Lattice Boltzmann for flow and transport phenomena

2. The lattice Boltzmann for porous flow and transport

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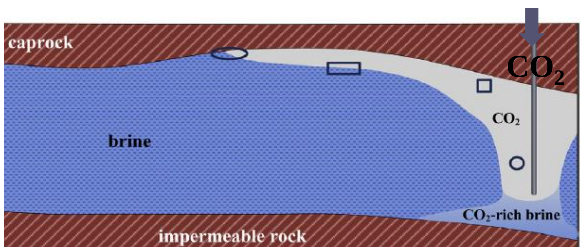
ResearchID: P-4886-2014

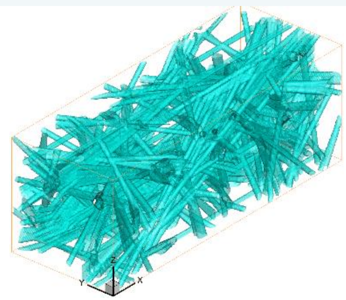
Content

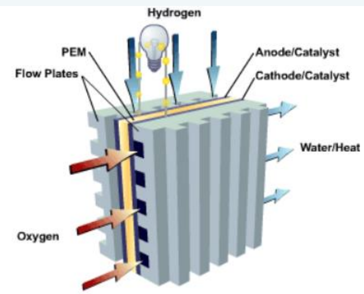
- 2.1 Background
- 2.2 Structural characteristics of porous media
- 2.3 Continuum-scale governing equation for porous media
- 2.4 Pore-scale simulation: reconstruction of porous media
- 2.5 Pore-scale simulation: LB for fluid flow
- 2.6 Pore-scale simulation: LB for heat transfer

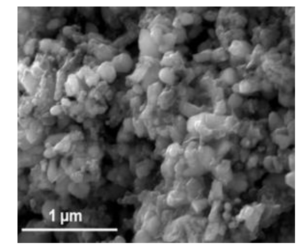
2.1 Examples of porous media

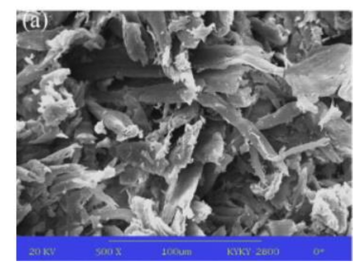
- Transport processes in porous media are widely encountered in scientific and engineering problems
- **Natural porous systems**: enhanced hydrocarbon and geothermal energy recovery, CO_2 geological sequestration, groundwater contaminant transport and bioremediation, nuclear waste disposal…
- **Artificial porous systems**: fuel cell, reactor, catalysts, building material…











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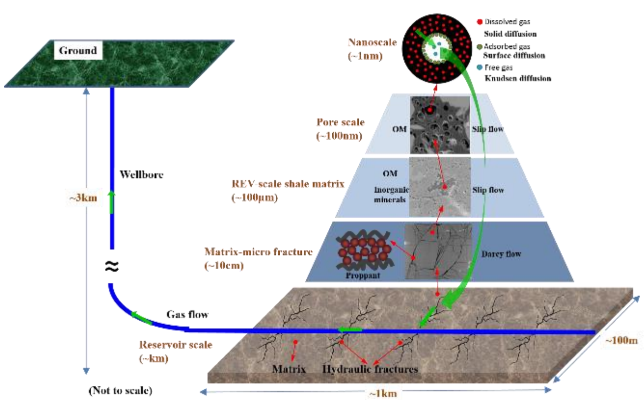
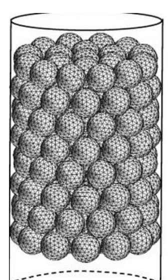
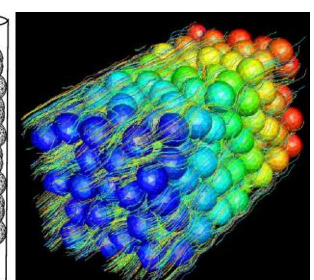
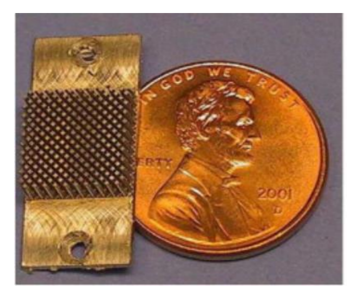




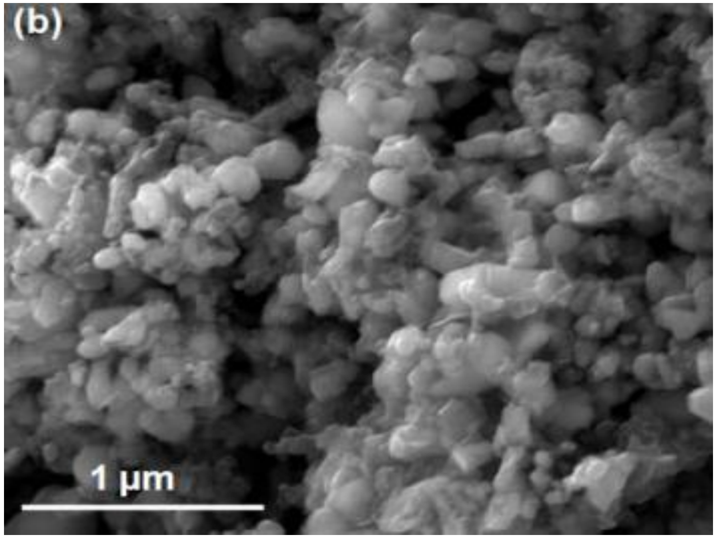




Stone

Carbon fiber

Metal foam



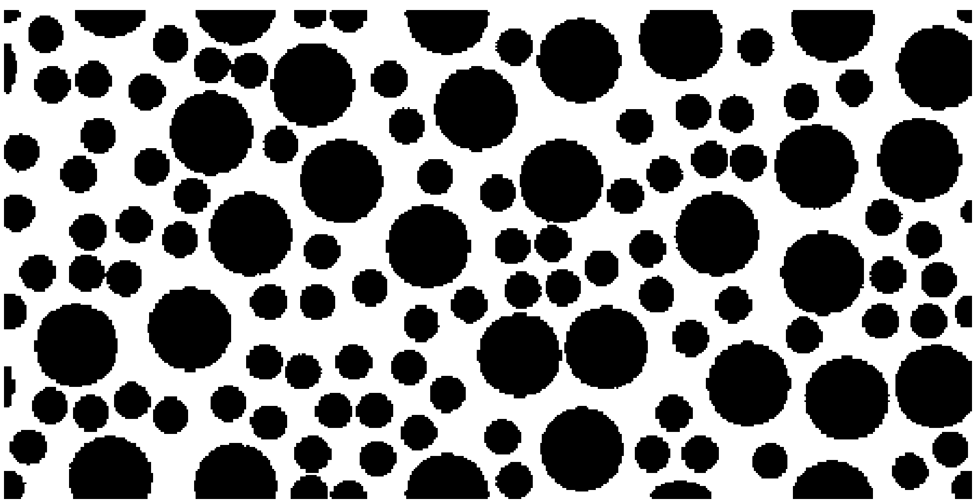
Catalyst

Content

2.2 Structural characteristics of porous media

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

- **Two necessary elements: skeleton and pores; Skeleton: maintain the shape; Pores: provide pathway for fluid flow through**



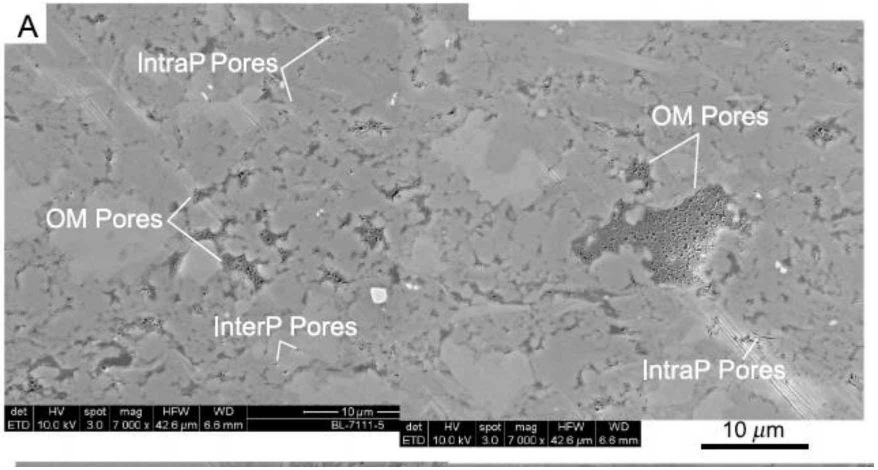
Black: solid
White: pores

2.2.1 Porosity

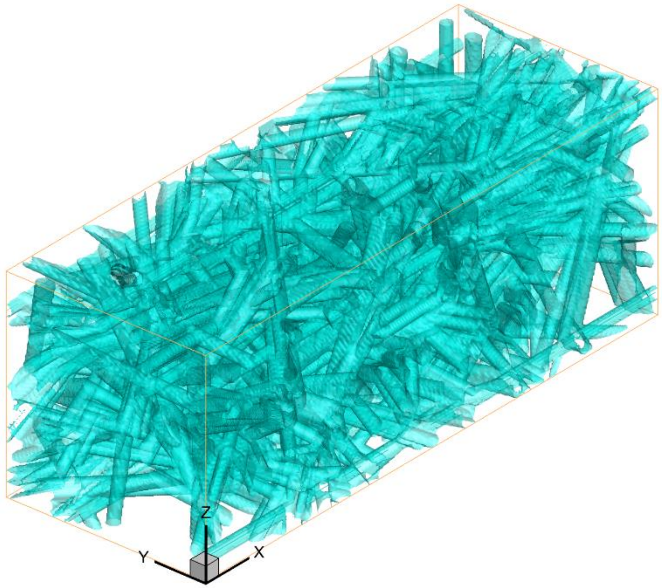
- The volume ratio between pore volume and total volume

