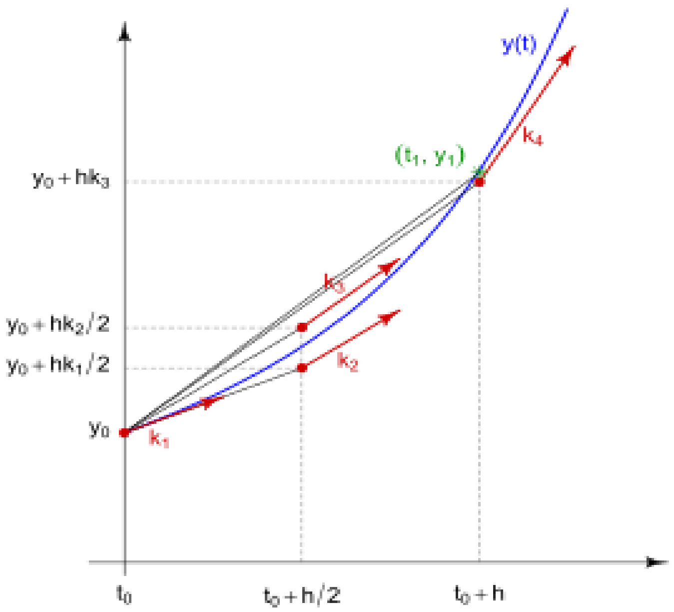
Energy (Heat) equation with source term

$$\frac{\partial T}{\partial t} + \nabla\cdot(\boldsymbol{U}T) = \nabla\cdot(\alpha\nabla T) + T\left[1 - \frac{1}{\rho c_v}\left(\frac{\partial P}{\partial T}\right)_\rho\right]\nabla\cdot\boldsymbol{U}$$

Directly solve with FDM method

$$\frac{\partial T}{\partial t} = -\boldsymbol{u}\cdot\nabla T + \frac{1}{\rho c_v}\nabla\cdot(k\nabla T) - \frac{T}{\rho c_v}\left(\frac{\partial p_{\mathrm{EOS}}}{\partial T}\right)_\rho \nabla\cdot\boldsymbol{u},$$

Source term which responsible for phase change



4th order Runge-Kutta Method

$$T^{t+\delta_t} = T^t + \frac{\delta_t}{6}(h_1 + 2h_2 + 2h_3 + h_4),$$

$$h_1 = K(T^t), h_2 = K\left(T^t + \frac{\delta_t}{2}h_1\right), h_3 = K\left(T^t + \frac{\delta_t}{2}h_2\right), h_4 = K(T^t + \delta_t h_3)$$

Benchmark Tests

Test 1 : Phase segregation (↓)
→ Validation of thermodynamic consistency
(Matching separated density with EOS value)

Test 2 : Wetting method (→)
→ Validation of interfacial wetting method

$$\psi_{interfacial} = \psi_{x,y<0} = G_w \psi_{x,y=0}$$

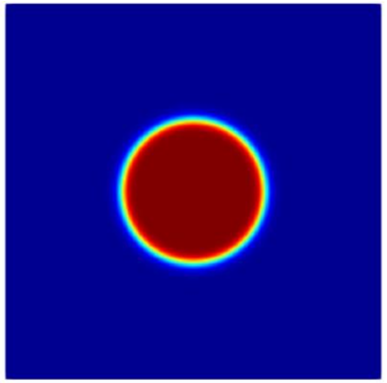


Fig. Droplet (Isothermal)

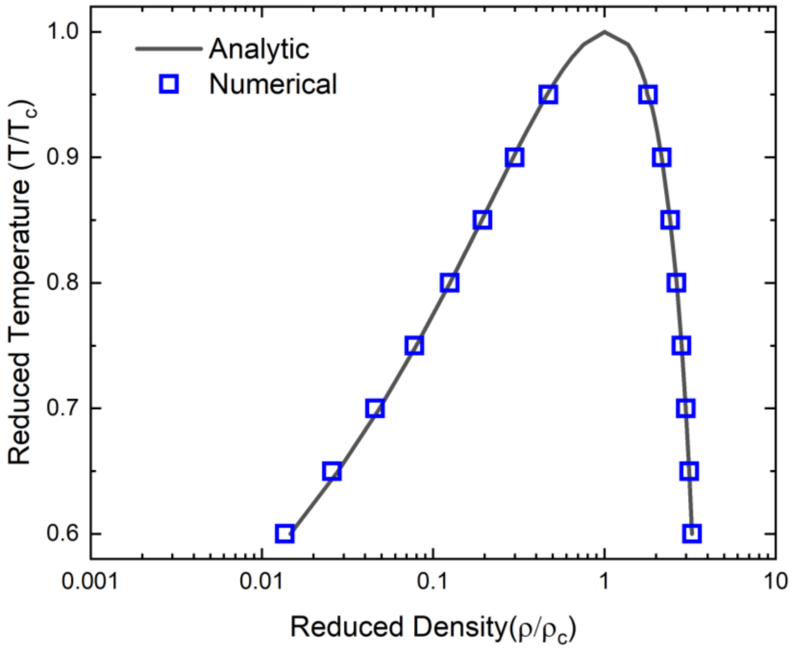
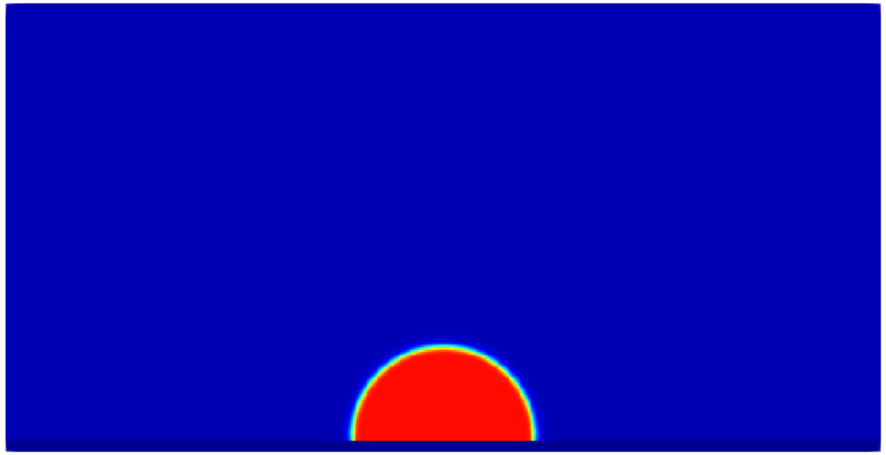


Fig. Thermodynamic consistency

Fig. Solid droplet on flat surface



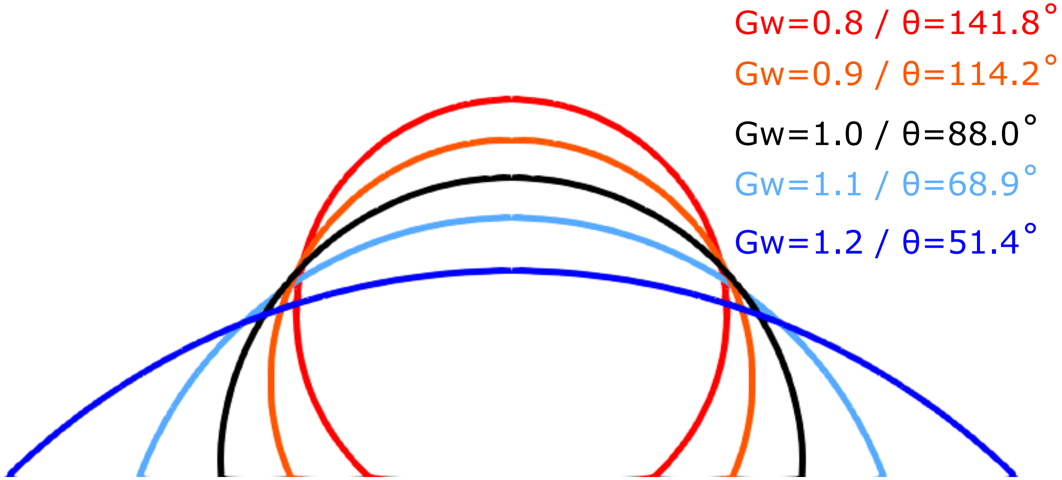


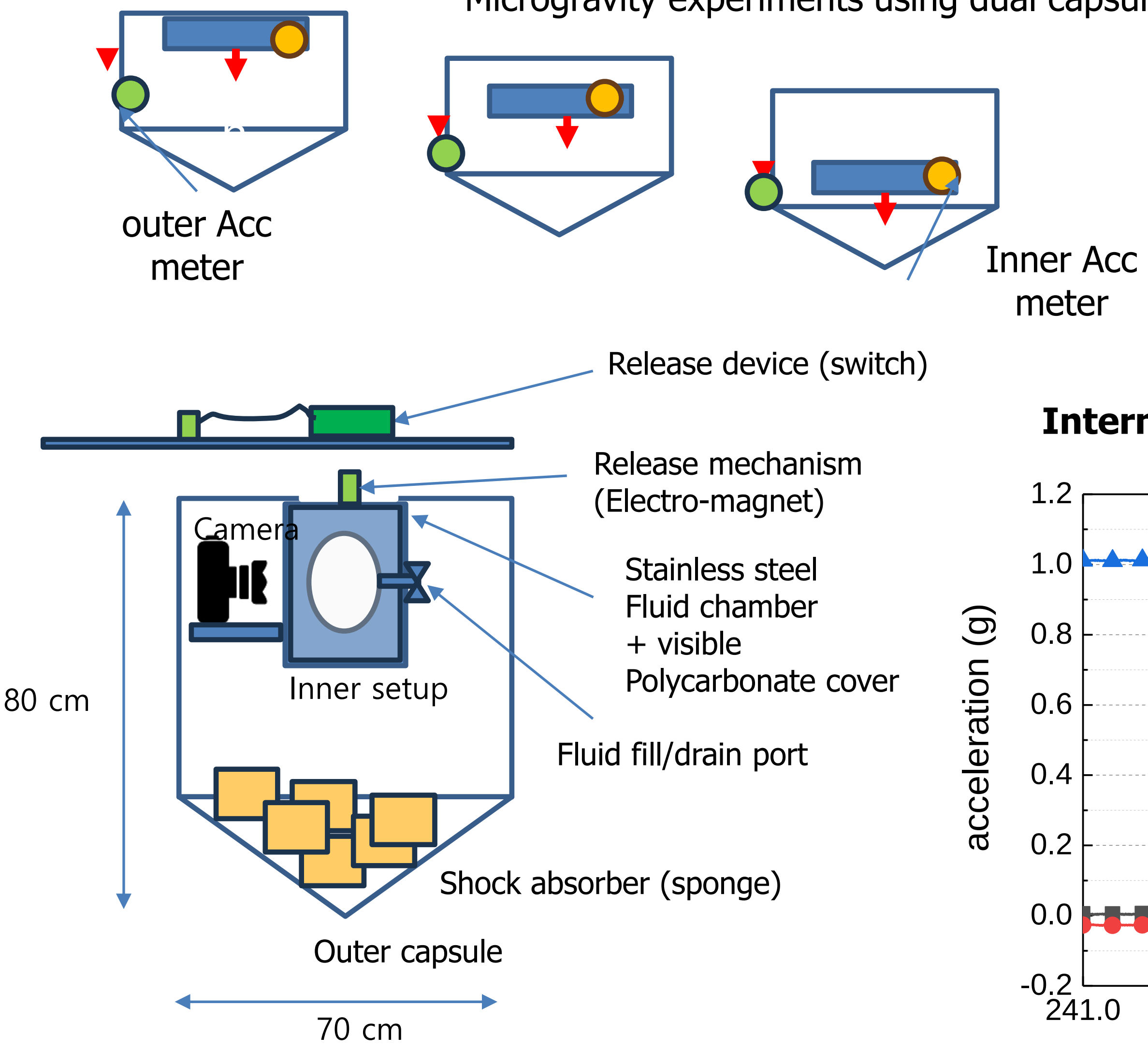
Fig. Contact angle with interfacial wetting method

