Lattice Boltzmann for flow and transport phenomena

3. The lattice Boltzmann for multiphase flow

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- 3.2 Important parameters for multiphase flow
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3.1 Background

Multiphase fluid flows are ubiquitous in natural, scientific and engineering systems

A phase refers to gas, liquid or solid state of matter. A multiphase flow is the flow of a mixture of phases such as gas (bubbles) in a liquid, or liquid (droplets) in a gas, and so on.

Same component:

Liquid water and water vapor system

Multiple components:

Small density: water and oil system

Large density ratio: water and air system

Crown

Simulation of multiphase flows is a problem encountered often in scientific and industrial applications, and has long been regarded as a challenging task.

Microscopically, the interfacial behaviors of multiphase flows result from the interactions among the constituent molecules.

↔

Conventional method:
Level set method
Volume of Fluid
VOSET
Additional techniques to track the phase interface

A need for alternative approaches to understand the connection between the macroscopic phenomena and the underlying microscopic dynamics at a much more fundamental level

Molecular dynamics

Microscopic numerical methods such as molecular dynamics are suitable for capturing the microscopic interactions. However, they are often too computationally demanding to be applied to macroscopic scales of engineering interest.

The lattice Boltzmann method

The LBM can be considered as a mesoscopic method, occupying the middle ground between the microscopic molecular dynamics and macroscopic fluid dynamics. The main strength of the LBM is that it behaves like a solver for the conservation equations such as Navier-Stokes equation in the bulk flow yet its mesoscopic nature provides a viable way to include the microscopic dynamics at the fluid-fluid and fluid-solid interfaces.

3.2 Fundamental definitions

Saturation: ratio between the volume of one phase to the total volume of void space

$$S_i = \frac{V_i}{V_{\text{void}}}$$

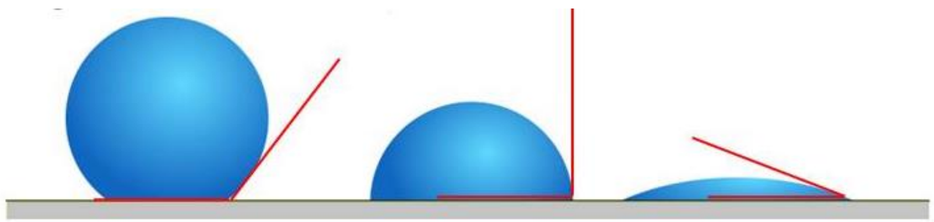
Surface tension: refers to the tensile force exists at the phase interface separating two fluids, arise due to a mutual attraction between molecules near the interface

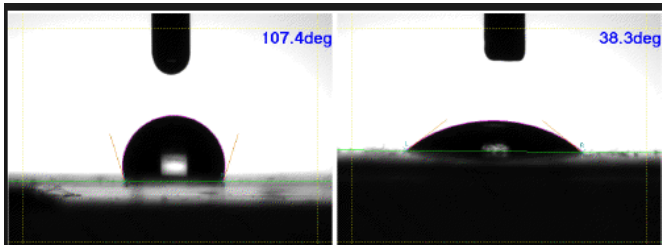
unit: N/m **Typical value**: water-air: 0.0725 N/m

Contact angle: is a measurement of the surface wettability. The angle of the triple-phase line. **Hydrophilic surface** with angle less than 90, liquid tends to spread. **Hydrophobic surface** with angle higher than 90, liquid tends to form droplet. **Neutral surface** with angle as 90.

Contact angle

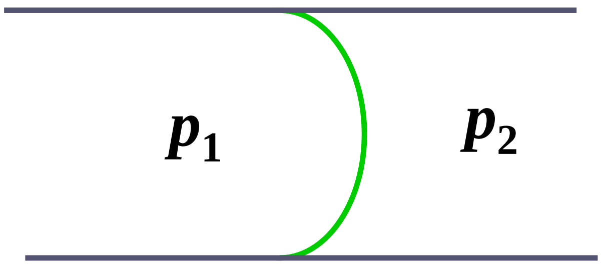
θ>90 θ=90 θ<90





Capillary pressure: pressure difference across a phase interface

$$P_C = P_1 - P_2 = \frac{\sigma\cos\theta}{r}$$



3.3 LB multiphase flow models

Due to its kinetic nature, LB does not need to track the phase interface, where the interface can be maintained automatically. Interface is a post-result of density field.

Several LB multiphase models:

1. Color-gradient model by Gunstense et al. 1991

A.K. Gunstensen, D.H. Rothman, S. Zaleski, G. Zanetti, Lattice Boltzmann model of immiscible fluids, Phys. Rev. A, 43 (8) (1991), pp. 4320–4327

2. Pseudopotential model by Shan and Chen 1993

X. Shan, H. Chen, Lattice Boltzmann model for simulating flows with multiple phases and component, Phys. Rev. E, 47 (3) (1993), pp. 1815–1819

3. Free energy model by Swift 1995

M.R. Swift, W.R. Osborn, J.M. Yeomans, Lattice Boltzmann simulation of nonideal fluids, Phys. Rev. Lett., 75 (5) (1995), pp. 830–833

The pseudo-potential LB model

Proposed by Shan and Chen in 1993.

[1] X. Shan, H. Chen, Lattice Boltzmann model for simulating flows with multiple phases and components, Phys. Rev. E, 47 (1993) 1815-1819

[2] X. Shan, H. Chen, Simulation of nonideal gases and liquid-gas phase transitions by the lattice Boltzmann equation, Physical Review E, 49(4) (1994) 2941-2948.

[3] X. Shan, G. Doolen, Multicomponent lattice-Boltzmann model with interparticle interaction, Journal of Statistical Physics, 81 (1995) 379-393.

[4] X. Shan, H. Chen, Diffusion in a multicomponent lattice Boltzmann equation model, Phys. Rev. E, 47 (1996) 3614-3620.

To the best of the authors' knowledge, this model is the most widely used LB multiphase model due to its simplicity and versatility

The basic idea is to represent the microscopic molecular interactions at the mesoscopic scale using a pseudo-potential (also often called effective mass) depending on the local density.

With such interactions, a single component system or a multicomponent system will spontaneously segregates into two phases if the interaction is properly calculated.

***: Such automatic phase separation is an attractive characteristic of the pseudopotential model, as the phase interface is no longer a mathematical boundary and no explicit interface-tracking or interface-capturing technique is needed.**

The phase interface is a post-processed quantity that can be characterized through monitoring the variation of the fluid densities.

3.3.1 The single component pseudopotential LBM

$$f_{\sigma,\alpha}(\mathbf{x}+c\mathbf{e}_\alpha\Delta t,t+\Delta t)-f_{\sigma,\alpha}(\mathbf{x},t)=-\frac{1}{\tau_{\sigma,\upsilon}}\left(f_{\sigma,\alpha}(\mathbf{x},t)-f_{\sigma,\alpha}^{eq}(\mathbf{x},t)\right)+F_{\sigma,\alpha}(\mathbf{x},t)$$

$$f_{\sigma,\alpha}^{\mathrm{eq}}=\omega_\alpha\rho_\sigma\left[1+\frac{3}{c^2}(\mathbf{e}_\alpha\cdot\mathbf{u})+\frac{9}{2c^4}(\mathbf{e}_\alpha\cdot\mathbf{u})^2-\frac{3}{2c^2}\mathbf{u}^2\right]$$

$$\rho_\sigma=\sum_\alpha f_{\sigma,\alpha}$$

$$\rho_\sigma\mathbf{u}_\sigma=\sum_\alpha f_{\sigma,\alpha}\mathrm{e}_\alpha$$

$$\upsilon_\sigma=c_s^2(\tau_{\sigma,\upsilon}-0.5)\Delta t$$

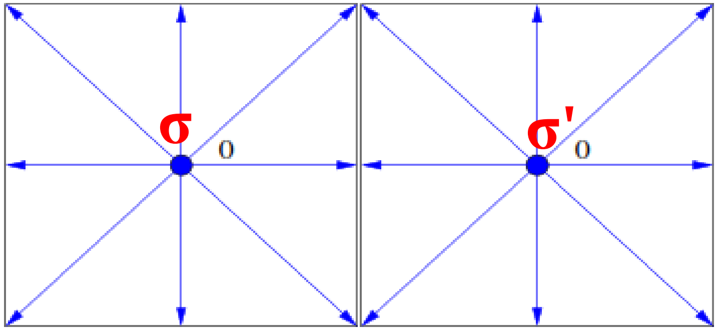
Equation of State

$$p=\rho c_s^{\ 2}$$

Ideal gas!

In order to introduce nonlocal interaction among particles, Shan and Chen defined the force experienced by the particles of component σ at *x* from the particles σ' at *x'* as the following form

$$\mathbf{F}(\mathbf{x},\mathbf{x}') = -G(|\mathbf{x}-\mathbf{x}'|)\psi_{\sigma}(\mathbf{x})\psi_{\sigma}(\mathbf{x}')(\mathbf{x}'-\mathbf{x})$$



Law of universal gravitation $\dfrac{Gm_1m_2}{r^2}$

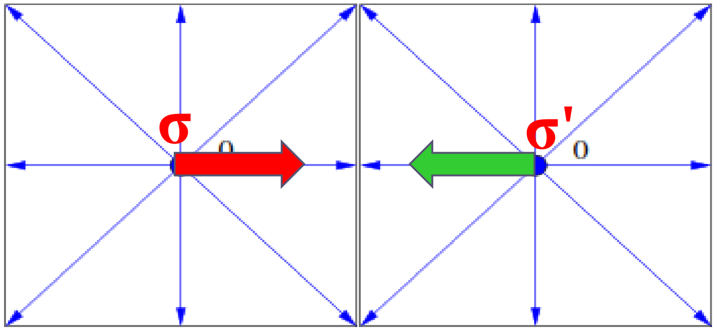
$$\mathbf{F}(\mathbf{x}',\mathbf{x}) = -G(|\mathbf{x}'-\mathbf{x}|)\psi_{\sigma}(\mathbf{x})\psi_{\sigma}(\mathbf{x}')(\mathbf{x}-\mathbf{x}')$$

***Ψ* is the effective mass, or the pseudopotential.**

$$\mathbf{F}(\mathbf{x},\mathbf{x}') = -G(|\mathbf{x}-\mathbf{x}'|)\psi_\sigma(\mathbf{x})\psi_\sigma(\mathbf{x}')(\mathbf{x}'-\mathbf{x})$$

$$\mathbf{F}(\mathbf{x}',\mathbf{x}) = -G(|\mathbf{x}'-\mathbf{x}|)\psi_\sigma(\mathbf{x})\psi_\sigma(\mathbf{x}')(\mathbf{x}-\mathbf{x}')$$

The most general one that meets the Newton's third law and conserves momentum globally



Such interaction force does not conserve the local momentum during the collision process because the force behaves as an external force acting on the site. The total momentum of the system is conserved and no net momentum is introduced into the system

$$\mathbf{F}(\mathbf{x},\mathbf{x}') = -G(|\mathbf{x}-\mathbf{x}'|)\psi_{\sigma}(\mathbf{x})\psi_{\sigma}(\mathbf{x}')(\mathbf{x}'-\mathbf{x})$$

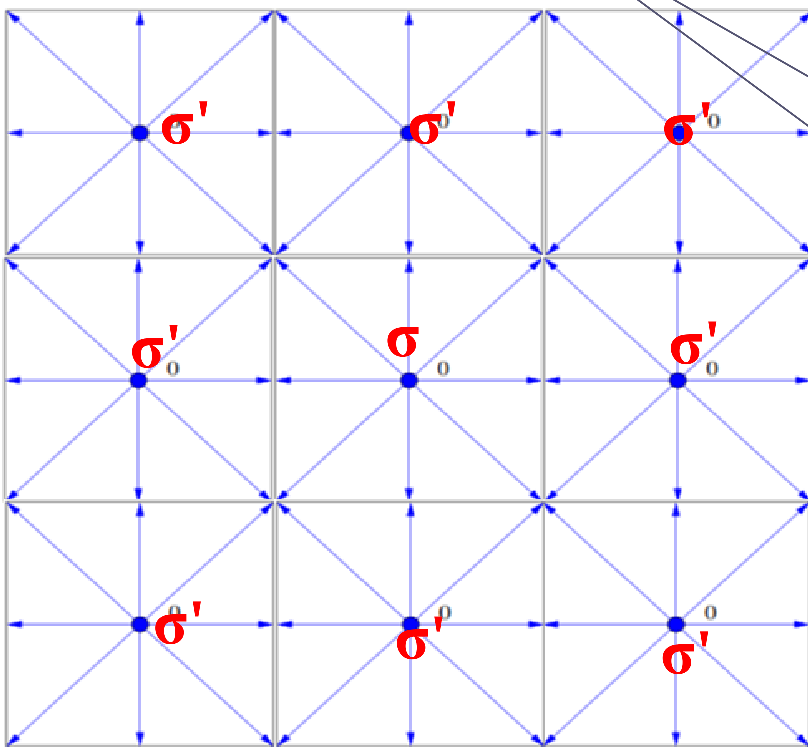
Total force

$$\mathbf{F}(\mathbf{x}) = -\psi(\mathbf{x})\sum G(|\mathbf{x}-\mathbf{x}'|)\psi(\mathbf{x}')(\mathbf{x}'-\mathbf{x})$$

$$\mathbf{F}(\mathbf{x}) = -g\psi(\mathbf{x})c_s^2\sum_{\alpha=1}^{N} w(|\mathbf{e}_\alpha|^2)\psi(\mathbf{x}+\mathbf{e}_\alpha)\mathbf{e}_\alpha$$

Interaction strength

Distance weight



$$\mathbf{F}(\mathbf{x}) = -g\psi(\mathbf{x})c_s^2 \sum_{\alpha=1}^{N} w(|\mathbf{e}_\alpha|^2)\psi(\mathbf{x}+\mathbf{e}_\alpha)\mathbf{e}_\alpha$$

Three important elements

- The interaction strength, *g*
- The effective mass, *Ψ*
- Determination of the neighbor sites, *N* and *w*

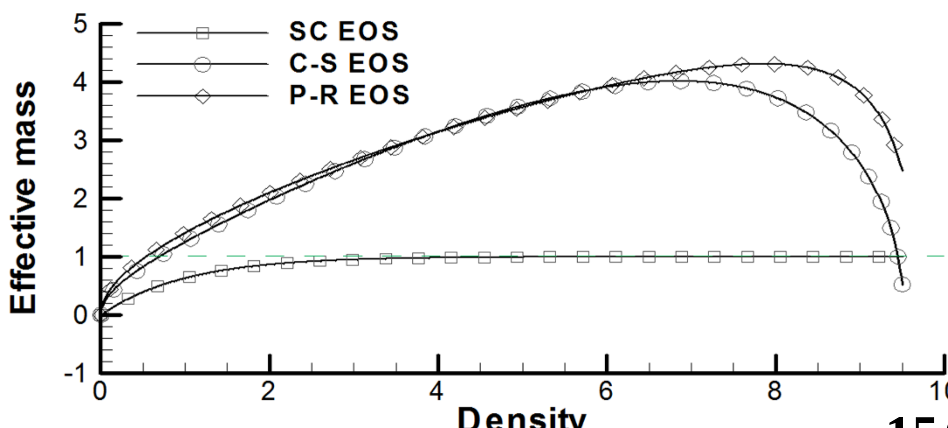
$$w(|\mathbf{e}_\alpha|^2) = 1/3, \quad |\mathbf{e}_\alpha|^2 = 1$$

$$w(|\mathbf{e}_\alpha|^2) = 1/12, \quad |\mathbf{e}_\alpha|^2 = 2$$

Ψ in the original work of Shan and Chen is as follows

$$\psi = \rho_0 (1 - \exp(-\frac{\rho}{\rho_0}))$$

ρ->∞, *Ψ*->1



$$\mathbf{F}(\mathbf{x}) = -g\psi(\mathbf{x})c_s^2\sum_{\alpha=1}^{N} w(|\mathbf{e}_\alpha|^2)\psi(\mathbf{x}+\mathbf{e}_\alpha)\mathbf{e}_\alpha$$