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

- **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%

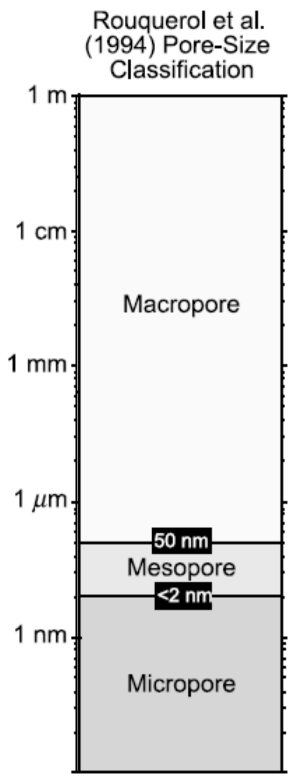
2.2.2 Pore size

Pore size terminology of IUPAC

International Union of Pure and Applied Chemistry

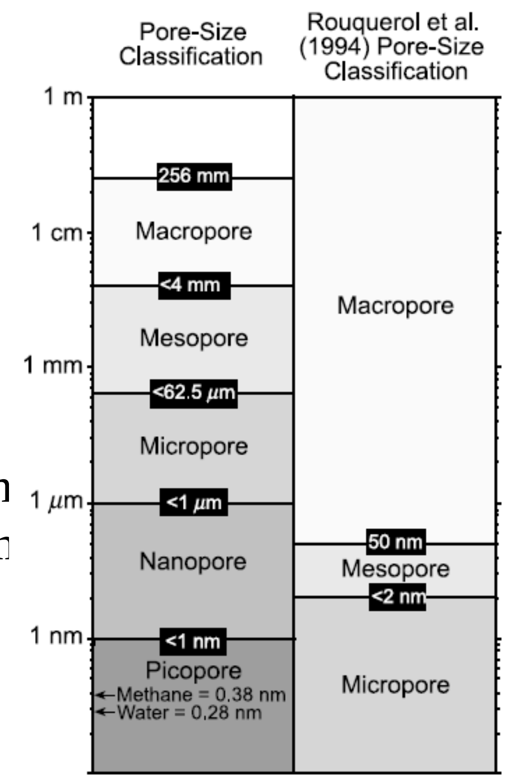
Rouquerol et al. (1994) *Membrane*

Micropores, <2nm
Mesopores, 2~50nm
Macropores, >50nm



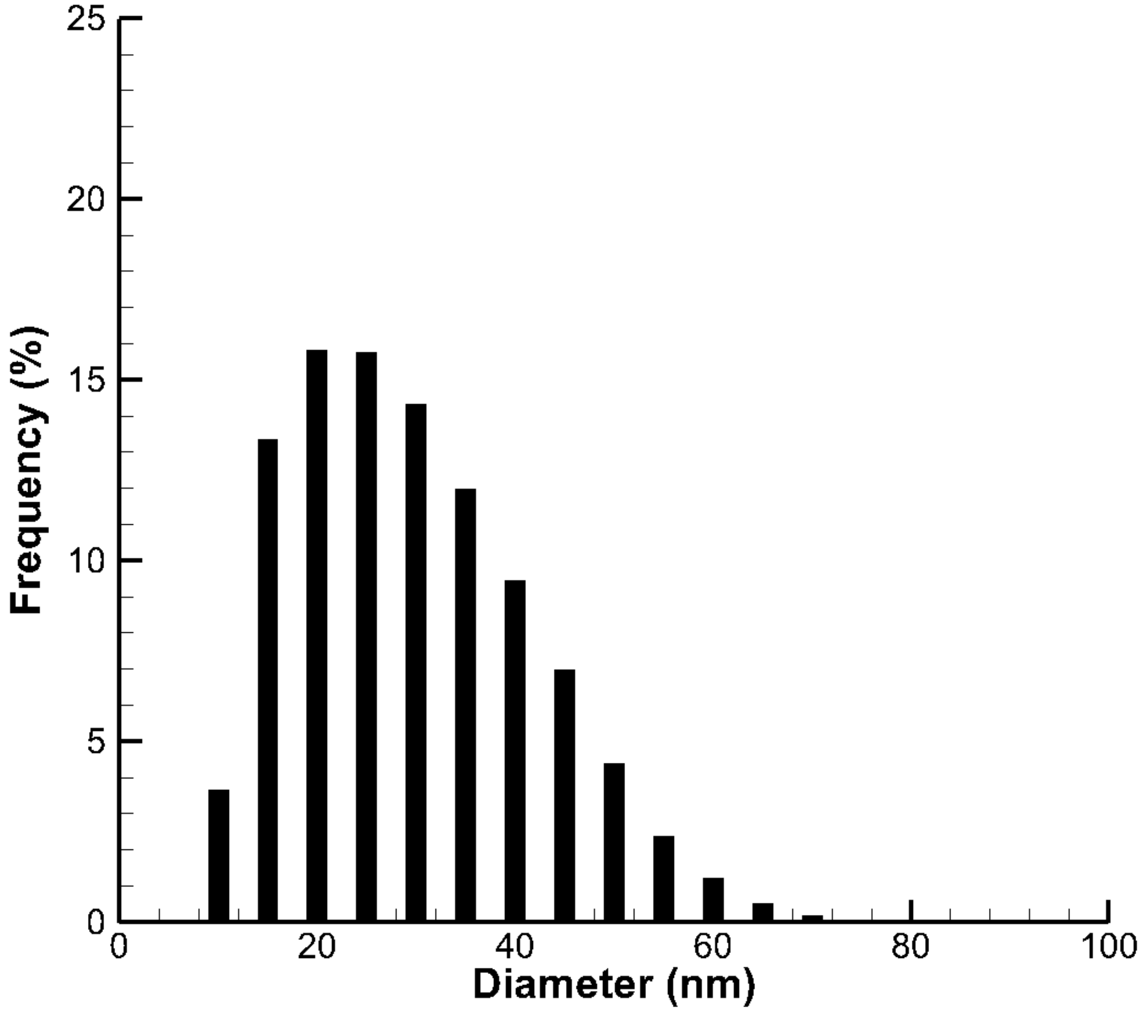
Choquette and Pray (1970)*Carbonate rock*

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.

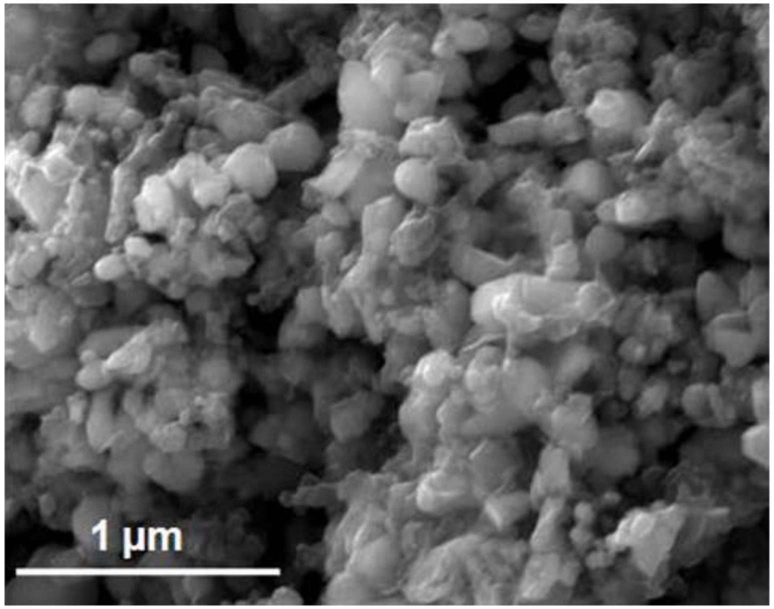
Pore size distribution



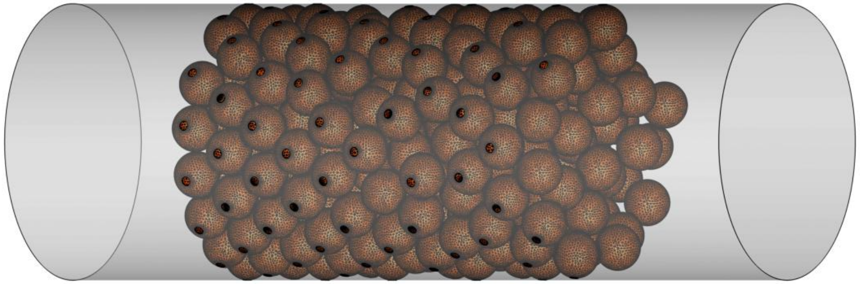
2.2.3 Specific surface area

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

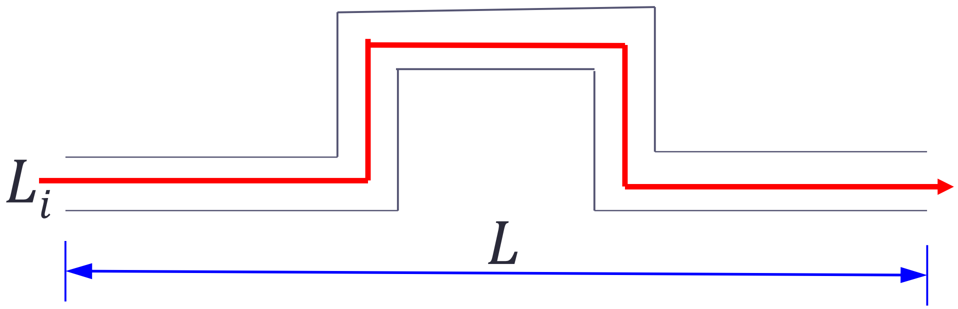


Packed-bed reactor

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"**

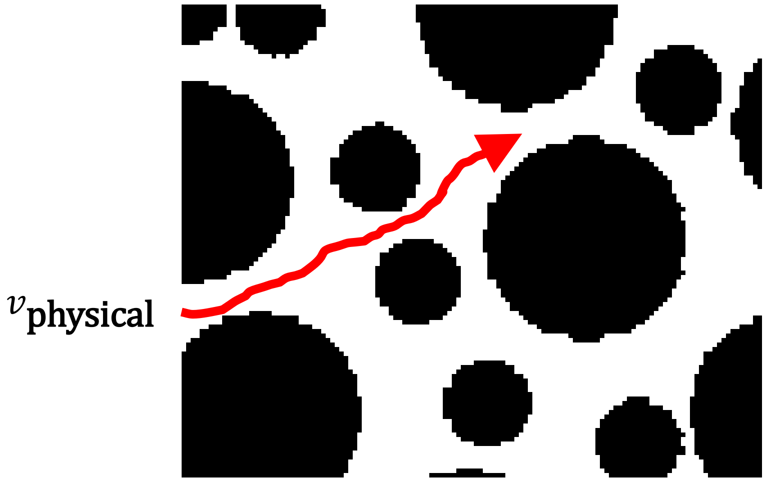
Except for some very simple porous structures, there is no clear consensus on the relation between these definitions.

Content

Two velocity definition in a porous medium:

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

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.

Original continuity and momentum equation

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

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + (\mathbf{u} \cdot \nabla)(\rho \mathbf{u}) = -\nabla p + \eta \nabla^2 \mathbf{u}$$

Continuity equation for porous media:

$$\frac{\partial (\varepsilon \rho)}{\partial t} + \nabla \cdot (\varepsilon \rho \mathbf{u}_{\text{physical}}) = 0$$

As the total mass of fluid is $\rho V_f = \rho \varepsilon V_{total} = \rho \varepsilon \Delta x \Delta y \Delta z$

Fluent uses superficial velocity as the default velocity.

$$\frac{\partial (\varepsilon \rho)}{\partial t} + \nabla \cdot (\rho \mathbf{u}_{\text{superficial}}) = 0$$

Momentum equation for porous media:

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

Total force due to porous media

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

For incompressible steady state problem:

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

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

The fluid-solid interaction is strong in porous media. Porous media are modeled by adding a momentum source term:

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

The first term is the viscous loss term （黏性项） or the Darcy term.

The second term is inertial loss term (惯性项） or the Forchheimer term.