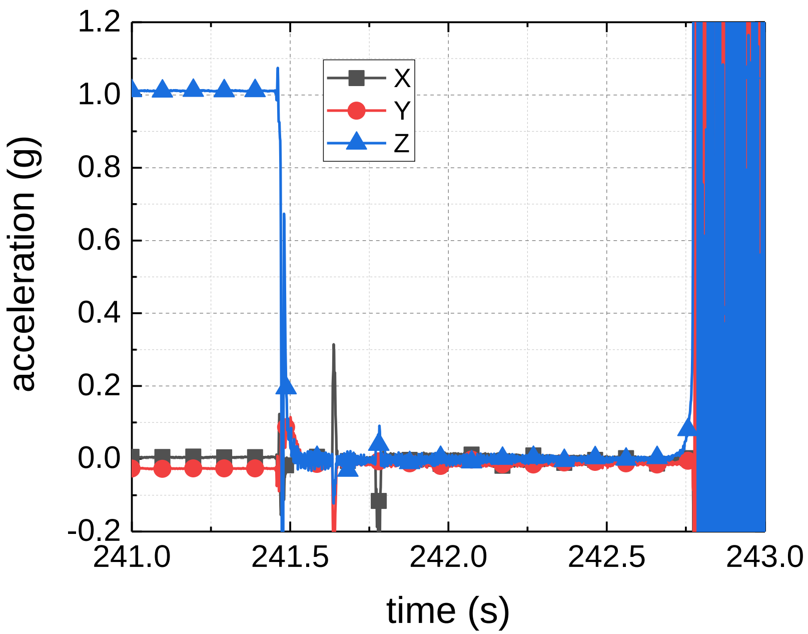
CHAPTER

III Microgravity Boiling Results

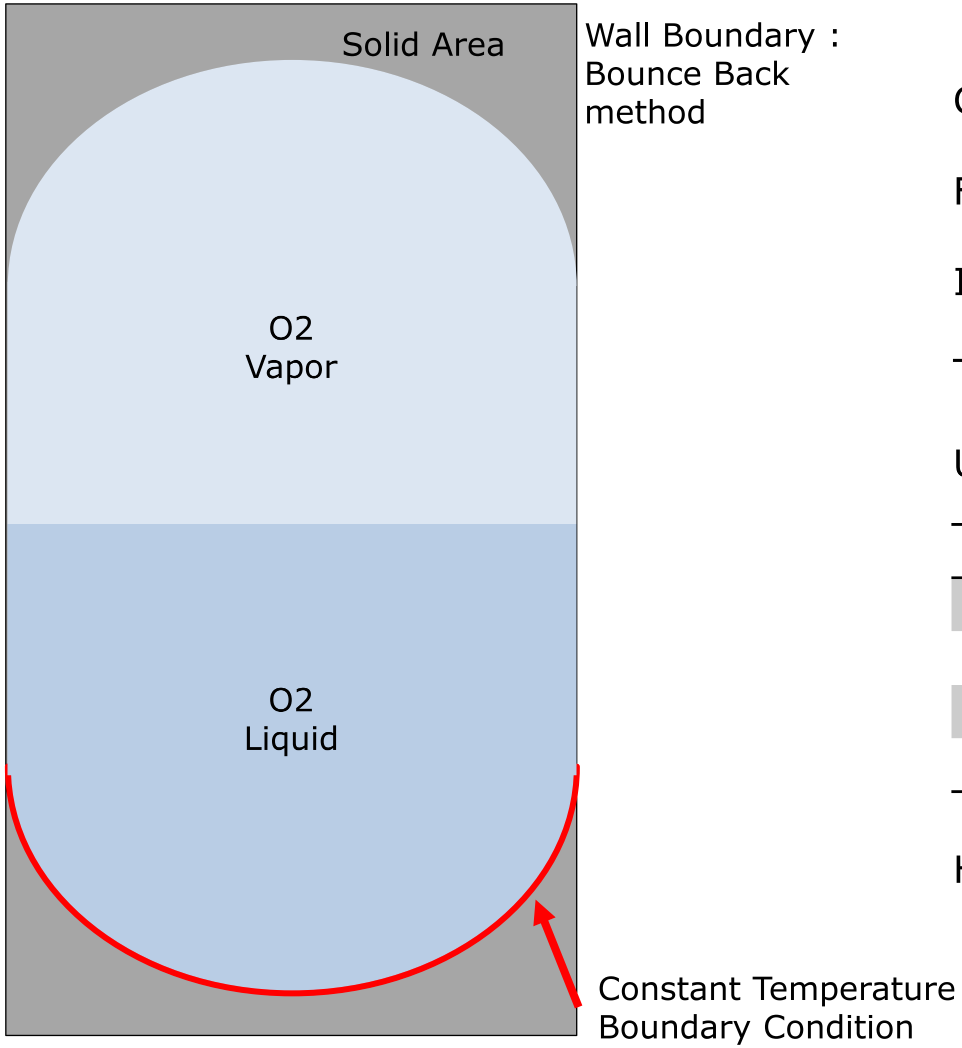
Drop tower test

Micrgravity experiments using dual capsule (7 m, 1.2 s drop)





Simulation Setup



Wetting method : Interfacial method (Gw=1.2)

Collision method : Central Moment (CM) collision with comprehensive scheme

Forcing method : Saito's enhanced forcing scheme

Interaction force : shan-chen interaction force with D2Q25 isotropic scheme

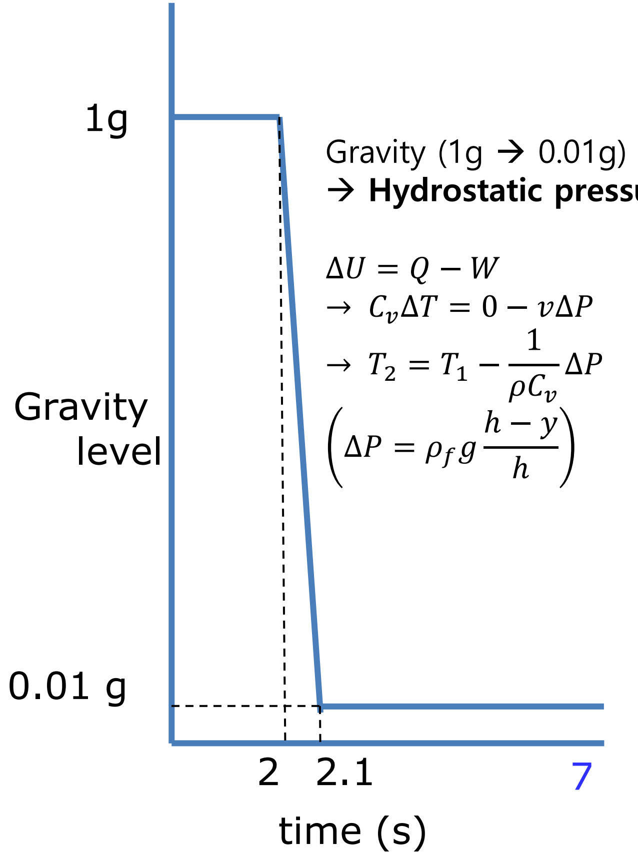
Temperature : Direct solve with FDM, space : D2Q25 isotropic, time : RK4

Unit conversion : Necessary method

Properties	Physical unit	Conversion Factor	Lattice unit
Channel diameter	0.03 m	$C_L = 3.33 \times 10^{-5}$ m	900
Time	0.025s	$C_t = 7.96 \times 10^{-6}$ s	3142
Viscosity	$1.\times10^{-7}\ m^2/s$	$C_v = 4.42 \times 10^{-6}\ m^2/s$	0.0226
Gravity	$9.81\ \mathrm{m}/s^2$	$C_g = 5.27 \times 10^5\ \mathrm{m}/s^2$	1.86×10^{-6}

Hydrostatic pressure change → Internal energy change

Simulation Case _ No Boiling (Subcooled)



Gravity (1g → 0.01g)
→ **Hydrostatic pressure decrease**

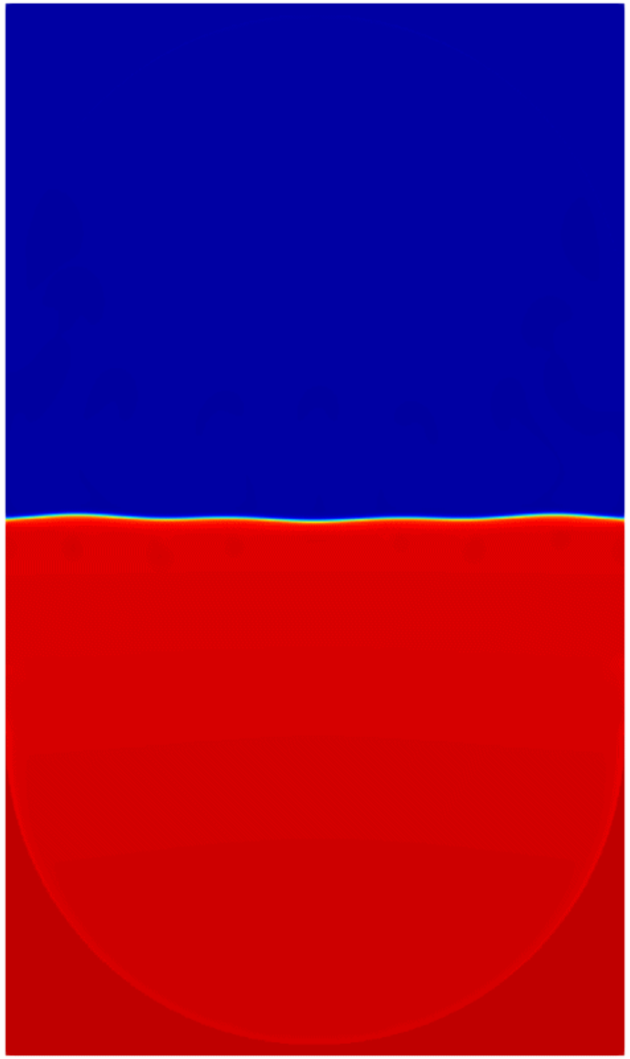
$\Delta U = Q - W$

$\rightarrow C_v \Delta T = 0 - v\Delta P$

$\rightarrow T_2 = T_1 - \frac{1}{\rho C_v}\Delta P$

$\left(\Delta P = \rho_f g \frac{h-y}{h}\right)$

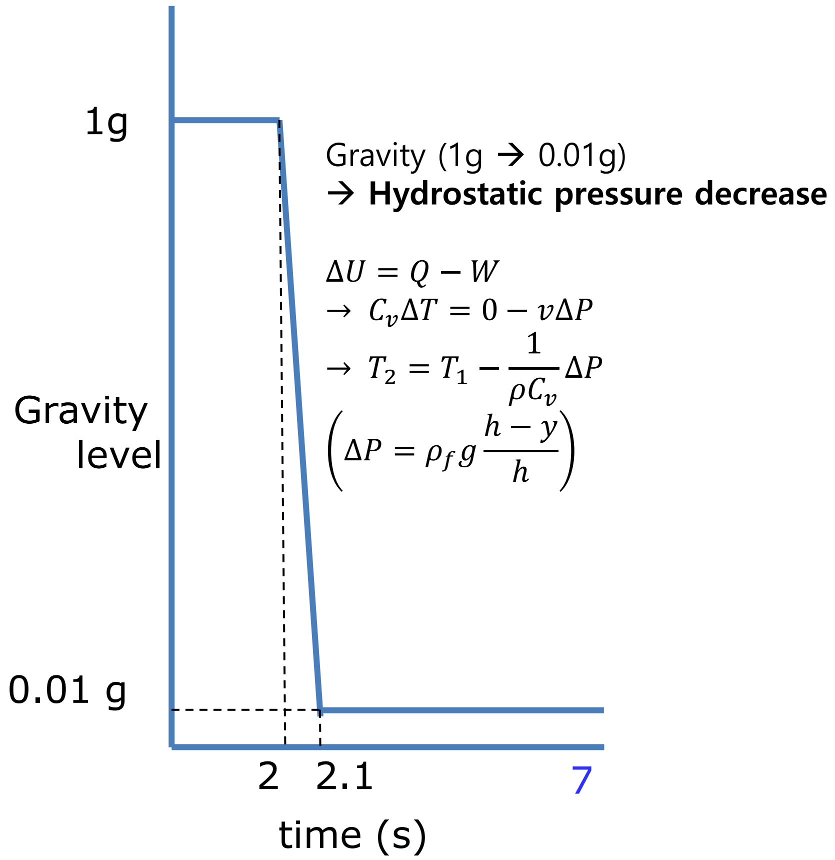
Fig. Gravity change over simulation time



