Technische Universität Braunschweig

Modeling Evaporation Mechanism with Lattice Boltzmann Multiphase Models

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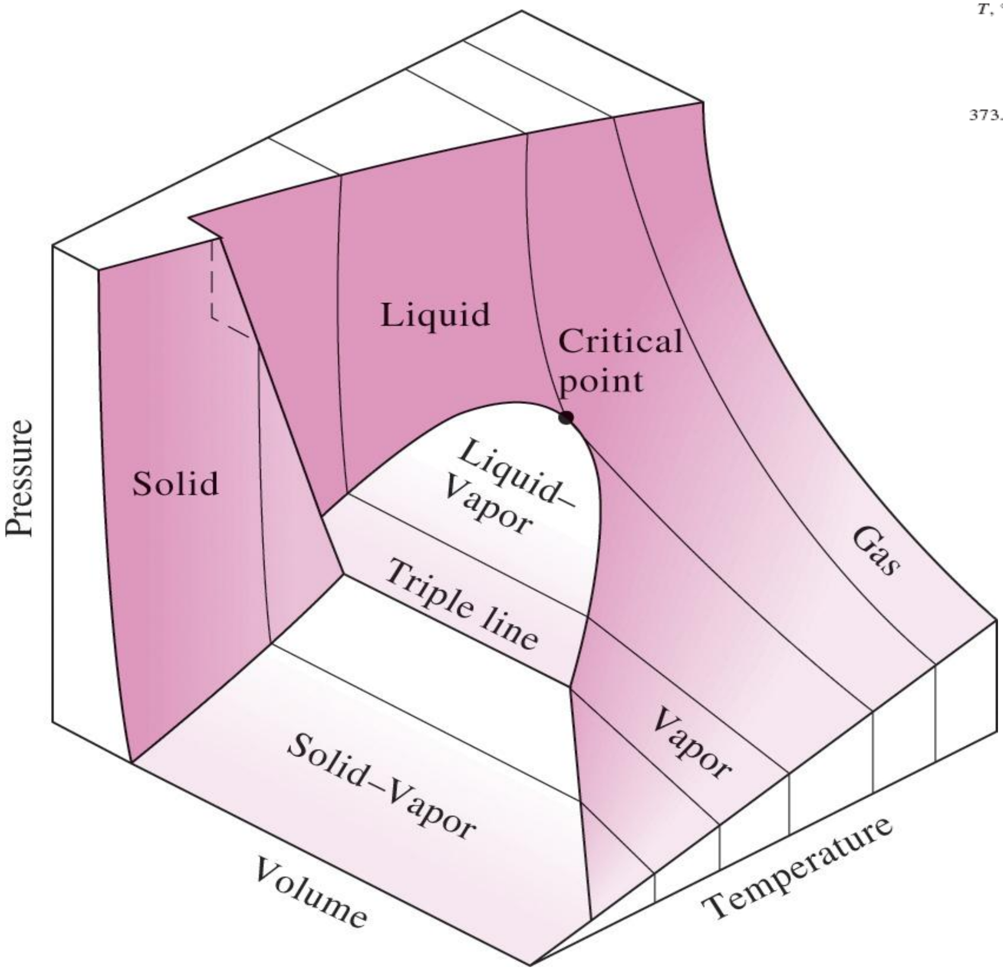
Outline

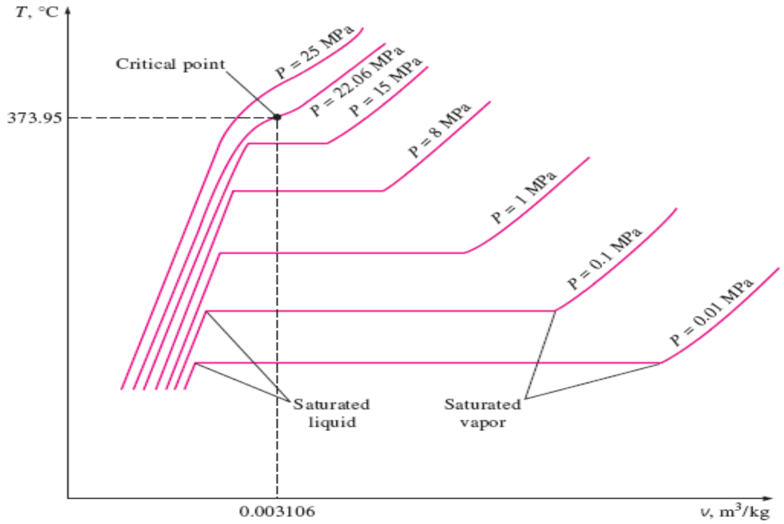
- Mathematical modeling of evaporation
  - Van der Waals equation of state
  - Thermo-, mechanical and chemical equilibria
  - Interfacial behavior

