Lattice Boltzmann for flow and transport phenomena

2. The lattice Boltzmann for porous flow and transport

Li Chen

XJTU, 2021/03/30

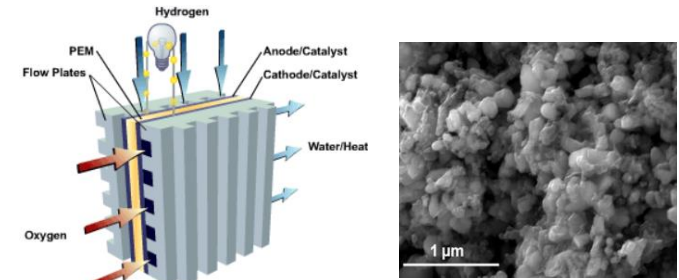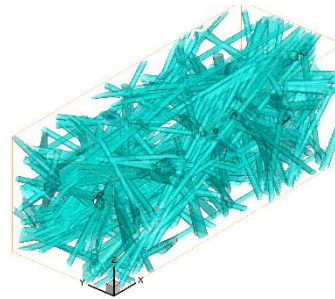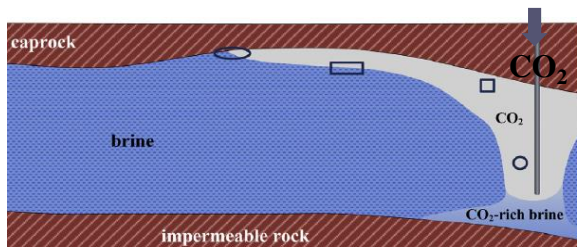**Mail:** lichennht08@mail.xjtu.edu.cn

Webpage: http://gr.xjtu.edu.cn/web/lichennht08
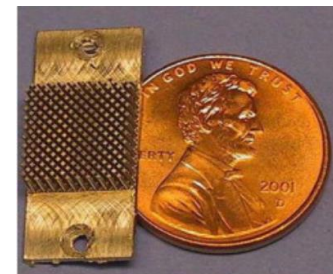
ResearchID: P-4886-2014

Content

2.1 Examples of porous media

o **Natural porous systems**: enhanced hydrocarbon and geothermal energy recovery, CO_2 geological sequestration,

o **Artificial porous systems**: fuel cell, reactor, catalysts, building material…

多孔介质内
传热传质

Stone

Carbon fiber

Metal foam
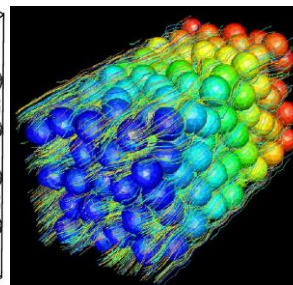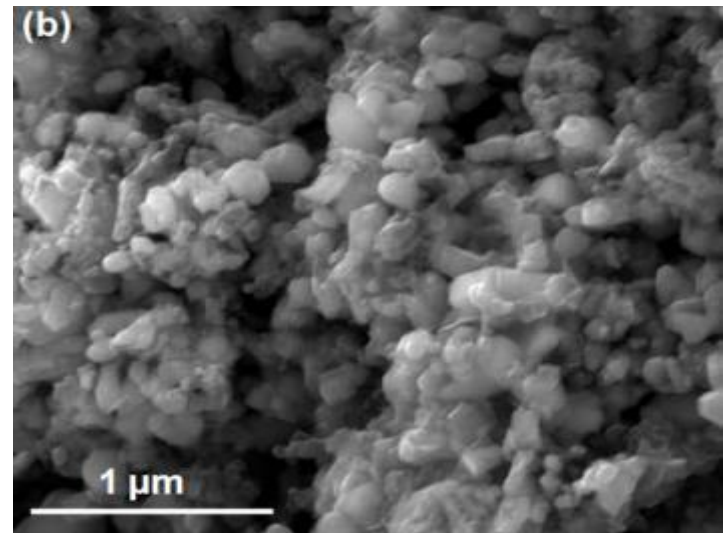
Catalyst

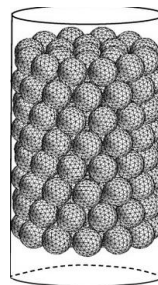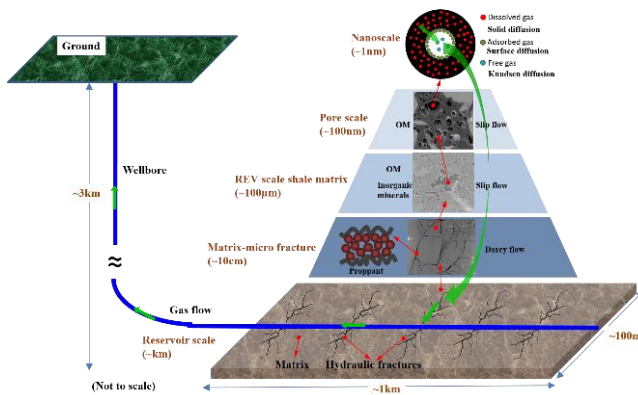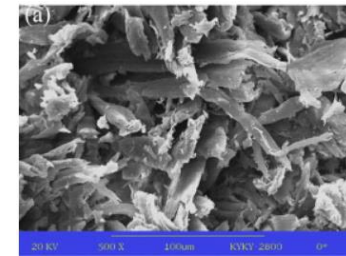# Content

- **2.1 Examples of porous media**

- **2.2 Structural characteristics of porous media**

- **2.3 Continuum-scale governing equation for porous media**

- **2.4 Pore-scale simulation: reconstruction of porous media**

- **2.5 Pore-scale simulation: LB for fluid flow**

- **2.6 Pore-scale simulation: LB for heat transfer**

2.2 Structural characteristics of porous media

o **A material that contains plenty of pores (or voids) between solid skeleton through which fluid can transport.**

o **Two necessary elements: skeleton and pores; Skeleton:**

maintain the shape; Pores: provide pathway for fluid flow through
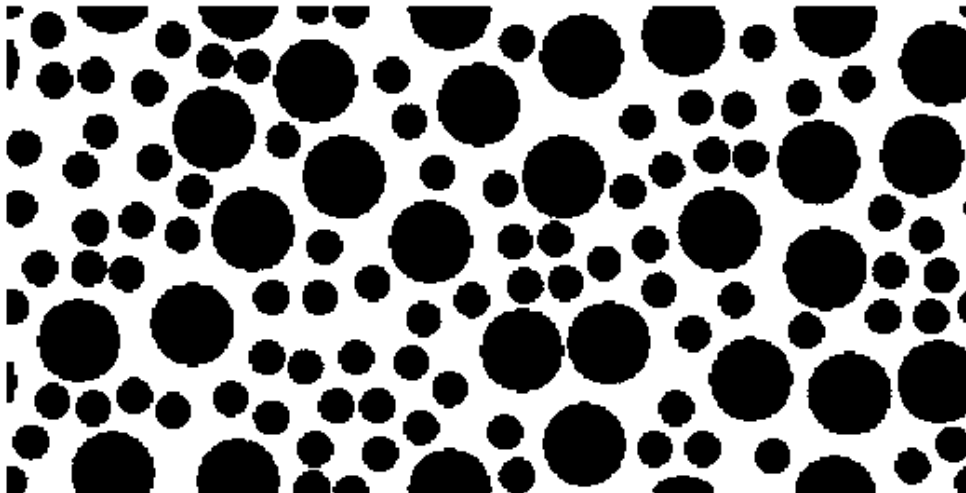
Black: solid
White: pores

2.2.1 Porosity

o **The volume ratio between pore volume and total volume**

$$\varepsilon = \frac{V_{\text{pore}}}{V_{\text{total}}}$$

o **Porosity maybe vary from near zero to almost unity.** Shale has low porosity, around 5%. Fiber-based porous media can have a porosity as high as 90%.
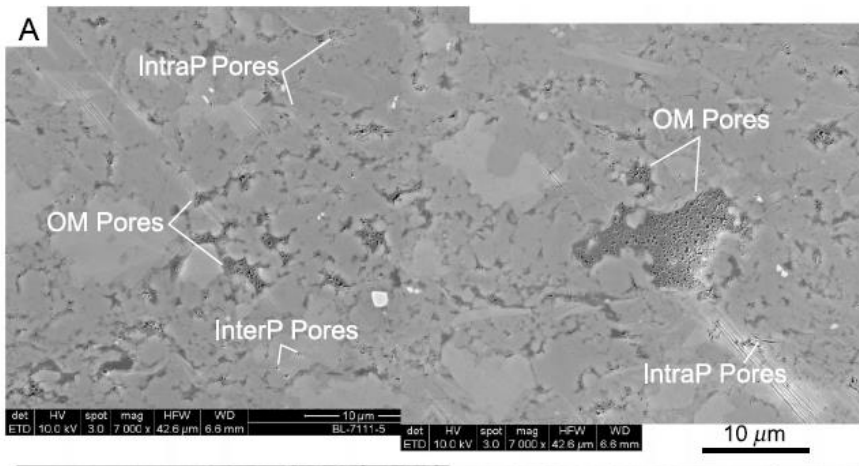
Shale: <10%
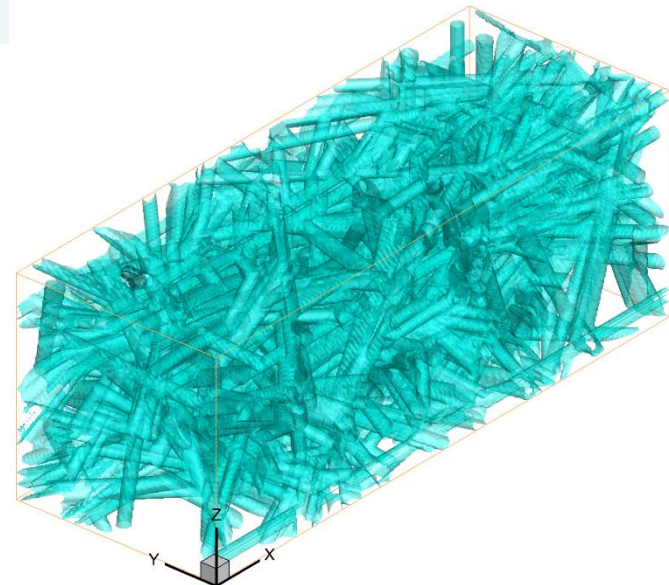
GDL: >70%