Subcooled liquid fluid motion in 0g (Fluid: O2)

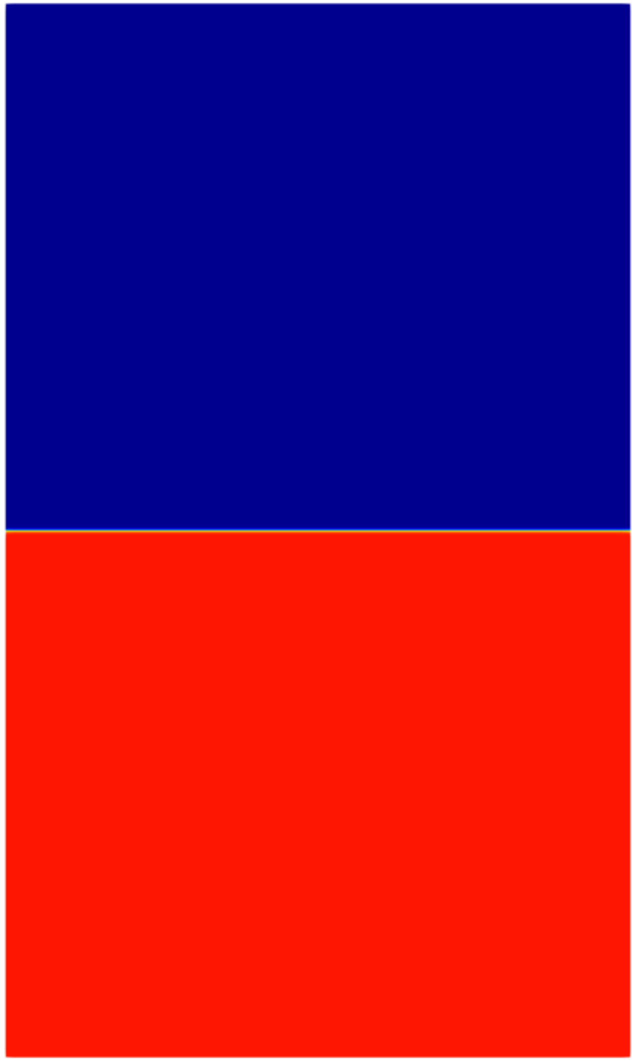
Subcooled liquid fluid motion in 0g (Fluid: Novec)

Simulation Case _ Boiling (Saturation)

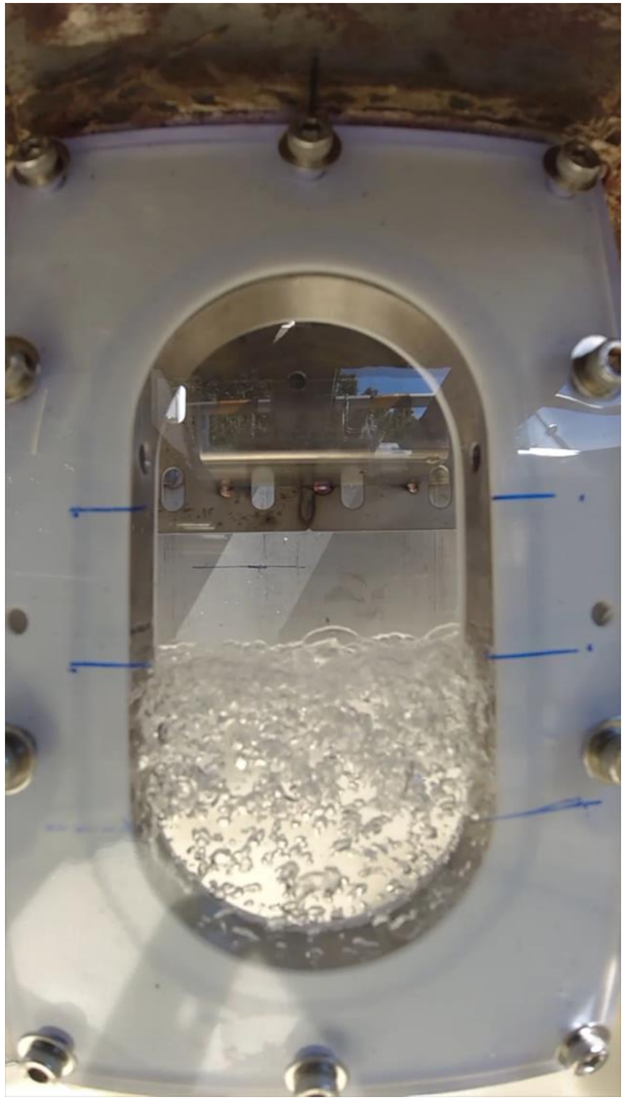


$$\Delta U = Q - W$$
$$\rightarrow C_v \Delta T = 0 - v\Delta P$$
$$\rightarrow T_2 = T_1 - \frac{1}{\rho C_v}\Delta P$$
$$\left(\Delta P = \rho_f g \frac{h-y}{h}\right)$$

Fig. Gravity change over simulation time

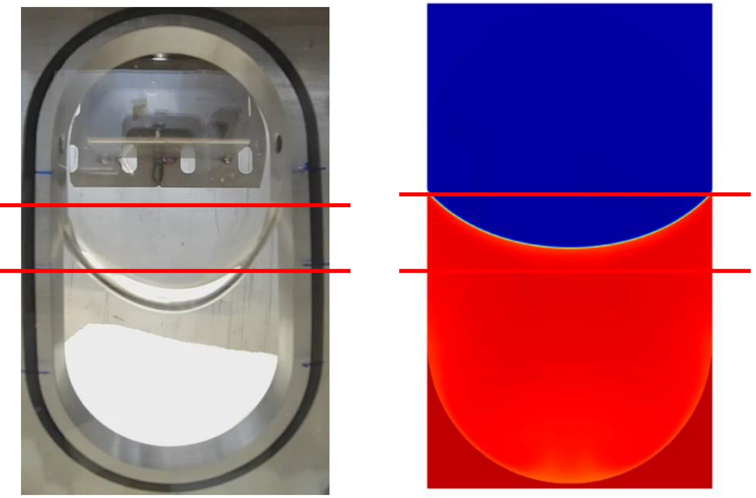


Saturated liquid fluid motion in 0g (Fluid: O2)



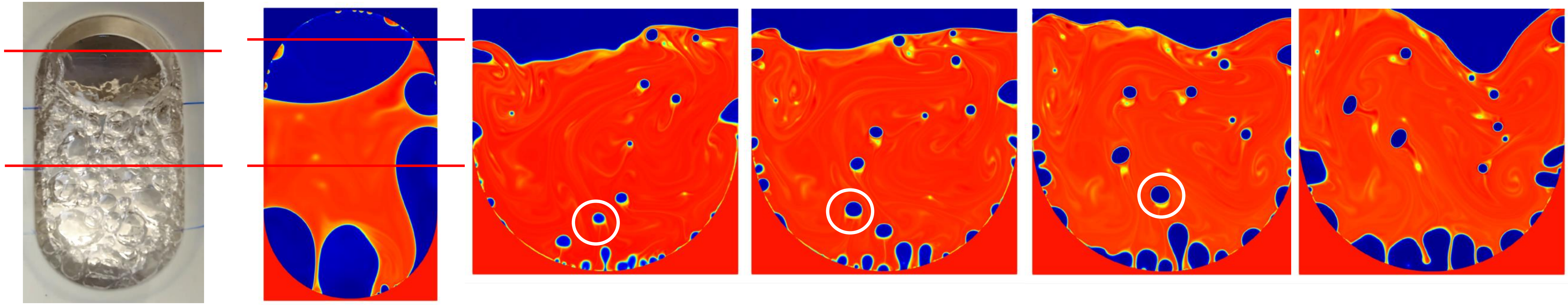
Saturated liquid fluid motion in 0g (Fluid: Novec)

Results Comparison



1. Liquid level change
   - Subcooled and saturated liquid shows different liquid level after gravity change
   - Similar liquid level is shown in LBM simulation results compared with experimental results

2. Bubble size change
   - Size of both bubbles attached to the bottom and departing into the bulk flow are increased as gravity changes
   - LBM could reproduce this phenomena



CHAPTER

IV Conclusion

Conclusion

0. cryogenic propellants are the promising candidates for the more upper stage of space exploration. However, due to its extreme thermophysical properties, further studies should be responsible.

1. LBM is adopted for the cryogenic boiling simulation due to its kinetic characteristics

2. Boiling under the microgravity is reproduced through the drop tower test and numerical simulation with LBM

3. LBM could reproduce boiling phenomena under the microgravity

Thank you !

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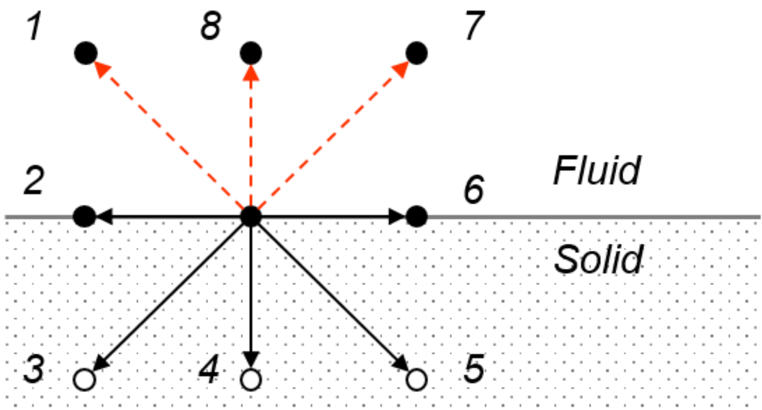
4. Boundary Condition - Wall Boundary Treatment