Taylor expansion

$$\mathbf{F} = -g\left(c_s^2\psi\nabla\psi + \frac{c_s^4}{2}\psi\nabla(\Delta\psi) + \ldots\right)$$

Two major ingredients of non-ideal fluids are captured: a non-ideal EOS relating to the first term and the surface tension

$$p = \rho c_s^2 + \frac{g}{2}c_s^2\psi^2$$

Force implementation: velocity shift scheme proposed by Shan and Chen

$$f_{\sigma,\alpha}(\mathbf{x}+c\mathbf{e}_\alpha\Delta t, t+\Delta t)-f_{\sigma,\alpha}(\mathbf{x},t)=-\frac{1}{\tau_{\sigma,\upsilon}}(f_{\sigma,\alpha}(\mathbf{x},t)-f_{\sigma,\alpha}^{eq}(\mathbf{x},t))$$

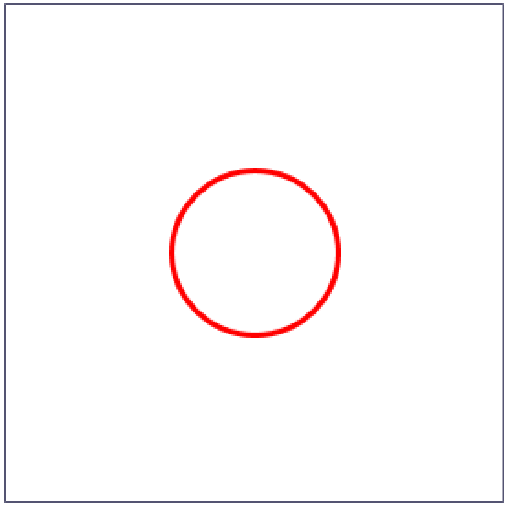
$$\mathbf{u}^{\mathrm{eq}}=\mathbf{u}+\frac{\tau}{\rho}\mathbf{F}\Delta t$$

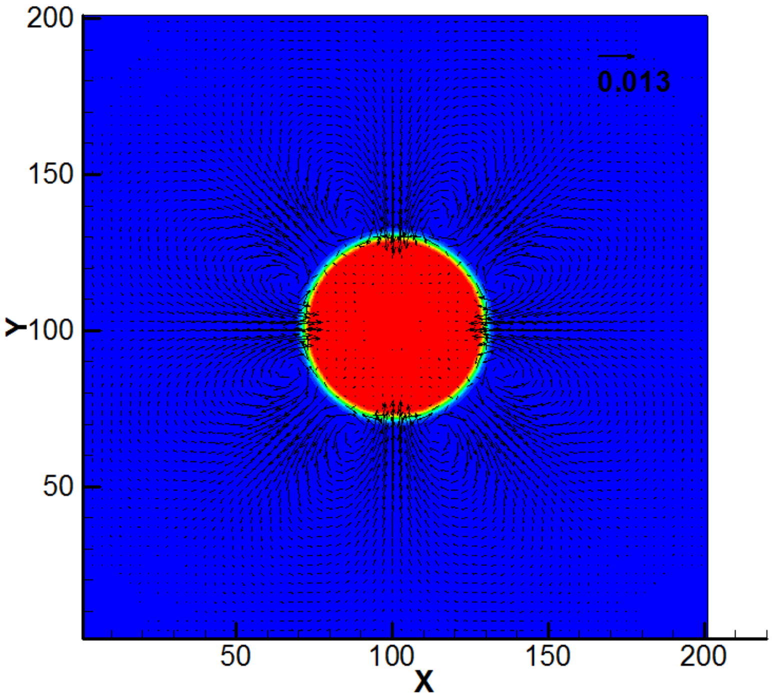
$$f_{\sigma,\alpha}^{\mathrm{eq}}=\omega_\alpha\rho_\sigma\left[1+\frac{3}{c^2}\left(\mathbf{e}_\alpha\cdot\mathbf{u}^{\mathbf{eq}}\right)+\frac{9}{2c^4}\left(\mathbf{e}_\alpha\cdot\mathbf{u}^{\mathbf{eq}}\right)^2-\frac{3}{2c^2}(\mathbf{u}^{\mathbf{eq}})^2\right]$$

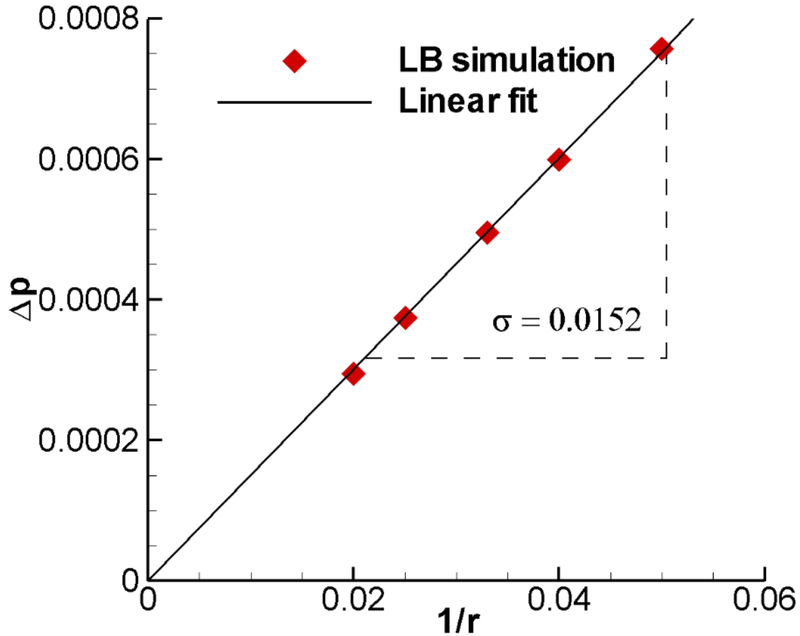
$$\mathbf{F}(\mathbf{x})=-g\psi(\mathbf{x})c_s^2\sum_{\alpha=1}^{N}w(|\mathbf{e}_\alpha|^2)\psi(\mathbf{x}+\mathbf{e}_\alpha)\mathbf{e}_\alpha$$

$$\mathbf{u}_{\mathrm{p}}=\mathbf{u}+\frac{1}{2\rho}\mathbf{F}\Delta t$$

Bubble test (Laplace law)







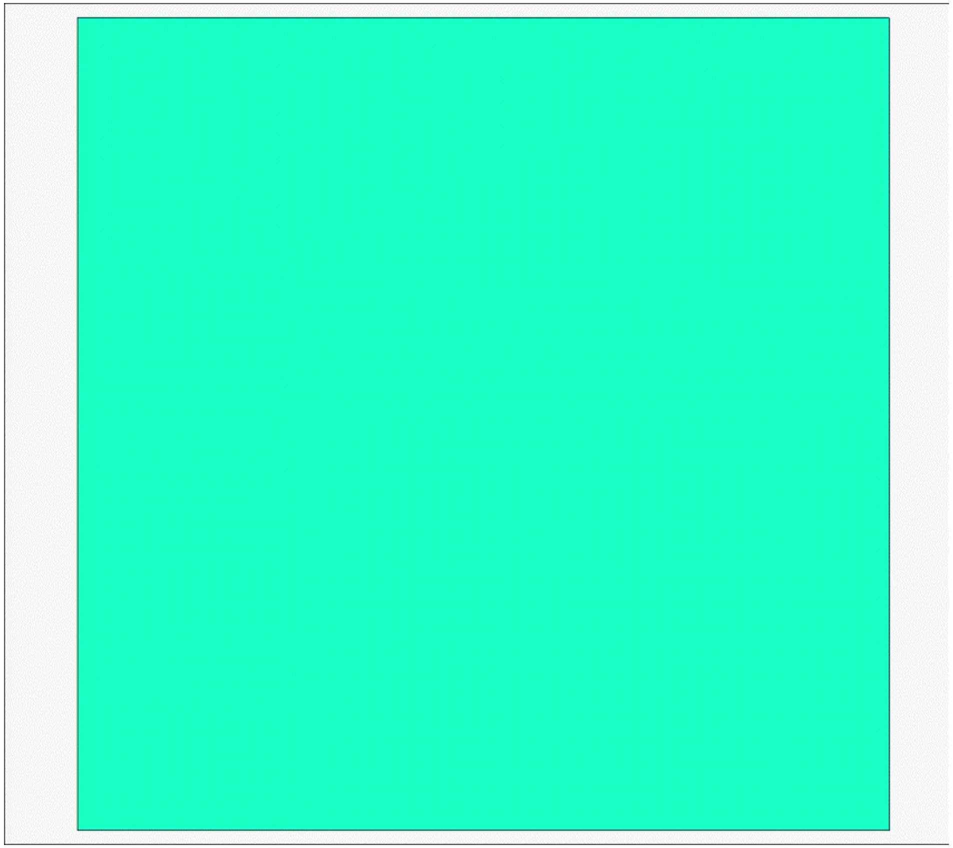
Laplace law

$$\nabla p = p_{\text{in}} - p_{\text{out}} = \frac{\sigma}{r}$$

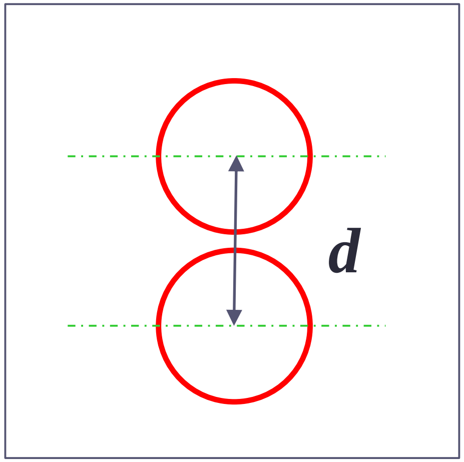
First phase transition

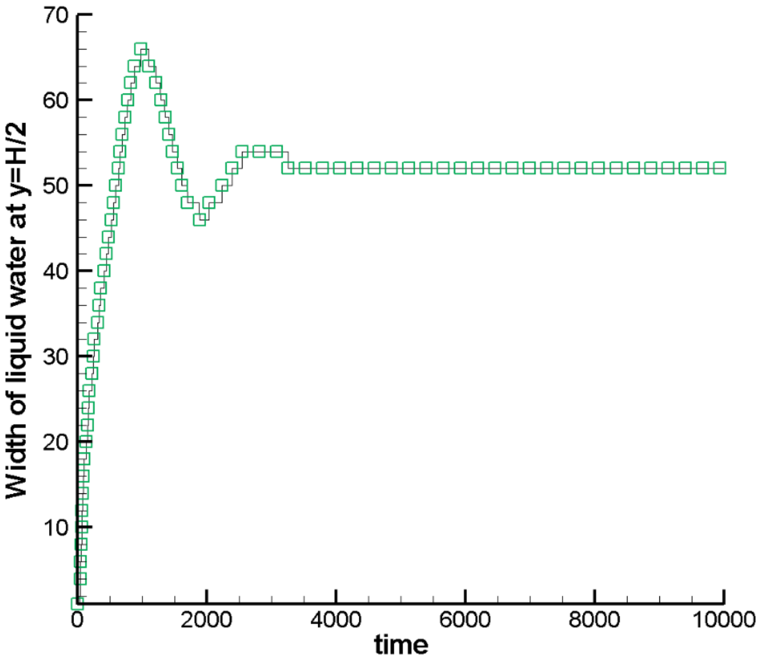
t=0, uniform density field

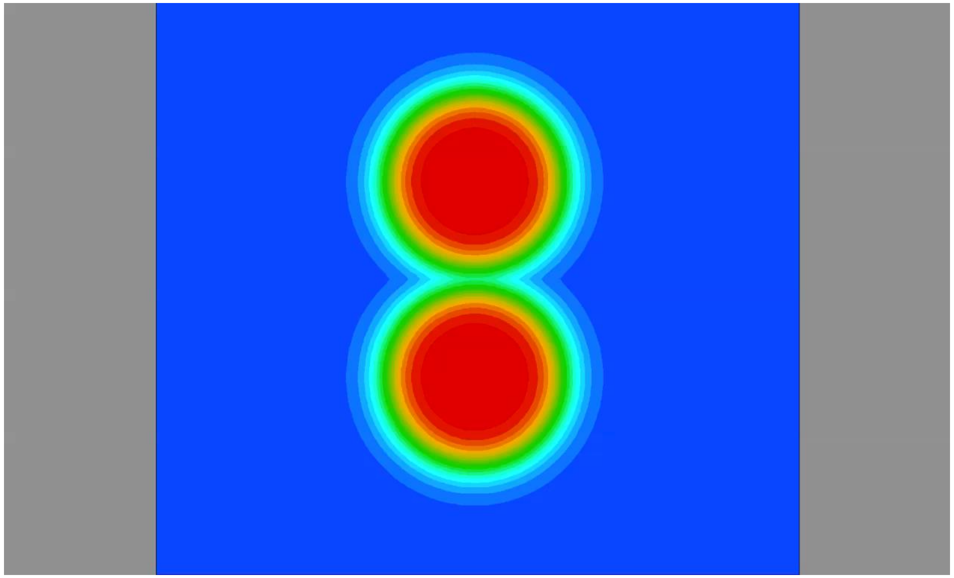
A small disturbance is added: δρ<5%.



Droplet coalesce







3.3.2 The limitation of SC original model

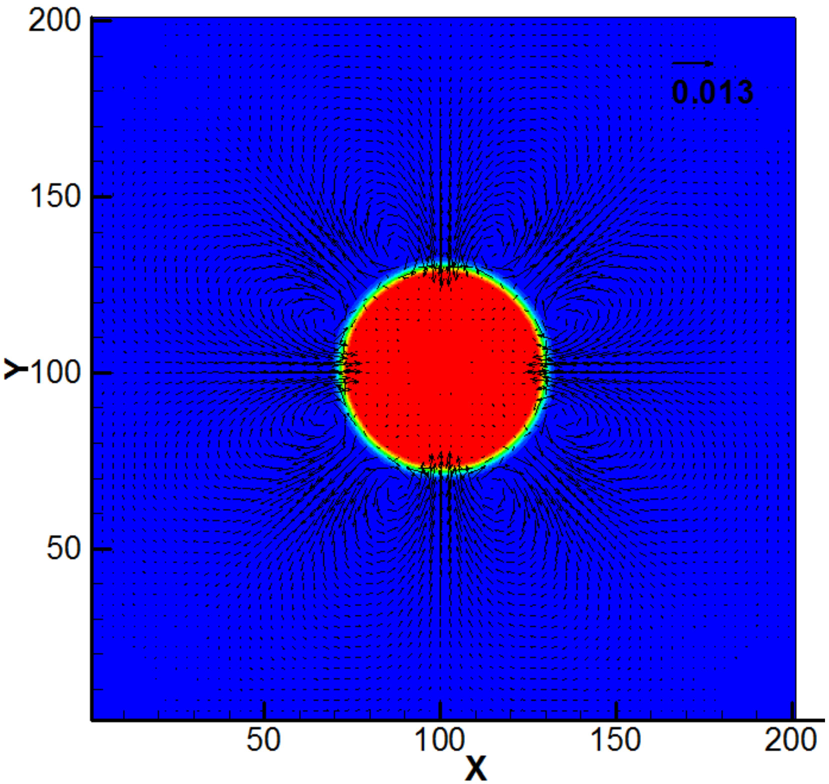
The original SC model suffers from some limitations.