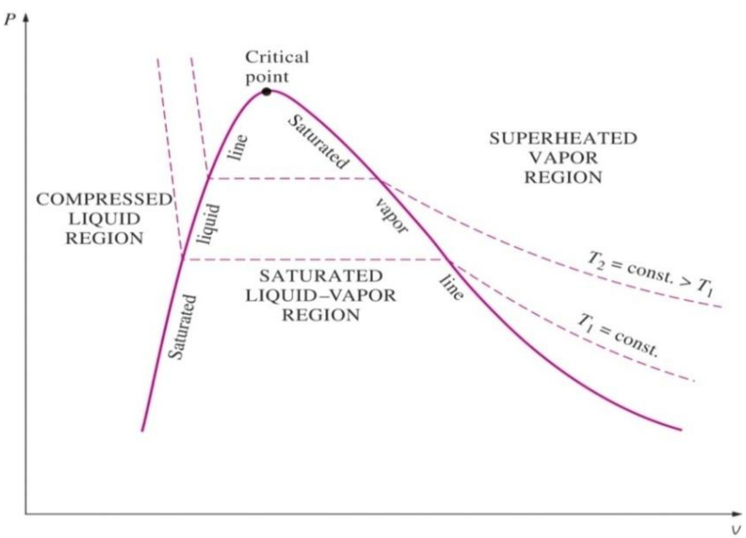
- Lattice Boltzmann method multiphase models
  - The immiscible fluid multiphase model (R-K model)
  - Lee’s multiphase model
  - Computational results

- Conclusions and outlook

The P-V-T Surface







Cengel, Y. A. and. Boles, M. A. Thermodynamics - An engineering approach. *McGraw-Hill*, 1989.

Van der Waals Equation of State (EOS)

- Free Energy

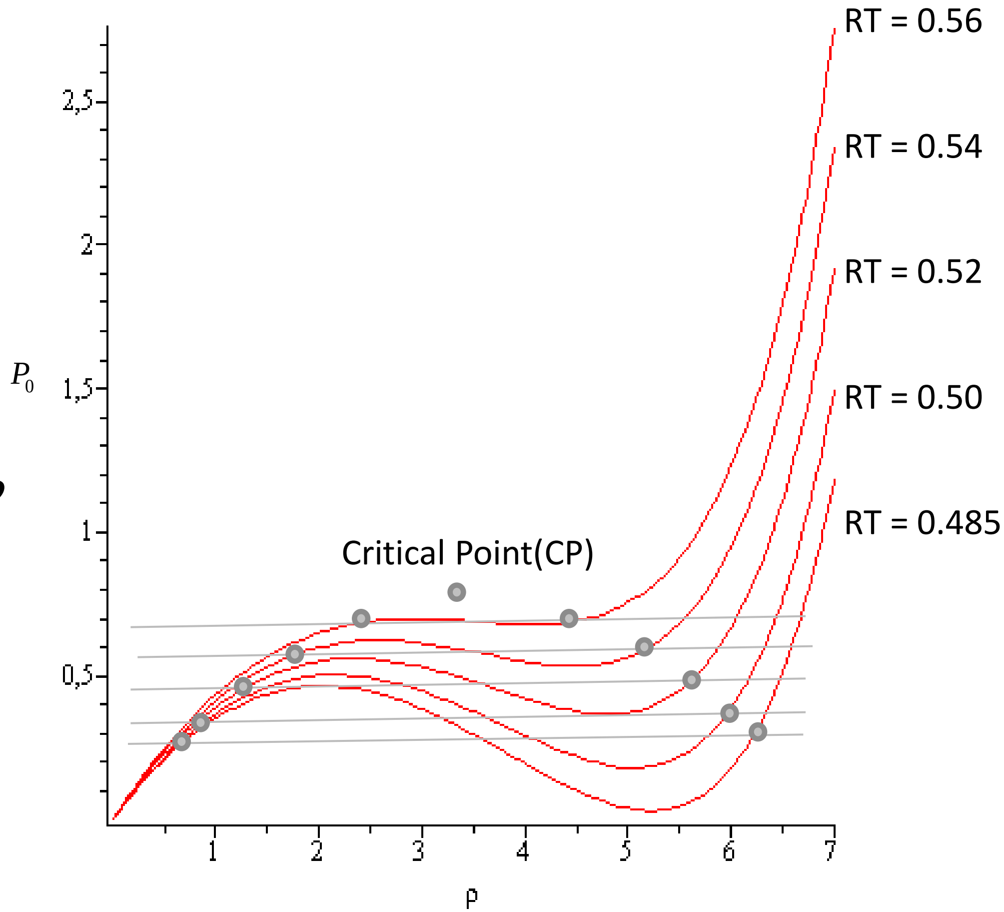
$$E_0 = \rho RT \ln\left(\frac{\rho}{1-b\rho}\right) - a\rho^2$$

- Chemical Potential

$$\mu_0 = \frac{\partial E_0}{\partial \rho} = RT\ln\left(\frac{\rho}{1-b\rho}\right) + \frac{RT}{(1-b\rho)} - 2a\rho$$

- Thermodynamic Pressure

$$P_0 = \rho\mu_0 - E_0 = \frac{\rho RT}{(1-b\rho)} - a\rho^2$$



Equilibria for Liquid-Vapor Coexistence

Flat surface

- Thermal equilibrium

$$T_v = T_l = T_{sat}$$

- Mechanical equilibrium

$$P_v = P_l = P_{sat}$$

- Chemical equilibrium

$$\mu_{0,l} = \mu_{0,v} = \mu_{0,eq}$$

Curved surface (e.g., capillary rise)