After colliding and streaming, Unknown distribution should be defined
+ Force term should correctly be included in the wall boundary treatment

$$\rho_k = \sum_{3,4,5} f_i\,,\ \rho_0 = \sum_{0,2,6} f_i\,,\ \rho_{uk} = \sum_{1,7,8} f_i$$

$$\rho = \rho_k + \rho_0 + \rho_{uk} \ \ and\ \rho u_1 = \rho_{uk} - \rho_k + 0.5F_1,$$

$$\rho = \frac{1}{1-u_1}(2\rho_k + \rho_0 - 0.5F_1)$$

a. Zou-He (Non-equilibrium Bonce-back method) $f_{\bar{i}}^{neq}(\boldsymbol{x}_b,t) = f_i^{neq}(\boldsymbol{x}_b,t) - (\boldsymbol{n}\cdot\boldsymbol{c}_i)N_n - (\boldsymbol{t}\cdot\boldsymbol{c}_i)N_t\ (\boldsymbol{c}_{\bar{i}} = -\boldsymbol{c}_i)$

only replace unknown distributions

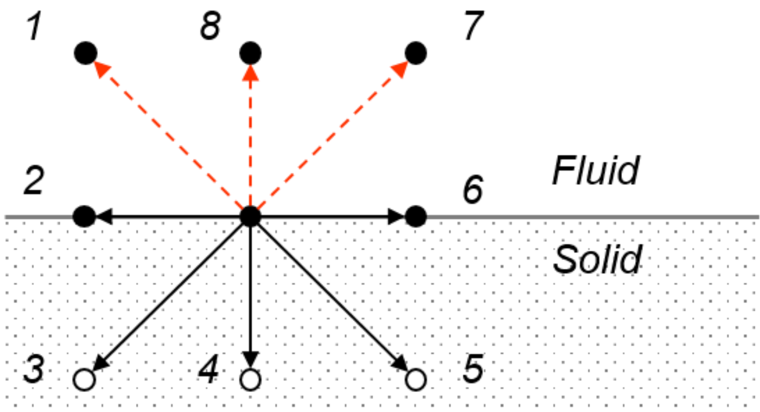
$$\begin{cases} f_8^{neq} = f_4^{neq} + N_y \\ f_1^{neq} = f_5^{neq} + N_y - N_x \\ f_7^{neq} = f_3^{neq} + N_y + N_x \end{cases} \rightarrow \begin{cases} f_8 = f_4 + \dfrac{2\rho u_y}{3c} + N_y \\ f_1 = f_5 + \dfrac{\rho(-u_x + u_y)}{6c} + N_y - N_x \\ f_7 = f_3 + \dfrac{\rho(u_x + u_y)}{6c} + N_y + N_x \end{cases}$$

$$f_8 = f_4 + \frac{2\rho u_y}{3c} - \frac{F_y}{6},$$
$$f_1 = f_5 + \frac{(f_6 - f_2)}{2} - \frac{\rho u_x}{2} + \frac{\rho u_y}{6} + \frac{F_x}{4} - \frac{F_y}{6}$$
$$f_7 = f_3 - \frac{(f_6 - f_2)}{2} + \frac{\rho u_x}{2} + \frac{\rho u_y}{6} - \frac{F_x}{4} - \frac{F_y}{6}.$$

4. Boundary Condition - Wall Boundary Treatment

b. Regularized boundary method *replace all of distributions*

$\boldsymbol{Q}_i = \boldsymbol{c}_i\boldsymbol{c}_i - c_s^2\boldsymbol{I},$



$$f_i^{neq} = -\frac{t_i}{c_s^2\omega}\left(\boldsymbol{Q}_i:\rho\vec{\nabla}_1\vec{u} - \vec{c}_i\vec{\nabla}_1:\rho\vec{u}\vec{u} + \frac{1}{2c_s^2}(\vec{c}_i\cdot\vec{\nabla}_1)(\boldsymbol{Q}_i:\rho\vec{u}\vec{u})\right) - \frac{1}{2}\frac{t_i}{c_s^2}\vec{c}_i\cdot\vec{F} - \frac{t_i}{4c_s^4}\boldsymbol{Q}_i:(\vec{F}\vec{u}+\vec{u}\vec{F})$$

$$\Pi_{\alpha\beta}^{(1)} = \sum_i Q_{i\alpha\beta}(R_{i\gamma\delta} + I_{i\gamma\delta}) = \sum_i t_i Q_{i\alpha\beta}Q_{i\gamma\delta}T_{\gamma\delta} + 0 = c_s^4(T_{\alpha\beta} + T_{\beta\alpha}).$$

$$\boldsymbol{Q}_i:\boldsymbol{\Pi}^{(1)} = c_s^4\boldsymbol{Q}_i:(\boldsymbol{T}+\boldsymbol{T}^T) = 2c_s^4\boldsymbol{Q}_i:\boldsymbol{T}$$

Regularized boundary method :

$$f_i^{neq} \approx \bar{f}_i^{(1)} = R_i = \frac{t_i}{2c_s^4}\boldsymbol{Q}_i:\boldsymbol{\Pi}^{(1)}$$

With NEBB method:

density and momentum are only conserved during collision

$$\boldsymbol{\Pi}^{(1)} = \sum_i \boldsymbol{Q}_i f_i^{(1)}$$

***With Finite Difference method:**

$$\boldsymbol{\Pi}^{(1)} = -\frac{2c_s^2}{\omega}\rho\boldsymbol{S} - \frac{1}{2}(\vec{F}\vec{u}+\vec{u}\vec{F}) \text{ where } \boldsymbol{S} = \frac{1}{2}(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^{\mathrm{T}}).$$

4. Boundary Condition - Wall Boundary Treatment

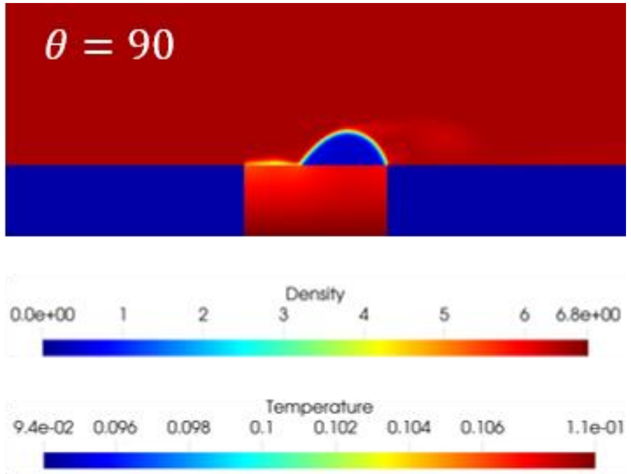


Fig. Flow boiling

Wall boundary treatment method affects to the bubble dynamics near the boundary

→ NEBB method makes undesired high numerical error
→ This leads divergence of simulation (Unstable)

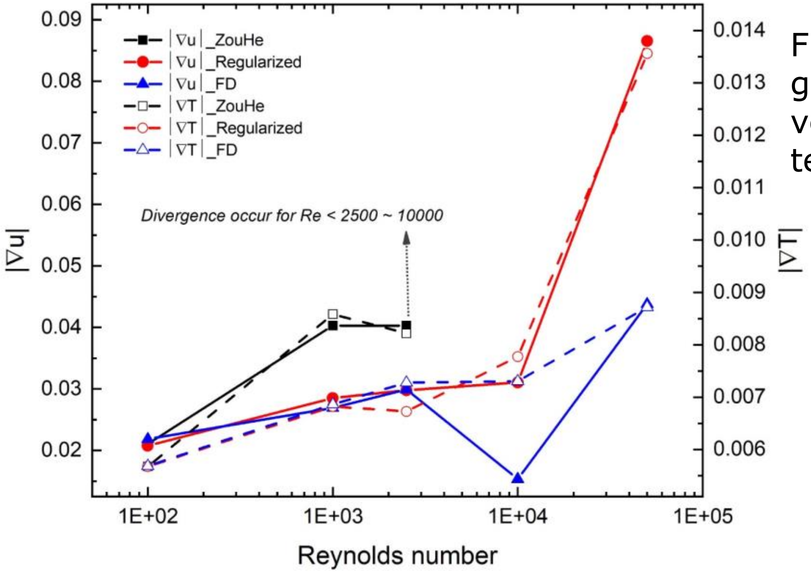


Fig. Magnitude gradient term of velocity and temperature

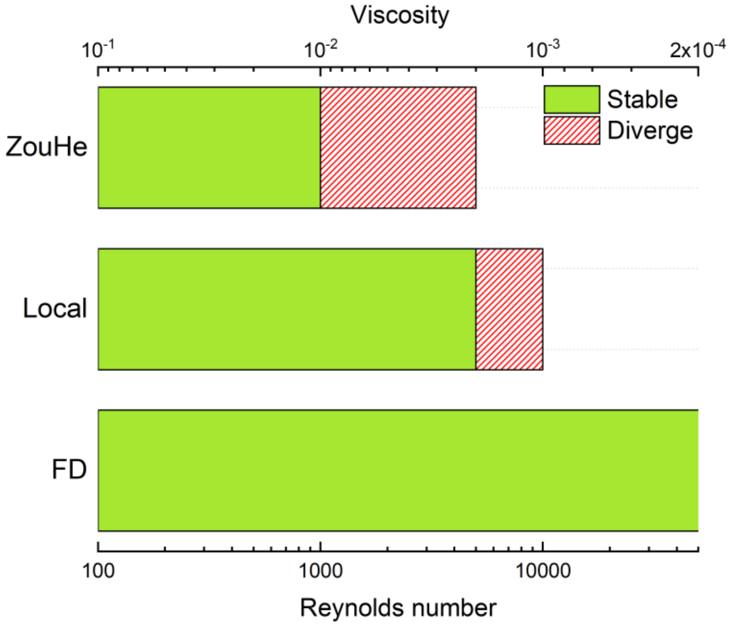


Fig. Maximum achievable Reynolds number

4. Boundary Condition - Outlet Boundary Treatment

$x = N$

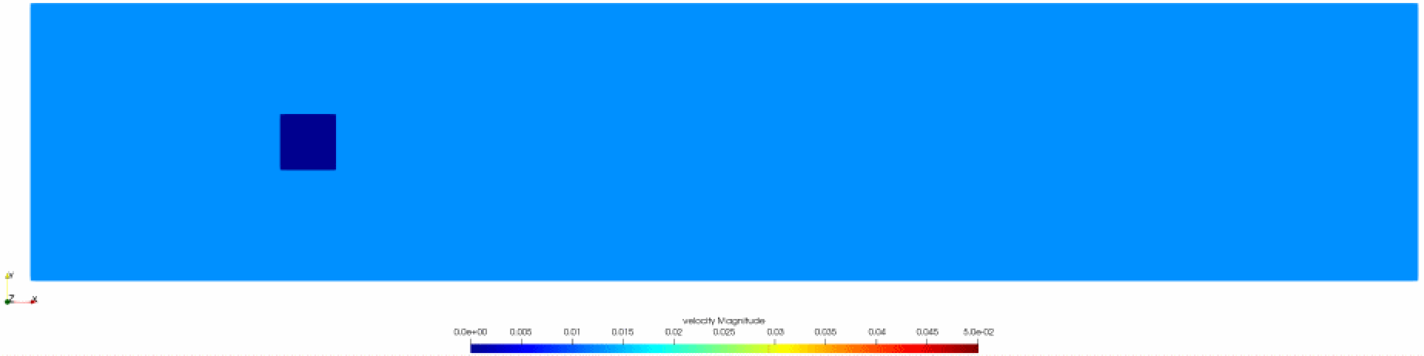
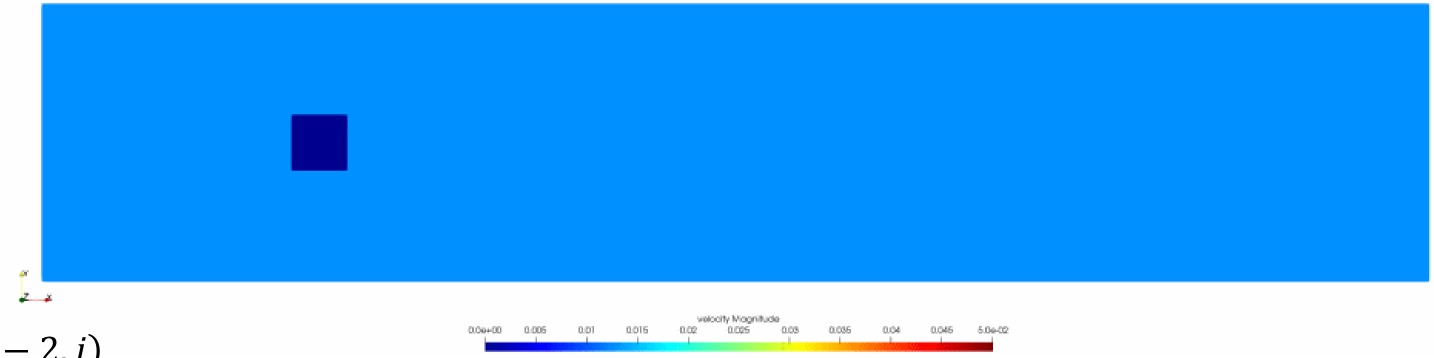