Some of the limitations are inherent to this particular model and others are common problems shared by other multiphase flow models

- **Relatively large spurious current**
- **Thermodynamic inconsistency**
- **Low density and viscosity ratio**
- **Coupling between EOS and surface tension force**
- **Dependence of surface tension and density ratio on the viscosity.**

Spurious current

The spurious current denotes the non-zero vortex-like fluid velocity in the vicinity of phase interface

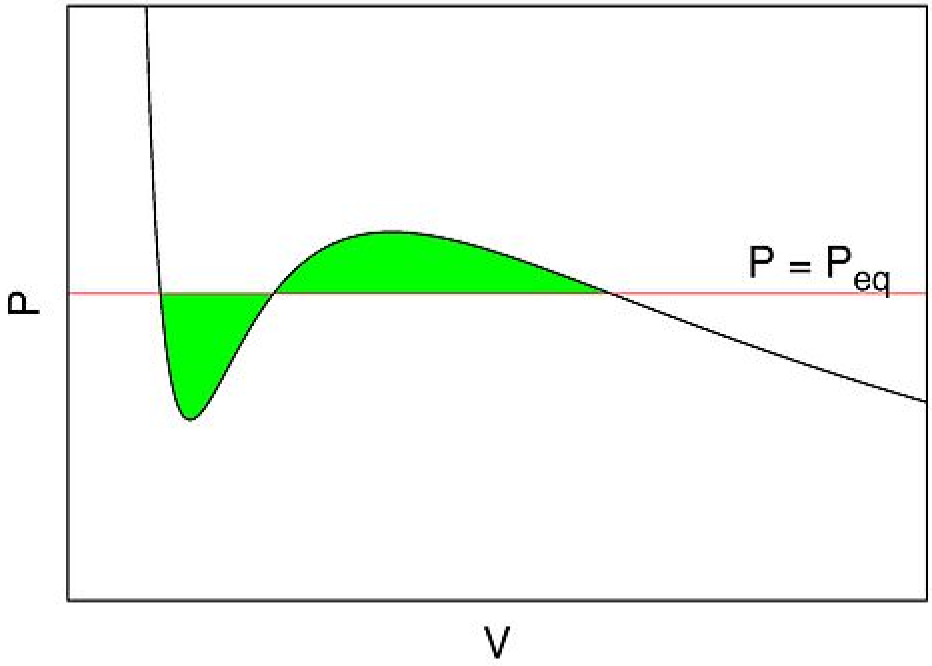


Physically, the droplet and its surrounding gas are at rest and the pressure difference inside and outside the droplet should be balanced by the surface tension force.

Due to the limited discretization in calculating the corresponding gradient, the pressure difference and surface tension are not exactly balanced, leading to the artificial vortex-like velocity.

Thermodynamic inconsistency

Maxwell construction

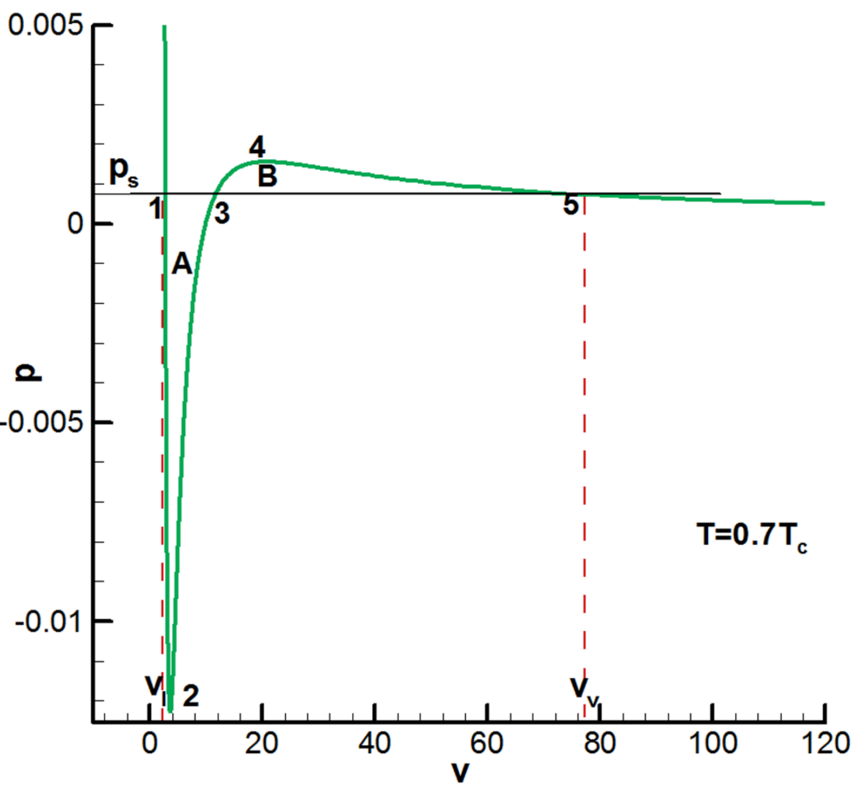


$$\int_{v_l}^{v_v} p\,dv = p_s (v_v - v_l)$$

$$\int_{v_l}^{v_v} (p - p_s)\,dv = 0$$

$$p = \rho RT \frac{1 + b\rho/4 + (b\rho/4)^2 - (b\rho/4)^3}{(1 - b\rho/4)^3} - a\rho^2$$

$a=0.4963(RT_c)^2/p_c$, $b=0.1873RT_c/p_c$



Maxwell construction

$$\int_{v_l}^{v_v} p\,dv = p_s(v_v - v_l)$$

$$\int_{v_l}^{v_v} (p - p_s)\,dv = 0$$

$$\int_{\rho_v}^{\rho_l} \left(p_s - \rho c_s^2 - \frac{g}{2} c_s^2 \psi^2\right) \frac{1}{\rho^2}\,d\rho = 0$$

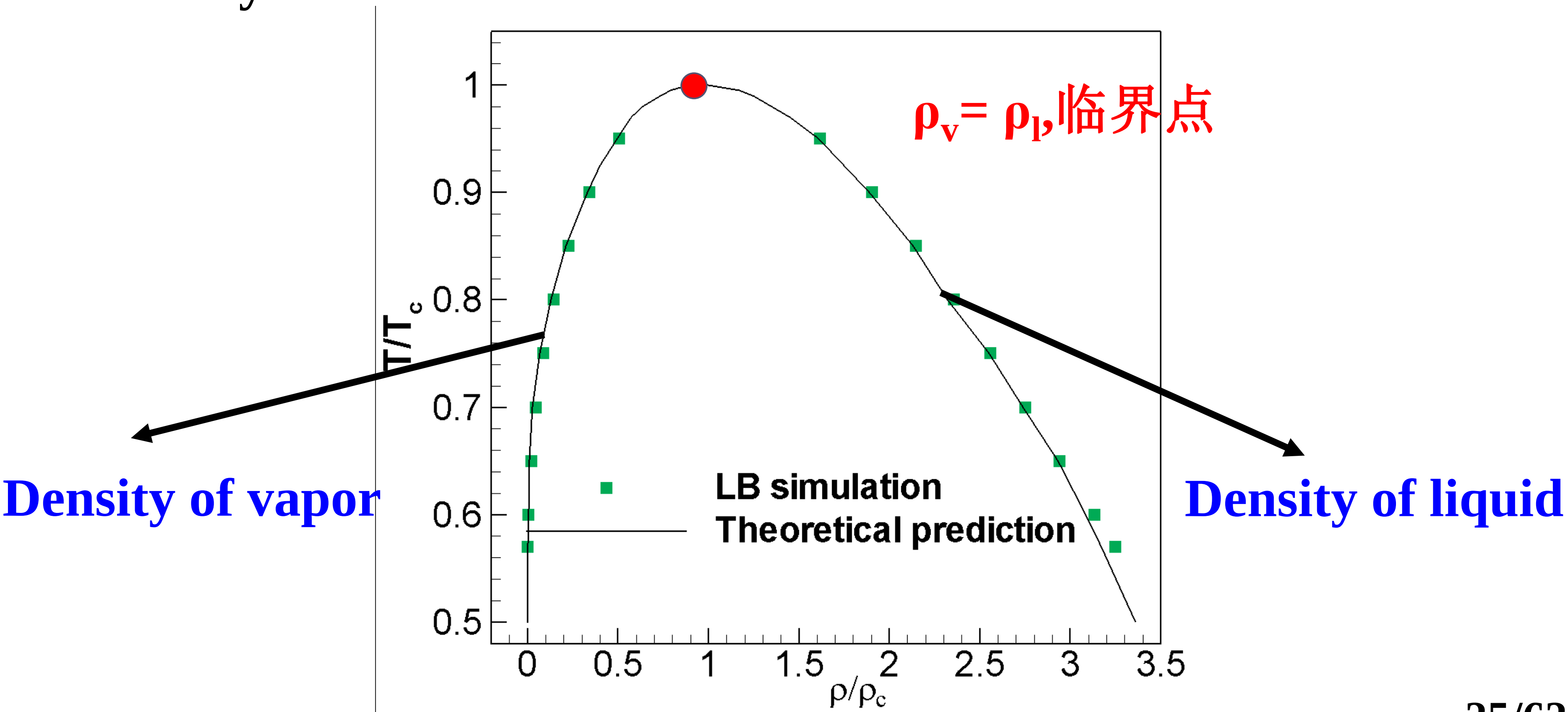
$$\int_{\rho_v}^{\rho_l} \left(p_s - \rho c_s^2 - \frac{g}{2} c_s^2 \psi^2\right) \frac{\psi'}{\psi}\,d\rho = 0$$

$$\psi \propto \exp(-1/\rho)$$

Thermodynamic inconsistency

$$\psi \propto \exp(-1/\rho)$$

Any other choices of effective mass will violate the thermodynamic consistency.



Limited density and viscosity ratio

Original SC model, density ratio ~10, viscosity ratio ~1

Coupling between some properties

Density and surface tension cannot be adjusted separately.
Dependence of density and surface tension on viscosity.

***Remark 1*: in real world, the various aspects of a multiphase system, e.g., the strength of the surface tension, the thickness of the interface, the EOS and its associated properties, are all manifestations of a single microscopic origin, i.e., the interaction potential, and therefore are "coupled together" naturally.**

***Remark 2*: however, as a practical numerical tool for simulating engineering problems, it is desirable for those macroscopic properties to be adjustable separately**

3.3.3 The improvement of pseudopotential model

Several techniques/schemes/methods have been developed to alleviate the above limitations of the original pseudo-potential model and to improve its performance.

- Incorporating realistic EOS into the model
- Increasing the isotropy order of the interaction force
- Modifying the interaction force
- Improving the force scheme to incorporate the interaction force

Incorporating realistic EOS

Equations of state in a lattice Boltzmann model

P Yuan, L Schaefer - Physics of Fluids, 2006 - aip.scitation.org

In this paper we consider the incorporation of various equations of state into the single-component multiphase lattice Boltzmann model. Several cubic equations of state, including the van der Waals, Redlich-Kwong, and Peng-Robinson, as well as a noncubic equation of state (Carnahan-Starling), are incorporated into the lattice Boltzmann model. The details of phase separation in these nonideal single-component systems are presented by comparing the numerical simulation results in terms of density ratios, spurious currents, and ...

Equations of state in a lattice Boltzmann model

Peng Yuan[a)] and Laura Schaefer
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(Received 4 August 2005; accepted 16 February 2006; published online 3 April 2006)

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[DOI: 10.1063/1.2187070]

$$p = \rho c_s^2 + \frac{g}{2} c_s^2 \psi^2$$

vdW EOS

$$p = \frac{\rho RT}{1 - b\rho} - a\rho^2$$

R-K EOS

$$p = \frac{\rho RT}{1 - b\rho} - \frac{a\rho^2}{\sqrt{T}(1 + b\rho)}$$

P-R EOS

$$p = \frac{\rho RT}{1 - b\rho} - \frac{a\alpha(T)\rho^2}{1 + 2b\rho - b^2\rho^2}$$

C-S EOS

$$p = \rho RT \frac{1 + b\rho/4 + (b\rho/4)^2 - (b\rho/4)^3}{(1 - b\rho/4)^3} - a\rho^2$$

$$p = \rho c_s^2 + \frac{g}{2} c_s^2 \psi^2$$

$$\psi = \sqrt{\frac{2}{g c_s^2} (p - \rho c_s^2)}$$

vdW EOS

$$p = \frac{\rho R T}{1 - b\rho} - a\rho^2$$

Pseudo-potential

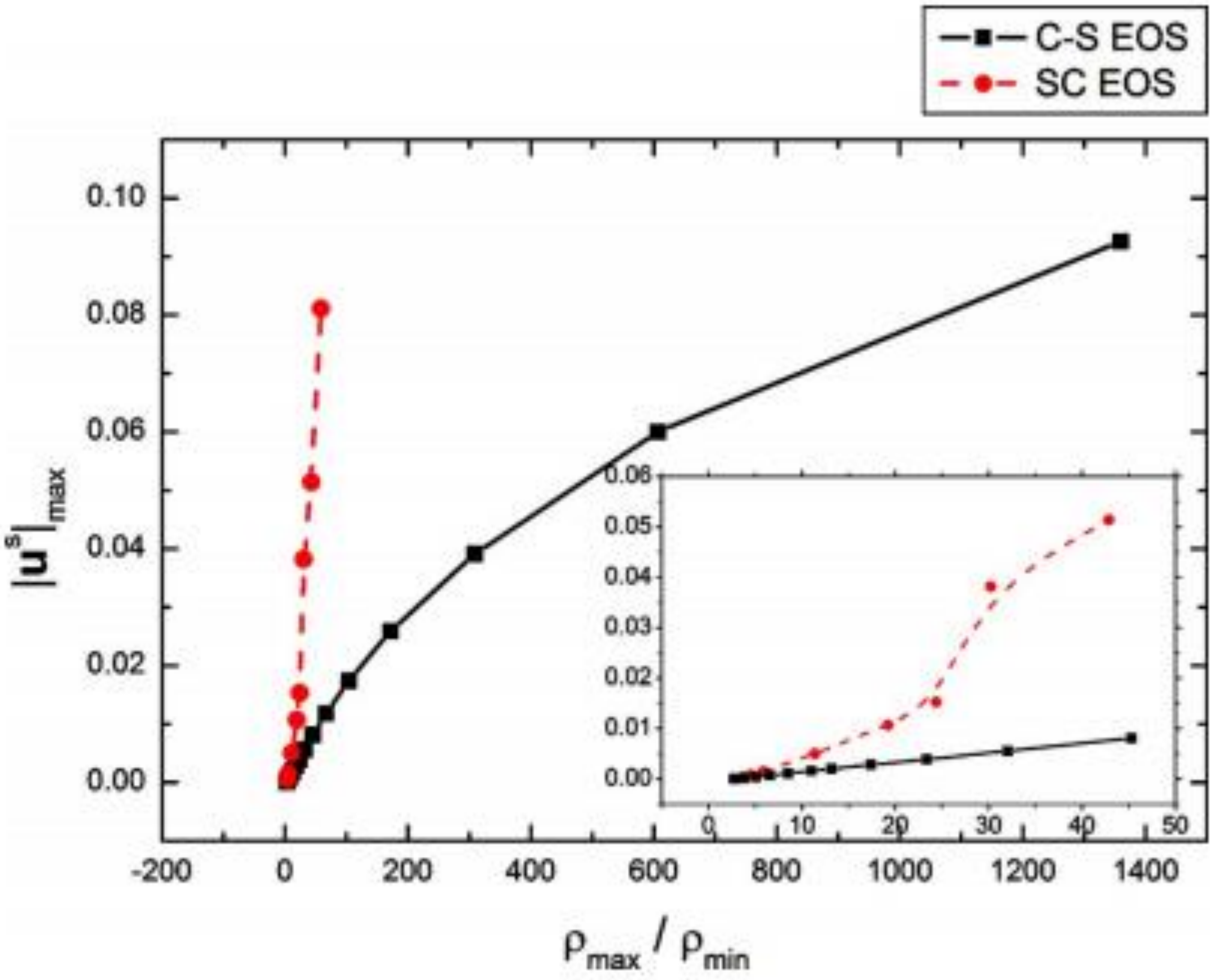
$$\psi = \sqrt{\frac{2}{g c_s^2} (\frac{\rho R T}{1 - b\rho} - a\rho^2 - \rho c_s^2)}$$