2.2.2 Pore size

Pore size terminology of IUPAC

International Union of Pure and Applied Chemistry

Rouquerol et al. (1994) *Membrane*

Micropores, <2nm
Mesopores, 2~50nm
Macropores, >50nm
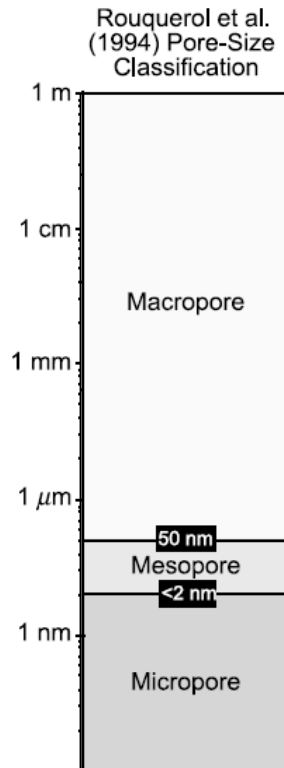
Choquette and Pray (1970)*Carbonate rock*

Micropores, <62.5 μm
Mesopores, 62.5 μm~4mm
Macropores, 4mm~256mm
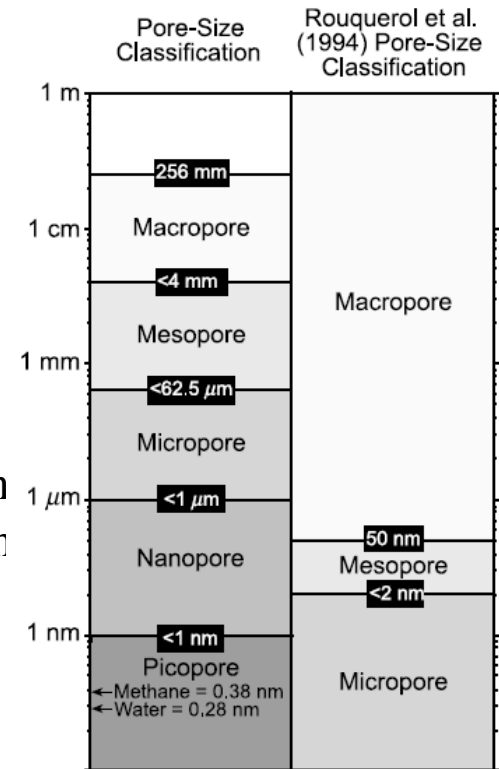
Rouck et al. 2012, further added picopore and nanopore for study of shale.

Pore size distribution
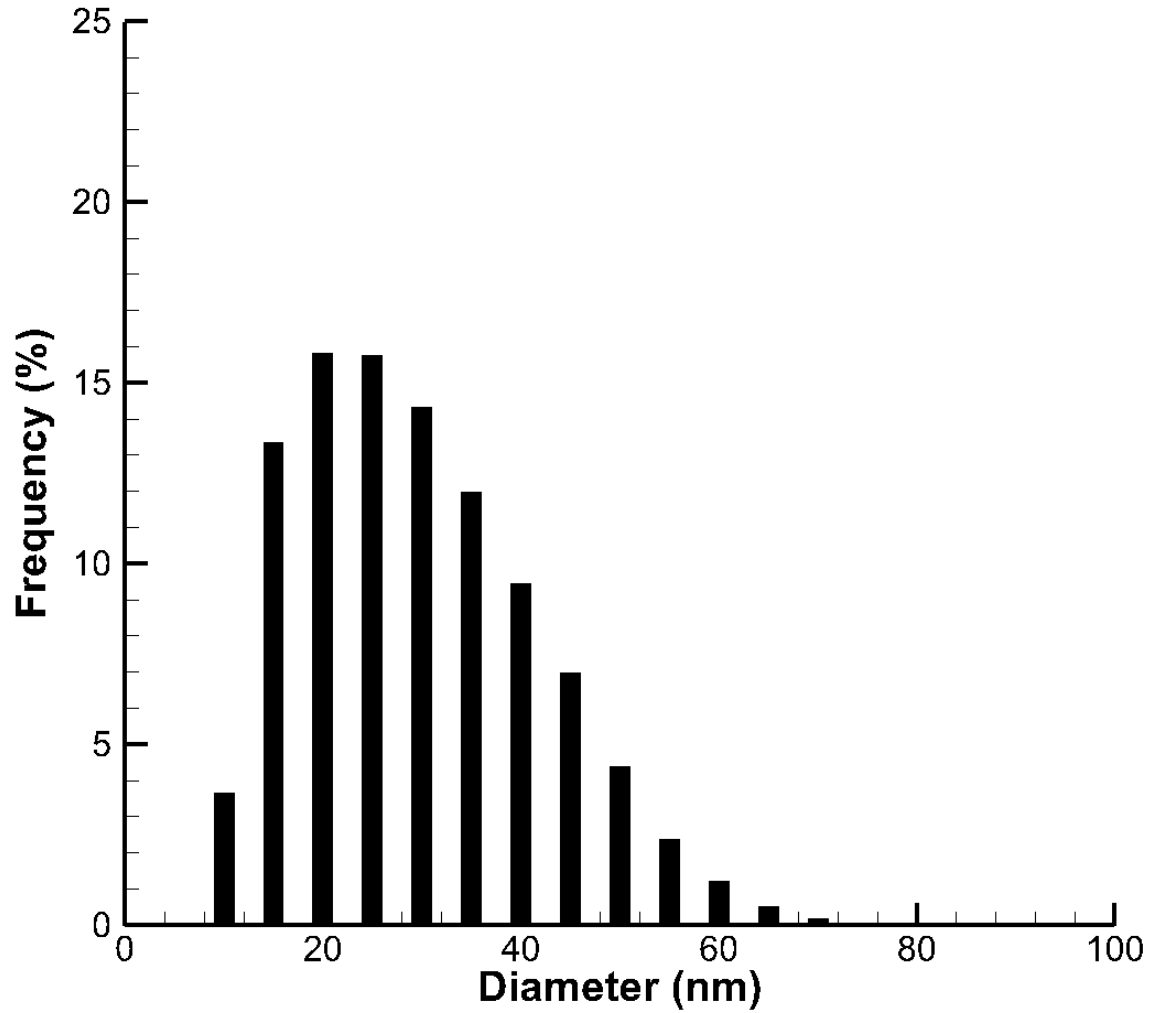
2.2.3 Specific surface area

Defined as the ratio between total surface area to the total volume.

An important parameter for porous media as one of the important type of porous media is catalyst, which requires high specific surface area for reaction.
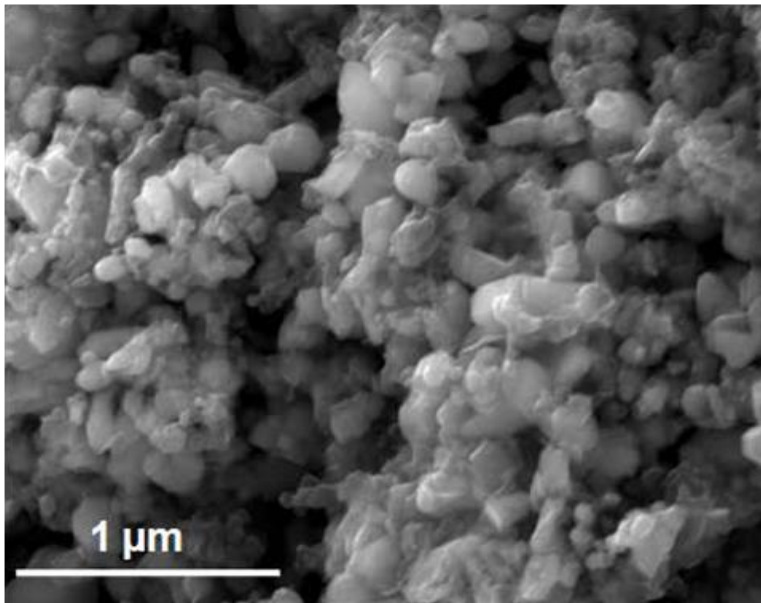
Catalyst of Fuel cell
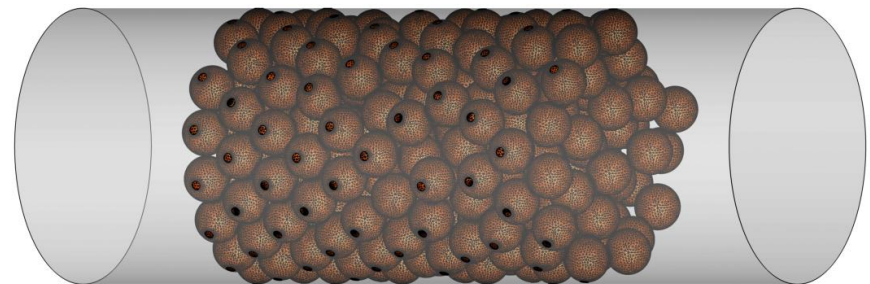
Packed-bed reactor

2.2.4 Tortuosity

Tortuosity: defined as the actual length traveled by a particle to the length of the media

$$\tau = \frac{L_i}{L}$$
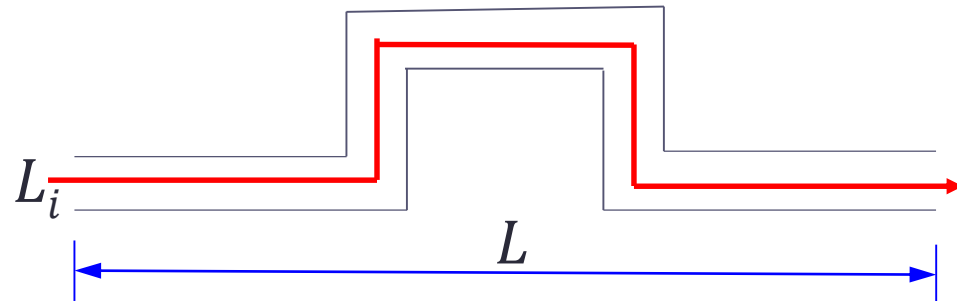
Tortuosity is thus transport dependent, including flow, diffusion, heat transfer, electrical conduct, acoustic transport.