Fig. Vortex shedding onto square box, Re=10,000, (a) Pressure BC, (b) Convective BC



~~0. Periodic boundary condition~~

Connect inlet and outlet boundary as continuous domain
→ Improper for investigation about certain domain

1. Pressure Boundary condition

Gives constant pressure (density) at the outlet boundary

2. Outflow boundary condition

2-1 Neumann condition

$$\frac{\partial f}{\partial x} = 0$$

$$\rightarrow f(N,j) = f(N-1,j)$$

2-2 Extrapolation condition

$$\frac{\partial^2 f}{\partial x^2} = 0$$

$$\rightarrow f(N,j) = 2f(N-1,j) - f(N-2,j)$$

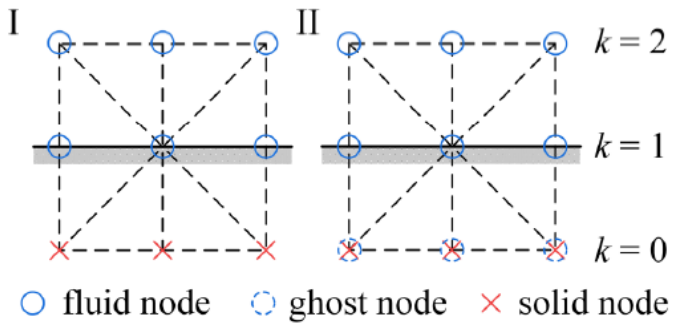
2-3 Convective condition

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = 0$$

$$\rightarrow f(N,j,t+\delta t) = \frac{f(N,j,\delta t) + U(N-1,j,t+\delta t)f(N-1,j,t+\delta t)}{1 + U(N-1,j,t+\delta t)}$$

4. Boundary Condition - Wetting Method

Fig. Type of wetting method [1]



Wetting method in pseudopotential LBM

: Mimic solid-fluid interaction force

Type 1 : Virtual density (potential) method

Type 2 : Solid-Fluid interaction force method

Method a. Modified pseudopotential method (Type 2) $\boldsymbol{F}_{ads}(\boldsymbol{x}) = -G_w\psi(\boldsymbol{x})\sum_{i=0}^{8} w_m(|\boldsymbol{c}_i|^2)\psi(\boldsymbol{x})s(\boldsymbol{x}+\boldsymbol{c}_i)\boldsymbol{c}_i$

Method b. Geometric pseudopotential method (Type 1) $\psi_{x,y=-1} = \psi_{x,1} + \sqrt{(\psi_{x+1,0}-\psi_{x-1,0})^2}\tan\left(\frac{\pi}{2}-\theta_d\right)$

***Method c. Interfacial pseudopotential method (Type 1)** $\psi_{interfacial} = \psi_{x,y<0} = G_w\psi_{x,y=0},$

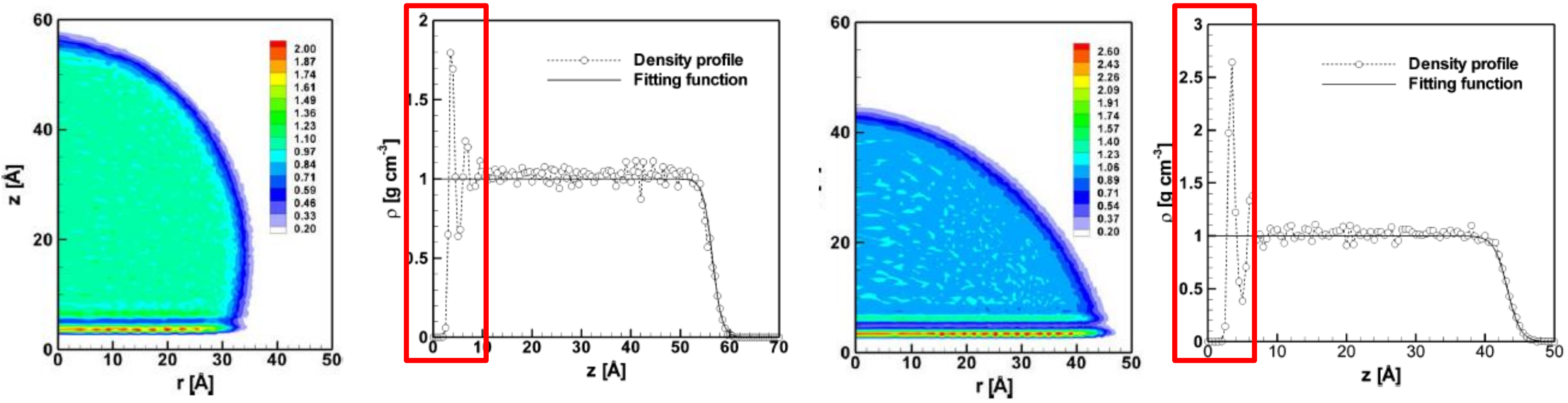


Fig. Interfacial density distribution with MD method [2]

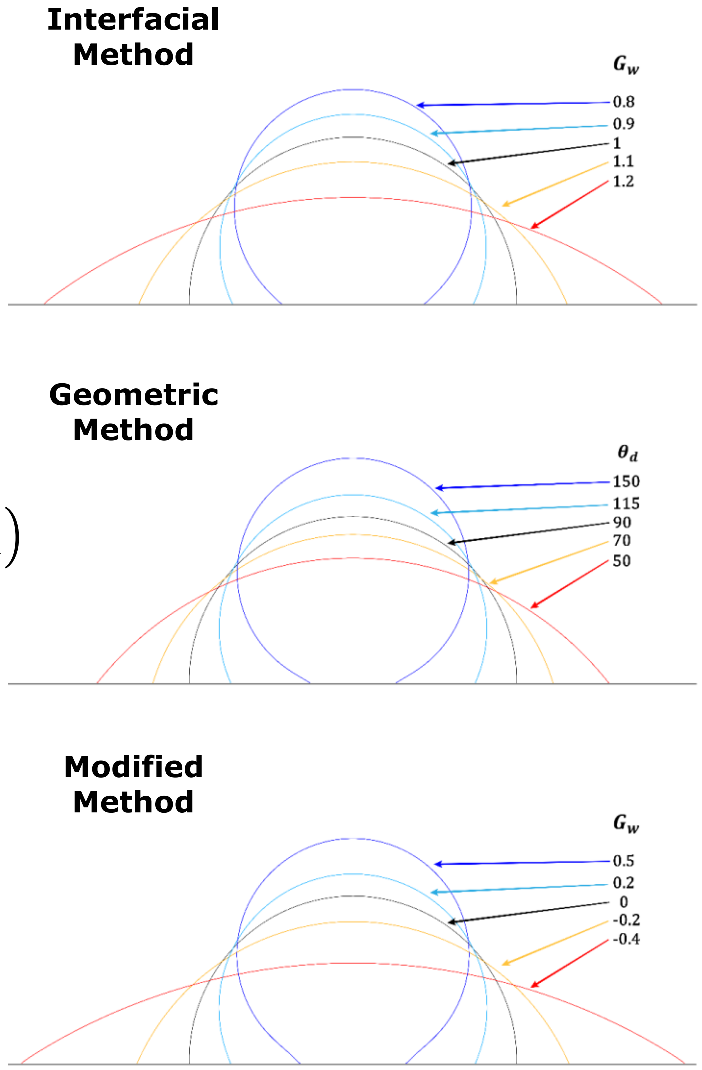


Fig. Various contact angles

[1] Wu, Suchen, Yongping Chen, and Long-Qing Chen. "Three-dimensional pseudopotential lattice Boltzmann model for multiphase flows at high density ratio." *Physical Review E* 102.5 (2020): 053308.
[2] Do Hong, Seung, Man Yeong Ha, and S. Balachandar. "Static and dynamic contact angles of water droplet on a solid surface using molecular dynamics simulation." *Journal of colloid and interface science* 339.1 (2009): 187-195.

4. Boundary Condition - Wetting Method

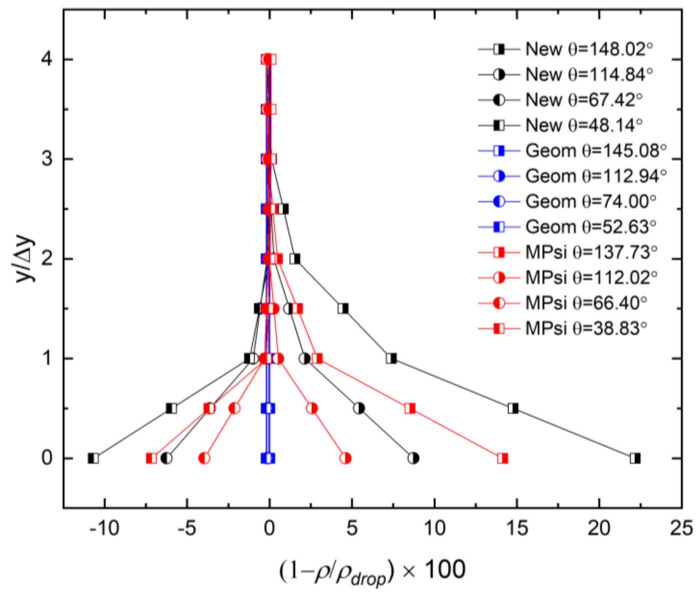


Fig. Density profile of liquid droplet (LBM)

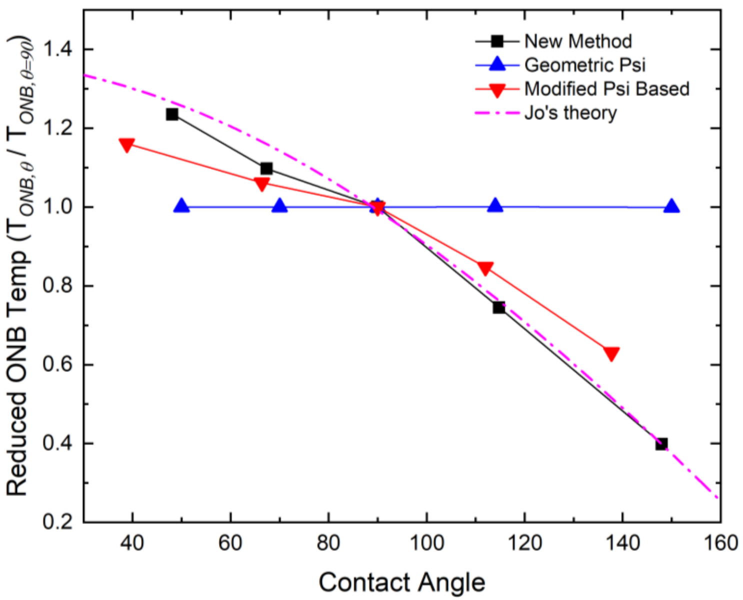


Fig. Reduced ONB results (LBM)

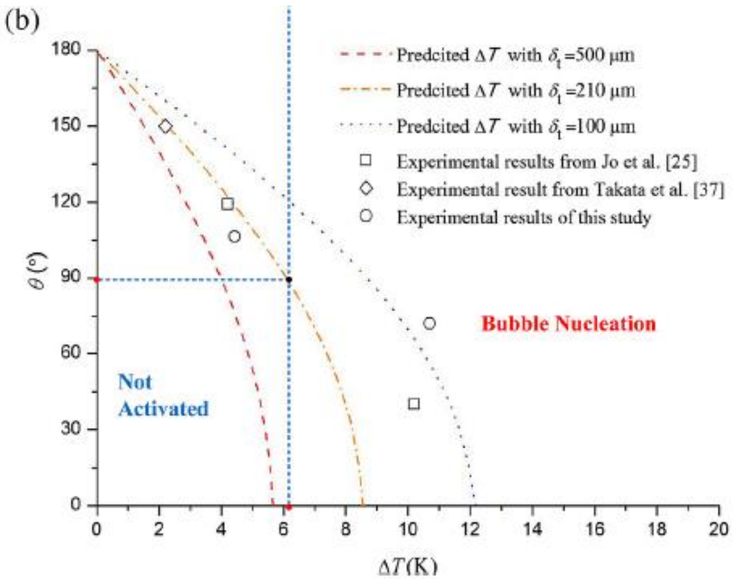


Fig. Predicted superheat [1]

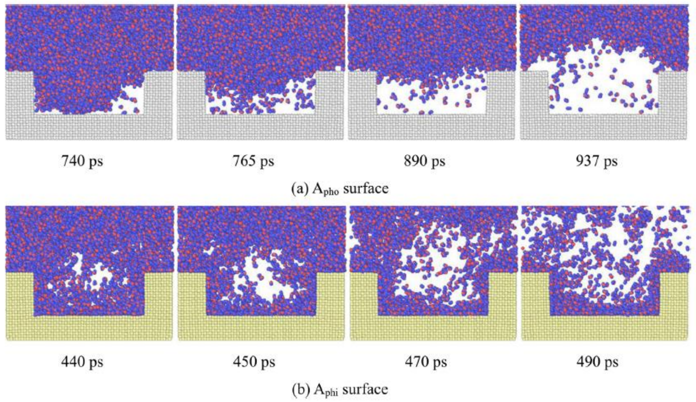
Interfacial and modified pseudopotential based methods reproduce similar density trends with MD result

Interfacial and modified pseudopotential based methods could reproduce similar ONB trends with analytic models.