Yuan and Schaefer assessed different EOS in terms of four criteria

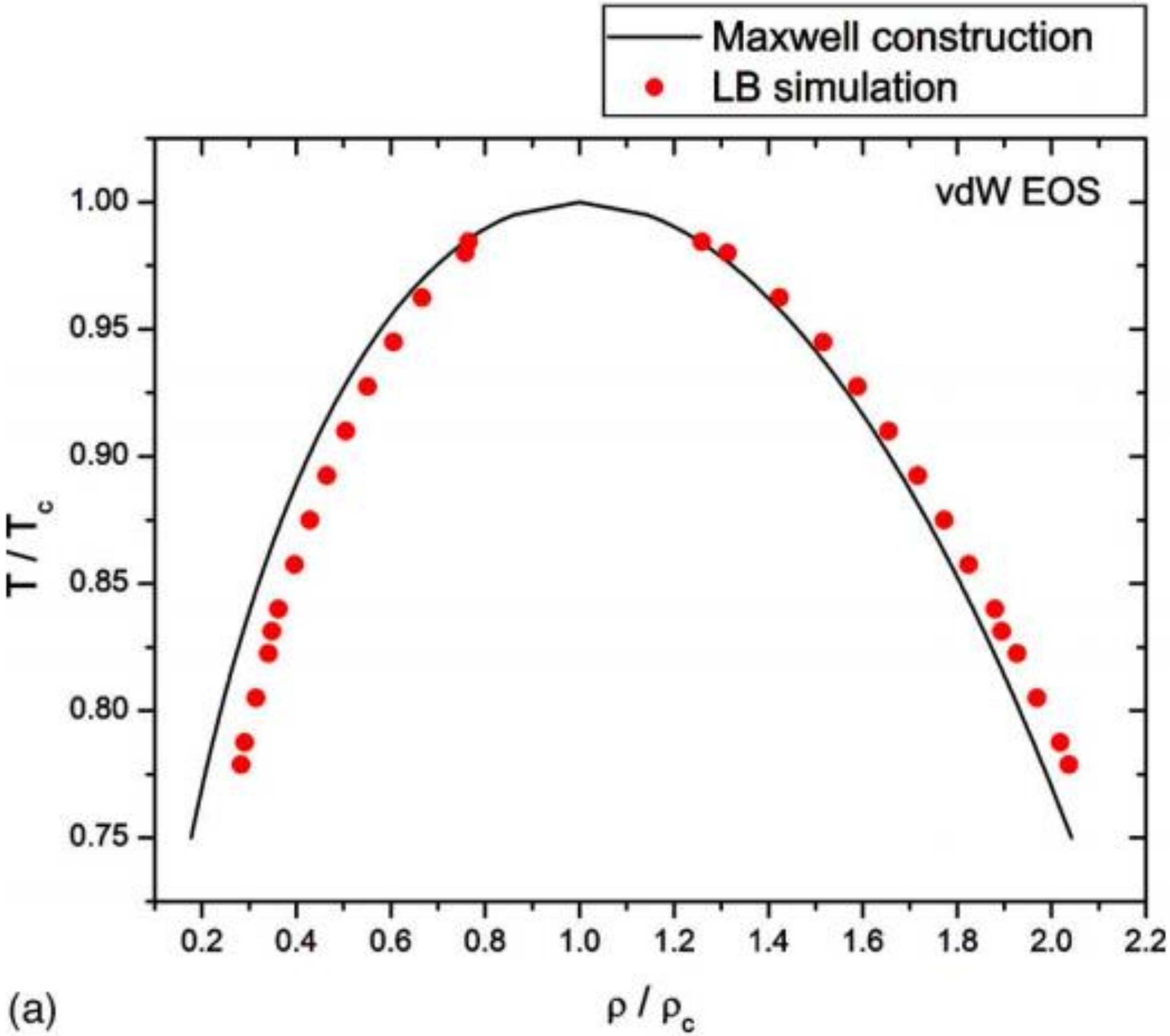
- The maximum density ratio
- The lowest spurious current
- The widest temperature range
- The thermal consistency

$$\psi = \sqrt{\frac{2}{g c_s^2}\left(p - \rho c_s^2\right)}$$

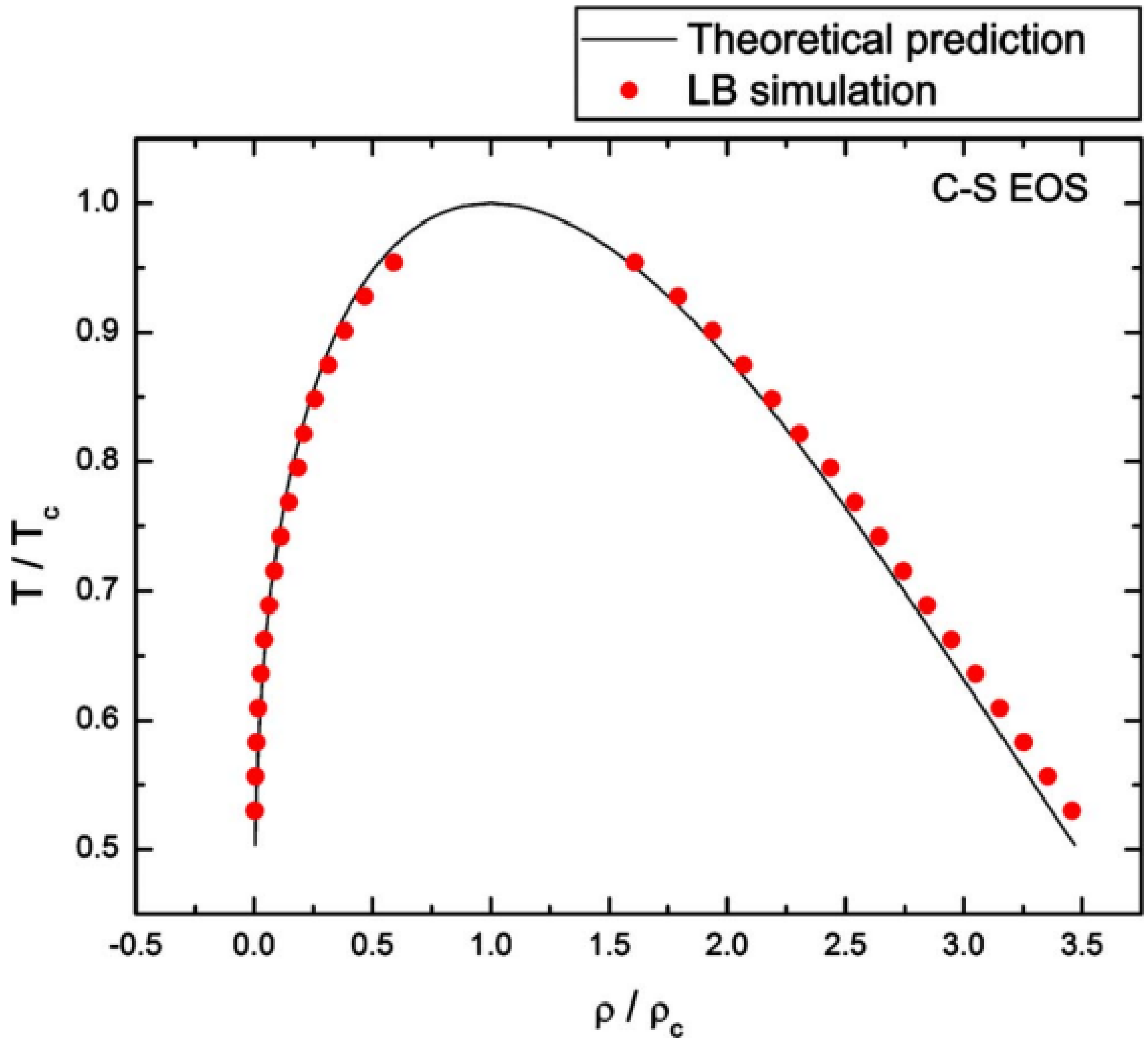
$$\psi \propto \exp(-1/\rho)$$



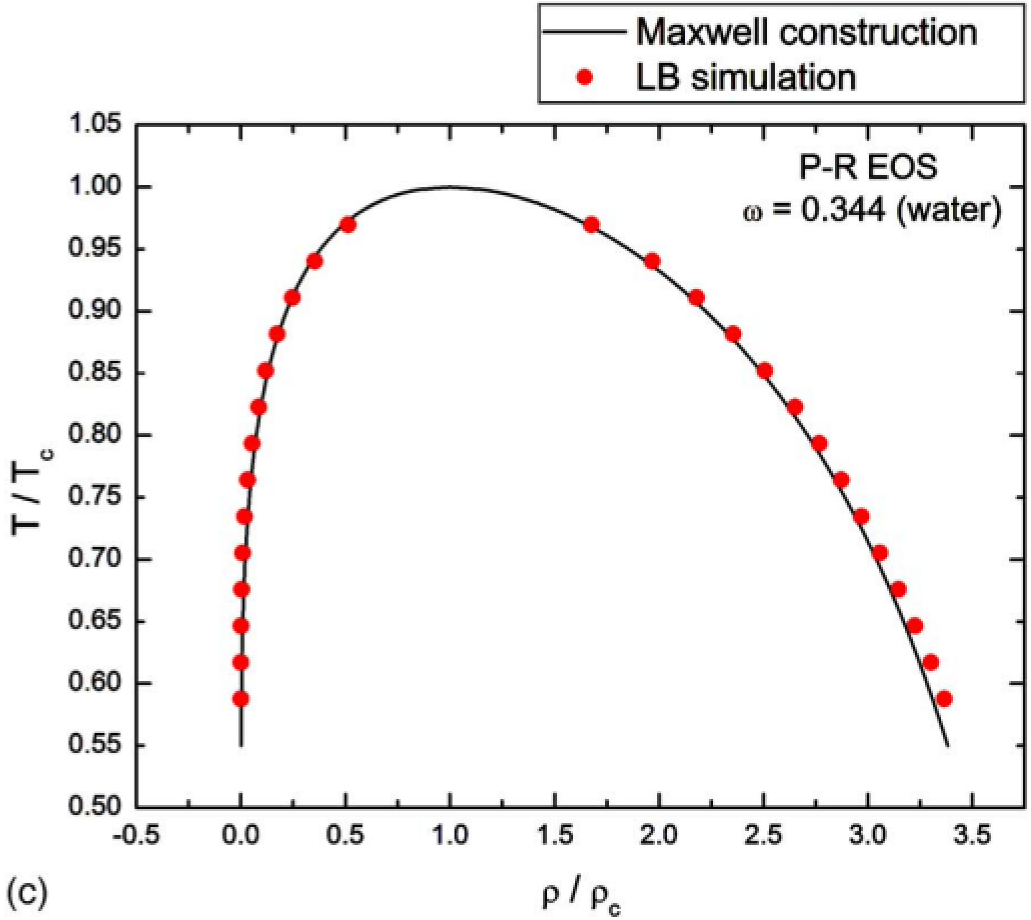
Spurious current



Density ratio, lowest temperature and thermal consistency



Density ratio, lowest temperature and thermal consistency



Density ratio, lowest temperature and thermal consistency

High order

Analysis and reduction of the spurious current in a class of multiphase lattice Boltzmann models

X Shan - Physical Review E, 2006 - APS

We show that the spurious current present near a curved interface in a class of multiphase lattice Boltzmann (LB) models is due to the insufficient isotropy of the discrete gradient operator. A method of obtaining highly isotropic gradient operators on a lattice is given. Numerical simulations show that both the magnitude and the spatial extent of the spurious current are significantly reduced as gradient operators of increasingly higher order of isotropy is adopted in multiphase LB models.