- **For fluid flow it is "hydraulic tortuosity"**
- **For diffusion it is "diffusivity tortuosity"**
- **For electron transport, it is "conductivity tortuosity"**

Except for some very simple porous structures, there is no clear consensus on the relation between these definitions.

Content

- **2.1 Examples of porous media**

- **2.2 Structural characteristics of porous media**

- **2.3 Continuum-scale governing equation for porous media**

- **2.4 Pore-scale simulation: reconstruction of porous media**

- **2.5 Pore-scale simulation: LB for fluid flow**

- **2.6 Pore-scale simulation: LB for heat transfer**

Two velocity definition in a porous medium:

$$v_{\text{superficial}} = \varepsilon v_{\text{physical}}$$

v_{physical}

Porosity
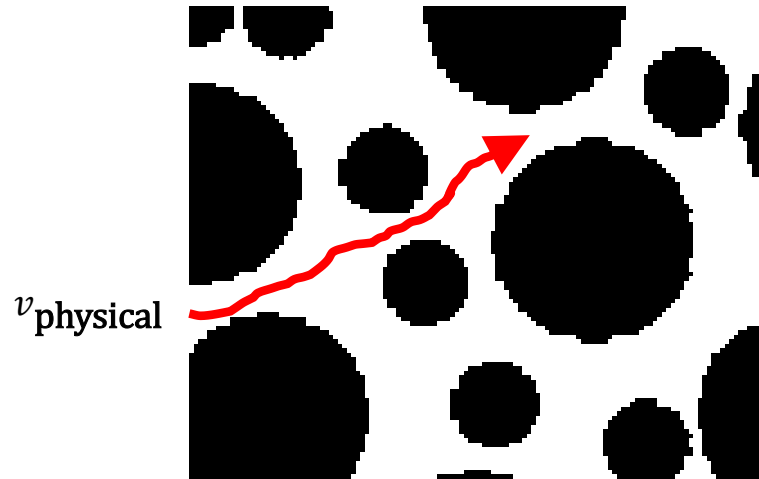
V_{physical}： **the actual flow velocity in the pores.**

$V_{\text{superficial}}$ **（表观速度）： the averaged velocity in the entire domain.**

$$V_{\text{superficial}} < V_{\text{physical}}$$

Fluent uses superficial velocity as the default velocity.

Continuum-scale equations for porous flow

$$\nabla \cdot \mathbf{u}_{\text{superficial}} = 0$$

$$(\frac{\mathbf{u}_{\text{superficial}}}{\varepsilon} \cdot \nabla)(\mathbf{u}_{\text{superficial}}) = -\frac{1}{\rho}\varepsilon\nabla(p) + \eta\nabla^2(\mathbf{u}_{\text{superficial}}) + \mathbf{F}$$

$$\mathbf{F} = -\frac{\varepsilon\upsilon}{k}\mathbf{u} - \frac{\varepsilon F_\varepsilon}{\sqrt{k}}|\mathbf{u}|\mathbf{u}$$

$$\frac{\partial((\rho C_p)_{\text{eff}}T)}{\partial t} + (u_{\text{superficial}} \cdot \nabla)(\rho C_p T) = \lambda_{\text{eff}}\nabla^2 T + S_{\text{eff}}$$

$$\lambda_{\text{eff}} = (1-\varepsilon)\lambda_s + \varepsilon\lambda_f$$

Content

2.4 Reconstruction

The first step towards pore-scale modeling using the LBM is structure reconstruction.

For a **nD** problem, where D is dimension, and n is 2 and 3 for two and three dimensional space, respectively, a **nD matrix is defined**

$$S=(nx, ny, nz)$$

nx, ny and *nz* is the mesh size of the domain in *x, y* and *z* direction.

In this matrix, $S_{i,j,k}=0$ **represents fluid and 1 stands for solid**. In such way the solid structure is defined and can be imported into the LB code.

Digitalized Structures
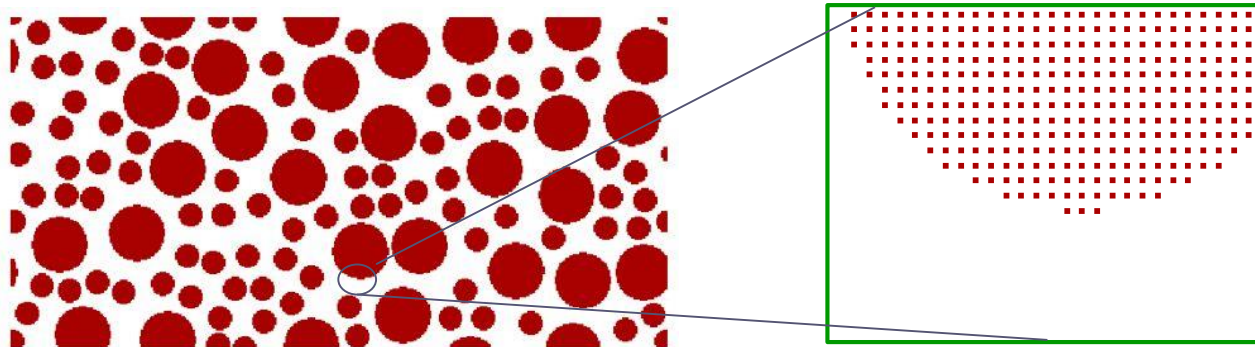
A 2D matrix is adopted to represent the porous media, with 1 as solid and 0 as fluid.

1 1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1 1	0 0 0 0 0 0 0 0 0
0 1 1 1 1 1 1 1 0	0 0 0 0 0 0 0 0 0	0 0 0 1 1 1 0 0 0
0 0 1 1 1 1 1 0 0	0 0 0 0 0 0 0 0 0	0 0 0 1 1 1 0 0 0
0 0 0 1 1 1 0 0 0	0 0 0 0 0 0 0 0 0	0 0 0 1 1 1 0 0 0
0 0 0 0 0 0 0 0 0	1 1 1 1 1 1 1 1 1	0 0 0 0 0 0 0 0 0

a. Quartet (四参数） structure generation set (QSGS) proposed by Wang et al. (2007)

Suppose a 2D domain with two constituents α and β (成分）

1. Randomly locate the cores of β in the domain based on a distribution probability, c_d, which is smaller than the volume fraction of β, ε_β. A random number within (0,1) will be assigned to each node in the domain, and if the random number is no greater than c_d the node is selected as a core.

Wang, M., J. Wang, N. Pan, and S. Chen (2007), Mesoscopic predictions of the effective thermal conductivity for microscale random porous media, *Phys. Rev. E*, 75(036702), doi: 10.1103/PhysRevE.75.036702.
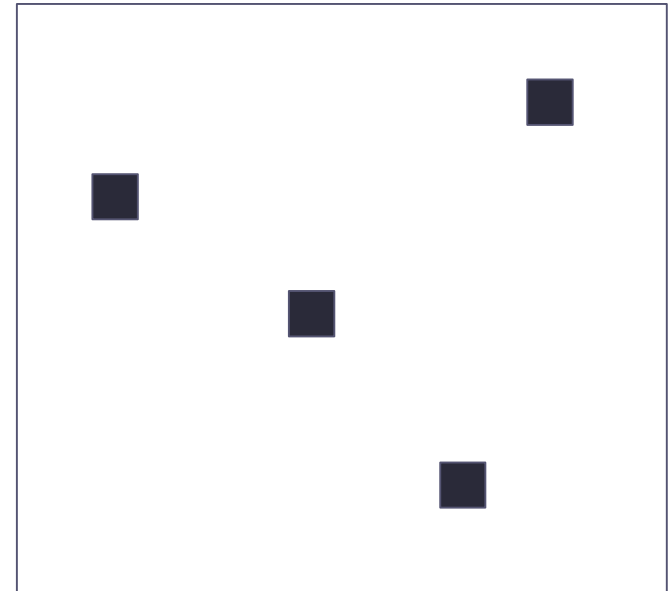
2. Grow an existing β node to its neighboring nodes based on another probability P_i with i representing the direction. In the present study only the nearest neighboring nodes are considered, namely four in the main direction (1,2,3,4) and the other four in the diagonal directions (5,6,7,8). For each direction, a new random number is generated, and if it is no greater than P_i the neighboring node in i direction becomes β.