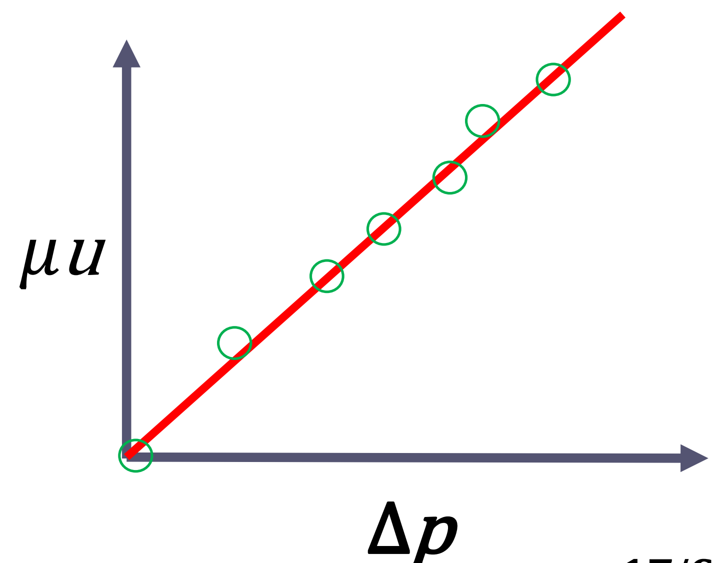
k **is the permeability (渗透率) of a porous media, one of the most important parameter of a porous media**

Permeability (渗透率)

In 1856, Darcy (法国工程师) noted that for laminar flow through porous media, the flow rate <*u*> is linearly proportional to the applied pressure gradient Δ*p*, thus he introduced **permeability to describe the conductivity of the porous media**. The Darcy' law is as follows

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

***k* is permeability** with unit of m^2



In Fluent, this force source term is expressed as

$$\mathbf{F} = -\frac{\mu}{k}\mathbf{u} - C_2 \frac{1}{2}\rho |\mathbf{u}| \mathbf{u}$$

***k*: permeability;** **C_2: inertial resistance factor**

The second term can be canceled if the fluid flow is slow

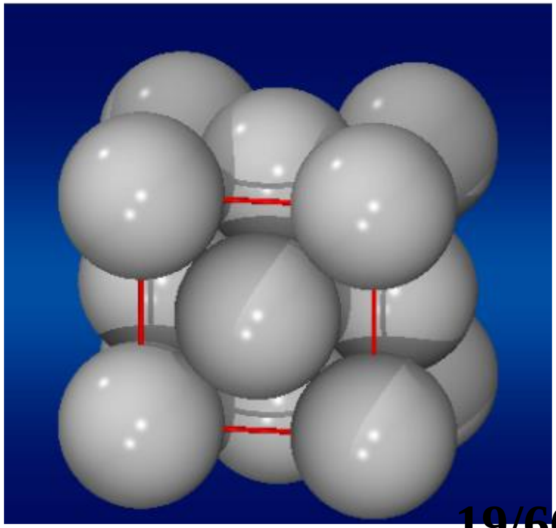
$$\mathbf{F} = -\frac{\mu}{k}\mathbf{u} - \cancel{C_2 \frac{1}{2}\rho |\mathbf{u}| \mathbf{u}}$$

u is small, thus u*u is smaller.

There have been lots of experiments in the literature to determine the relationship between pressure drop and velocity of different kinds of porous media, and thus to determine permeability.

Ergun equation is one of the most adopted empirical equations (经验公式) for packed bed porous media.

$$\frac{\Delta P}{l}=\frac{150\mu}{D_p^2}\frac{(1-\varepsilon)^2}{\varepsilon^3}u+\frac{1.75\rho}{D_p}\frac{(1-\varepsilon)}{\varepsilon^3}u^2$$



Diameter of solid particle

$$\mathbf{F}=-\frac{\mu}{k}\mathbf{u}-C_2\frac{1}{2}\rho|\mathbf{u}|\mathbf{u}$$

$$\frac{\Delta P}{l} = \frac{150\mu}{D_p^2}\frac{(1-\varepsilon)^2}{\varepsilon^3}u + \frac{1.75\rho}{D_p}\frac{(1-\varepsilon)}{\varepsilon^3}u^2$$

$$\mathbf{F} = -\frac{\mu}{k}\mathbf{u} - C_2\frac{1}{2}\rho|\mathbf{u}|\mathbf{u}$$

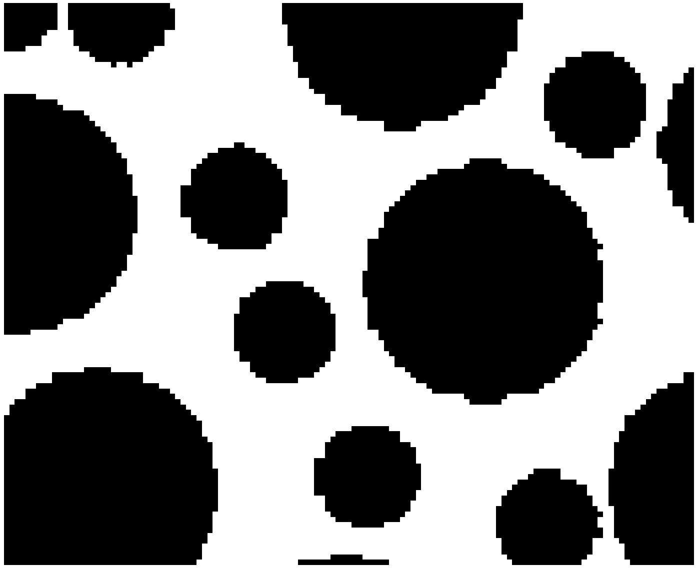
Comparing the two equations, you can obtain C_2.

$$k = \frac{D_p^2}{150}\frac{\varepsilon^3}{(1-\varepsilon)^2}$$

$$C_2 = \frac{3.5}{D_p}\frac{(1-\varepsilon)}{\varepsilon^3}$$

Original energy equation:

$$\frac{\partial(\rho C_p T)}{\partial t} + (\mathbf{u}\cdot\nabla)(\rho C_p T) = \lambda\nabla^2\mathbf{T} + \mathbf{S}$$



For porous media:

Heat transfer in fluid phase as well as in solid phase.

There are two models for heat transfer:

Equilibrium thermal model

Non-Equilibrium thermal model

Equilibrium thermal model

Assume solid phase and fluid phase are in thermal equilibrium. At the fluid-solid phase, temperature and heat flux are continuous.

Original

$$\frac{\partial(\rho C_p T)}{\partial t} + (\mathbf{u}\cdot\nabla)(\rho C_p T) = \lambda\nabla^2 T + S$$

For the first term:

$$\rho C_p T V = (1-\varepsilon)V(\rho C_p)_{\text{solid}} T_{\text{solid}} + \varepsilon V(\rho C_p)_{\text{fluid}} T_{\text{fluid}}$$
$$= \left[(1-\varepsilon)(\rho C_p)_{\text{solid}} + \varepsilon(\rho C_p)_{\text{fluid}}\right] V T$$

$$\rho C_p T = \left[(1-\varepsilon)(\rho C_p)_{\text{solid}} + \varepsilon(\rho C_p)_{\text{fluid}}\right] T$$

For the second term:

$$(\mathbf{u}\cdot\nabla)(\varepsilon\rho C_p T)$$

As convective term is only for fluid phase!

For the diffusion term:

$$\lambda\nabla^2 TV = V(1-\varepsilon)\lambda_s\nabla^2 T_s + V\varepsilon\lambda_f\nabla^2 T_f$$

$$= \left[V(1-\varepsilon)\lambda_s + V\varepsilon\lambda_f\right]\nabla^2 T$$

$$\lambda\nabla^2 T = \left[(1-\varepsilon)\lambda_s + \varepsilon\lambda_f\right]\nabla^2 T$$

For the source term

$$SV = (1-\varepsilon)\mathrm{V}\,S_s + \varepsilon V S_f$$

$$\frac{\partial\left(\left[(1-\varepsilon)(\rho C_p)_{\text{solid}}+\varepsilon(\rho C_p)_{\text{fluid}}\right]T\right)}{\partial t}+(\mathbf{u}\cdot\nabla)(\varepsilon\rho C_p T)$$
$$=\left[(1-\varepsilon)\lambda_s+\varepsilon\lambda_f\right]\nabla^2 T+\left[(1-\varepsilon)S_s+\varepsilon S_f\right]$$

$$(\rho C_p)_{\text{eff}}=\left[(1-\varepsilon)(\rho C_p)_{\text{solid}}+\varepsilon(\rho C_p)_{\text{fluid}}\right]$$

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

The final energy equation for porous media

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

Continuum-scale equations for porous flow

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

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

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

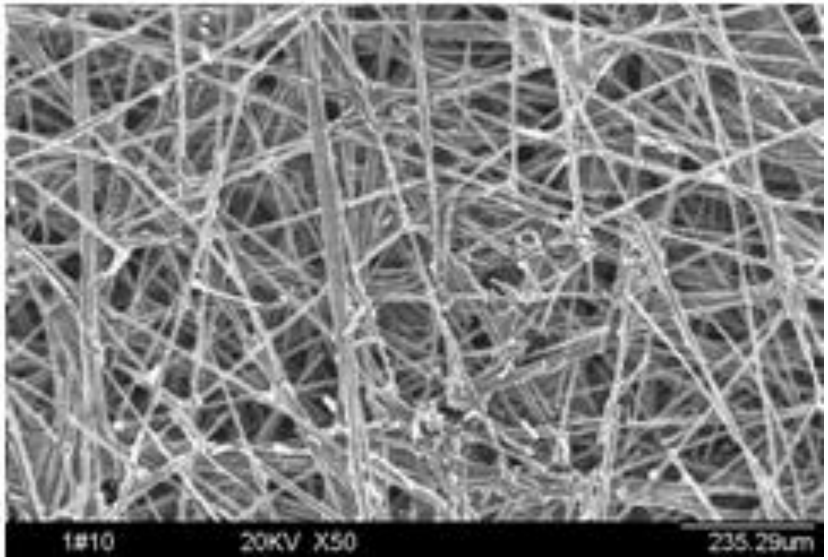
$$\frac{\partial((\rho C_p)_{\text{eff}} T)}{\partial t} + (\mathbf{u}_{\text{superficial}} \cdot \nabla)(\rho C_p T) = \lambda_{\text{eff}}\nabla^2 T + S_{\text{eff}}$$

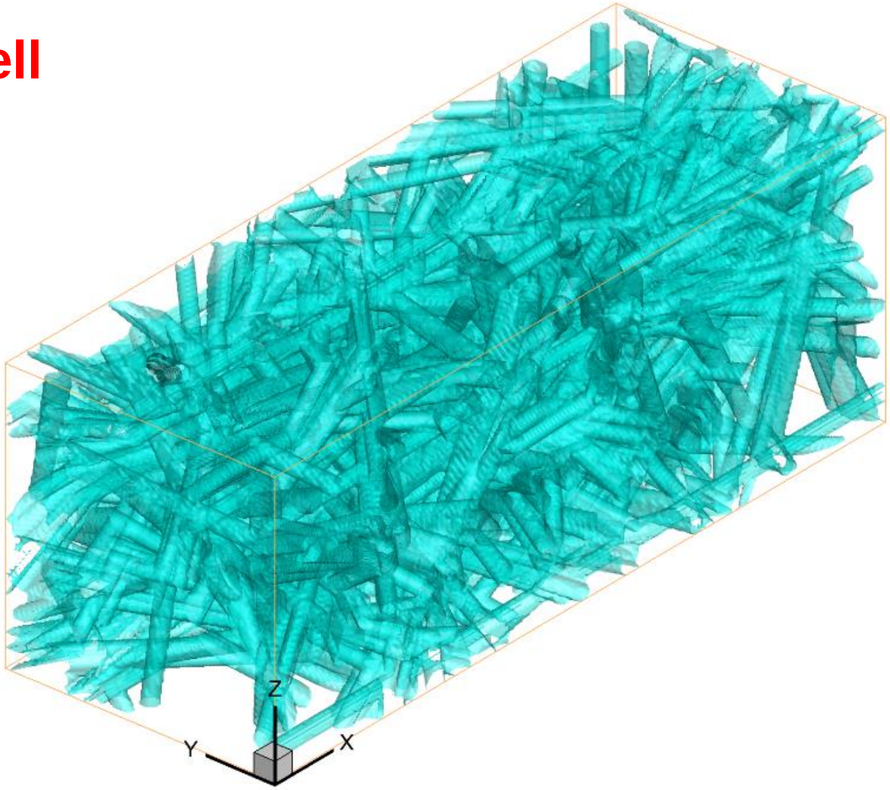
$$\lambda_{\text{eff}} = (1-\varepsilon)\lambda_s + \varepsilon\lambda_f$$