- Thermal equilibrium

$$T_v = T_l = T$$

- Mechanical equilibrium

$$P_l = P_v + \frac{2\sigma}{R}$$

$$P_{sat,T} - P_v = \left(\frac{V_l}{V_l - V_{v,sat}}\right)\left(\frac{2\sigma}{R}\right)$$

$$P_{sat,T} - P_l = \left(\frac{V_{v,sat}}{V_l - V_{v,sat}}\right)\left(\frac{2\sigma}{R}\right)$$

$$P_v \cong P_{sat,T}, \quad P_l \cong P_{sat,T} + \frac{2\sigma}{R}$$

- Chemical equilibrium

$$\mu_{0,l} = \mu_{0,v} = \mu_{0,eq}$$

Jump Mass Balance Condition

- Interface between liquid saturated water and saturated water vapor

$$\rho_{v,eq} = \frac{1}{V_{v,eq}} \quad \rho_{l,eq} = \frac{1}{V_{l,eq}}$$

- -> binary system, two phases(water liquid + gas),
  two components (gas = air + water vapor)

$$C = \rho_{p,eq} / \rho_w, \quad p \in \{l, v\}, \quad \rho_w = 1000 \frac{kg}{m^3}, \quad \rho_a$$

$$\rho = C\rho_w + (1-C)\rho_a$$

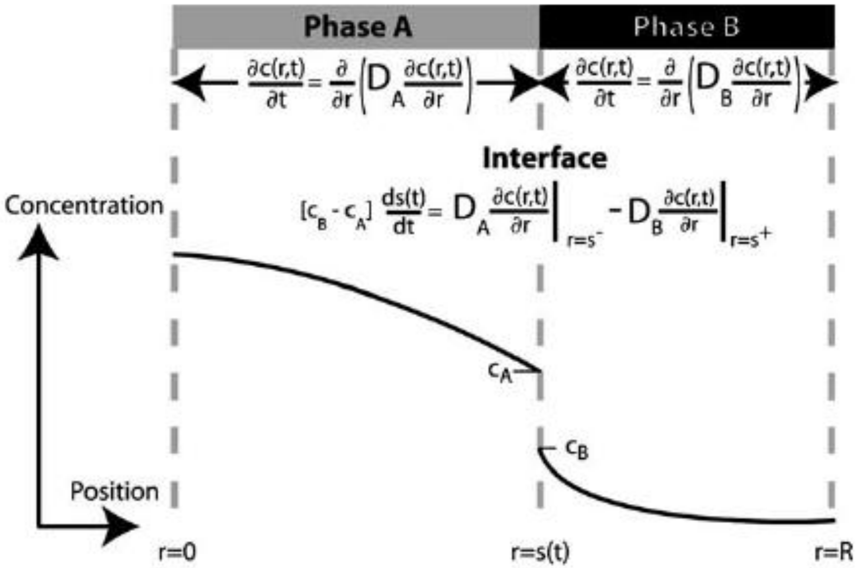
- A sharp interface technique can be used to simulate a one-dimensional isothermal binary system from unsaturated state towards equilibrium state, i.e., to compute the dynamic saturated water-vapor interface.

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial r}(D_l \frac{\partial C}{\partial r}), \quad 0 \le r \le s(t)$$

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial r}(D_v \frac{\partial C}{\partial r}), \quad s(t) \le r \le L$$

$$(C_v - C_l)\frac{\partial s(t)}{\partial t} = D_l \frac{\partial C}{\partial r}\bigg|_{r = s(t)^-} - D_v \frac{\partial C}{\partial r}\bigg|_{r = s(t)^+}$$

Diffusion-Controlled Phase Change



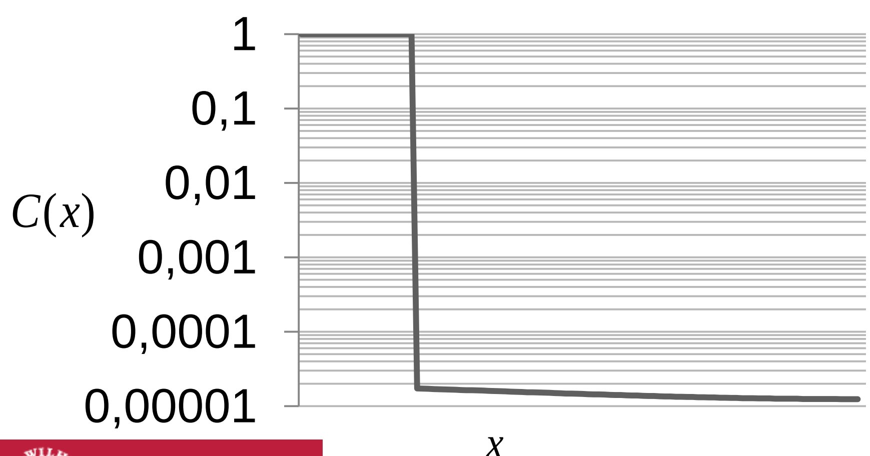
Illingworth, T. & Golosnoy, I.
Numerical solutions of diffusion-controlled moving boundary problems which conserve solute. *Journal of Computational Physics,* **2005**, *209*, 207 - 225