Interfacial method gives more precise results

[1] Jo, HangJin, et al. "Heterogeneous bubble nucleation on ideally-smooth horizontal heated surface." International Journal of Heat and Mass Transfer 71 (2014): 149-157.

4. Boundary Condition - Wetting Method



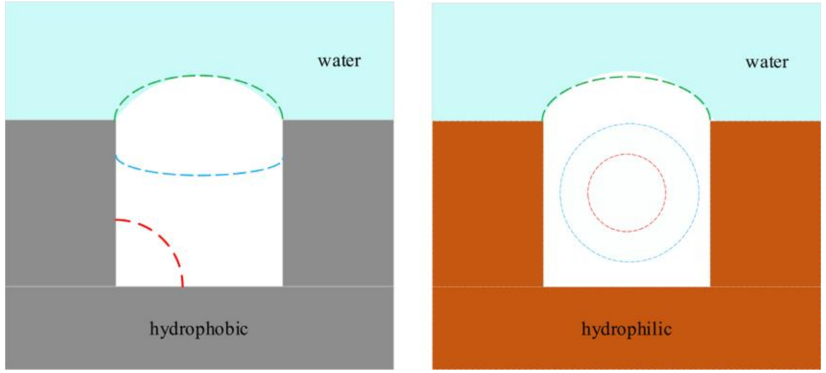


Fig. Bubble nucleation at the nano-groove with MD [1]

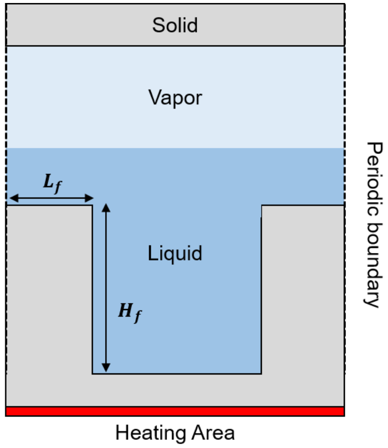


Fig. Pool boiling domain with corner

The constant temperature boundary condition is applied at the bottom wall

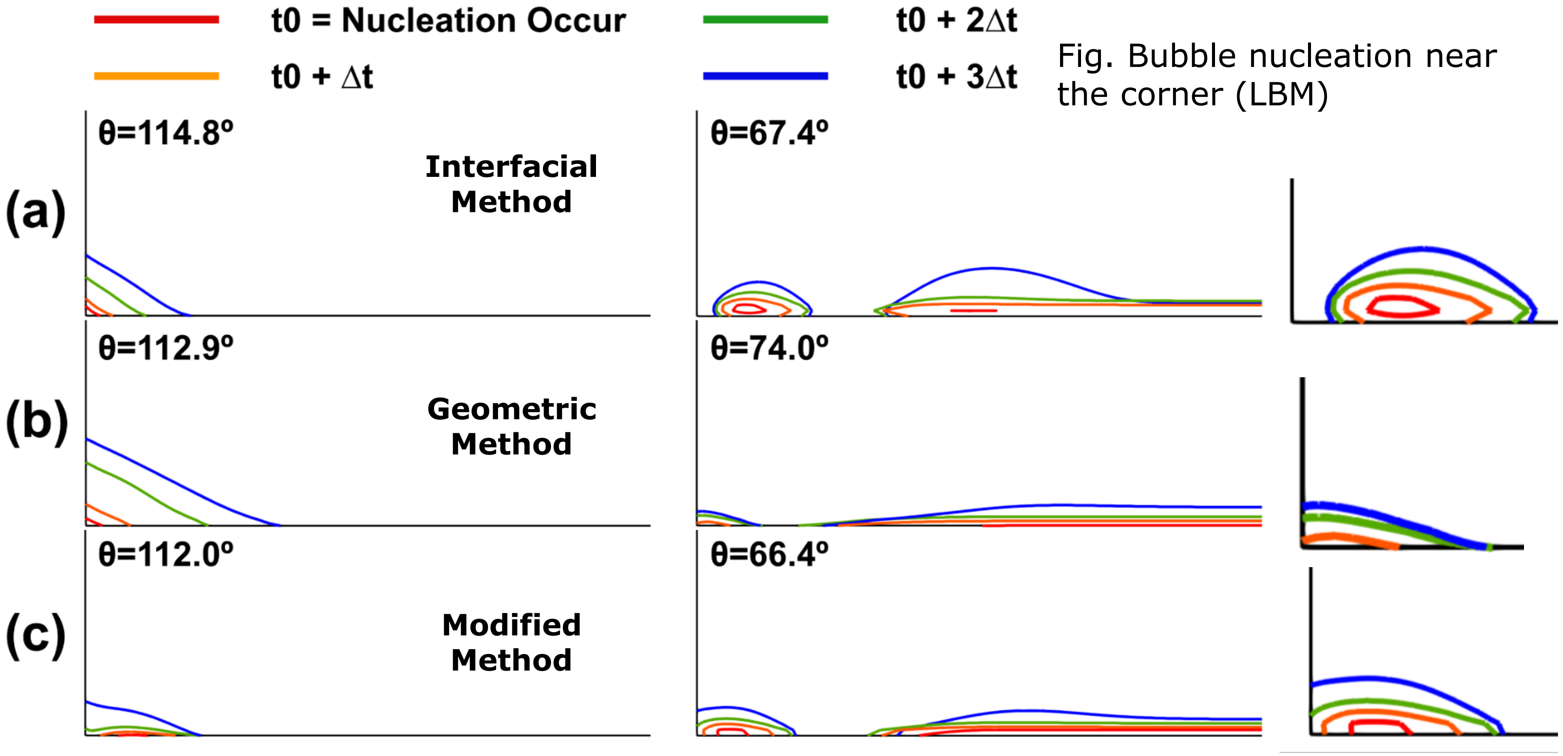


Fig. Bubble nucleation near the corner (LBM)

Three different wetting methods are applied

For higher contact angle (Left) :

Nucleation occurs at the corner

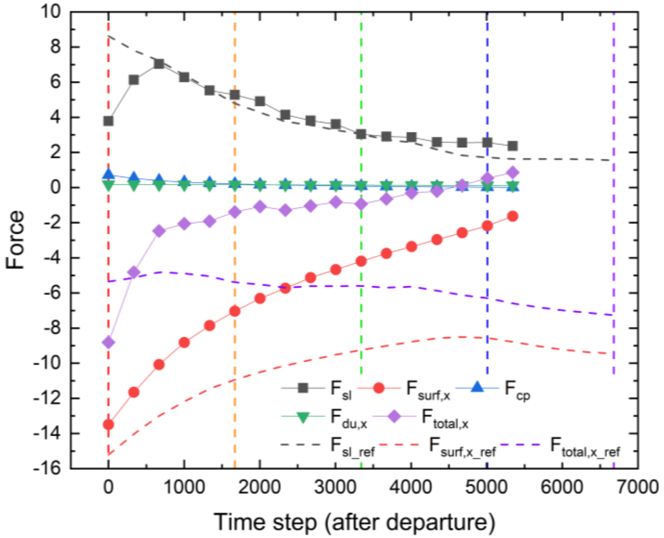
For lower contact angle (Right) :

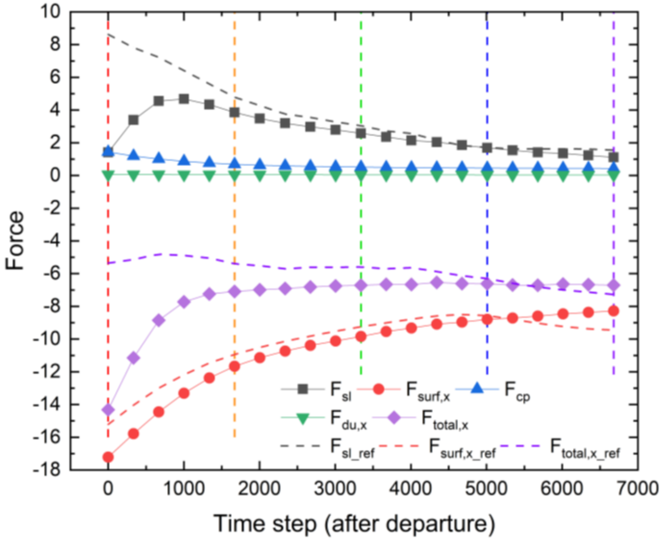
(a) Nucleation occurs away from the bottom wall (agreed with MD results)

(b),(c) Nucleation occurs at the bottom wall

[1] Zhao, Hui, Leping Zhou, and Xiaoze Du. "Bubble nucleation on grooved surfaces with hybrid wettability: molecular dynamics study under a transient temperature boundary condition." International Journal of Heat and Mass Transfer 166 (2021): 120752..