P_i

P_i

Seed   **Grow**
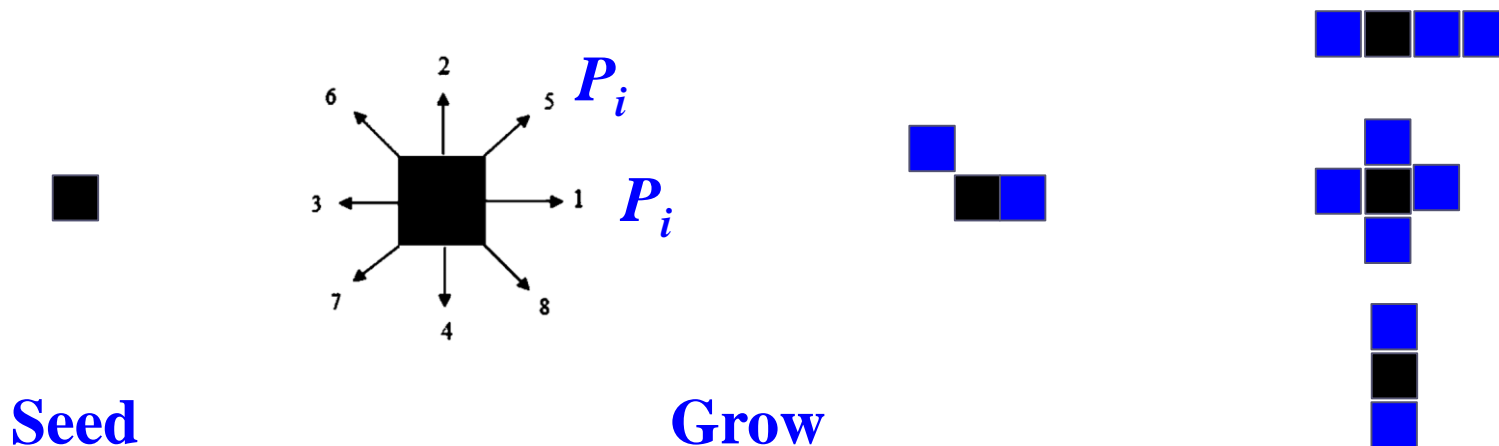
3. Repeating 1 and 2, until the volume fraction is obtained.
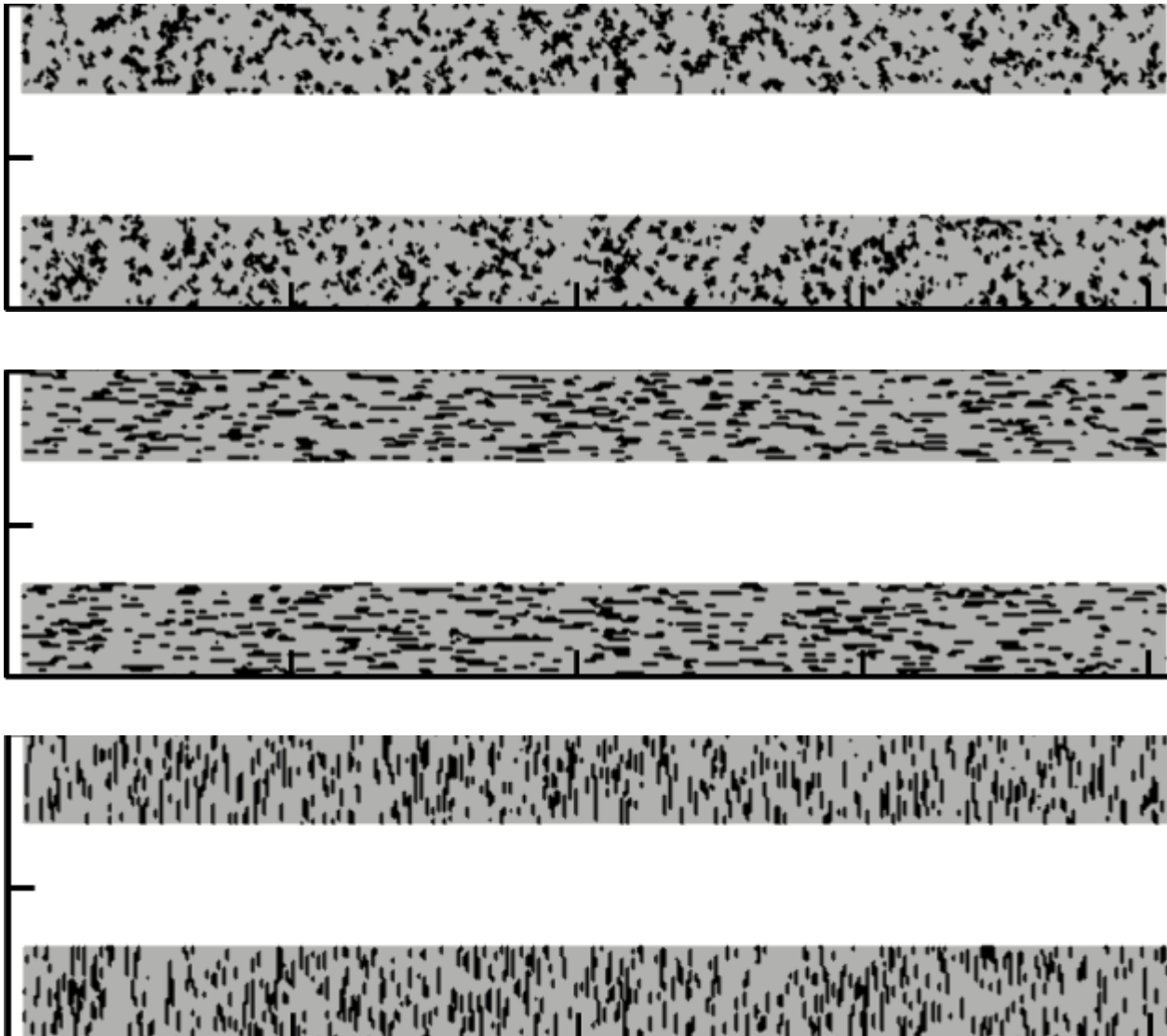
Schematic of the porous structures using QSGS

b. Reconstruction of fibrous porous media

Fiber porous media in PEM fuel cell
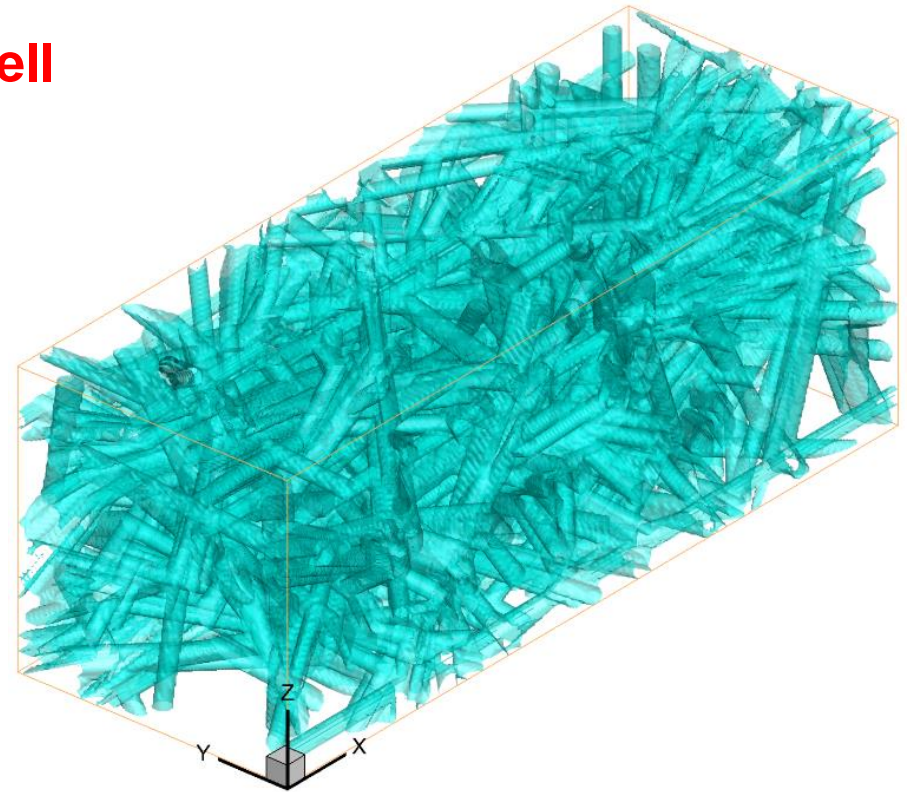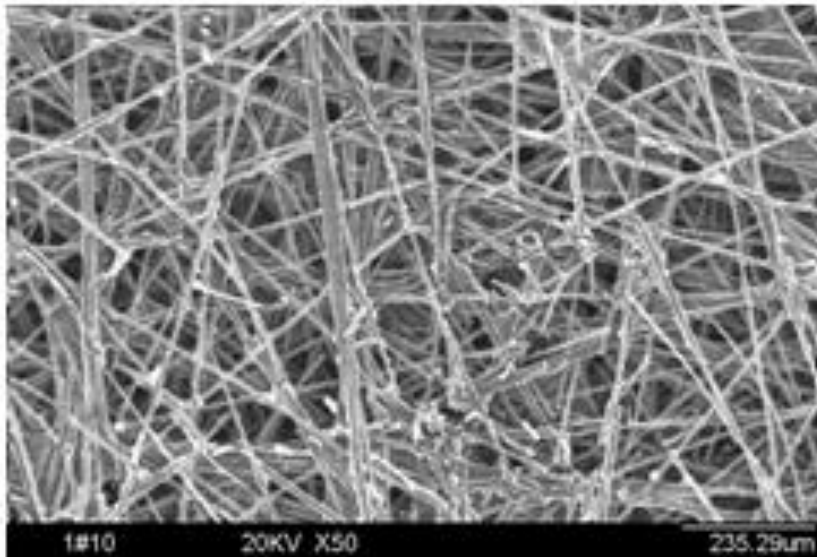
1. **L Chen**, YL He, WQ Tao, P Zelenay, R Mukundan, Q Kang, Pore-scale study of multiphase reactive transport in fibrous electrodes of vanadium redox flow batteries, , Electrochimica Acta 248, 425-439;
2. **L. Chen***, H.B. Luan, Y.-L. He, W.-Q. Tao, Pore-scale flow and mass transport in gas diffusion layer of proton exchange membrane fuel cell with interdigitated flow fields, 2012, 51, 132-144, International journal of thermal science

c. Random spheres with uniform gap

(d)
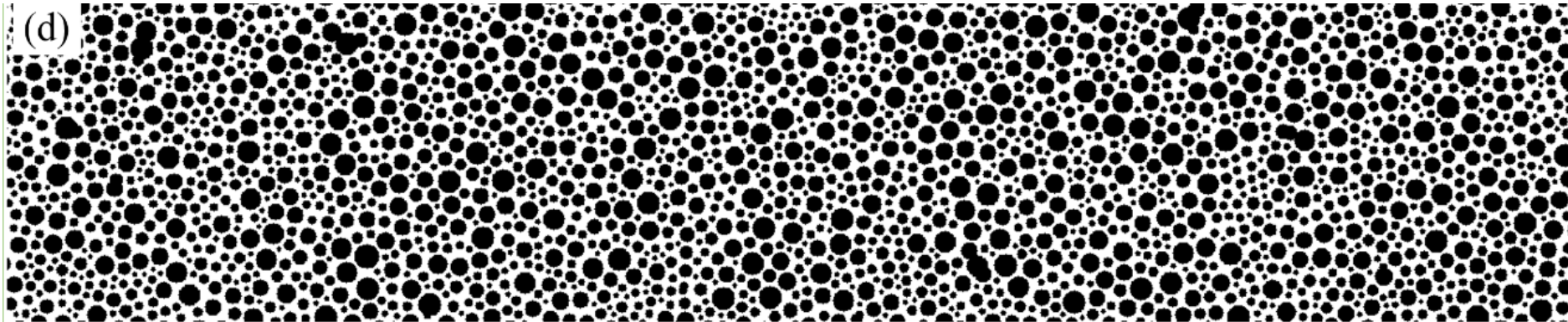
Li Chen, et al. Pore-scale study of effects of macroscopic pores and their distributions on reactive transport in hierarchical porous media, Chemical Engineering Journal, 2018,