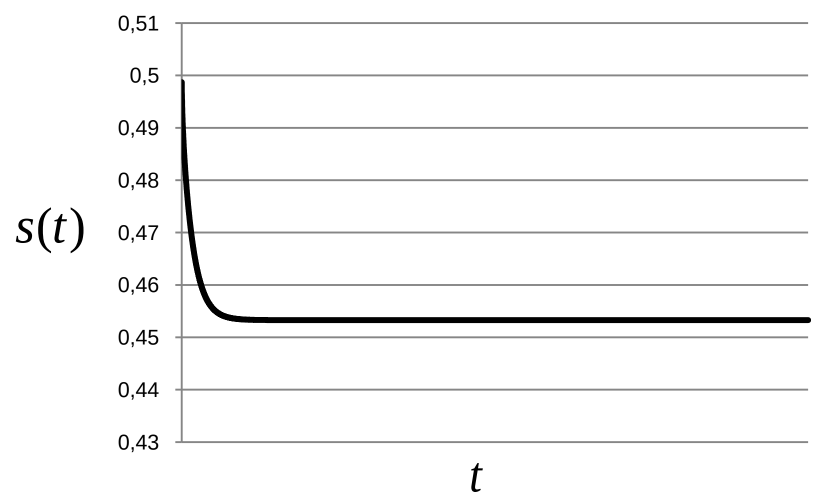
$$T = 20^oC$$

$$\rho_w = 1000\frac{kg}{m^3}$$

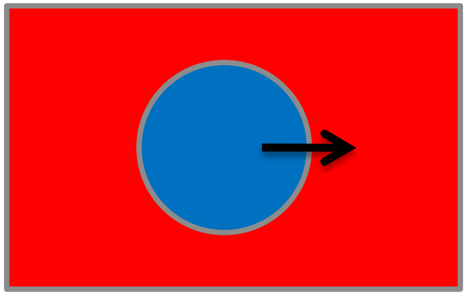
$$\tilde{\rho}_{l,eq} = \frac{1}{v_{l,eq}} = \frac{1}{0.001002} = 998.00 \quad C_l = \frac{998.00}{1000} = 99.8\%$$

$$\tilde{\rho}_{v,eq} = \frac{1}{v_{v,eq}} = \frac{1}{57.79} = 0.0173 \quad C_v = \frac{0.0173}{1000} = 0.00173\%$$

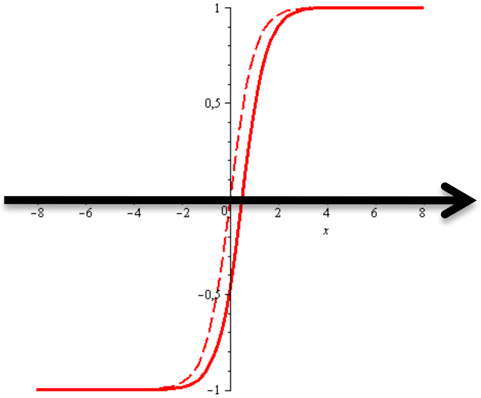




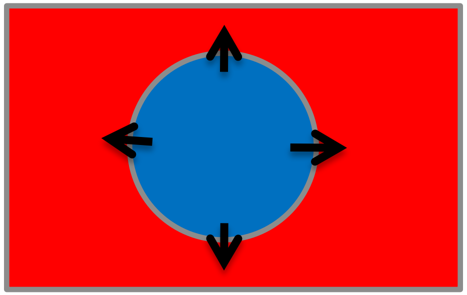
Evaporation with the R-K Model



- Assumption: The phase field generates the hyperbolic tangent profile in the normal direction of the interface.



- The 1D transformation of the phase field into a reference coordinate is used to change the water phase status, i.e., from liquid into vapor.



- The process of evaporation is therefore equivalent to displacement of water by gas.