4. Boundary Condition - Wetting Method





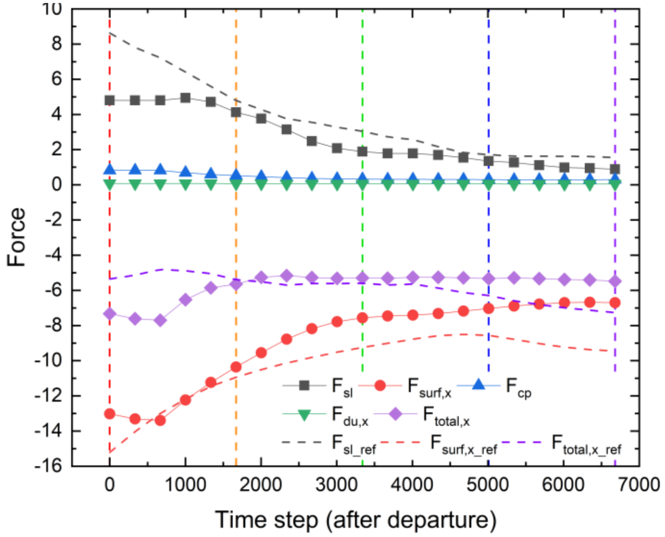


Fig. Force analysis of departing bubble (~70˚)

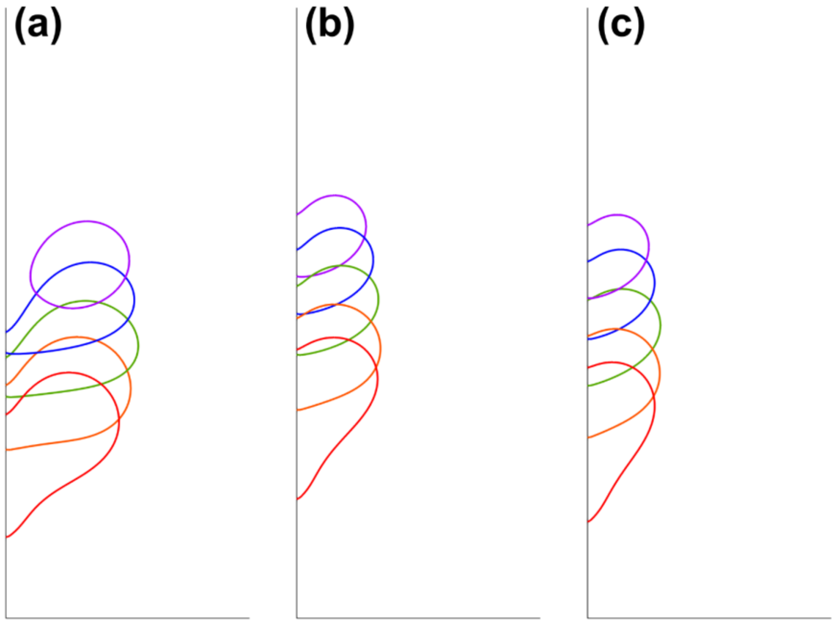


Fig. Departing bubble motion (~70˚)

Dotted line represents force exerted to the departing bubble for reference contact angle case (90˚)

Shear lift force and surface tension force are dominant (same with experimental result)

Only interfacial wetting method makes different force trend with reference case
→ Bubble lift-off occurs during sliding (total force > 0)

Interfacial method is proper for boiling with corner configuration

5. Proper Unit Conversion

Unit conversion in LBM $Q_{pu} = C_Q \times Q_{lu}$, same with 'Buckingham π theorm'

Difficulties of unit conversion in LBM

1. Velocity limitation from chapman-enskog analysis

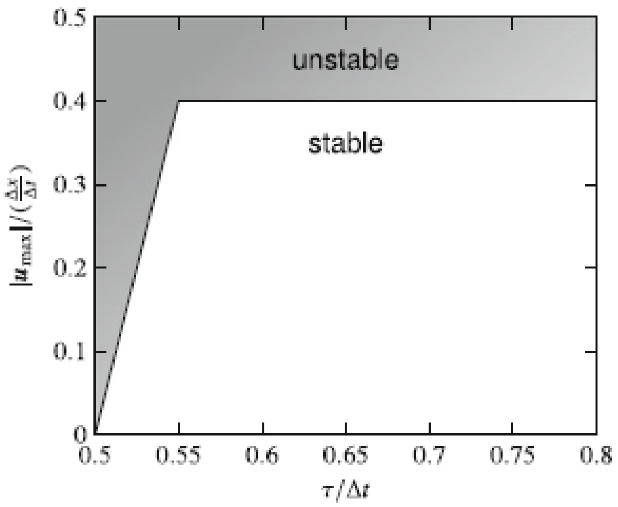
$$\Pi_{\alpha\beta}^{(1)} = -\rho c_s^2 \tau \left(\partial_\beta^{(1)} u_\alpha + \partial_\alpha^{(1)} u_\beta\right) + \tau \partial_\gamma^{(1)} (\rho u_\alpha u_\beta u_\gamma)$$

negligible if $u^2 \ll c_s^2$ → LBM is valid for "weakly compressible" flow

2. Sufficient stability condition : Non negative distribution

$$\left(\tau - \frac{\Delta t}{2}\right) > 0$$

3. Relaxation time stability limit from *von Neumann* analysis



+3. Properties relation with EOS

$$p_{EOS} = \frac{\rho RT}{1 - b\rho} - \frac{a\varphi(T)\rho^2}{1 + 2b\rho - b^2\rho^2},$$

$$\varphi(T) = \left[1 + \left(0.37464 + 1.54226\omega_{acentric} - 0.26992\omega_{acentric}^2\right)\left(1 - \sqrt{T/T_c}\right)\right]^2$$

a : *attraction parameter* b : *repulsion parameter*

Arbitrary choice of lattice value is impossible

Equation of State and Surface Tension

$F = \kappa \rho \nabla \Delta \rho.$ **Surface tension in diffuse interface model**

Divergence of Pressure tensor

$$\begin{aligned}\partial_\alpha p_b - F_\alpha &= \partial_\alpha p_b - \kappa \rho \partial_\alpha \partial_\gamma \partial_\gamma \rho = \partial_\alpha p_b - \kappa \partial_\alpha (\rho \partial_\gamma \partial_\gamma \rho) + \kappa (\partial_\alpha \rho) \partial_\gamma \partial_\gamma \rho \\ &= \partial_\alpha p_b - \kappa \partial_\alpha (\rho \partial_\gamma \partial_\gamma \rho) + \kappa \partial_\gamma \left((\partial_\alpha \rho)(\partial_\gamma \rho) \right) - \kappa (\partial_\gamma \rho) \partial_\alpha \partial_\gamma \rho \\ &= \partial_\alpha p_b - \kappa \partial_\alpha (\rho \partial_\gamma \partial_\gamma \rho) + \kappa \partial_\gamma \left((\partial_\alpha \rho)(\partial_\gamma \rho) \right) - \frac{\kappa}{2} \partial_\alpha \left((\partial_\gamma \rho)^2 \right)\end{aligned}$$

$$= \partial_\beta \left[\left(p_b - \frac{\kappa}{2} (\partial_\gamma \rho)^2 - \kappa \rho \partial_\gamma \partial_\gamma \rho \right) \delta_{\alpha\beta} + \kappa (\partial_\alpha \rho)(\partial_\beta \rho) \right]$$

Equation of state *Surface tension*

$$= \partial_\beta P_{\alpha\beta}.$$

$$\mathbf{P}_{FE} = \left(p_{EOS} - k \rho \nabla^2 \rho - \frac{\kappa}{2} |\nabla \rho|^2 \right) \mathbf{I} + k \nabla \rho \nabla \rho$$

Equation of state *Surface tension*

Standard free energy functional pressure tensor

Taylor expansion

Discretized interaction force : $F^{SC}(x) = -\psi(x) G \sum_i w_i \psi(x + c_i \Delta t) c_i \Delta t$

Continuum form of **Shan-Chen force** : $F^{SC}(x) = -G\psi(x)(c_s^2 \Delta t^2 \nabla \psi(x) + \frac{c_s^4 \Delta t^4}{2} \nabla \Delta \psi(x))$

Divergence of Pressure tensor

$$\nabla \cdot \boldsymbol{P}^{SC} = \nabla (c_s^2 \rho) - \boldsymbol{F}^{SC}$$

Pressure tensor from SC interaction force (Continuum term)

$$\mathbf{P}_c = \left(\rho c_s^2 + \frac{Gc^2}{2} \psi^2 + \frac{Gc^4}{12} |\nabla \psi|^2 + \frac{Gc^4}{6} \psi \nabla^2 \psi \right) \mathbf{I} - \frac{Gc^4}{6} \nabla \psi \nabla \psi$$

Equation of state *Surface tension*

Pressure tensor from SC interaction force (Discrete term)

$$\mathbf{P} = \left(\rho c_s^2 + \frac{Gc^2}{2} \psi^2 + \frac{Gc^4}{12} \psi \nabla^2 \psi \right) \mathbf{I} + \frac{Gc^4}{6} \psi \nabla \nabla \psi.$$

Mechanical stability condition

Shan-chen interaction force $F(\mathbf{x},t) = -G\psi(\mathbf{x})\sum_{\alpha} w_\alpha \psi(\mathbf{x}+\mathbf{e}_\alpha\delta_t)\mathbf{e}_\alpha$

Equation of state

Pressure tensor $\nabla\cdot\mathbf{P} = \nabla\cdot(\rho c_s^2\mathbf{I}) - \mathbf{F}$ $\quad \mathbf{P} = \rho c_s^2\mathbf{I} + \frac{G}{2}\psi(\mathbf{x})\sum_{\alpha} w_\alpha \psi(\mathbf{x}+\mathbf{e}_\alpha\delta_t)\mathbf{e}_\alpha\mathbf{e}_\alpha = \left(\rho c_s^2 + \frac{Gc^2\psi^2}{2}\right)\mathbf{I} + \frac{G\psi}{2}\sum_{\alpha} w_\alpha[\psi(\mathbf{x}+\mathbf{e}_\alpha\delta_t) - \psi(\mathbf{x})]\mathbf{e}_\alpha\mathbf{e}_\alpha$

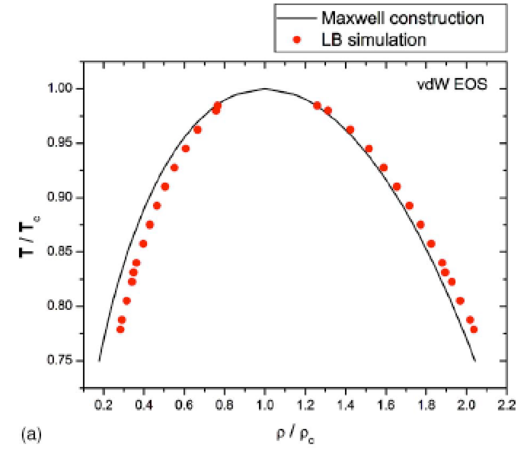
Pressure tensor from SC interaction force

$$\mathbf{P} = \left(\rho c_s^2 + \frac{Gc^2}{2}\psi^2 + \frac{Gc^4}{12}\psi\nabla^2\psi\right)\mathbf{I} + \frac{Gc^4}{6}\psi\nabla\nabla\psi$$

Standard free energy functional pressure tensor

$$\mathbf{P}_{FE} = \left(p_{EOS} - k\rho\nabla^2\rho - \frac{k}{2}|\nabla\rho|^2\right)\mathbf{I} + k\nabla\rho\nabla\rho$$

Defining density ratio



Normal Pressure tensor (interface) $P_n = \rho c_s^2 + \frac{Gc^2}{2}\psi^2 + \frac{Gc^4}{4}\psi\frac{d^2\psi}{dn^2}$

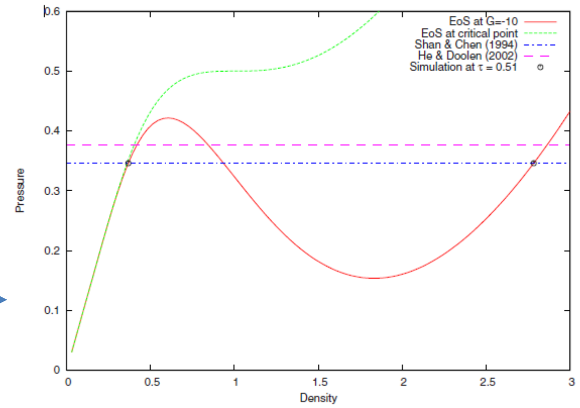
$$P_n - \rho c_s^2 - \frac{Gc^2}{2}\psi^2 = \frac{Gc^4}{8}\frac{\psi}{\psi'}\frac{d}{d\rho}\left[\psi'^2\left(\frac{d\rho}{dn}\right)^2\right]$$

diffusive interface

Mechanical stability $\int_{\rho_g}^{\rho_l}\left(p_b - \rho c_s^2 - \frac{Gc^2}{2}\psi^2\right)\frac{\psi'}{\psi}d\rho = 0$

$$p_b = p_{EOS}(\rho_l) = p_{EOS}(\rho_g)$$

compute phase change density



Define G by Mechanical stability condition

Thermodynamic consistency

MRT Forcing scheme

$$f_\alpha(\mathbf{x} + \mathbf{e}_\alpha \delta_t, t + \delta_t) = f_\alpha(\mathbf{x}, t) - \bar{\Lambda}_{\alpha\beta}\left(f_\beta - f_\beta^{eq}\right)\big|_{(\mathbf{x},t)} + \delta_t(S_\alpha - 0.5\bar{\Lambda}_{\alpha\beta}S_\beta)\big|_{(\mathbf{x},t)}, \quad (1)$$

$$\mathbf{m}^* = \mathbf{m} - \mathbf{\Lambda}(\mathbf{m} - \mathbf{m}^{eq}) + \delta_t\left(\mathbf{I} - \frac{\mathbf{\Lambda}}{2}\right)\bar{\mathbf{S}},$$