L Chen, M Wang, Q Kang, W Tao, Pore scale study of multiphase multicomponent reactive transport during CO2 dissolution trapping, Advances in Water Resources, 2018, 116, 208-218
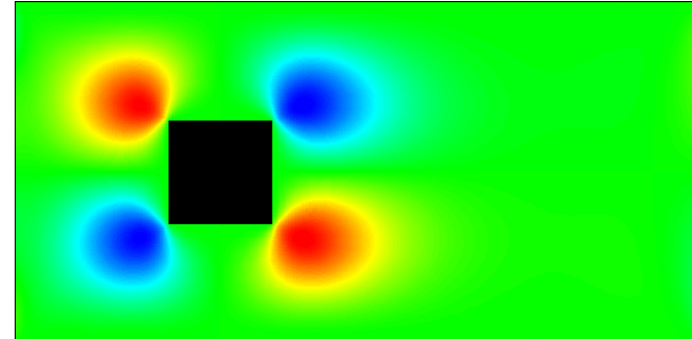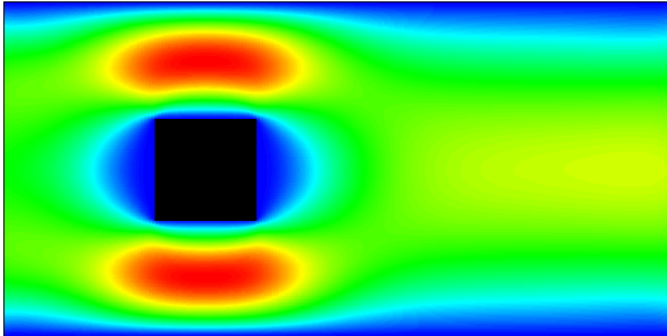
Content

Case A: flow around a square


```fortran
!=====================================================================-=
SUBROUTINE SOLID_STRUCTURE
USE START_L
   ! ls represents the porous structure: 0 denotes nodes of void space, 1 denotes solid node.
   ls=0
   ls(:,ny:ny+1)=1
   ls(:,0:1)=1
   icenter=61
   jcenter=ny/2+1
   ls(icenter-15:icenter+15,jcenter-15:jcenter+15)=1
   walls=.false.
   do j=0,ny+1
   do i=0,nx+1
      if(ls(i,j).eq.1) then
         walls(i,j)=.true.
      endif
   enddo
   enddo
RETURN
END SUBROUTINE
!=====================================================================
```

Case B: flow around a cylinder
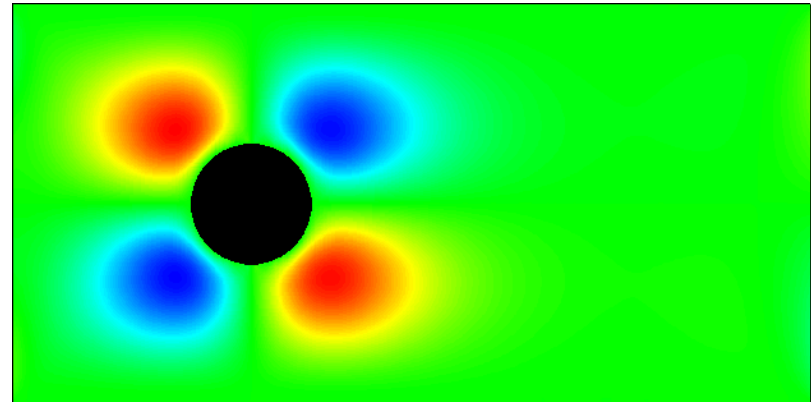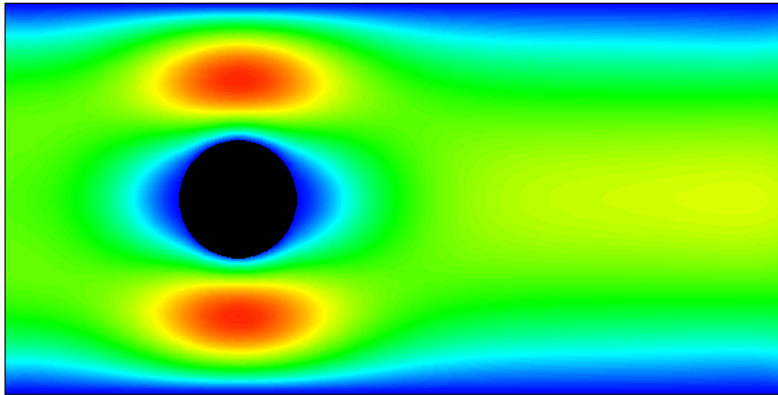

```fortran
SUBROUTINE SOLID_STRUCTURE
USE START_L
double precision::radius
    ! ls represents the porous structure: 0 denotes nodes of void space, 1 denotes solid node.
    ls=0
    ls(:,ny:ny+1)=1
    ls(:,0:1)=1
    icenter=61
    jcenter=ny/2+1
    walls=.false.
    do j=0,ny+1
    do i=0,nx+1
        radius=sqrt(float(i-icenter)**2.+float(j-jcenter)**2.)
        if(radius.le.15.d0) then
            ls(i,j)=1
        endif
        if(ls(i,j).eq.1) then
            walls(i,j)=.true.
        endif
    enddo
    enddo
RETURN
END SUBROUTINE
!===================================================================
```

Permeability

- **Permeability**, an indictor of the capacity of a porous medium for fluid flow through

- **In 1856, Darcy noted that for laminar flow through porous media, the flow rate <u> is linearly proportional to the applied pressure gradient Δp, he introduced permeability to describe the conductivity of the porous media. The Darcy' law is as follows**

  - leakage in the test
  - too high *Re* number
  - fluid is not viscous.

$$< u >= -\frac{k}{\mu}\frac{\Delta p}{l}$$

μu

Δp

- *q* flow rate (m/s), *μ* the viscosity, pressure drop Δp, length of the porous domain *l*, *k* is the permeability.
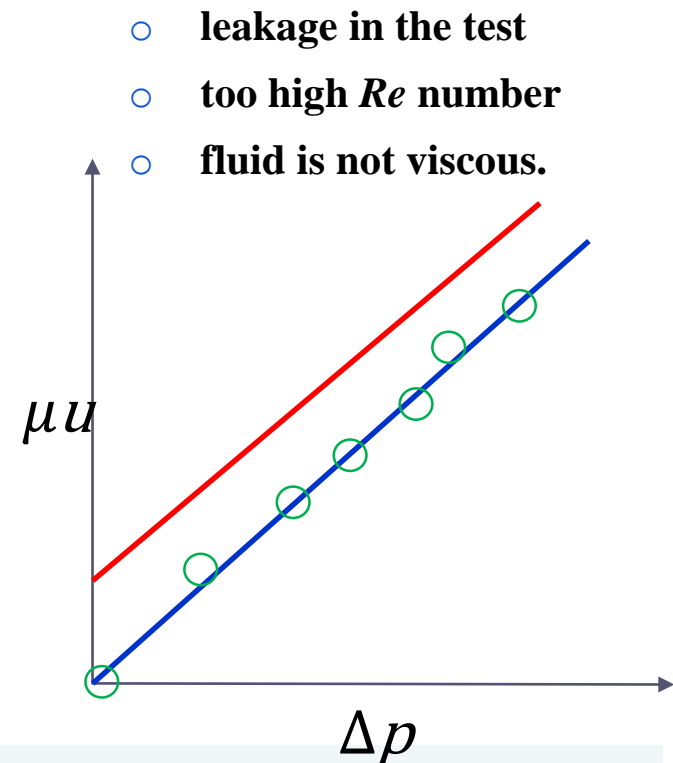
Pore-scale modeling of fluid flow