Content

2.4 Reconstruction

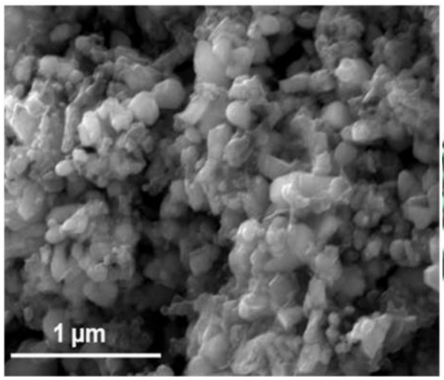
Fiber porous media in PEM fuel cell

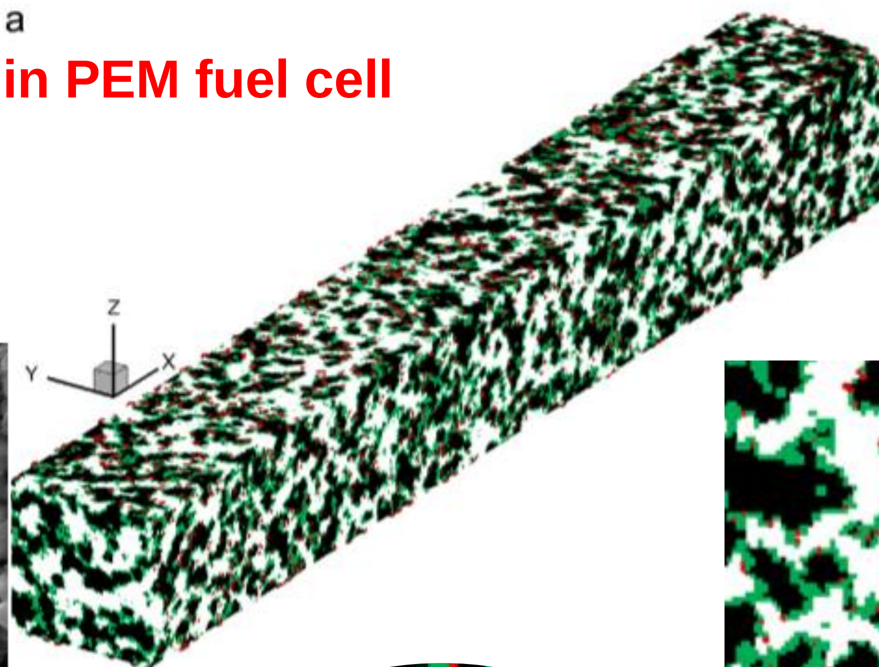


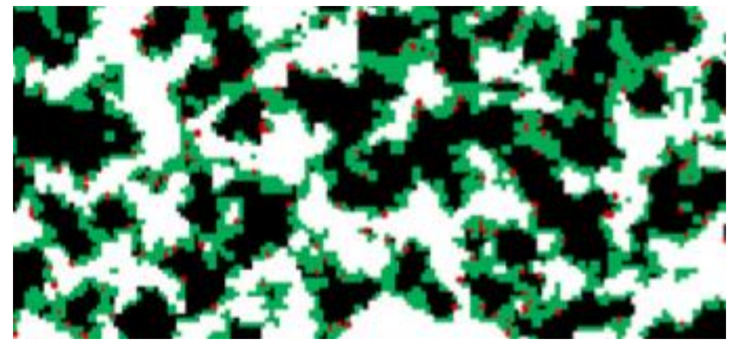


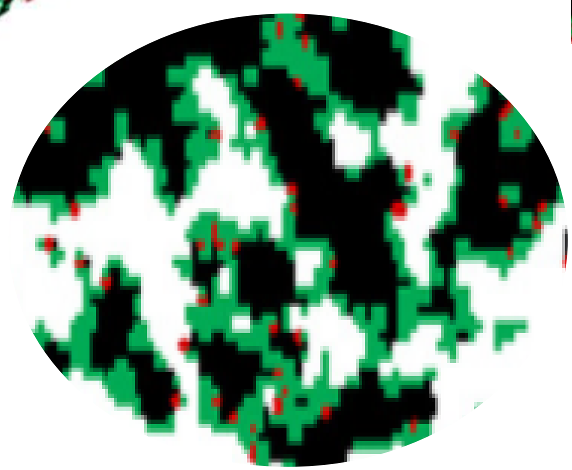
1. **L Chen**, YL He, WQ Tao, P Zelenay, R Mukundan, Q Kang, Pore-scale study of multiphase reactive transport in fibrous electrodes of vanadium redox flow batteries, , Electrochimica Acta 248, 425-439;
2. **L. Chen***, H.B. Luan, Y.-L. He, W.-Q. Tao, Pore-scale flow and mass transport in gas diffusion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

Catalyst layer in PEM fuel cell



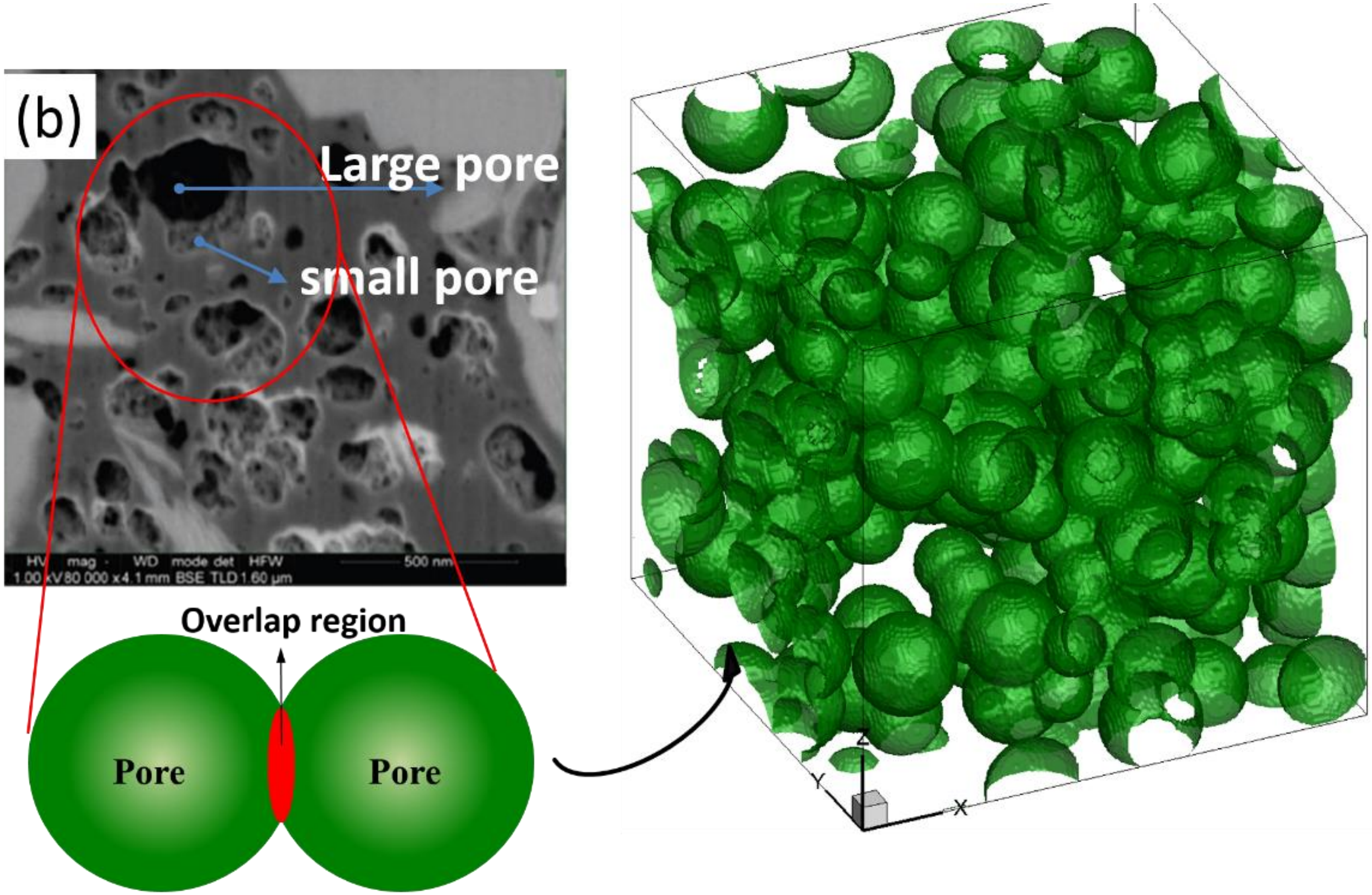






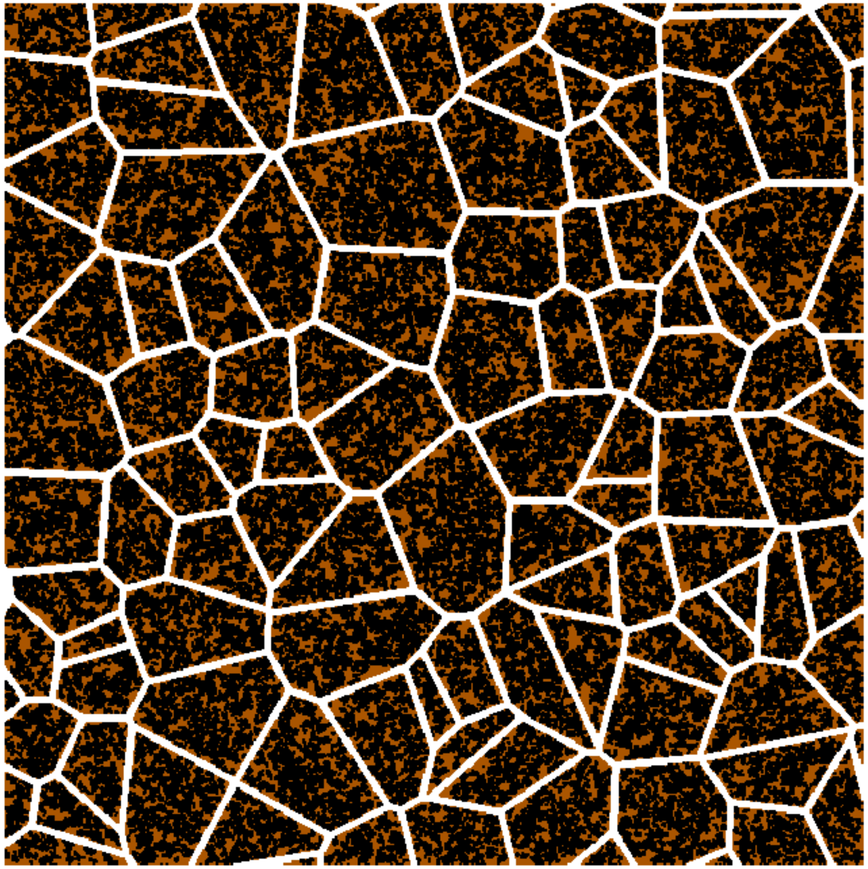
L. Chen, G. Wu, E. Holby, P. Zelenay, W.Q. Tao, Q. Kang, Lattice Boltzmann Pore-Scale Investigation of Coupled Physical-electrochemical Processes in C/Pt and Non-Precious Metal Cathode Catalyst Layers in Proton Exchange Membrane Fuel Cell, 2015, 158, 175-186, Electrochimica Acta