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Analysis and reduction of the spurious current in a class of multiphase lattice Boltzmann models

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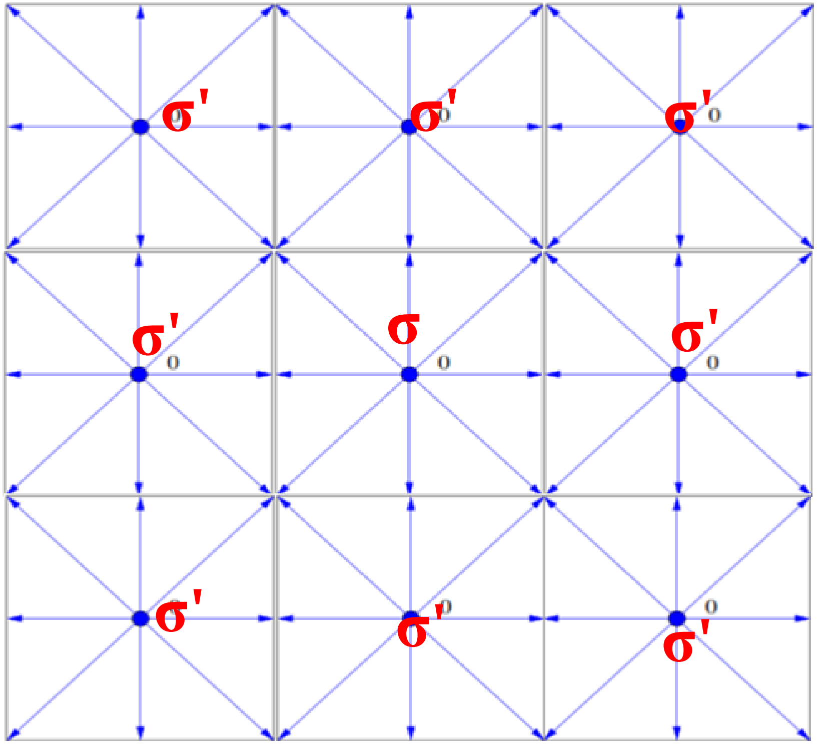
(Received 20 December 2005; published 6 April 2006)

We show that the spurious current present near a curved interface in a class of multiphase lattice Boltzmann (LB) models is due to the insufficient isotropy of the discrete gradient operator. A method of obtaining highly isotropic gradient operators on a lattice is given. Numerical simulations show that both the magnitude and the spatial extent of the spurious current are significantly reduced as gradient operators of increasingly higher order of isotropy is adopted in multiphase LB models.

$$\mathbf{F}(\mathbf{x}) = -g\psi(\mathbf{x})c_s^2 \sum_{\alpha=1}^{N} w(|\mathbf{e}_\alpha|^2)\psi(\mathbf{x}+\mathbf{e}_\alpha)\mathbf{e}_\alpha$$

$$w(|\mathbf{e}_\alpha|^2) = 1/3, \quad |\mathbf{e}_\alpha|^2 = 1$$

$$w(|\mathbf{e}_\alpha|^2) = 1/12, \quad |\mathbf{e}_\alpha|^2 = 2$$



$$F_x = -g\psi(i,j)c_s^2 \left[\frac{1}{3}(\psi(i+1,j)-\psi(i-1,j)) + \frac{1}{12}(\psi(i+1,j+1)-\psi(i-1,j+1)) + \frac{1}{12}(\psi(i+1,j-1)-\psi(i-1,j-1)) \right]$$

$$F_x = -g\psi(i,j)c_s^2 \left[\frac{1}{3}(\psi(i+1,j)-\psi(i-1,j)) + \frac{1}{12}(\psi(i+1,j+1)-\psi(i-1,j+1)) + \frac{1}{12}(\psi(i+1,j-1)-\psi(i-1,j-1)) \right]$$

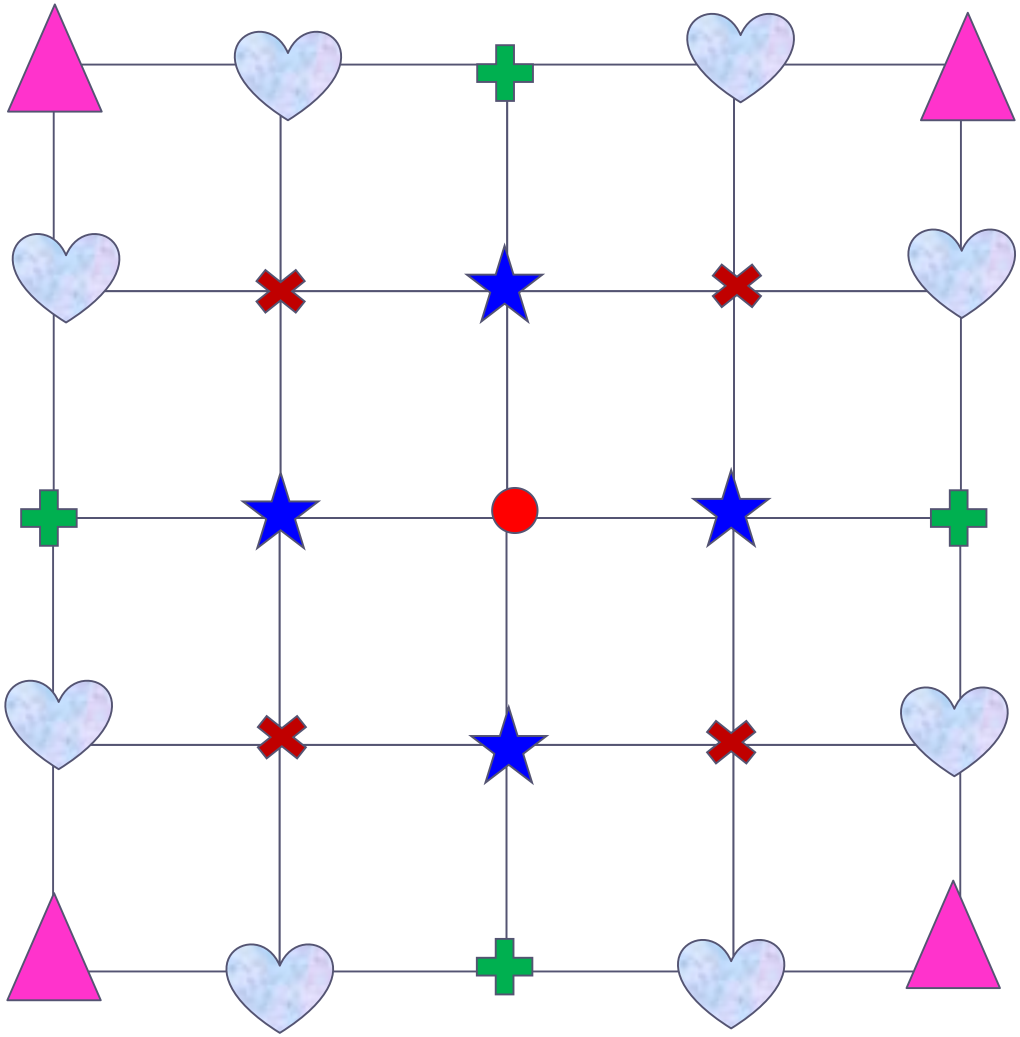
$$F_y = -g\psi(i,j)c_s^2 \left[\frac{1}{3}(\psi(i,j+1)-\psi(i,j-1)) + \frac{1}{12}(\psi(i+1,j+1)-\psi(i+1,j-1)) + \frac{1}{12}(\psi(i-1,j+1)-\psi(i-1,j-1)) \right]$$

$$\mathbf{F}(\mathbf{x}) = -g\psi(\mathbf{x})c_s^2 \sum_{\alpha=1}^{N} w(|\mathbf{e}_\alpha|^2)\psi(\mathbf{x}+\mathbf{e}_\alpha)\mathbf{e}_\alpha$$

$$\mathbf{F} = -g\psi(\mathbf{x})c_s^2 \sum_{n=0}^{\infty} \frac{1}{n!}\nabla^{(n)}\psi(\mathbf{x}) : E^{(n+1)}$$

$$E^{(n)}_{i_1 i_2 \ldots i_n} = \sum_{\alpha=1}^{N} w(|\mathbf{e}_\alpha|^2)(\mathbf{e}_\alpha)_{i_1} \ldots (\mathbf{e}_\alpha)_{i_n}$$

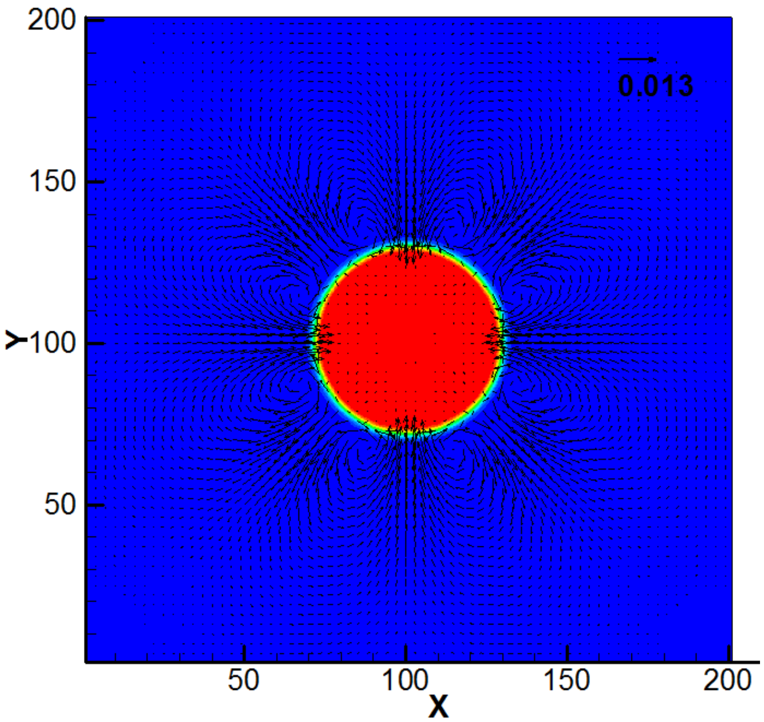
Tensor	w(1)	w(2)	w(3)	w(4)	w(5)	w(6)	w(7)	w(8)
E4	1/3	1/12	-	-	-	-	-	-
E6	4/15	1/10	-	1/120	-	-	-	-
E8	4/21	4/45	-	1/60	2/315	-	-	1/5040



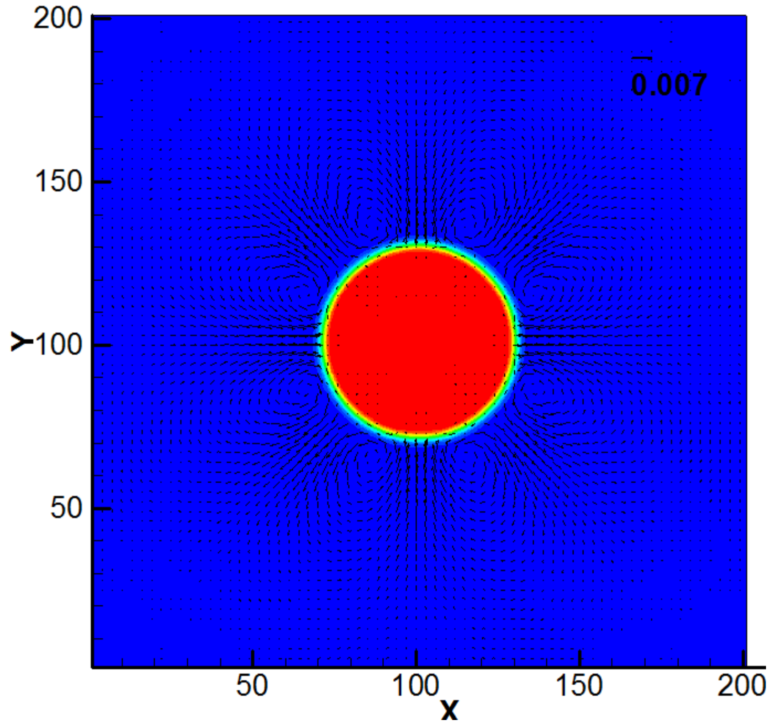
Tensor	w(1)	w(2)	w(3)	w(4)	w(5)	w(6)	w(7)	w(8)
E8	4/21	4/45	-	1/60	2/315	-	-	1/5040

$$F_x = -g\psi(i,j)c_s^2 \left[\begin{array}{l} \frac{4}{21}(\psi(i+1,j)-\psi(i-1,j)) + \frac{4}{45}(\psi(i+1,j+1)-\psi(i-1,j+1)) + \\ \frac{4}{45}(\psi(i+1,j-1)-\psi(i-1,j-1)) + \frac{1}{60}(2\psi(i+2,j)-2\psi(i-2,j)) + \\ \frac{2}{315}(2\psi(i+2,j+1)-2\psi(i-2,j+1)) + \frac{2}{315}(2\psi(i+2,j-1)-2\psi(i-2,j-1)) + \\ \frac{2}{315}(\psi(i+1,j+2)-\psi(i-1,j+2)) + \frac{2}{315}(\psi(i+1,j-2)-\psi(i-1,j-2)) + \\ \frac{1}{5040}(2\psi(i+2,j+2)-2\psi(i-2,j+2)) + \frac{1}{5040}(2\psi(i+2,j-2)-2\psi(i-2,j-2)) \end{array} \right]$$

$$F_y = -g\psi(i,j)c_s^2 \left[\begin{array}{l} \frac{4}{21}(\psi(i,j+1)-\psi(i,j-1)) + \frac{4}{45}(\psi(i+1,j+1)-\psi(i+1,j-1)) + \\ \frac{4}{45}(\psi(i-1,j+1)-\psi(i-1,j-1)) + \frac{1}{60}(2\psi(i,j+2)-2\psi(i,j-2)) + \\ \frac{2}{315}(\psi(i+2,j+1)-\psi(i+2,j-1)) + \frac{2}{315}(\psi(i-2,j+1)-\psi(i-2,j-1)) + \\ \frac{2}{315}(2\psi(i+1,j+2)-2\psi(i+1,j-2)) + \frac{2}{315}(2\psi(i-1,j+2)-2\psi(i-1,j-2)) + \\ \frac{1}{5040}(2\psi(i+2,j+2)-2\psi(i+2,j-2)) + \frac{1}{5040}(2\psi(i-2,j+2)-2\psi(i-2,j-2)) \end{array} \right]$$


200
150
100
50
Y
50
100
150
200
X
0.013

E4


200
150
100
50
Y
50
100
150
200
X
0.007

E8

Force scheme

$$f_{\sigma,\alpha}(\mathbf{x}+c\mathbf{e}_\alpha\Delta t, t+\Delta t) - f_{\sigma,\alpha}(\mathbf{x},t) = -\frac{1}{\tau_{\sigma,\upsilon}}\left(f_{\sigma,\alpha}(\mathbf{x},t) - f_{\sigma,\alpha}^{eq}(\mathbf{x},t)\right) + F_{\sigma,\alpha}(\mathbf{x},t)$$

$$f_{\sigma,\alpha}^{\text{eq}} = \omega_\alpha\rho_\sigma\left[1+\frac{3}{c^2}\left(\mathbf{e}_\alpha\cdot\mathbf{u}^{\mathbf{eq}}\right)+\frac{9}{2c^4}\left(\mathbf{e}_\alpha\cdot\mathbf{u}^{\mathbf{eq}}\right)^2-\frac{3}{2c^2}(\mathbf{u}^{\mathbf{eq}})^2\right]$$

Velocity shifting scheme

$$\mathbf{u}^{\text{eq}} = \mathbf{u} + \frac{\tau}{\rho}\mathbf{F}\Delta t$$

$$\mathbf{u}_{\text{p}} = \mathbf{u} + \frac{1}{2\rho}\mathbf{F}\Delta t$$

Exact difference method

$$F_\alpha = f_\alpha^{\text{eq}}(\rho, \mathbf{u}+\mathbf{F}\Delta t/\rho) - f_\alpha^{\text{eq}}(\rho,\mathbf{u})$$

$$\mathbf{u}_{\text{p}} = \mathbf{u} + \frac{1}{2\rho}\mathbf{F}\Delta t$$

Guo's force scheme

$$F_\alpha = (1-\frac{1}{2\tau})\omega_\alpha\left(\frac{\mathbf{e}_\alpha-\mathbf{u}^{\text{eq}}}{c_s^2}+\frac{\mathbf{e}_\alpha\mathbf{u}^{\text{eq}}}{c_s^4}\right)\cdot\mathbf{F}\Delta t$$

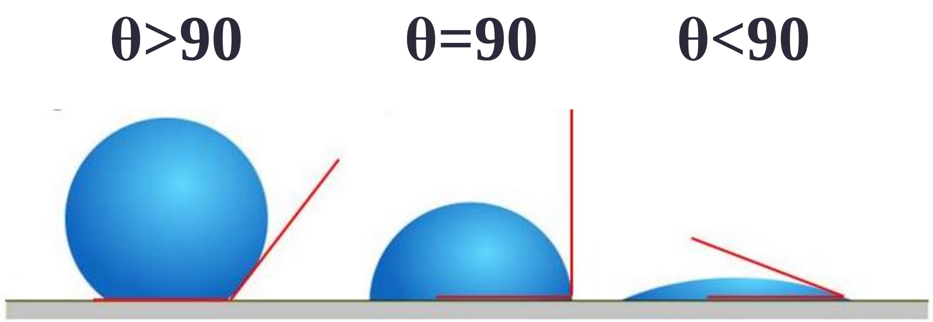
$$\mathbf{u}_{\text{p}} = \mathbf{u}^{\text{eq}} = \mathbf{u} + \frac{1}{2\rho}\mathbf{F}\Delta t$$

1. For the dependence of the surface tension and density on the kinematic viscosity, i.e., the relaxation time, **both the EDM and Guo's force scheme lead to independence**, while in the velocity shift scheme the surface force and density change with the kinetic viscosity;

2. For the stable temperature range, Guo's force scheme leads to a relatively narrow temperature range. For example, at τ=1 for C-S EOS, the minimum Tmin achieved is only Tmin =0.777Tc. The velocity shifting scheme and the EDM scheme are demonstrated to perform almost the same.