Evaporation with Different Contact Angels

$\theta = 45^o$

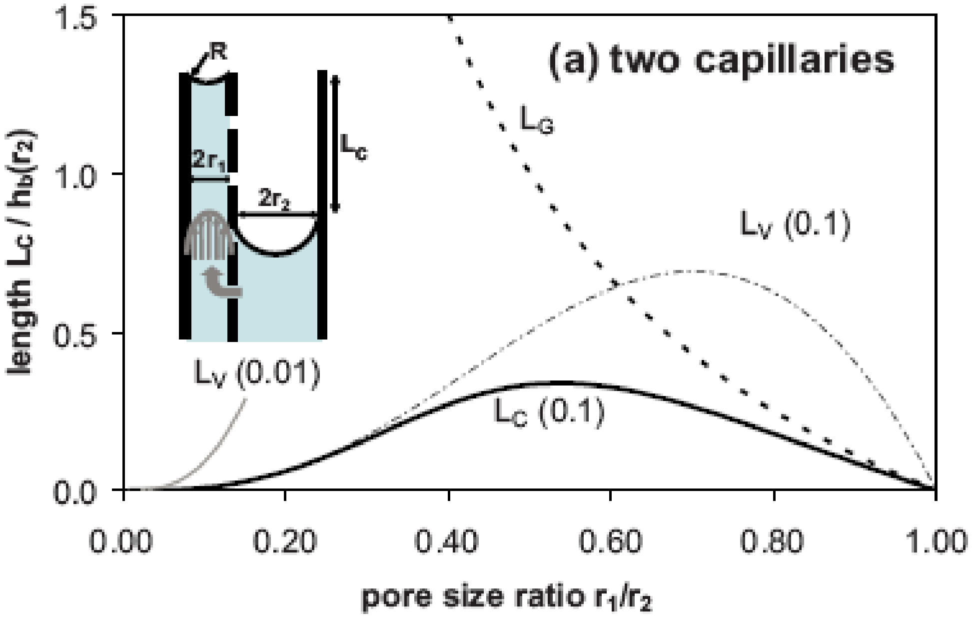
$\theta = 90^o$

$\theta = 135^o$

$\theta = 180^o$

Characteristic Length for Vaporization from Capillaries

P. Lehmann, S. Assouline, and D. Or, Phys. Rev. E **77, 056309** 2008.



$$L_G = \frac{2\sigma}{\rho g}\left(\frac{1}{r_1} - \frac{1}{r_2}\right)$$

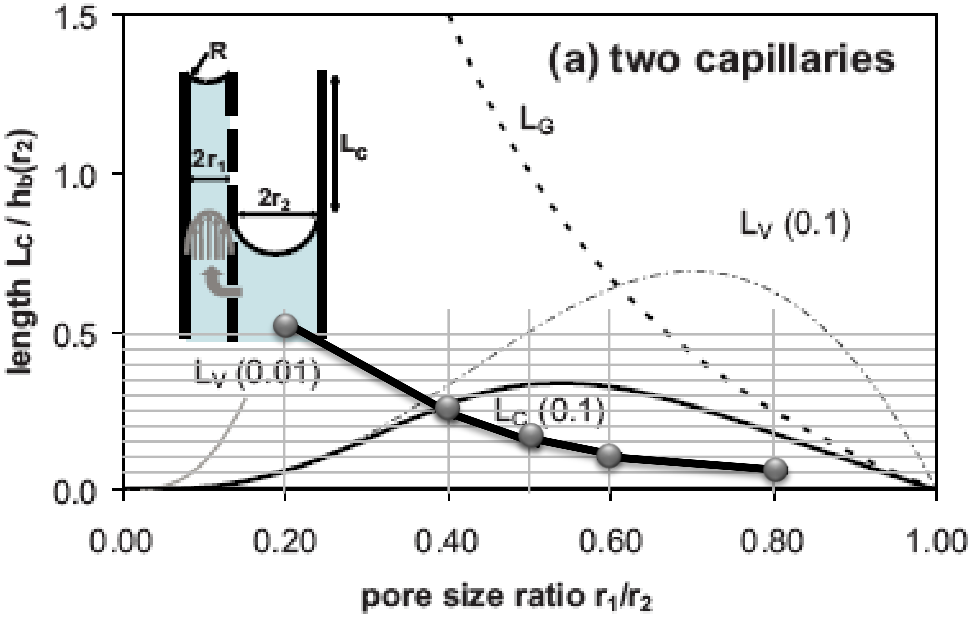
$$L_V = \frac{\rho g r_1^4}{8 e_0 \eta (r_1^2 + r_2^2)} L_G$$

$$L_C = \frac{L_G}{\frac{L_G}{L_V} + 1}$$

For real porous media, a reasonable drying rate can be captured from a dimensionless approach.

Characteristic Length for Vaporization from Capillaries

P. Lehmann, S. Assouline, and D. Or, Phys. Rev. E **77, 056309** 2008.



$$L_G = \frac{2\sigma}{\rho g}\left(\frac{1}{r_1} - \frac{1}{r_2}\right)$$

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$$L_C = \frac{L_G}{\frac{L_G}{L_V} + 1}$$

- The previous example with the radii ratio 0.4 matches fortunately the analytical characteristic capillary length.
- Right, but almost without the viscous effect
    - Decrease evaporation rate
    - Other combination of parameters of LBM

The Lee's Multiphase Model

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla f_\alpha = -\frac{f_\alpha - f_\alpha^{eq}}{\lambda} + \frac{(\mathbf{e}_\alpha - \mathbf{u}) \cdot (\mathbf{F} + \mathbf{G})}{\rho c_s^2} f_\alpha^{eq}$$

$$\mathbf{F} = \nabla \rho c_s^2 - \nabla p_1 - C \nabla \mu \quad \mathbf{G} = -\rho g \nabla h$$

$$\frac{\partial g_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla g_\alpha = -\frac{g_\alpha - g_\alpha^{eq}}{\lambda} + (\mathbf{e}_\alpha - \mathbf{u}) \cdot \nabla \rho c_s^2 \big(\Gamma_\alpha(\mathbf{u}) - \Gamma_\alpha(\mathbf{0})\big)$$
$$- (\mathbf{e}_\alpha - \mathbf{u}) \cdot \big(C \nabla \mu + \rho g \nabla h\big) \Gamma_\alpha(\mathbf{u}) + \mathbf{e}_\alpha \cdot \rho_l g \nabla h \Gamma_\alpha(0)$$

$$\bar{g}_\alpha = g_\alpha + \frac{g_\alpha - g_\alpha^{eq}}{2\tau} - \frac{\delta t}{2}(\mathbf{e}_\alpha - \mathbf{u}) \cdot \nabla \rho c_s^2 \big(\Gamma_\alpha(\mathbf{u}) - \Gamma_\alpha(\mathbf{0})\big)$$
$$+ \frac{\delta t}{2}(\mathbf{e}_\alpha - \mathbf{u}) \cdot \big(C \nabla \mu + \rho g \nabla h\big) \Gamma_\alpha(\mathbf{u})$$
$$- \frac{\delta t}{2} \mathbf{e}_\alpha \cdot \rho_l g \nabla h \Gamma_\alpha(0)$$

$$\bar{g}_\alpha(t + \delta t, \mathbf{x} + \delta t \mathbf{e}_\alpha) - \bar{g}_\alpha(t, \mathbf{x})$$
$$= -\frac{g_\alpha - g_\alpha^{eq}}{\tau + 0.5} + \delta t (\mathbf{e}_\alpha - \mathbf{u}) \cdot \nabla \rho c_s^2 \big(\Gamma_\alpha(\mathbf{u}) - \Gamma_\alpha(\mathbf{0})\big)$$
$$- \delta t (\mathbf{e}_\alpha - \mathbf{u}) \cdot \big(C \nabla \mu + \rho g \nabla h\big) \Gamma_\alpha(\mathbf{u}) + \delta t \mathbf{e}_\alpha \cdot \rho_l g \nabla h \Gamma_\alpha(0)$$