Organic matter in shale gas



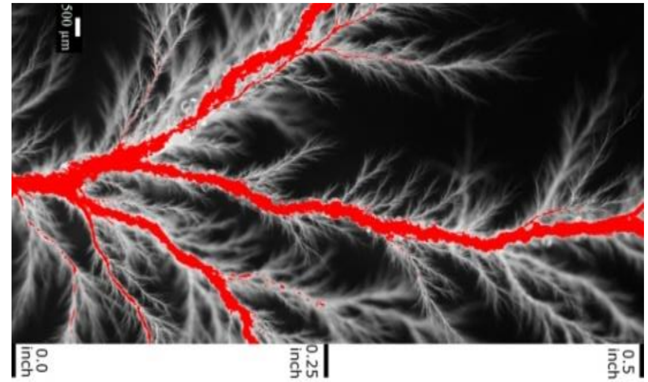
L. Chen, L Zhang, Q Kang, W.Q. Tao, Nanoscale simulation of shale transport properties using the lattice Boltzmann method: permeability and diffusivity, 2015, 5, 8089, Scientific Reports

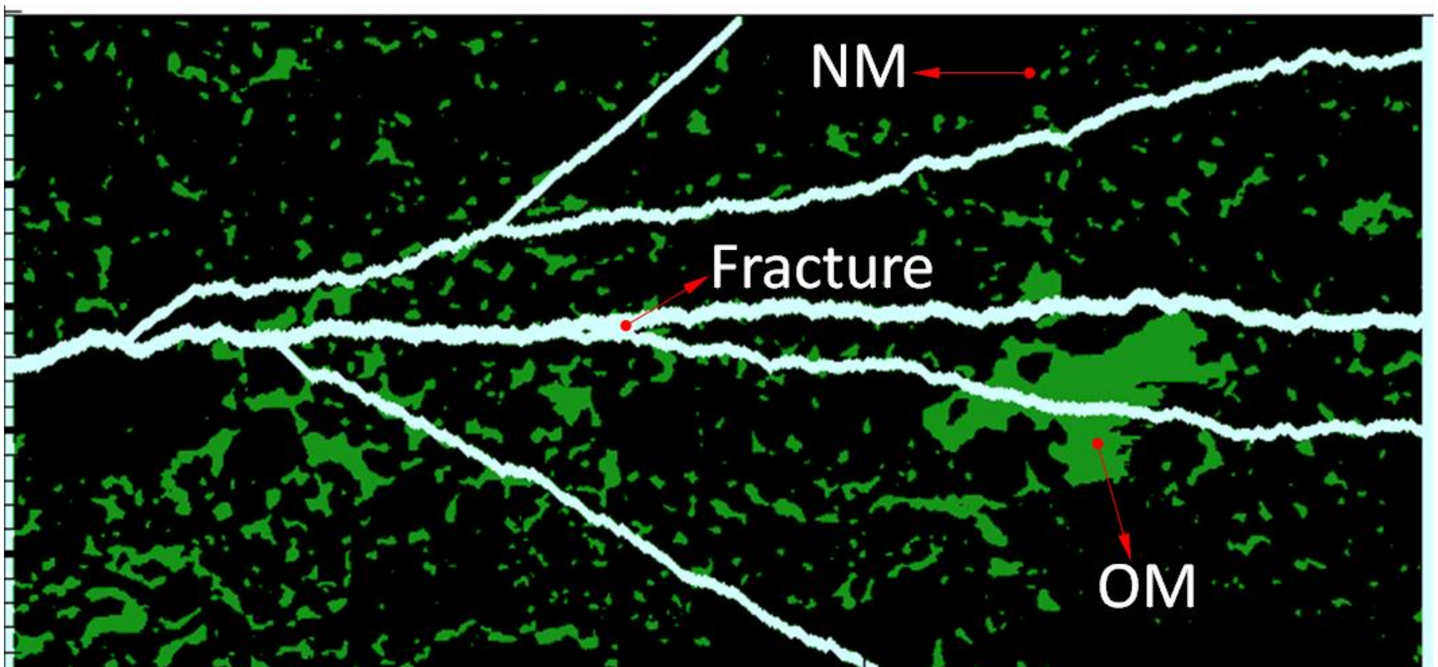
Porous rock



L. Chen, Q. Kang, H. Viswanathan, W.Q. Tao, Pore-scale study of dissolution-induced changes in hydrologic properties of rocks with binary minerals, 2014, 50 (12), WR015646, Water Resource Research

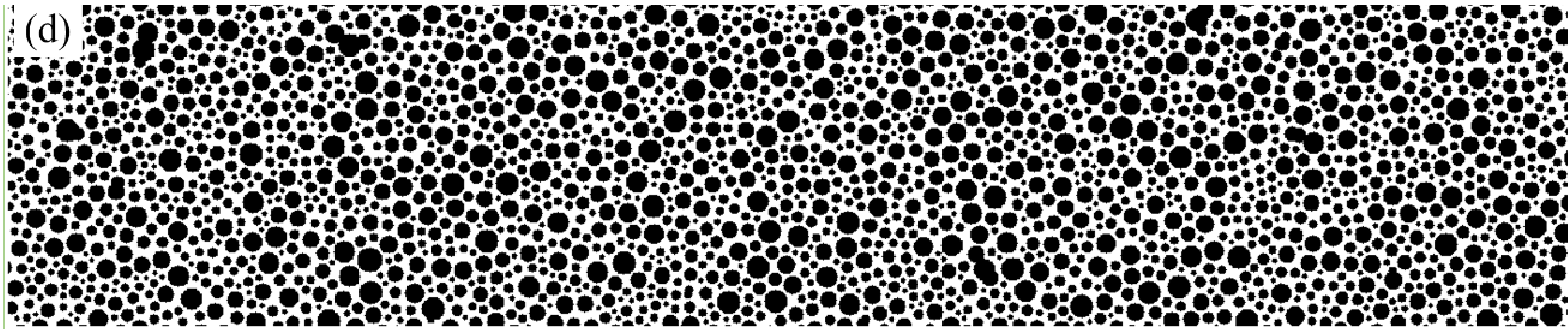
Fractures under subsurface





L. Chen, F Wang, Q, Kang, J. Hyman, H. Viswanathan, W. Tao, Generalized lattice Boltzmann model for flow through tight porous media with Klinkenberg's effect, 2015, 91(3), 033004, Physical Review E.

Random spheres with uniform gap



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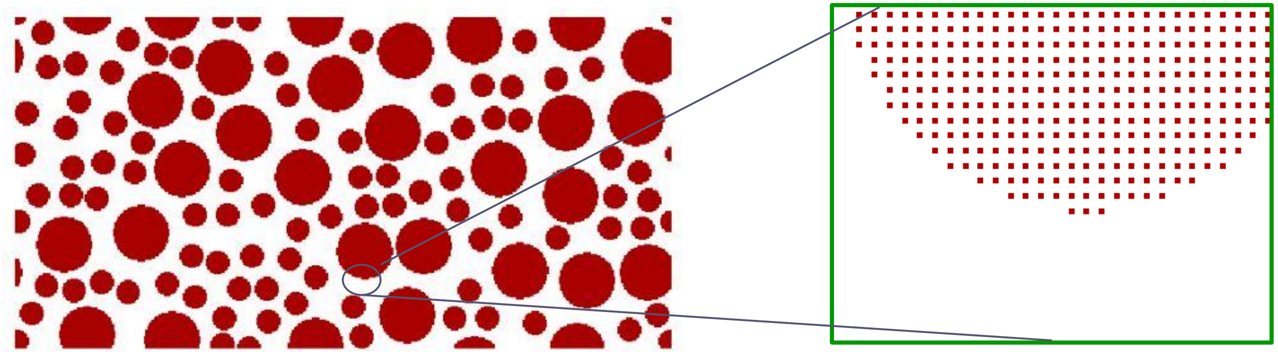
L Chen, M Wang, Q Kang, W Tao, Pore scale study of multiphase multicomponent reactive transport during CO2 dissolution trapping, *Advances in Water Resources*, 2018, 116, 208-218

Content

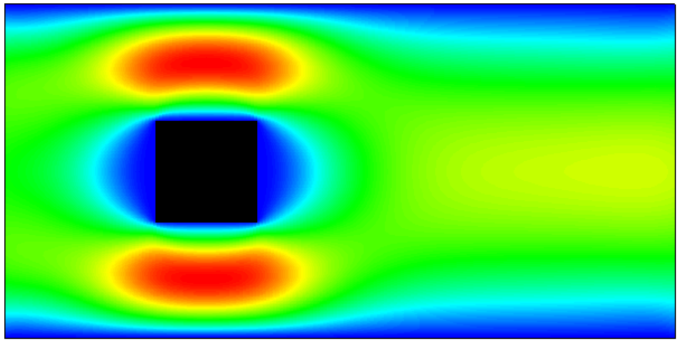
Digitalized Structures

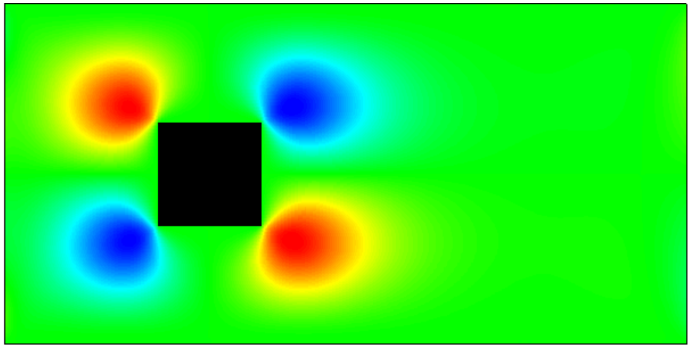


A 2D matrix is adopted to represent the porous media, with 1 as solid and 0 as fluid.