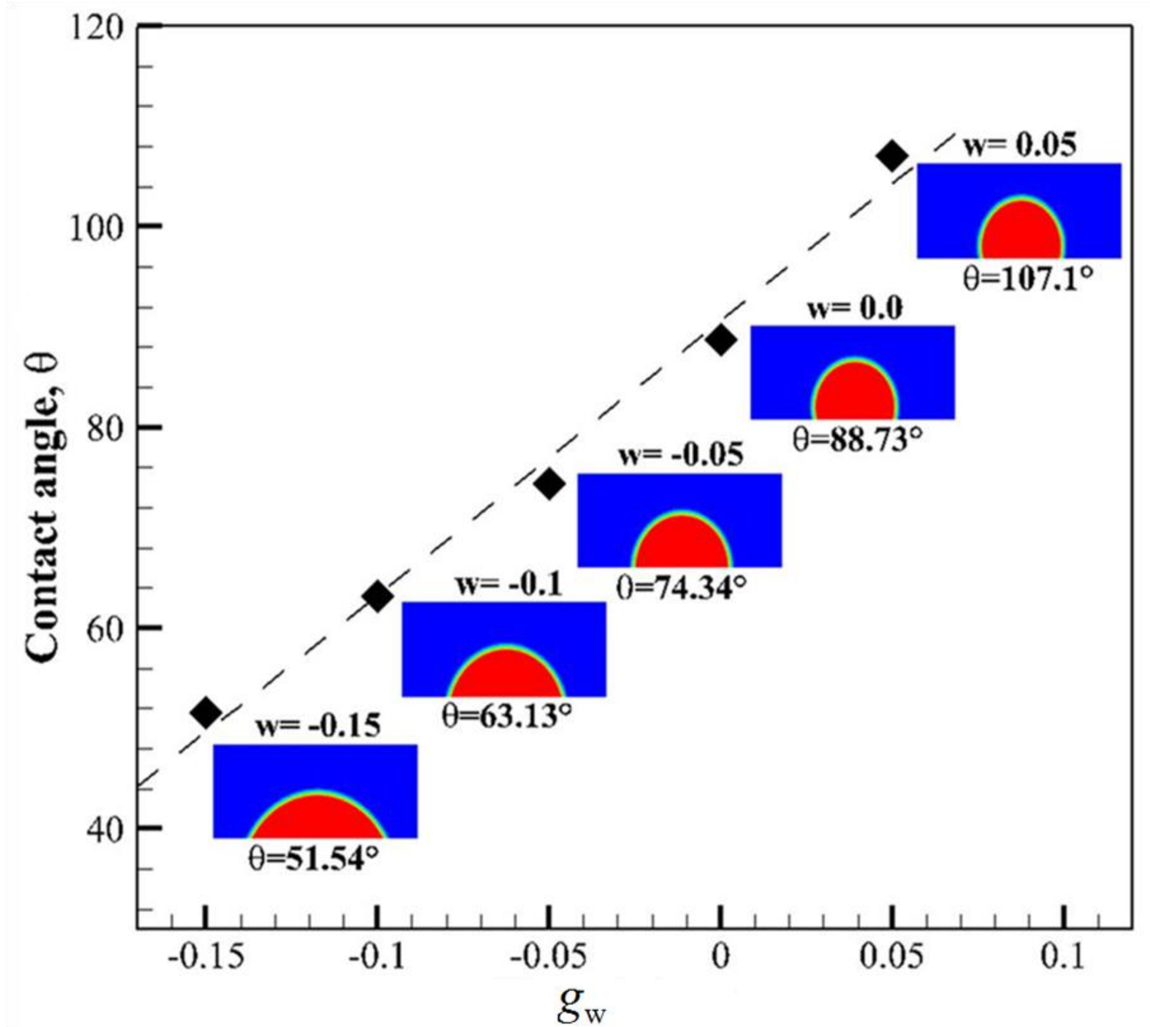
3. For the thermodynamic coexistence, Guo's model gives the best agreement. Discrepancy of EDM increases as temperature decreases.

3.3.4 Fluid-solid interaction



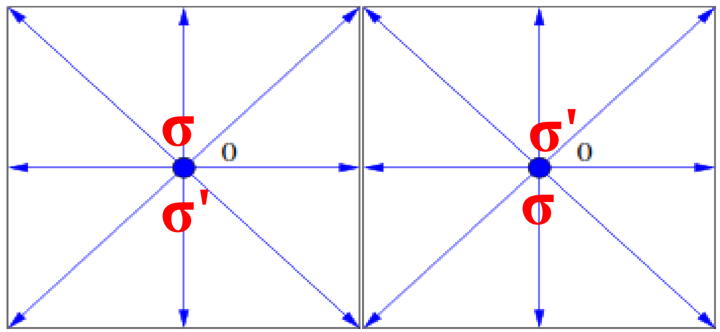
$$\mathbf{F}_{\mathrm{ads}}(\mathbf{x}) = -g_{\mathrm{w}}\psi(\mathbf{x})\sum_{\alpha=1}^{N} w(|\mathbf{e}_{\alpha}|^{2})\psi(\rho_{\mathrm{w}})s(\mathbf{x}+\mathbf{e}_{\alpha})\mathbf{e}_{\alpha}$$

s **is an indicator function that equals 1 for solid nodes and 0 for fluid nodes**


Contact angle, θ
120
100
80
60
40
-0.15
-0.1
-0.05
0
0.05
0.1
g_w
w= -0.15
θ=51.54°
w= -0.1
θ=63.13°
w= -0.05
θ=74.34°
w= 0.0
θ=88.73°
w= 0.05
θ=107.1°

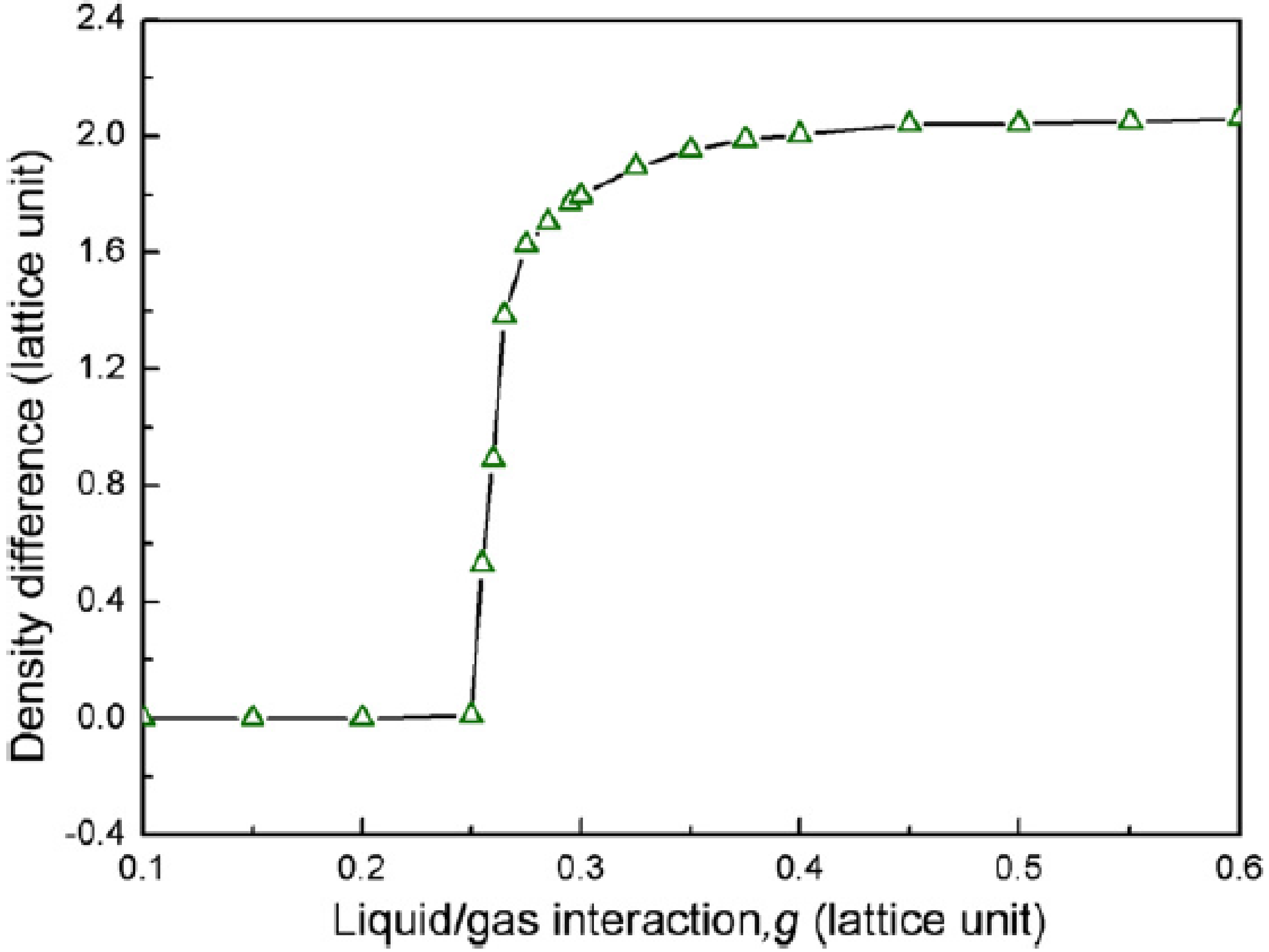
3.3.5 Multicomponent multiphase model

$$\mathbf{F}_{\sigma\bar{\sigma}}(\mathbf{x}) = -g_{\sigma\bar{\sigma}}\psi_{\sigma}(\mathbf{x})c_s^2\sum_{\alpha=1}^{N} w(|\mathbf{e}_{\alpha}|^2)\psi_{\bar{\sigma}}(\mathbf{x}+\mathbf{e}_{\alpha})\mathbf{e}_{\alpha}$$

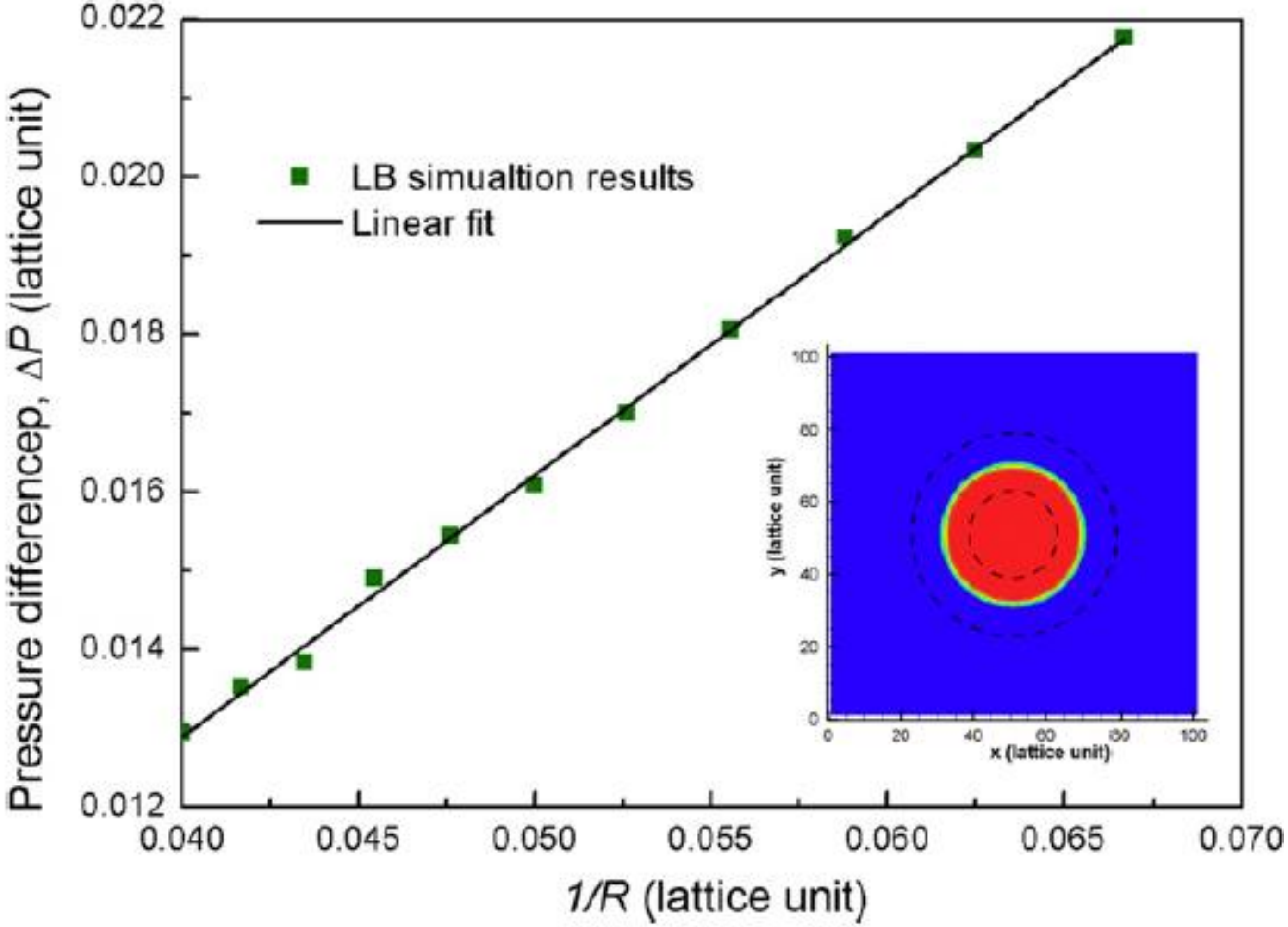


$$\mathbf{F}_{\sigma}(\mathbf{x}) = -g_{\sigma\sigma}\psi_{\sigma}(\mathbf{x})c_s^2\sum_{\alpha=1}^{N} w(|\mathbf{e}_{\alpha}|^2)\psi_{\sigma}(\mathbf{x}+\mathbf{e}_{\alpha})\mathbf{e}_{\alpha} - g_{\sigma\bar{\sigma}}\psi_{\sigma}(\mathbf{x})c_s^2\sum_{\alpha=1}^{N} w(|\mathbf{e}_{\alpha}|^2)\psi_{\bar{\sigma}}(\mathbf{x}+\mathbf{e}_{\alpha})\mathbf{e}_{\alpha}$$

$$\mathbf{F}_{\bar{\sigma}}(\mathbf{x}) = -g_{\bar{\sigma}\bar{\sigma}}\psi_{\bar{\sigma}}(\mathbf{x})c_s^2\sum_{\alpha=1}^{N} w(|\mathbf{e}_{\alpha}|^2)\psi_{\bar{\sigma}}(\mathbf{x}+\mathbf{e}_{\alpha})\mathbf{e}_{\alpha} - g_{\bar{\sigma}\sigma}\psi_{\bar{\sigma}}(\mathbf{x})c_s^2\sum_{\alpha=1}^{N} w(|\mathbf{e}_{\alpha}|^2)\psi_{\sigma}(\mathbf{x}+\mathbf{e}_{\alpha})\mathbf{e}_{\alpha}$$