$$\frac{\partial h_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla h_\alpha = -\frac{h_\alpha - h_\alpha^{eq}}{\lambda} + (\mathbf{e}_\alpha - \mathbf{u}) \cdot \nabla C \Gamma_\alpha(\mathbf{u}) + \nabla \cdot (M \nabla \mu) \Gamma_\alpha(\mathbf{u})$$
$$- \frac{1}{(\rho_l - \rho_g) c_s^2} (\mathbf{e}_\alpha - \mathbf{u}) \cdot \big(\nabla P + p_2 \nabla C\big) \Gamma_\alpha(\mathbf{u})$$
$$- \frac{1}{(\rho_l - \rho_g) c_s^2} (\mathbf{e}_\alpha - \mathbf{u}) \cdot \big(C \nabla \mu + (\rho - \rho_l) g \nabla h\big) \Gamma_\alpha(\mathbf{u})$$

$$\bar{h}_\alpha = h_\alpha + \frac{h_\alpha - h_\alpha^{eq}}{2\tau} - \frac{\delta t}{2}(\mathbf{e}_\alpha - \mathbf{u}) \cdot \nabla C \Gamma_\alpha(\mathbf{u}) - \frac{\delta t}{2} \nabla \cdot (M \nabla \mu) \Gamma_\alpha(\mathbf{u})$$
$$+ \frac{\delta t}{2(\rho_l - \rho_g) c_s^2} (\mathbf{e}_\alpha - \mathbf{u}) \cdot \big(\nabla P + p_2 \nabla C + C \nabla \mu + (\rho - \rho_l) g \nabla h\big) \Gamma_\alpha(\mathbf{u})$$

$$\bar{h}_\alpha(t + \delta t, \mathbf{x} + \delta t \mathbf{e}_\alpha) - \bar{h}_\alpha(t, \mathbf{x})$$
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$$+\frac{\delta t}{2} (\mathbf{e}_\alpha - \mathbf{u}) \cdot \big(C \nabla \mu + \rho g \nabla h\big) \Gamma_\alpha(\mathbf{u})$$
$$-\frac{\delta t}{2} \mathbf{e}_\alpha \cdot \rho_l g \nabla h \Gamma_\alpha(0)$$

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$$h_\alpha = \frac{f_\alpha - \rho_g \Gamma_\alpha(0)}{\rho_l - \rho_g}$$

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$$\mathbf{F} = \nabla \rho c_s^2 - \nabla p_1 - C\nabla\mu \quad \mathbf{G} = -\rho g \nabla h$$

$$C = \sum_\alpha \bar{h}_\alpha + \frac{\delta t}{2}\nabla\cdot(M\nabla C)$$

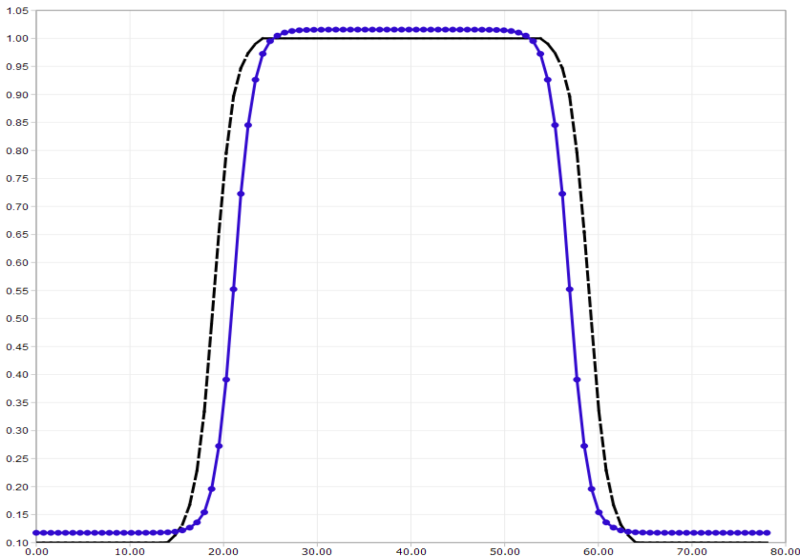
$$\rho\mathbf{u} = \frac{1}{c_s^2}\sum_\alpha \mathbf{e}_\alpha \bar{g}_\alpha - \frac{\delta t}{2} C\nabla\mu$$

$$P = \sum_\alpha \bar{g}_\alpha + \frac{\delta t}{2}\mathbf{u}\cdot\nabla\rho c_s^2$$