Schematic of Darcy's experiment

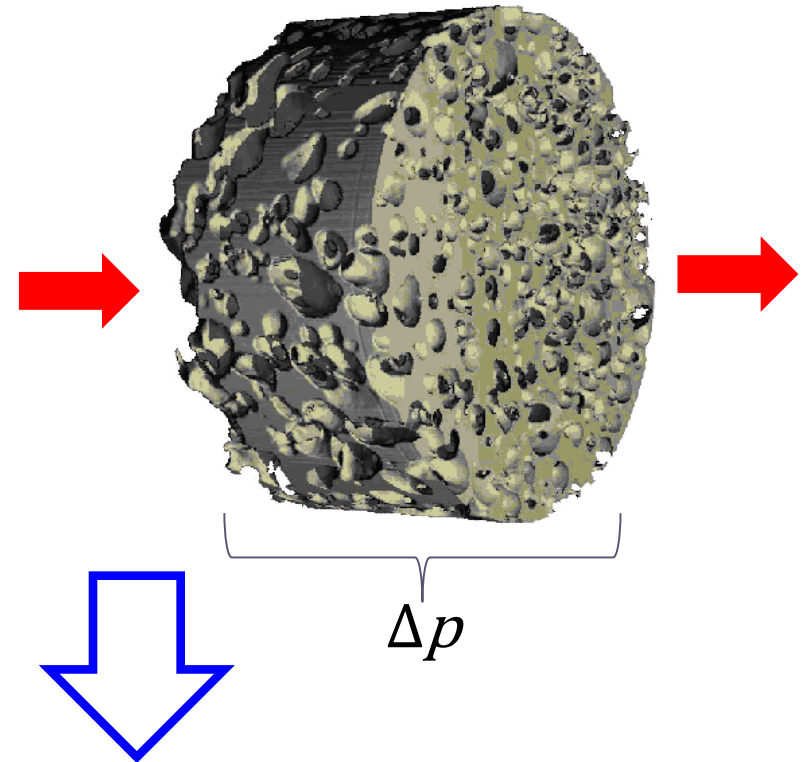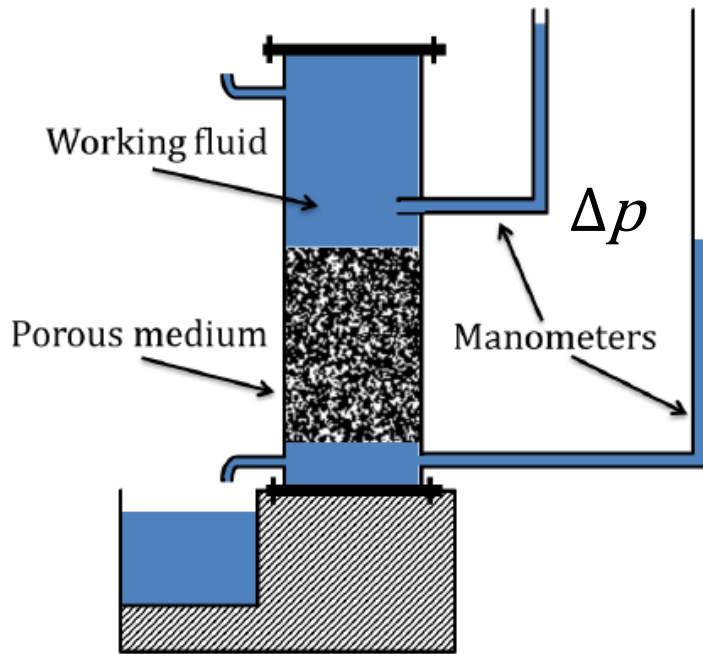**Simulation mimic the experiment**

Working fluid

Δp

Porous medium   Manometers

Δp

NS equation is solved at the pore scale. Non-slip boundary condition for the fluid-solid interface
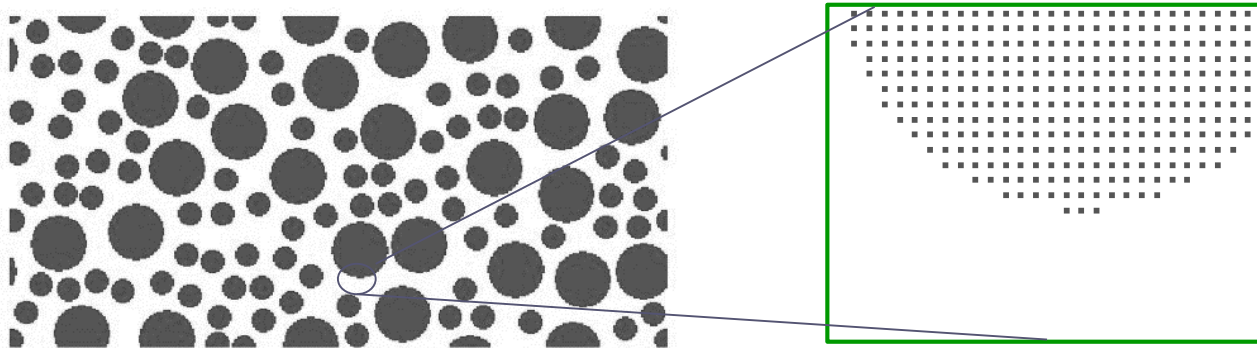
Bounce-back at the solid surface

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = -\frac{1}{\tau}(f_i(\mathbf{x}, t) - f_i^{\mathrm{eq}}(\mathbf{x}, t))$$

Collision

$$f_i'(\mathbf{x}, t) = -\frac{1}{\tau}(f_i(\mathbf{x}, t) - f_i^{\mathrm{eq}}(\mathbf{x}, t))$$

Streaming

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i'(\mathbf{x}, t)$$

Macroscopic variables calculation

$$\rho = \sum_{i=0} f_i, \quad \rho \mathbf{u} = \sum_{i=0} f_i \mathbf{e}_i.$$
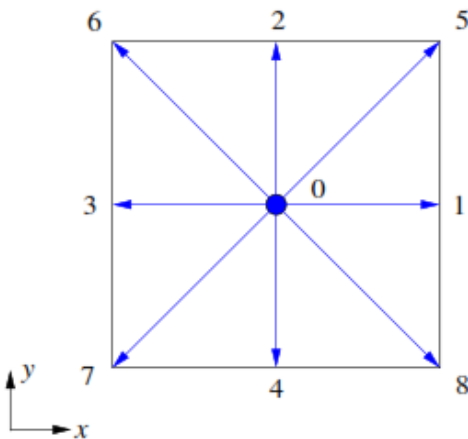
Pore-scale fluid flow in a 2D porous structure
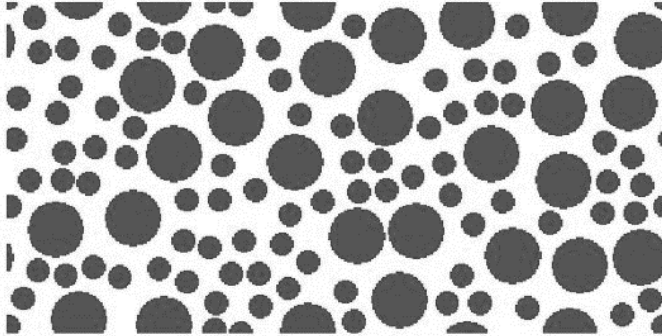
◆ **Bounce-back at the solid surface**

◆ **Pressure drop across *x* direction**

◆ **Periodic boundary condition *y***

◆ **Analyze the detailed flow field**

◆ **Calculate permeability based on Darcy equation.**

$$< u >= -\frac{k}{\mu}\frac{\Delta p}{l}$$
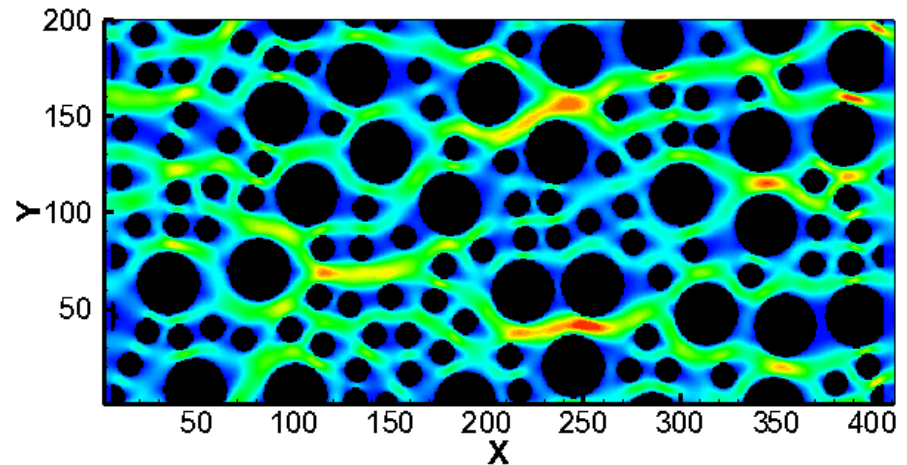
Permeability

o **One of the most famous empirical relationship between permeability and statistical structural parameters is proposed by Kozeny and Carman (KC) equation for beds of particle**

$$k = \frac{d^2}{180} \frac{\varepsilon^3}{(1-\varepsilon)^2}$$

L. Chen, L Zhang, Q Kang, W.Q. Tao, Nanoscale simulation of shale transport properties using the lattice Boltzmann method: permeability and diffusivity, 2015, 5, 8089, Scientific Reports
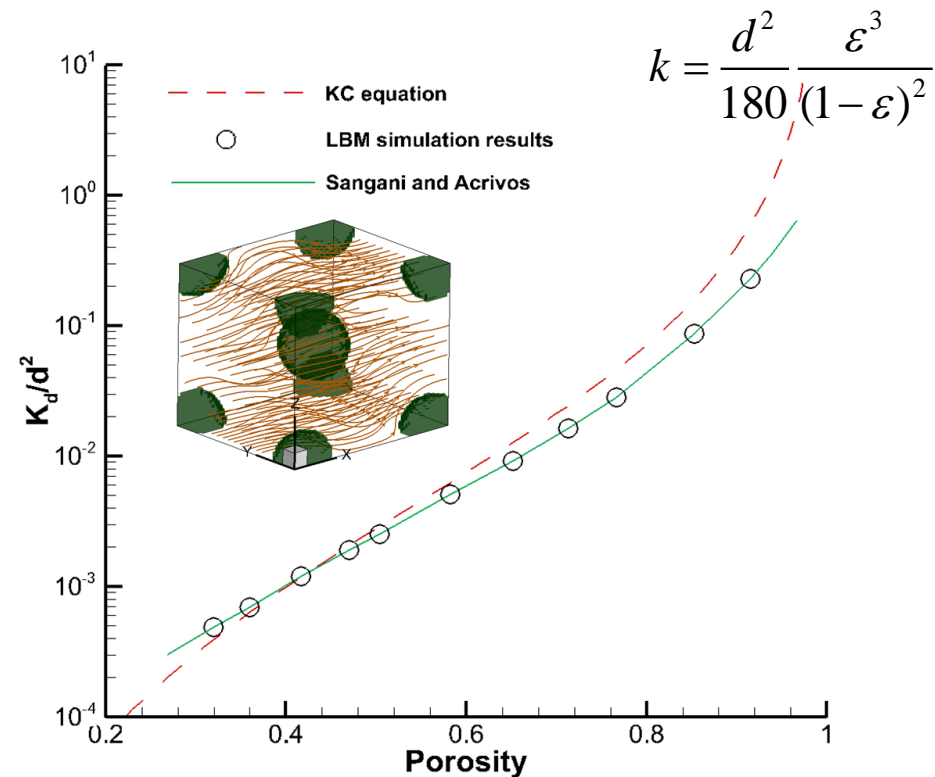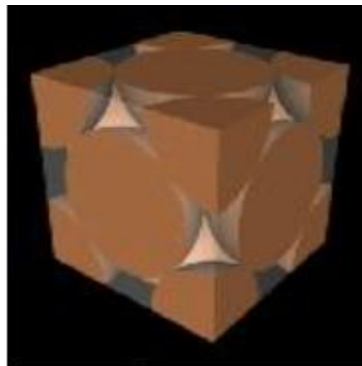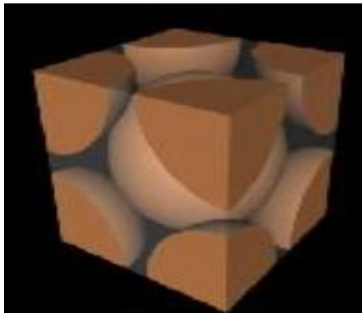
Permeability