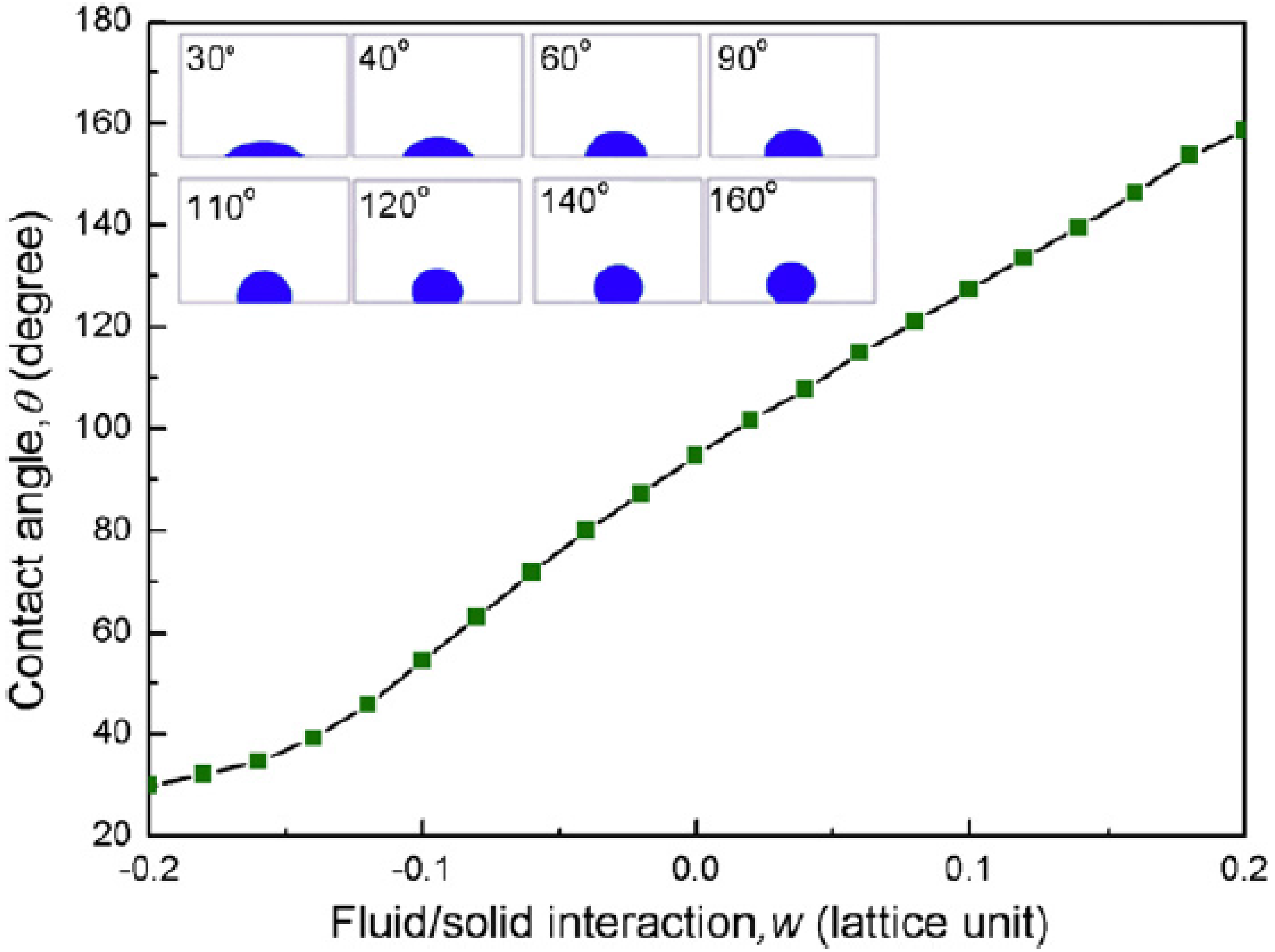


Water/air system



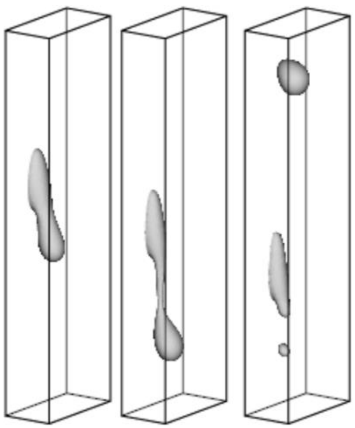
0.022
0.020
0.018
0.016
0.014
0.012
0.040
0.045
0.050
0.055
0.060
0.065
0.070
Pressure differencep, ΔP (lattice unit)
1/R (lattice unit)
LB simualtion results
Linear fit
y (lattice unit)
x (lattice unit)