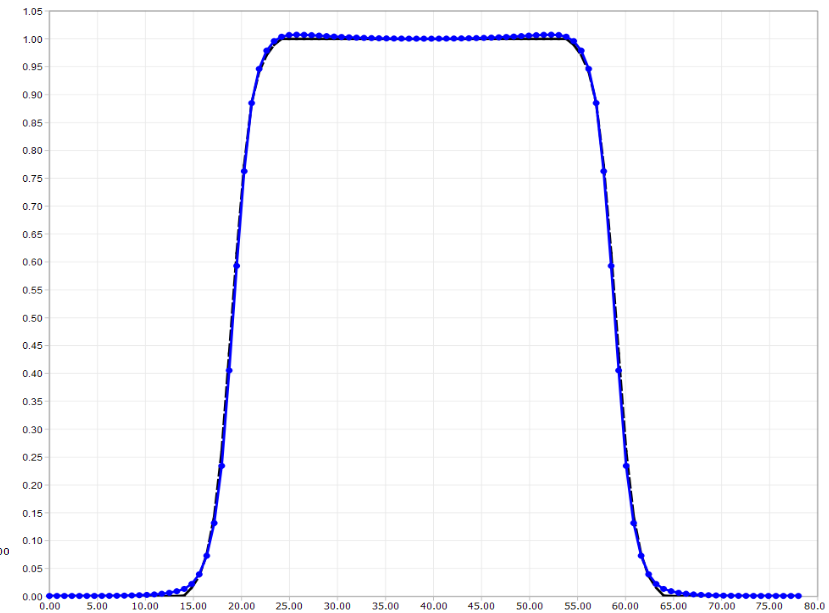
Static 3D Droplet Example

Laplace law of a 3D static droplet with SD and DD*

Initialization	Surface tension	2,17E-03	9,87E-03	1,08E-02	1,30E-02	1,52E-02	Initialization	1.0E-05
1.0	Density High	1,015653	1,02011	1,020106	1,01565	1,015652	1.0	1.0076
0.1	Density Low	0,117486	0,123265	0,123265	0,117485	0,117485	0.001	0.001
20	radius	18	17	17	18	18	20	20
	Young Laplace Law	3,04E-04	1,48E-03	1,62E-03	1,82E-03	2,13E-03		1.00E-06
	LBM	2,98E-04	1,43E-03	1,56E-03	1,79E-03	2,09E-03		1.04E-06
	Rel. Error	2,00%	3,23%	3,49%	1,97%	1,98%		3.79%



Lee's Model SD, 1:0.1

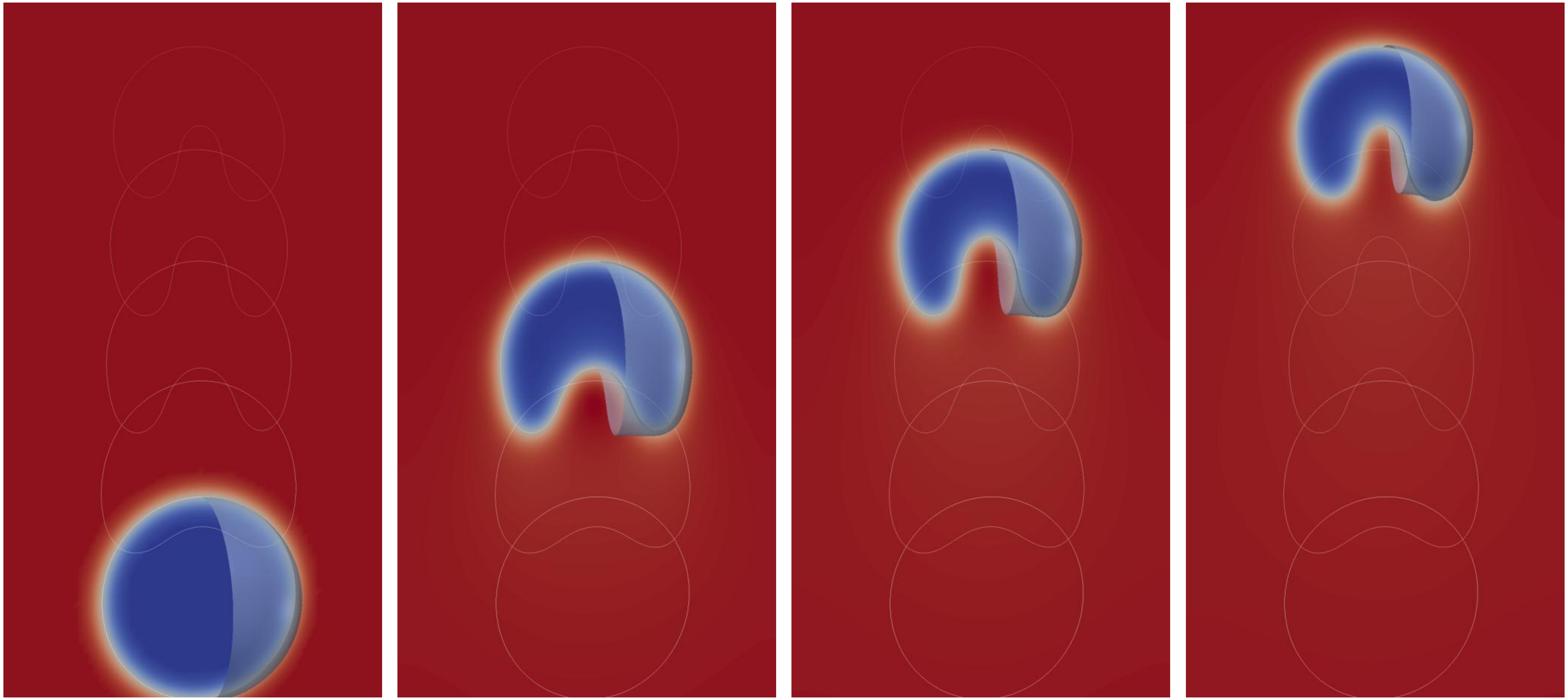


Lee's Model DD, 1:0.001

SD*: Lee's Model with single distribution function [1] DD*: Lee's Model with double distribution [2]