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

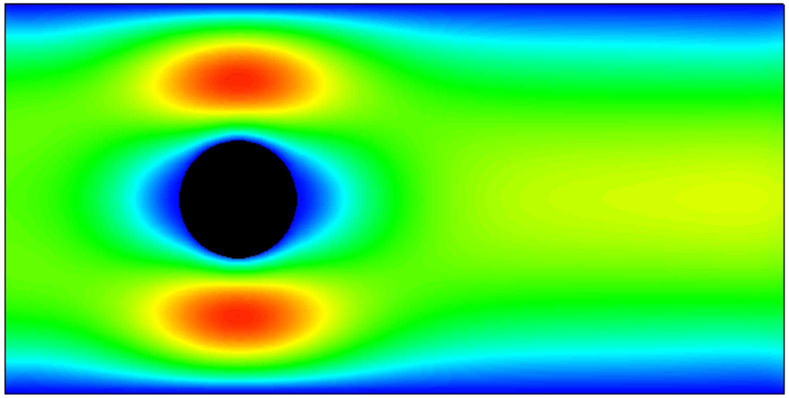
Flow around a square

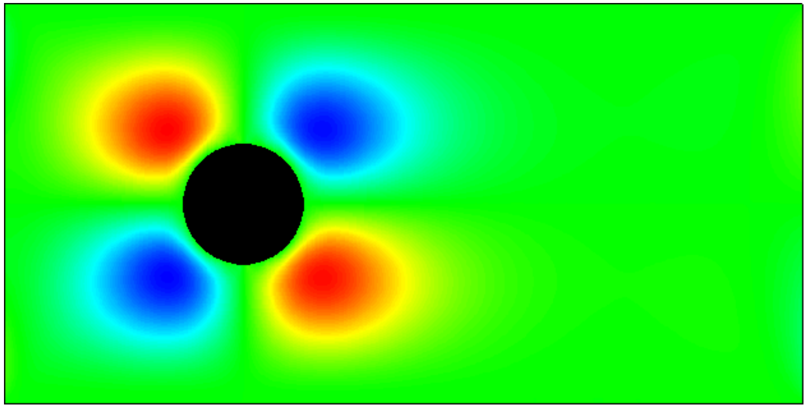




```
!===========================================================================-=
SUBROUTINE SOLID_STRUCTURE
USE START_L
   ! ls represents the porous structure: 0 denotes nodes of void space, 1 denotes solid node.
   ls=0
   ls(:,ny:ny+1)=1
   ls(:,0:1)=1
   icenter=61
   jcenter=ny/2+1
   ls(icenter-15:icenter+15,jcenter-15:jcenter+15)=1
   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
!============================================================================
```

Flow around a circle





```
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
!===========================================================================
```

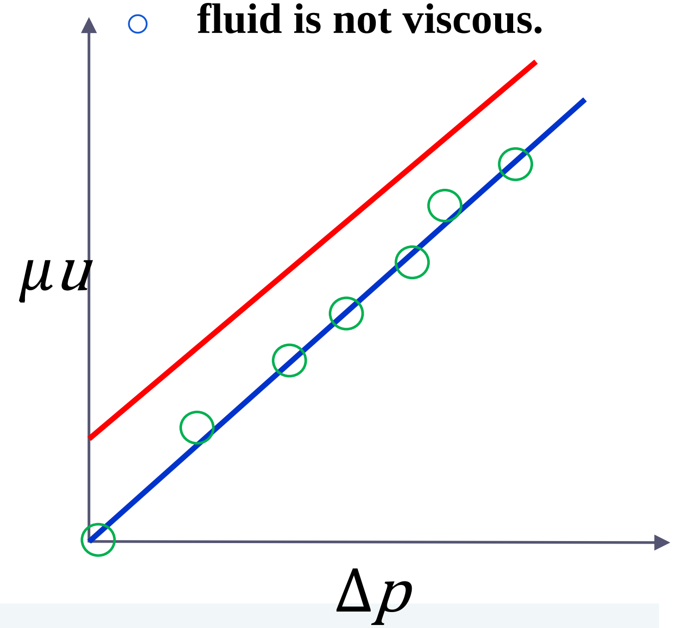
Permeability

- **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 Δ*p*, he introduced permeability to describe the conductivity of the porous media. The Darcy' law is as follows**

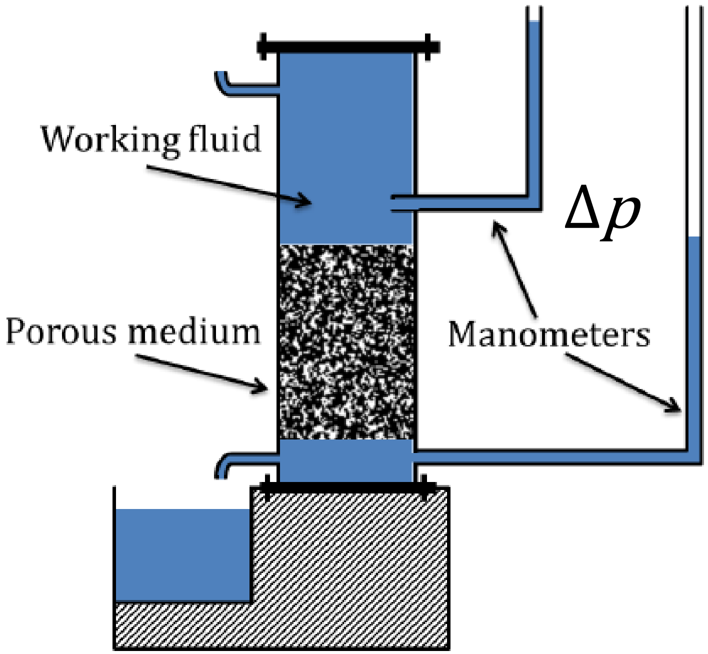
$$< u > = -\frac{k}{\mu}\frac{\Delta p}{l}$$

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

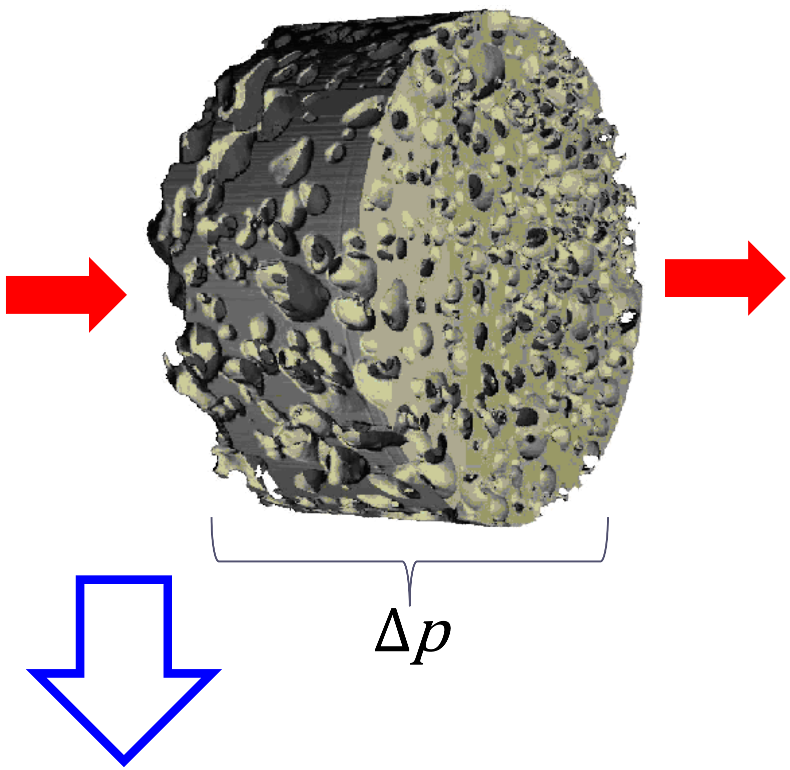


- ***q* flow rate (m/s), *μ* the viscosity, pressure drop Δ*p*, length of the porous domain *l*, *k* is the permeability.**

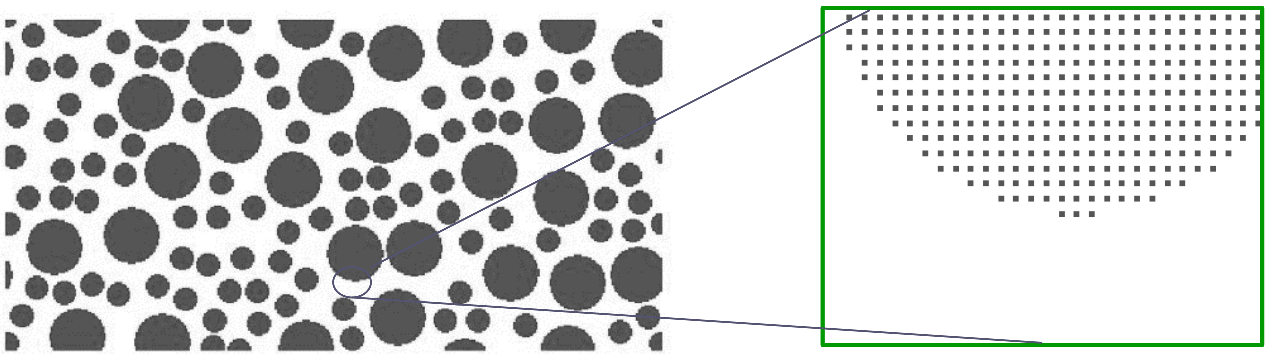
Schematic of Darcy's experiment



Simulation mimic the experiment

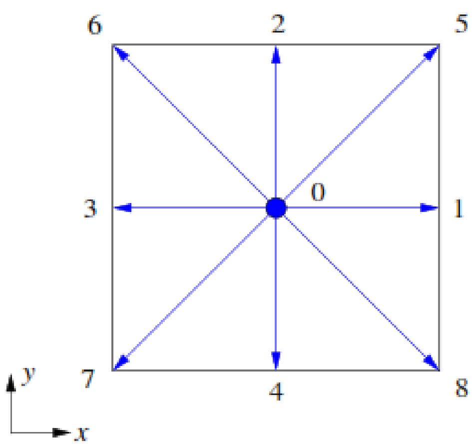


NS equation is solved at the pore scale. Non-slip boundary condition for the fluid-solid interface



Bounce-back at the solid surface

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



Collision

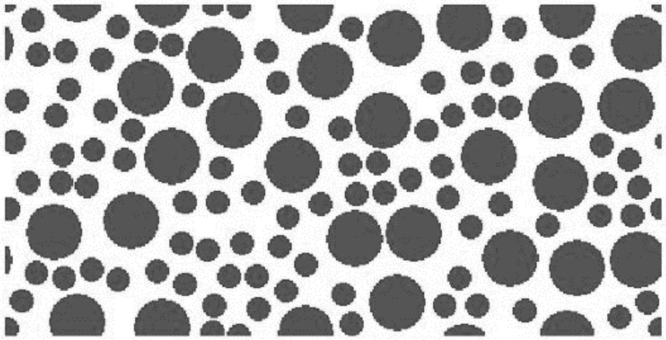
$$f_i^{'}(\mathbf{x},t) = -\frac{1}{\tau}\left(f_i(\mathbf{x},t) - f_i^{\mathrm{eq}}(\mathbf{x},t)\right)$$

Streaming

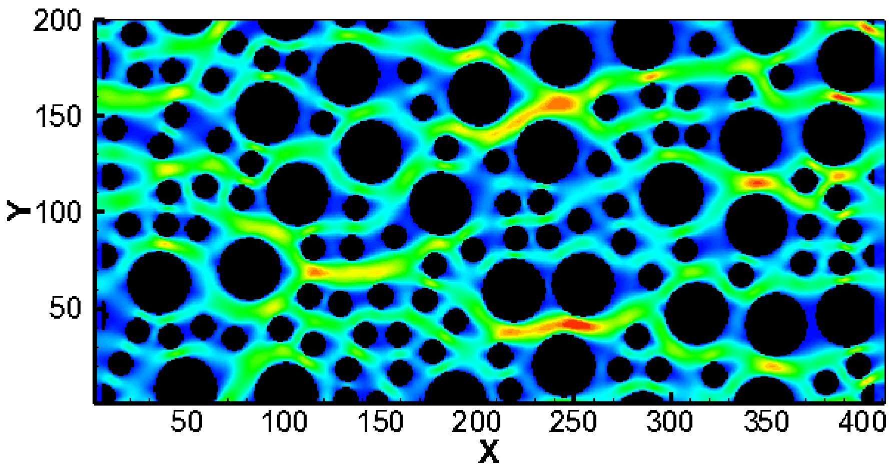
$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) = f_i^{'}(\mathbf{x},t)$$