○ **Fibrous beds have received special attention for its wide applications such as filter which can form stable structures of very high porosity.**

$$k = r^2 A(\sqrt{\frac{1-\varepsilon_c}{1-\varepsilon}} - 1)^B$$
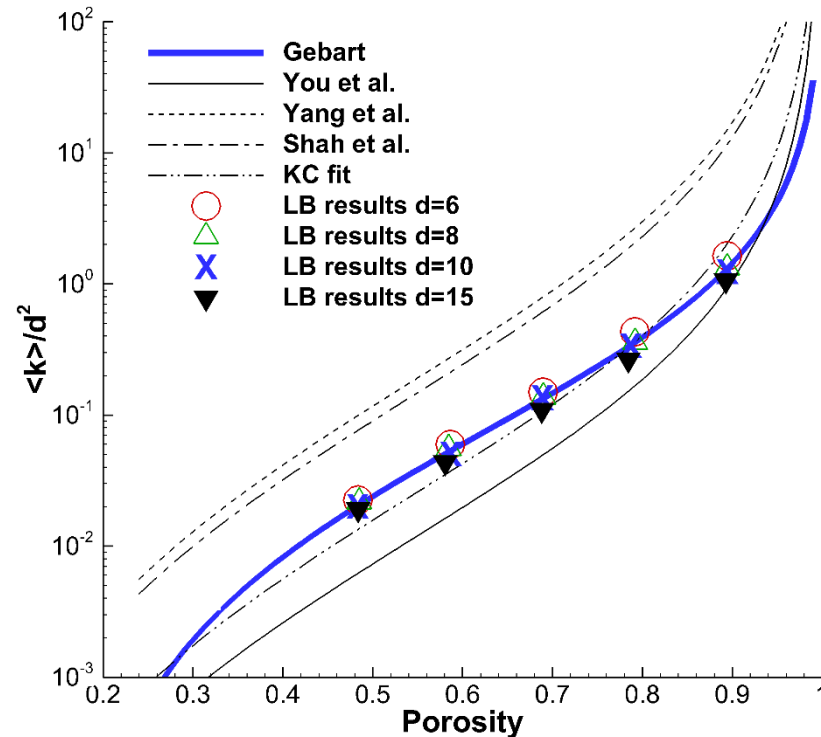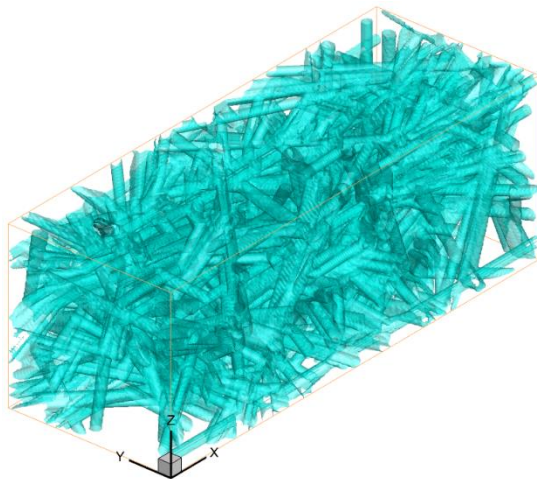
1. **L Chen**, YL He, WQ Tao, P Zelenay, R Mukundan, Q Kang, Pore-scale study of multiphase reactive transport in fibrous electrodes of vanadium redox flow batteries, , Electrochimica Acta 248, 425-439;

2. **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

Content

Content

LB model for heat transfer

Evolution equation

$$g_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) - g_i(\mathbf{x},t) = -\frac{1}{\tau}(g_i(\mathbf{x},t) - g_i^{eq}(\mathbf{x},t)) + \omega_i S(\mathbf{x},t)$$

Equilibrium distribution function

$$g_i^{eq} = \omega_i T(1 + 3\mathbf{c}_i \cdot \mathbf{u})$$

Temperature

$$T = \sum_i g_i$$

Thermal diffusivity

$$\alpha = \frac{\lambda}{\rho C_p} = \frac{1}{3}(\tau - 0.5)\frac{(\Delta x)^2}{\Delta t}$$

LB model for heat transfer

Standard energy governing equation

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \mathbf{u} T) = \nabla \cdot (\lambda \nabla T) + S$$

Energy equation recovered from LB

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \mathbf{u} T) = \nabla \cdot (\alpha \nabla \rho c_p T) + S$$

where

$$\alpha = \lambda / \rho c_p$$

thermal diffusivity of the material.

At the fluid-solid interface

$$T_f = T_s$$

$$-\lambda_f \frac{\partial (T)_f}{\partial n_f} = \lambda_s \frac{\partial (T)_s}{\partial n_s}$$
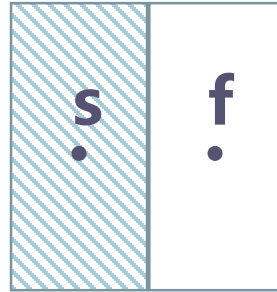
$$T_f = T_s$$

$$-\alpha_f \frac{\partial (\rho C_P T)_f}{\partial n_f} = \alpha_s \frac{\partial (\rho C_P T)_s}{\partial n_s}$$

Conjugate heat transfer

In LB

Satisfy Dirichlet- and Neumann-like boundary restriction at the same time

Only when heat capacity of the two materials is the same, the conjugate heat transfer condition form the LB is equal to practical case!

Heat conduction across two solids

FIG. 1. (Color online) Schematic of two-layer stratified medium.
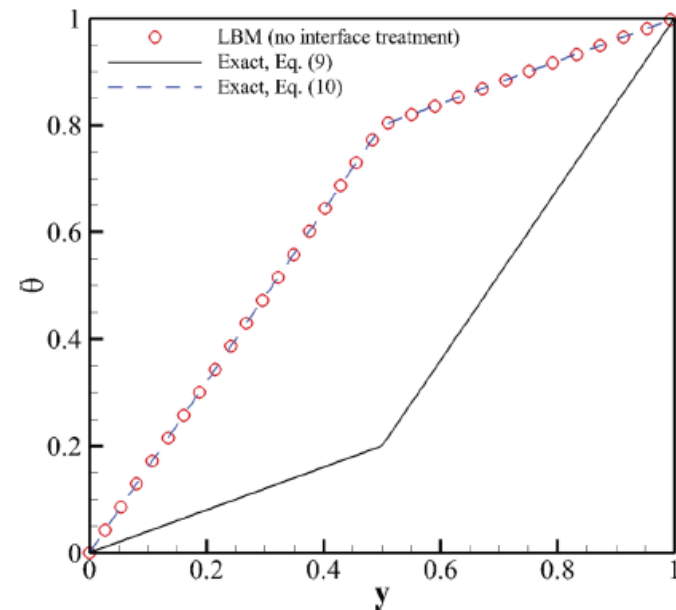
FIG. 2. (Color online) Comparison of LBM solution with analytical solutions for two-layered stratified medium.

$$\frac{\lambda_1}{\lambda_2} = 4$$

$$\frac{\alpha_1}{\alpha_2} = 4$$

LB model for predicting thermal conductivity

Standard energy governing equation

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \mathbf{u} T) = \nabla \cdot (\lambda \nabla T) + S$$