[1] Lee, T. & Fischer, P. F. Eliminating parasitic currents in the lattice Boltzmann equation method for non-ideal gases. *Phys. Rev. E, American Physical Society*, **2006**, *74*, 046709
[2] Amaya-Bower, L. & Lee, T. Single bubble rising dynamics for moderate Reynolds number using Lattice Boltzmann Method. Computers & *Fluids*, **2010**, *39*, 1191 - 1207

Skirted Bubble Regime with Smooth (SKS)



T = 0 | T =20000 | T =30000 | T =40000

Skirted with smooth (SKS) Bo = 340 Mo = 43 : Ut = 0.00417 Re = 10

Comparison of 3D Simulations with Experiments

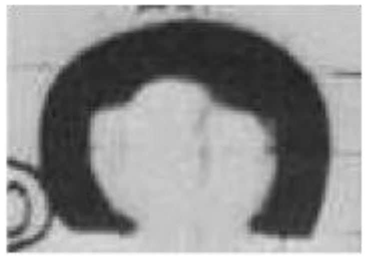
Experimental results by Bhaga and Weber

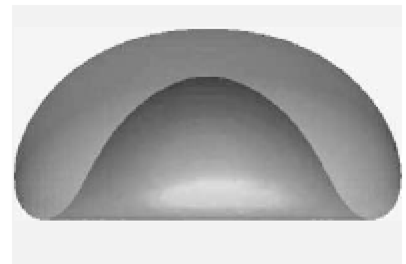
Previous simulation results by Amaya-Bower and Lee

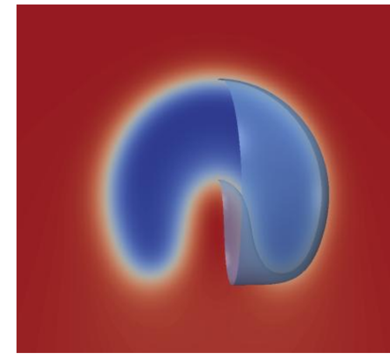
Current results

Skirted with smooth(SKS):

- Bo = 340
- Mo = 43







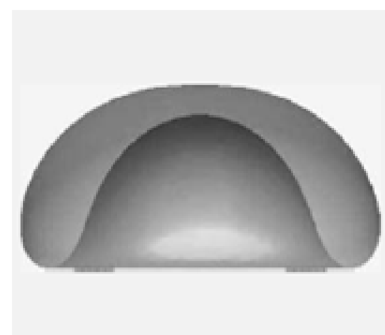
Re = 18.3

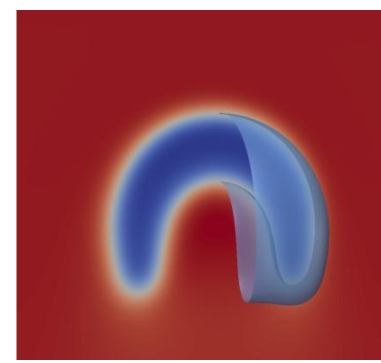
Re = 15.2

Re = 10

Skirted with wavy(SKW):

- Bo = 640,
- Mo = 43





Re = 30.3

Re = 26.8

Re = 27

Conclusions and Outlook

Mathematical modeling of evaporation formalism

Simulation of evaporation with the R-K multiphase model

- ☑ Mass und momentum conservation
- ✘ "Isothermal" evaporation rate; limited density ratio; spurious currents

Simulation of evaporation with the Lee's multiphase model

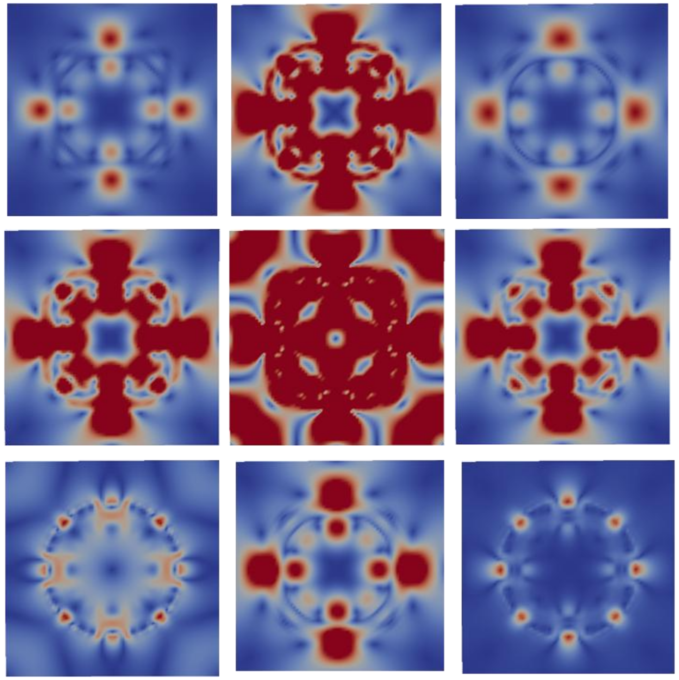
- ☑ Large density and viscosity ratio; phase separation combined with van der Waals EOS; vanished spurious currents
- ✘ Non local algorithm

Lee's multiphase model

- ❑ Simulate three phases interaction with different contact angles [3]
- ❑ Validation on GPU
- ❑ Comparison evaporation simulation with the experimental data of a real soil sample

[3] Lee, T. & Liu, L. Wall boundary conditions in the lattice Boltzmann equation method for non-ideal gases. *Phys. Rev. E, American Physical Society,* **2008**, *78*, 01770

Thank you for your attention.



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