Macroscopic variables calculation

$$\rho = \sum_{i=0} f_i, \quad \rho\mathbf{u} = \sum_{i=0} f_i\mathbf{e}_i.$$



- **Bounce-back at the solid surface**
- **Pressure drop across *x* direction**
- **Periodic boundary condition *y***

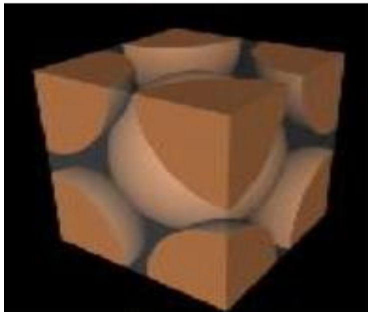


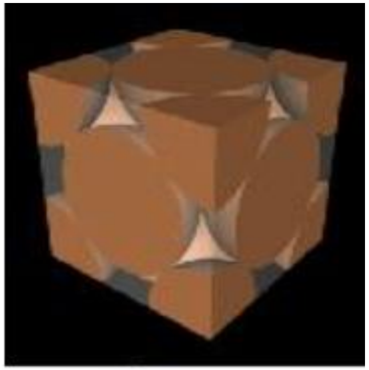
- **Analyze the detailed flow field**
- **Calculate permeability based on Darcy equation.**

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

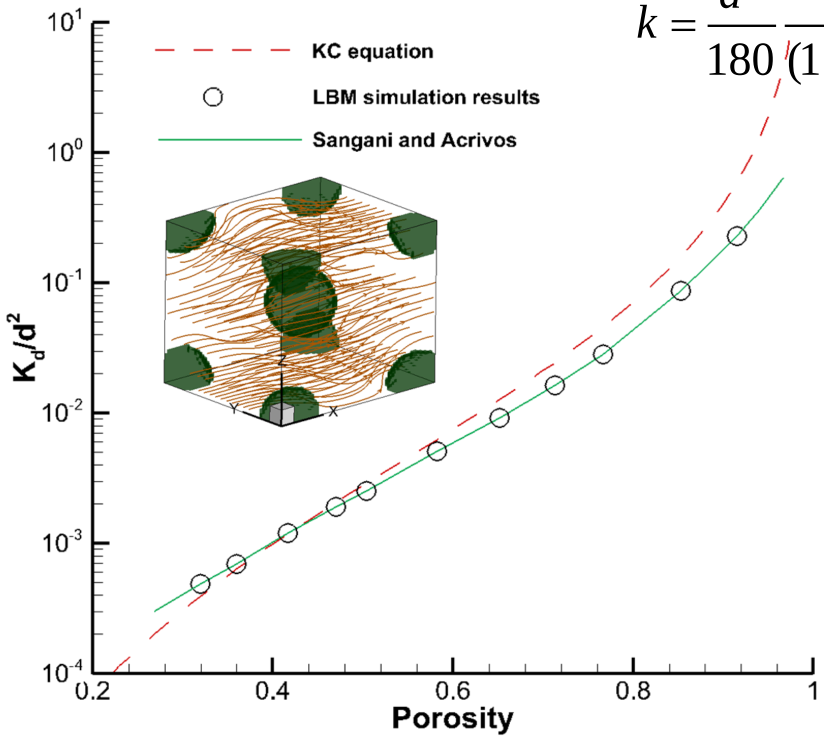
Permeability

- **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**





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

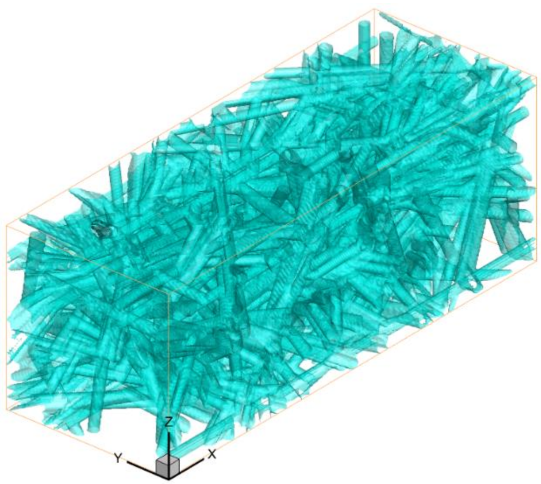


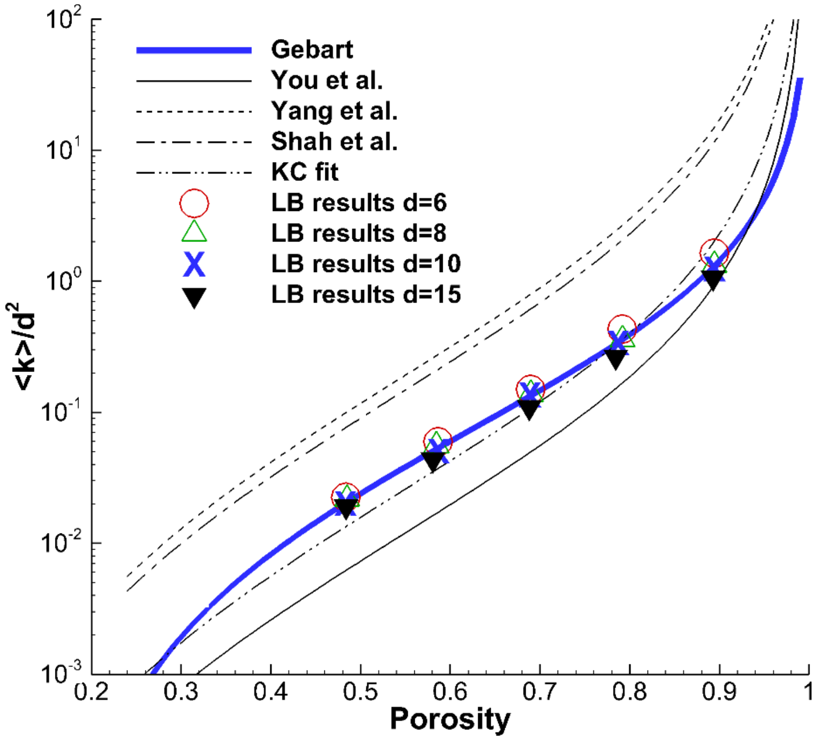
L. Chen, L Zhang, Q Kang, W.Q. Tao, Nanoscale simulation of shale transport properties using the lattice Boltzmann method: permeability and diffusivity, 2015, 5, 8089, Scientific Reports

Permeability

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

$$k = r^2 A\left(\sqrt{\frac{1-\varepsilon_c}{1-\varepsilon}} - 1\right)^B$$





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

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

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

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

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

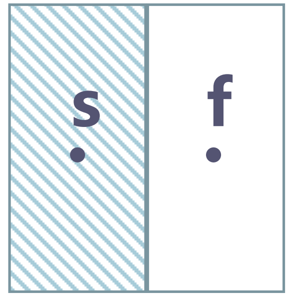
thermal diffusivity of the material.

At the fluid-solid interface

$$T_{\mathrm{f}} = T_{\mathrm{s}}$$

$$-\lambda_{\mathrm{f}} \frac{\partial (T)_{\mathrm{f}}}{\partial n_{\mathrm{f}}} = \lambda_{\mathrm{s}} \frac{\partial (T)_{\mathrm{s}}}{\partial n_{\mathrm{s}}}$$

Conjugate heat transfer



$$T_{\mathrm{f}} = T_{\mathrm{s}}$$

$$-\alpha_{\mathrm{f}} \frac{\partial (\rho C_{\mathrm{P}} T)_{\mathrm{f}}}{\partial n_{\mathrm{f}}} = \alpha_{\mathrm{s}} \frac{\partial (\rho C_{\mathrm{P}} T)_{\mathrm{s}}}{\partial n_{\mathrm{s}}}$$

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 one!!!!

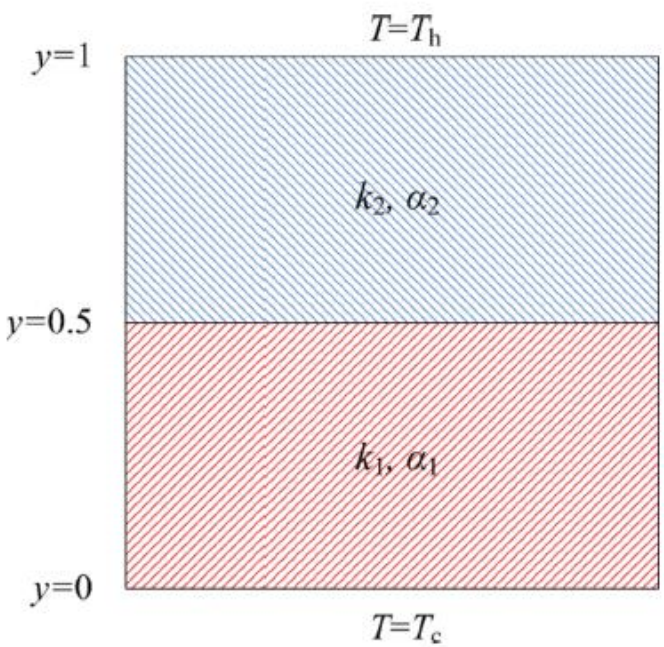


FIG. 1. (Color online) Schematic of two-layer stratified medium.

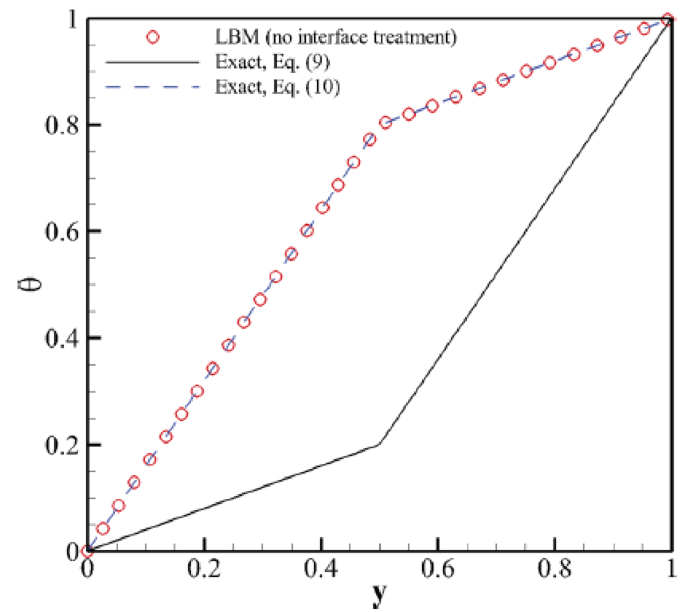


FIG. 2. (Color online) Comparison of LBM solution with analytical solutions for two-layered stratified medium.