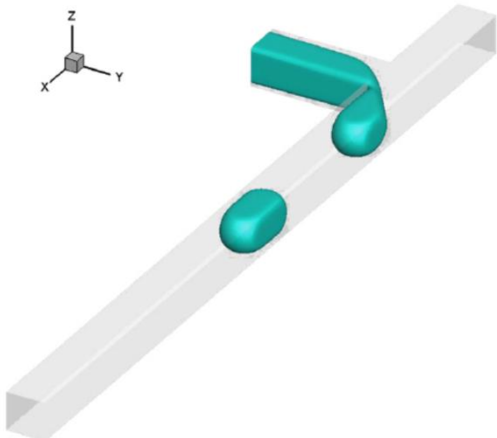
Laplace law

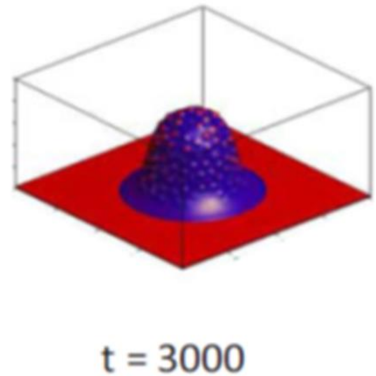


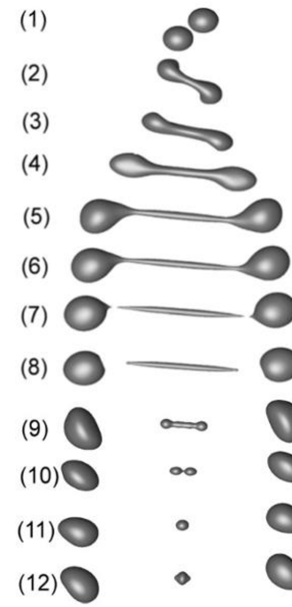
Contact angle

3.4 Application

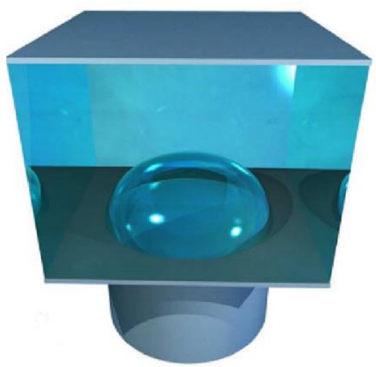


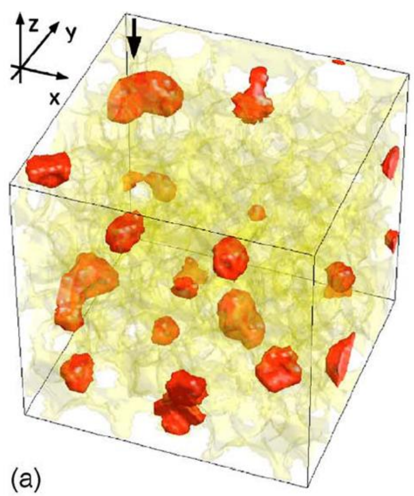


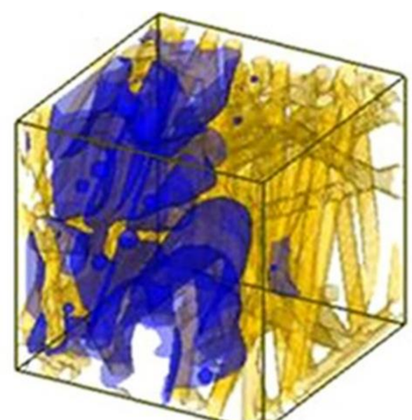




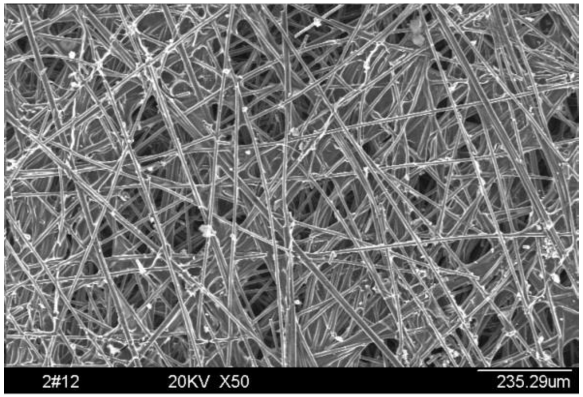
LB pseudopotential model

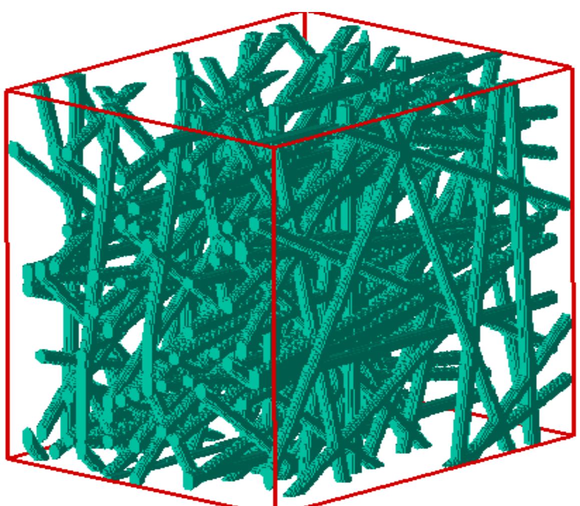


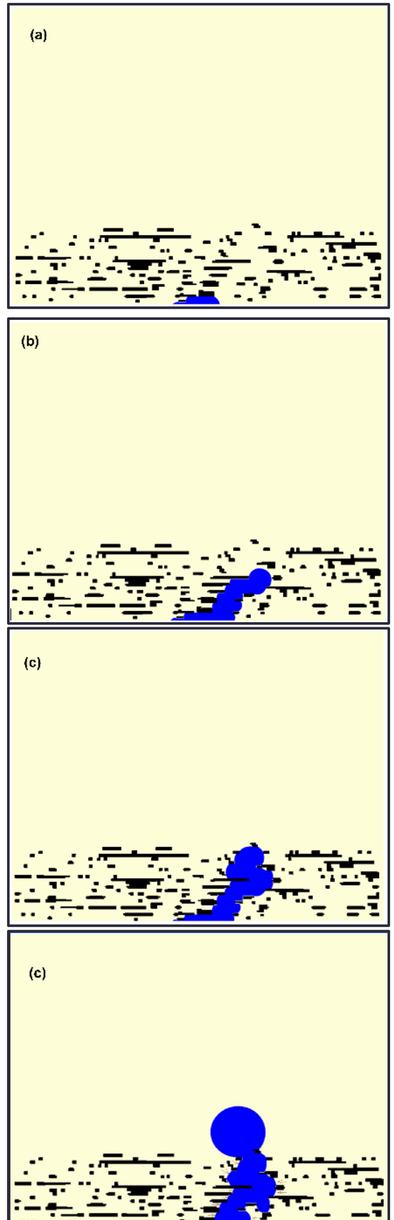


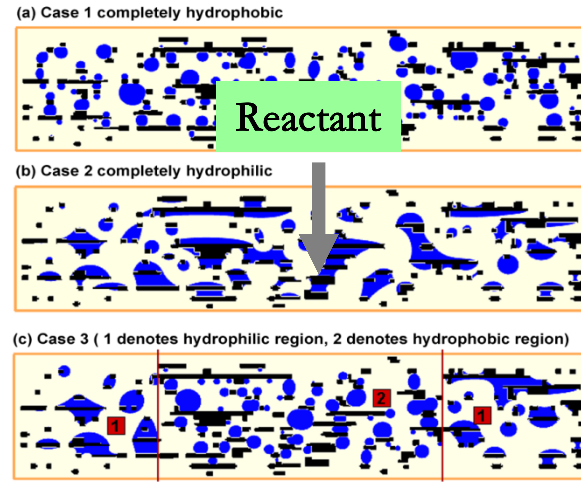


Two-phase in PEM fuel cell

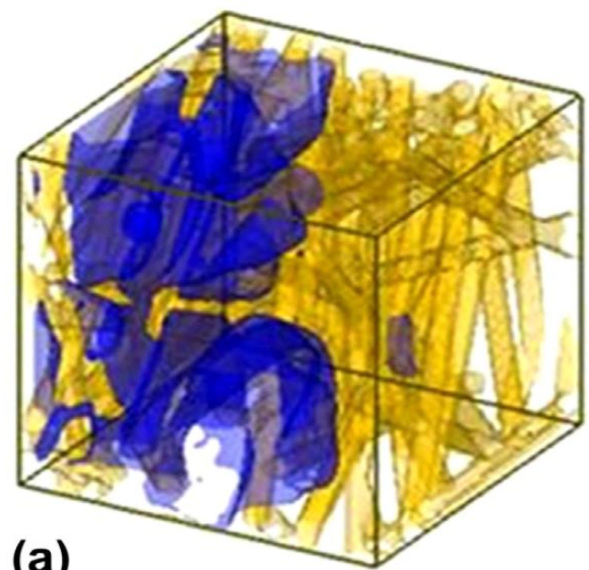






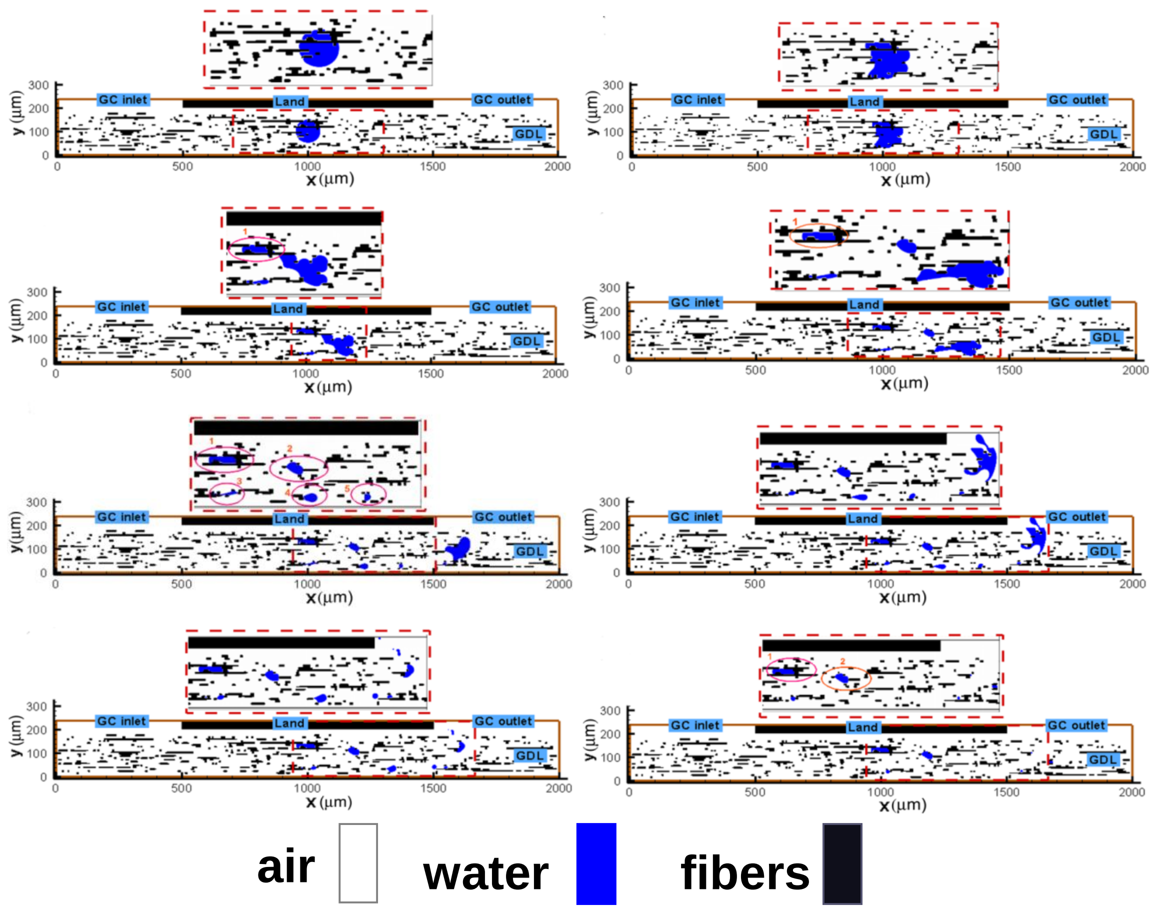


Mixed wettability

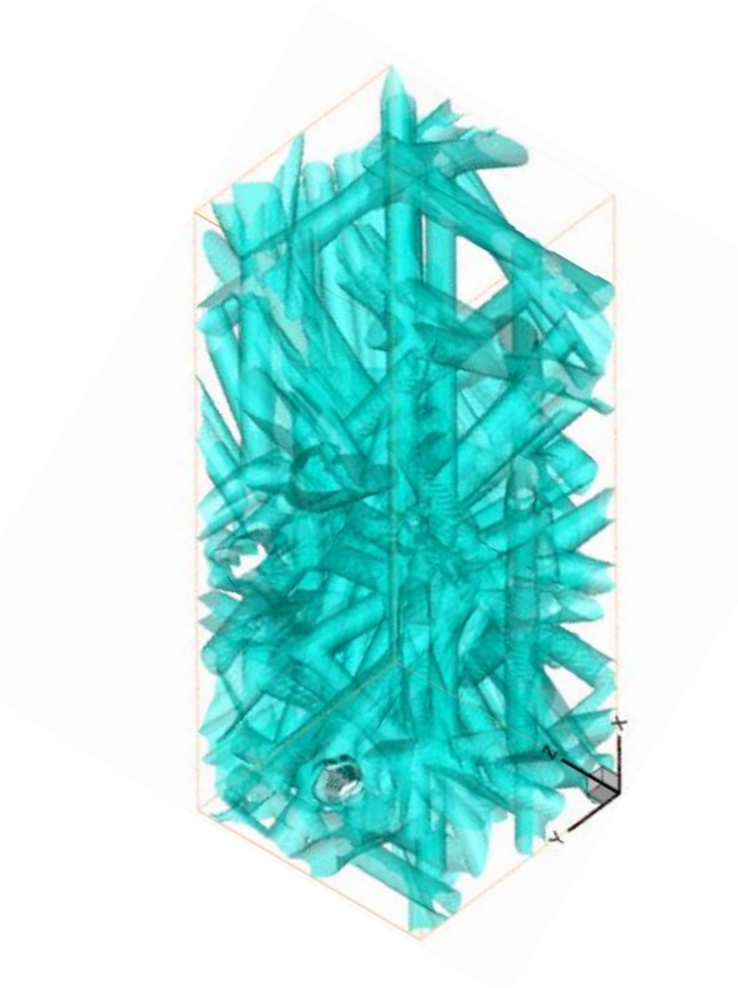


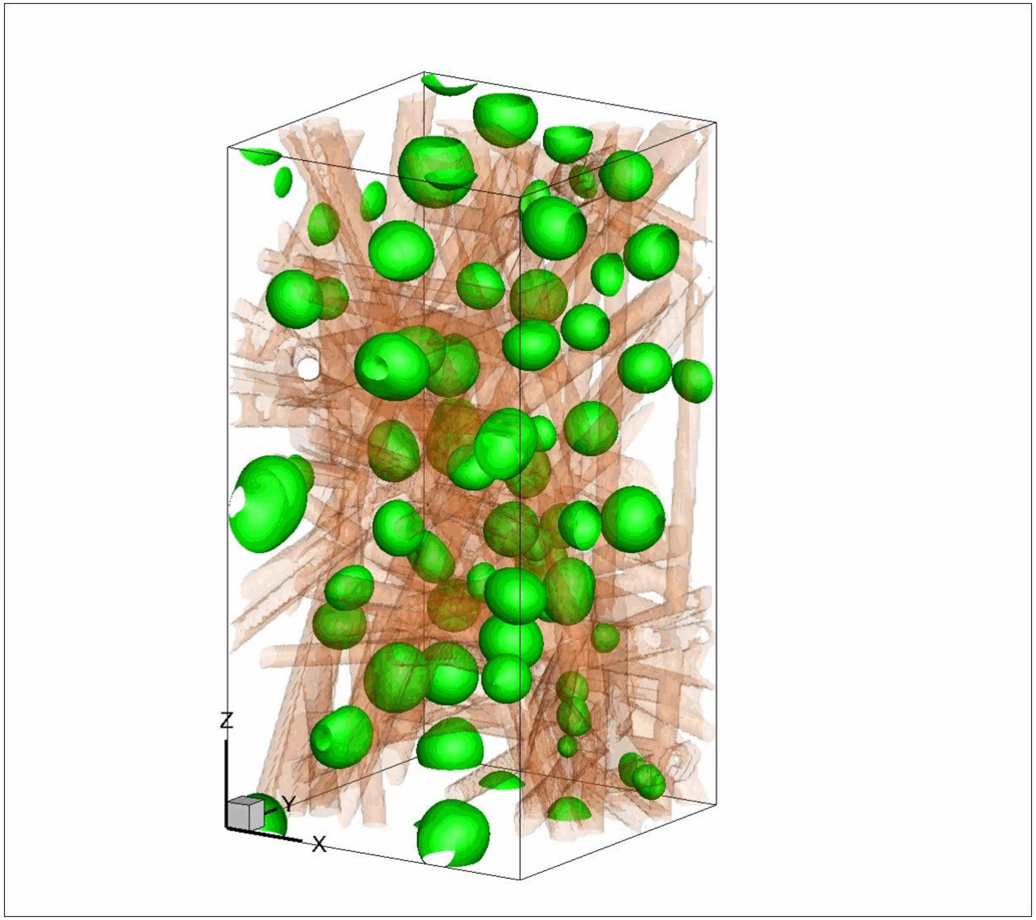
(a)

Droplet behaviors under air flow



L. Chen*, H.B. Luan, Y.-L. He, W.-Q. Tao, Pore-scale flow and mass transport in gas diffusion layer of proton exchange membrane fuel cell with interdigitated flow fields, 2012, 51, 132-144, International journal of thermal science

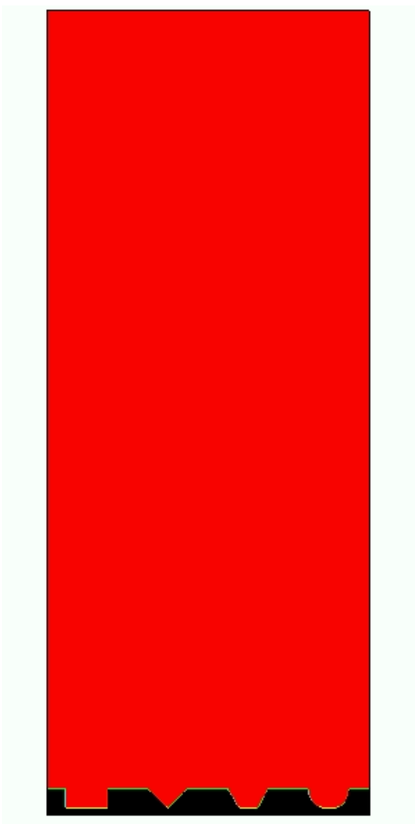




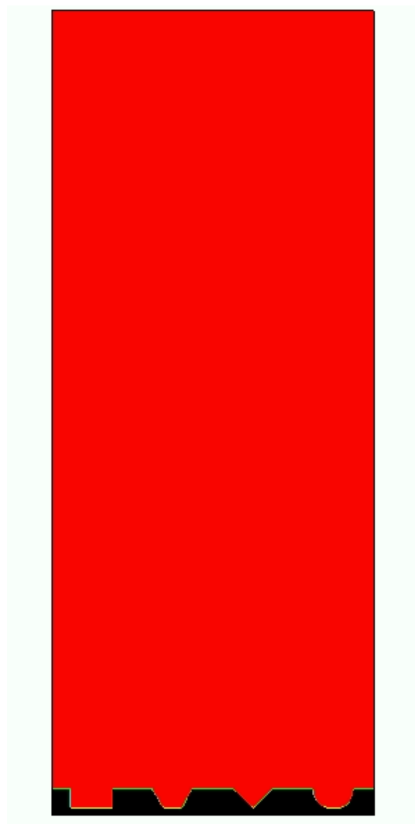
L Chen, YL He, WQ Tao, P Zelenay, R Mukundan, Q Kang, Pore-scale study of multiphase reactive transport in fibrous electrodes of vanadium redox flow batteries, , Electrochimica Acta 248, 425-439;

Boiling

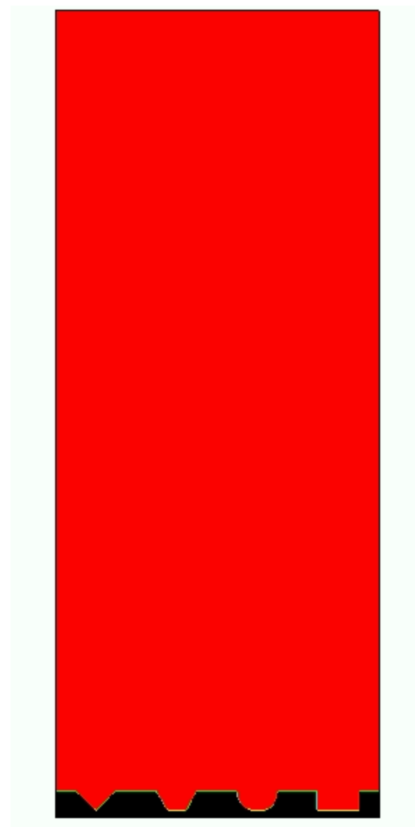
➢ Density distribution



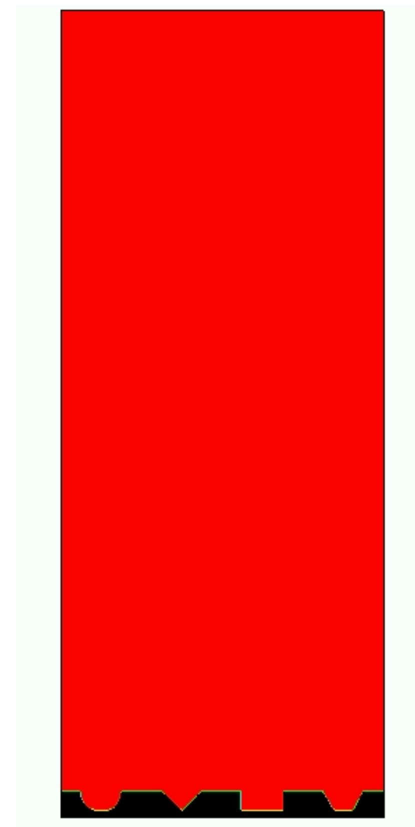
Case 1



Case 2



Case 3



Case 4

YT Mu, L Chen, YL He, QJ Kang, WQ Tao, Nucleate boiling performance evaluation of cavities at mesoscale level, International Journal of Heat and Mass Transfer 106, 708-719

International Journal of Heat and Mass Transfer 76 (2014) 210–236

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Review

A critical review of the pseudopotential multiphase lattice Boltzmann model: Methods and applications

CrossMark

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ABSTRACT

This article presents a critical review of the theory and applications of a multiphase model in the community of the lattice Boltzmann method (LBM), the pseudopotential model proposed by Shan and Chen (1993) [4], which has been successfully applied to a wide range of multiphase flow problems during the past two decades. The first part of the review begins with a description of the LBM and the original pseudopotential model. The distinct features and the limitations of the original model are described in detail. Then various enhancements necessary to improve the pseudopotential model in terms of decreasing the spurious currents, obtaining high density/viscosity ratio, reducing thermodynamic inconsistency, unraveling the coupling between surface tension and equations of state (EOS), and unraveling the coupling between viscosity and surface tension, are reviewed. Then the fluid–solid interactions are presented and schemes to obtain different contact angles are discussed. The final section of this part focuses on the multi-component multiphase pseudopotential model. The second part of this review describes fruitful applications of this model to various multiphase flows. Coupling of this model with other models for more complicated multiple physicochemical processes are also introduced in this part.


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中国科学技术信息研究所
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