Interaction force

Taylor expanding

$$\mathbf{F} = -G\psi(\mathbf{x})\sum_{\alpha=1}^{N} w(|\mathbf{e}_\alpha|^2)\psi(\mathbf{x} + \mathbf{e}_\alpha)\mathbf{e}_\alpha, \rightarrow \mathbf{F} = -Gc^2\left[\psi\nabla\psi + \tfrac{1}{6}c^2\psi\nabla(\nabla^2\psi) + \cdots\right], \quad (8)$$

Pressure tensor

$$\int(\nabla\cdot\mathbf{P})d\Omega = \int\nabla\cdot(\rho c_s^2\mathbf{I})\,d\Omega - \int\mathbf{F}d\Omega, \rightarrow \mathbf{P} = \left(\rho c_s^2 + \frac{Gc^2}{2}\psi^2 + \frac{Gc^4}{12}\psi\nabla^2\psi\right)\mathbf{I} + \frac{Gc^4}{6}\psi\nabla\nabla\psi.$$

Forcing term
(left) Original
(right) Improved

$$\bar{\mathbf{S}} = \begin{bmatrix} 0 \\ 6(v_xF_x + v_yF_y) \\ -6(v_xF_x + v_yF_y) \\ F_x \\ -F_x \\ F_y \\ -F_y \\ 2(v_xF_x - v_yF_y) \\ (v_xF_y + v_yF_x) \end{bmatrix}.$$

$$\bar{\mathbf{S}} = \begin{bmatrix} 0 \\ 6(v_xF_x + v_yF_y) + \frac{12\sigma|\mathbf{F}|^2}{\psi^2\delta_t(\tau_e - 0.5)} \\ -6(v_xF_x + v_yF_y) - \frac{12\sigma|\mathbf{F}|^2}{\psi^2\delta_t(\tau_\varsigma - 0.5)} \\ F_x \\ -F_x \\ F_y \\ -F_y \\ 2(v_xF_x - v_yF_y) \\ (v_xF_y + v_yF_x) \end{bmatrix},$$

Pressure tensor normal to interface

$$\mathbf{P}_{\text{new}} = \mathbf{P}_{\text{original}} + 2G^2c^4\sigma|\nabla\psi|^2\mathbf{I}.$$

$$P_n = \rho c_s^2 + \frac{Gc^2}{2}\psi^2 + \frac{Gc^4}{12}\left[\alpha\left(\frac{d\psi}{dn}\right)^2 + \beta\psi\frac{d^2\psi}{dn^2}\right], \quad (20)$$

$$P_n = \rho c_s^2 + \frac{Gc^2}{2}\psi^2 + \frac{Gc^4}{12}\left[(\alpha + 24G\sigma)\left(\frac{d\psi}{dn}\right)^2 + \beta\psi\frac{d^2\psi}{dn^2}\right],$$

$\alpha = 0, \beta = 3$ *for nearest neighbor* - isotropy에 의해 결정

Mechanical stability condition

Mechanical stability condition

$$\int_{\rho_g}^{\rho_l}\left(p_0-\rho c_s^2-\frac{Gc^2}{2}\psi^2\right)\frac{\psi'}{\psi^{1+\varepsilon}}\,d\rho=0,$$

$$\psi'/\psi^{1+\varepsilon}=1/\rho^2.$$

Maxwell area construction

$$\int_{\rho_g}^{\rho_l}\left(p_0-p_{\mathrm{EOS}}\right)\frac{1}{\rho^2}\,d\rho=0.$$

Equation of state $\psi(\rho)=\sqrt{\dfrac{2\left(p_{\mathrm{EOS}}-\rho c_s^2\right)}{Gc^2}}.$

Pressure tensor normal to interface

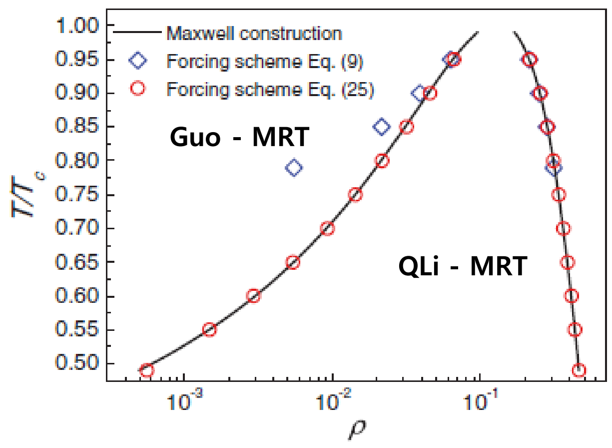
$$P_n=\rho c_s^2+\frac{Gc^2}{2}\psi^2+\frac{Gc^4}{12}\left[\alpha\left(\frac{d\psi}{dn}\right)^2+\beta\psi\frac{d^2\psi}{dn^2}\right],\quad(20)$$

$$\varepsilon=-2\alpha/\beta,$$

$$P_n=\rho c_s^2+\frac{Gc^2}{2}\psi^2+\frac{Gc^4}{12}\left[(\alpha+24G\sigma)\left(\frac{d\psi}{dn}\right)^2+\beta\psi\frac{d^2\psi}{dn^2}\right],$$

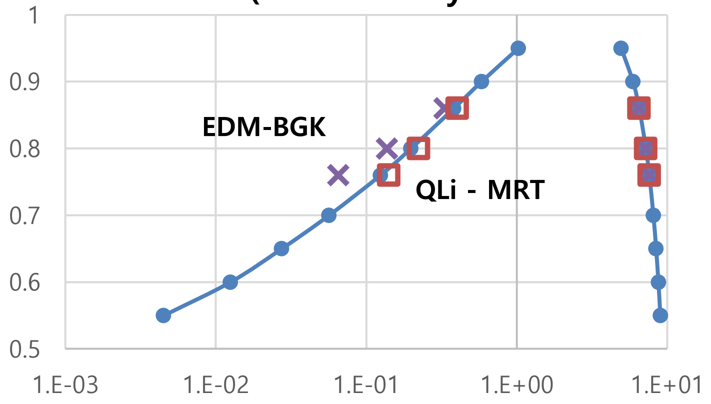
$$\varepsilon=-2(\alpha+24G\sigma)/\beta.$$

Paper – CS EOS



(b) $\tau_\upsilon=0.8$

Own – PR EOS (No boundary Interaction Force)



Equation of State and Energy Equation

Equation of state : $p_{eos} = \rho c_s^2 + \frac{G c_s^2}{2} \psi^2$ → Pseudopotential = $\sqrt{\frac{2(p - \rho c_s^2)}{Gc}}$

Peng-Robinson Equation of state

$$p = \frac{\rho R T}{1 - b\rho} - \frac{a\rho^2 \left[1 + (0.37464 + 1.54226\omega - 0.2699\omega^2)\left(1 - \sqrt{\frac{T}{T_c}}\right)\right]^2}{1 + 2b\rho - b^2\rho^2}.$$

chose $a = 2/49$, $b = 2/21$ and $R = 1$. $\omega: acentric\ factor = 0.344\ for\ water$

Temperature should be calculated to specify equation of state (Density can be calculated by LBM)

Thermodynamic relation of entropy $T\mathrm{d}s = c_v \mathrm{d}T + T\left(\frac{\partial p}{\partial T}\right)_v \mathrm{d}v = c_v \mathrm{d}T + T\left(\frac{\partial p}{\partial T}\right)_v \mathrm{d}\left(\frac{1}{\rho}\right) = c_v \mathrm{d}T - T\frac{1}{\rho^2}\left(\frac{\partial p}{\partial T}\right)_\rho \mathrm{d}\rho$

Entropy balance equation $\rho T \frac{\mathrm{d}s}{\mathrm{d}t} = \nabla \cdot (\lambda \nabla T)$ → $\frac{\mathrm{d}T}{\mathrm{d}t} = \nabla \cdot \left(\frac{\lambda}{\rho c_v} \nabla T\right) + \frac{T}{\rho^2 c_v}\left(\frac{\partial p}{\partial T}\right)_\rho \frac{\mathrm{d}\rho}{\mathrm{d}t}$

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{\partial T}{\partial t} + (\mathbf{U} \cdot \nabla) T$$

$$\frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{U}T) = \nabla \cdot (\alpha \nabla T) + \frac{T}{\rho^2 c_v}\left(\frac{\partial p}{\partial T}\right)_\rho \frac{\mathrm{d}\rho}{\mathrm{d}t} + T\nabla \cdot \mathbf{U}$$

Mass conservation $\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0$

$$\phi = T\left[1 - \frac{1}{\rho c_v}\left(\frac{\partial p}{\partial T}\right)_\rho\right] \nabla \cdot \mathbf{U}$$

From LBM

Energy (Heat) equation with source term $\frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{U}T) = \nabla \cdot (\alpha \nabla T) + \phi$

Source term which responsible for phase change

Energy equation with source term should be solved and coupled to specify equation of state

Finite Difference Method

From LBM

Energy (Heat) equation with source term

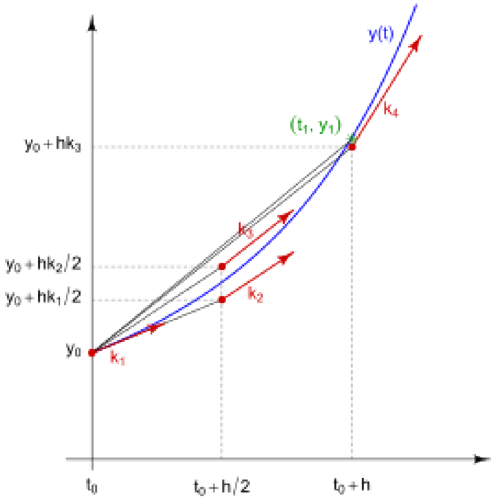
$$\frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{U} T) = \nabla \cdot (\alpha \nabla T) + \phi$$

$$\phi = T\left[1 - \frac{1}{\rho c_v}\left(\frac{\partial p}{\partial T}\right)_\rho\right] \nabla \cdot \mathbf{U}$$

Directly solve with FDM method

$$\partial_t T = -\mathbf{v} \cdot \nabla T + \frac{1}{\rho c_v} \nabla \cdot (\lambda \nabla T) - \frac{T}{\rho c_v} \left(\frac{\partial p_{\mathrm{EOS}}}{\partial T}\right)_\rho \nabla \cdot \mathbf{v}.$$

4th order Runge-Kutta Method



$$T^{t+\delta_t} = T^t + \frac{\delta_t}{6}(h_1 + 2h_2 + 2h_3 + h_4),$$

$$h_1 = K(T^t), h_2 = K\left(T^t + \frac{\delta_t}{2} h_1\right), h_3 = K\left(T^t + \frac{\delta_t}{2} h_2\right)$$

$$h_4 = K(T^t + \delta_t h_3).$$

- k_1 is the slope at the beginning of the interval, using y (Euler's method);
- k_2 is the slope at the midpoint of the interval, using y and k_1;
- k_3 is again the slope at the midpoint, but now using y and k_2;
- k_4 is the slope at the end of the interval, using y and k_3.

Solve the energy equation directly with FDM