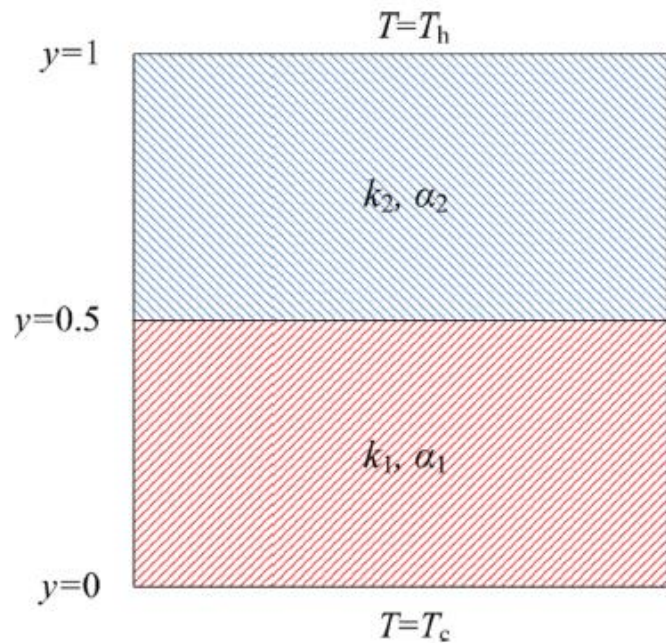$$\mathbf{f} \qquad \nabla \cdot (\rho c_p \mathbf{u} T) = \nabla \cdot (\lambda \nabla T)$$

$$\mathbf{s} \qquad 0 = \nabla \cdot (\lambda \nabla T)$$

"pseudo-capacity of solid phase" scheme

$$(\rho c_p)_f = (\rho c_p)_s$$

$$\mathbf{s} \quad 0 = \nabla \cdot \left(\frac{\lambda_s}{(\rho c_p)_f} \nabla T\right)$$

$$\frac{\alpha_f}{\alpha_s} = \frac{\lambda_f}{\lambda_s}$$

X. Chen, P. Han, A note on the solution of conjugate heat transfer problems using SIMPLE-like algorithms, Int. J. Heat Fluid Flow 21 (2000) 463–467.
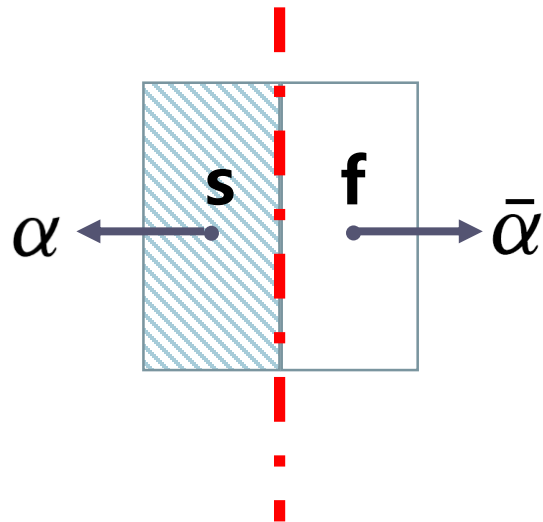
$$g_{\bar{\alpha}}(\mathbf{x}_f, t + \delta t) = \hat{g}_{\bar{\alpha}}(\mathbf{x}_s, t),$$

$$g_{\alpha}(\mathbf{x}_s, t + \delta t) = \hat{g}_{\alpha}(\mathbf{x}_f, t)$$

Half lattice node

$$g_{\alpha}(\mathbf{r} + \mathbf{e}_{\alpha}\delta_t) - g_{\alpha}(\mathbf{r}, t) = -\frac{1}{\tau_g}\left[g_{\alpha}(\mathbf{r}, t) - g_{\alpha}^{\text{eq}}(\mathbf{r}, t)\right]$$
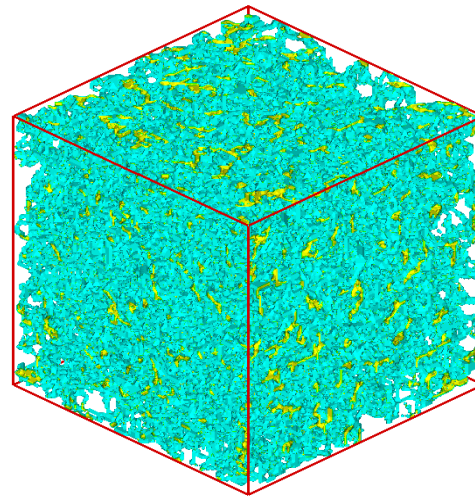
$$\tau_g = \frac{3}{2}\frac{\lambda}{\rho c_p c^2 \delta t} + 0.5$$

$$T = \sum_{\alpha} g_{\alpha}$$

Jinku Wang a, Moran Wang b, Zhixin Li, A lattice Boltzmann algorithm for fluid–solid conjugate heat transfer, 2007, 46, 228-234

Prediction of thermal conductivity of aerogel

Aerogel: low density and *k*

$$\lambda_{x,e} = \frac{\int q_x dA_x}{(\Delta T/L_x)A_x}$$

$$\lambda_{y,e} = \frac{\int q_y dA_y}{(\Delta T/L_y)A_y}$$
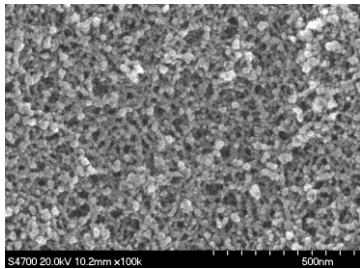
$$\lambda_{z,e} = \frac{\int q_z dA_z}{(\Delta T/L_z)A_z}$$

Different components with Large variations of *k*

Effective thermal conductivity

WZ Fang, L. Chen, JJ Gou, WQ Tao, Predictions of effective thermal conductivities for three-dimensional four-directional braided composites using the lattice Boltzmann method, International Journal of Heat and Mass Transfer, 2016, 92, 120-130
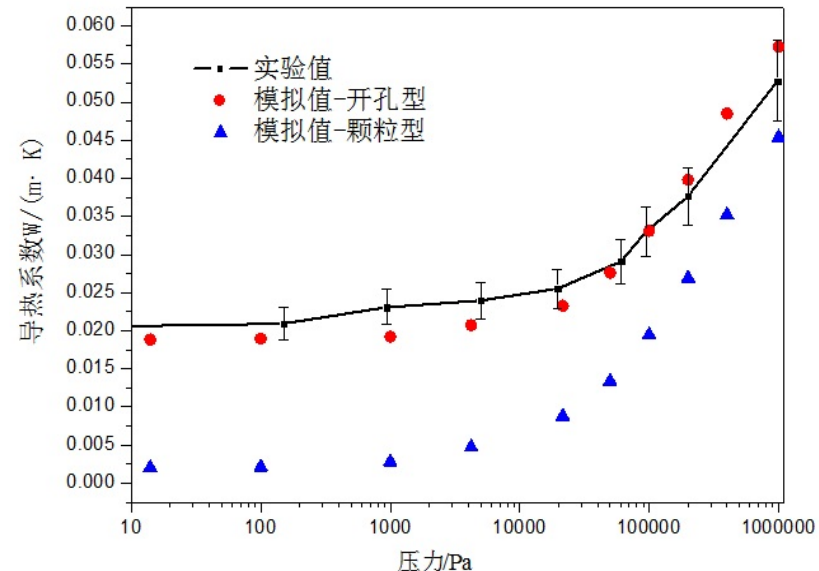
General case

    For general heat transfer process, the unsteady term should be considered, and thus the "pseudo-capacity of solid phase scheme" fails.

1. Treat the interface as boundary

    Treat the interface as boundary. Then the problem is changed to construct boundary condition at the phase interface.

2. Re-arrange the governing equation

    Re-arrange the energy equation and add additional source term into the governing equation.
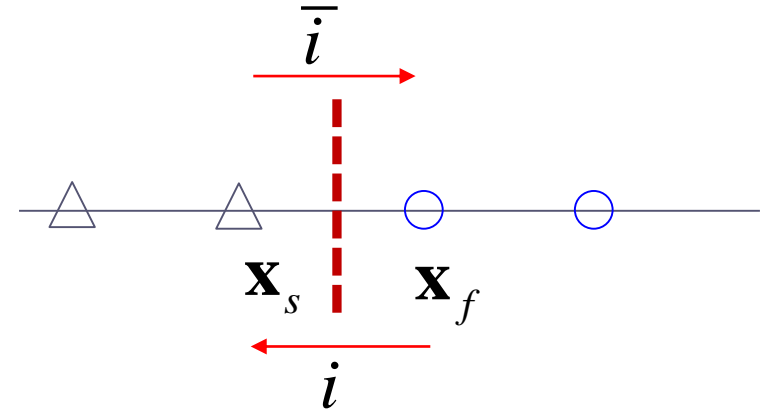
1. Treat the interface as boundary

Dirichlet condition

$$g_{\bar{i}}(\mathbf{x}_f, t + \Delta t) = -\widehat{g}_i(\mathbf{x}_f, t) + \varepsilon_{\mathrm{D}}\phi_{\mathrm{d}}$$

Neumann equation

$$g_{\bar{i}}(\mathbf{x}_f, t + \Delta t) = \widehat{g}_i(\mathbf{x}_f, t) + \frac{\Delta t}{\Delta x}J_d$$

$$g_{\bar{i}}(\mathbf{x}_f, t + \Delta t) = \left(\frac{1-\sigma}{1+\sigma}\right)\widehat{g}_i(\mathbf{x}_f, t) + \left(\frac{2\sigma}{1+\sigma}\right)\widehat{g}_{\bar{i}}(\mathbf{x}_s, t)$$

$$g_i(\mathbf{x}_s, t + \Delta t) = -\left(\frac{1-\sigma}{1+\sigma}\right)\widehat{g}_{\bar{i}}(\mathbf{x}_s, t) + \left(\frac{2}{1+\sigma}\right)\widehat{g}_i(\mathbf{x}_f, t)$$

$$\sigma = \frac{(\rho C_{\mathrm{p}})_{\mathrm{s}}}{(\rho C_{\mathrm{p}})_f}$$

Like Li, et al. PHYSICAL REVIEW E 89, 043308 (2014)

42/66

2. Re-arrange the governing equation

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \mathbf{u} T) = \nabla \cdot (\lambda \nabla T) + S$$

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \mathbf{u} T) = \nabla \cdot (\frac{\lambda}{\rho c_p} \rho c_p \nabla \ (\frac{\rho c_p T}{\rho c_p})) + S$$

$$\alpha \rho c_p \nabla \ (\frac{h}{\rho c_p}) = \alpha \rho c_p (\frac{1}{\rho c_p} \nabla h + h \nabla \frac{1}{\rho c_p})$$

$$= \alpha \nabla h + \alpha \rho c_p h \nabla \frac{1}{\rho c_p}$$

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \mathbf{u} T) = \nabla(\alpha \nabla h) + \nabla(\alpha \rho c_p h \nabla \frac{1}{\rho c_p}) + S \qquad S*$$

同舟共济
渡彼岸！