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

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

LB model for predicting thermal conductivity

Standard energy governing equation

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

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

s $\quad 0 = \nabla \cdot (\lambda \nabla T)$

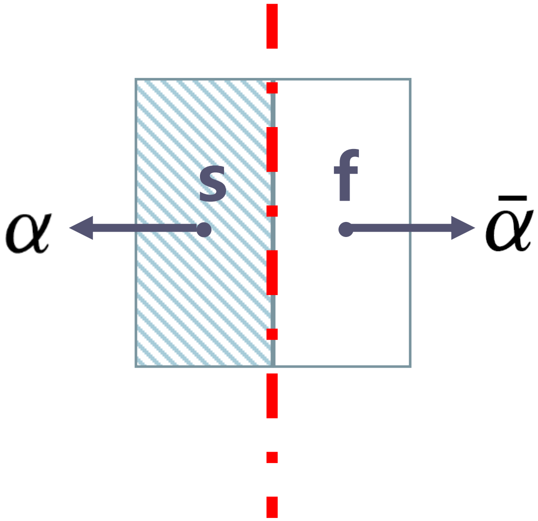
"pseudo-capacity of solid phase" scheme

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

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

$$g_\alpha(\mathbf{r}+\mathbf{e}_\alpha\delta_t) - g_\alpha(\mathbf{r},t) = -\frac{1}{\tau_g}\left[g_\alpha(\mathbf{r},t) - g_\alpha^{\mathrm{eq}}(\mathbf{r},t)\right]$$

$$\tau_g = \frac{3}{2}\frac{\lambda}{\rho c_p c^2 \delta t} + 0.5$$

SRT is employed. Thus cannot take into account anisotropic thermal conductivity

$$T = \sum_\alpha g_\alpha$$

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

MRT model

$$h_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta t, t+\delta t) - h_\alpha(\mathbf{x},t) = -\mathbf{M}^{-1}\mathbf{S}\mathbf{M}(h_\alpha - h_\alpha^{eq}) + \omega_\alpha S$$

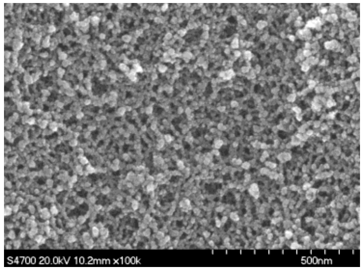
$$\mathbf{M} = \begin{bmatrix} 1, & 1, & 1, & 1, & 1, & 1, & 1 \\ 0, & 1, & -1, & 0, & 0, & 0, & 0 \\ 0, & 0, & 0, & 1, & -1, & 0, & 0 \\ 0, & 0, & 0, & 0, & 0, & 1, & -1 \\ 6, & -1, & -1, & -1, & -1, & -1, & -1 \\ 0, & 2, & 2, & -1, & -1, & -1, & -1 \\ 0, & 0, & 0, & 1, & 1, & -1, & -1 \end{bmatrix}$$

$$\mathbf{S}^{-1} = \begin{bmatrix} \tau_0, & 0, & 0, & 0, & 0, & 0, & 0 \\ 0, & \tau_{xx}, & \tau_{xy}, & \tau_{xz}, & 0, & 0, & 0 \\ 0, & \tau_{yx}, & \tau_{yy}, & \tau_{yz}, & 0, & 0, & 0 \\ 0, & \tau_{zx}, & \tau_{zy}, & \tau_{zz}, & 0, & 0, & 0 \\ 0, & 0, & 0, & 0, & \tau_4, & 0, & 0 \\ 0, & 0, & 0, & 0, & 0, & \tau_5, & 0 \\ 0, & 0, & 0, & 0, & 0, & 0, & \tau_6 \end{bmatrix}$$

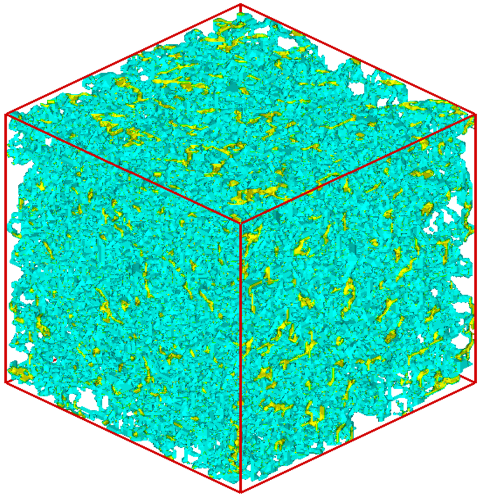
$$\tau_{ij} = \frac{1}{2}\delta_{ij} + \frac{\delta t}{\varepsilon(\delta x)^2} D_{ij}$$

Yoshida, H. and M. Nagaoka, Multiple-relaxation-time lattice Boltzmann model for the convection and anisotropic diffusion equation. Journal of Computational Physics, 2010. 229(20): p. 7774-7795.

For heterogeneous anisotropic materials.



Aerogel: low density and *k*

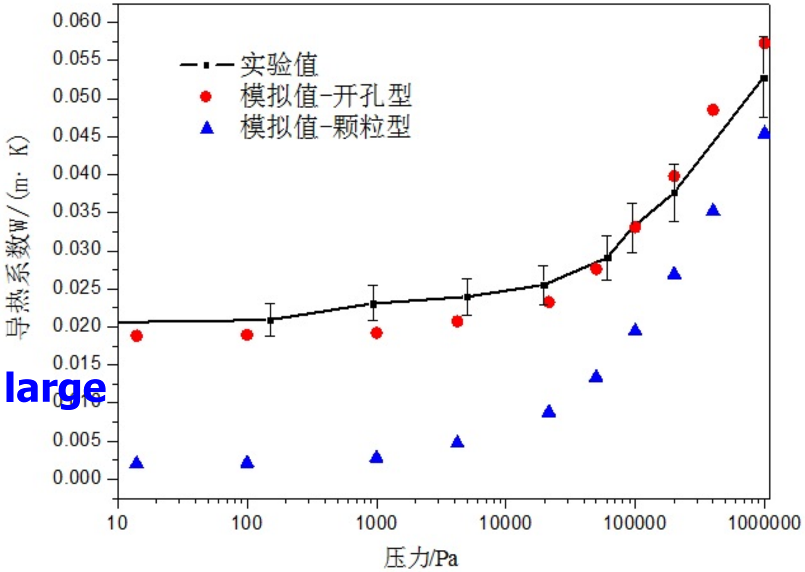


Different components with large variations of *k*

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

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

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



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.

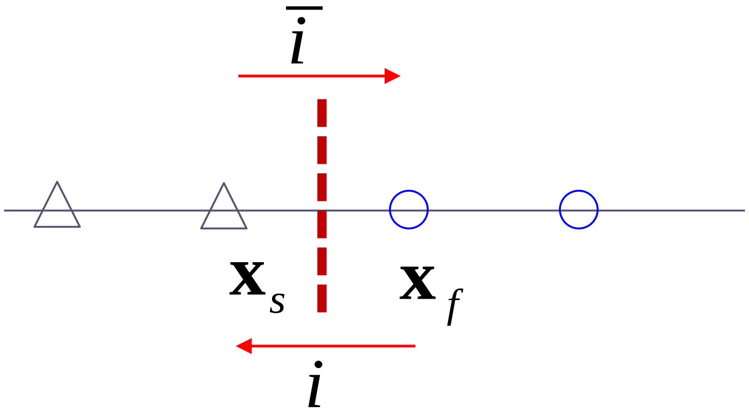
1. Treat the interface as boundary

Dirichlet condition

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

Neumann equation

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



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

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

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

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

2. Re-arrange the governing equation

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

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

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

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

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

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

2. Re-arrange the governing equation

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

$h^* = (\rho C_\mathrm{p})_0 T$ $\qquad$ $\sigma = \rho C_\mathrm{p} / (\rho C_\mathrm{p})_0$

$$\frac{\partial(\sigma h^*)}{\partial t} + \nabla \cdot (\sigma h^* \mathbf{u}) = \nabla \cdot (\lambda \nabla \frac{h^*}{(\rho C_\mathrm{p})_0})$$

$$\sigma \frac{\partial h^*}{\partial t} + h^* \frac{\partial \sigma}{\partial t} + \sigma \nabla \cdot (h^* \mathbf{u}) + h^* \mathbf{u} \nabla \cdot \sigma = \nabla \cdot (\lambda \nabla \frac{h^*}{(\rho C_\mathrm{p})_0})$$

$$\frac{\partial h^*}{\partial t} + \nabla \cdot (h^* \mathbf{u}) = \frac{1}{\sigma} \nabla \cdot (\lambda \nabla \frac{h^*}{(\rho C_\mathrm{p})_0}) - \frac{h^*}{\sigma} \mathbf{u} \nabla \cdot \sigma$$

$$\frac{\partial h^*}{\partial t}+\nabla\cdot(h^*\mathbf{u})=\frac{1}{\sigma}\frac{1}{(\rho C_p)_0}\nabla\cdot\left(\frac{\lambda}{\rho C_p}\rho C_p\nabla h^*\right)-\frac{h^*}{\sigma}\mathbf{u}\nabla\cdot\sigma$$

$$\frac{\partial h^*}{\partial t}+\nabla\cdot(h^*\mathbf{u})=\frac{1}{\sigma}\frac{1}{(\rho C_p)_0}\nabla\cdot(\alpha\rho C_p\nabla h^*)-\frac{h^*}{\sigma}\mathbf{u}\nabla\cdot\sigma$$

$$=\frac{1}{\sigma}\frac{1}{(\rho C_p)_0}\left[\rho C_p\nabla\cdot(\alpha\nabla h^*)+\alpha\nabla\cdot(\rho C_p\nabla h^*)\right]-\frac{h^*}{\sigma}\mathbf{u}\nabla\cdot\sigma$$

$$=\nabla\cdot(\alpha\nabla h^*)+\frac{1}{\sigma}\frac{1}{(\rho C_p)_0}\alpha\nabla\cdot(\rho C_p\nabla h^*)-\frac{h^*}{\sigma}\mathbf{u}\nabla\cdot\sigma$$

$$\frac{\partial h^*}{\partial t}+\nabla\cdot(h^*\mathbf{u})=\nabla\cdot(\alpha\nabla h^*)+\underbrace{\frac{1}{\sigma}\frac{1}{(\rho C_p)_0}\alpha\nabla\cdot(\rho C_p\nabla h^*)-\frac{h^*}{\sigma}\mathbf{u}\nabla\cdot\sigma}_{S^*}$$

Hamid Karani et al., PRE, 2015, 91, 023304

LB model for mass 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

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

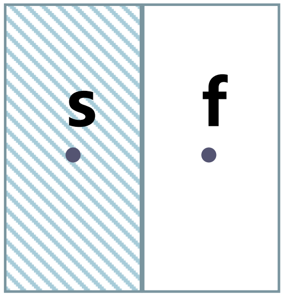
Concentration

$$C=\sum_i g_i$$

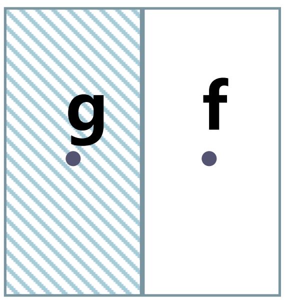
Diffusivity

$$D=\frac{1}{3}(\tau-0.5)\frac{(\Delta x)^2}{\Delta t}$$

At the fluid-solid interface

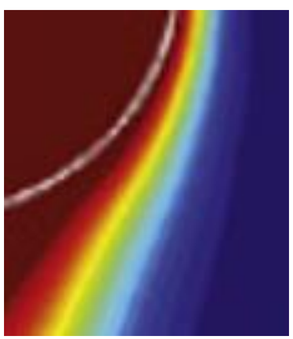


Mass transport does not take place inside the solid phase. Thus, only mass transport inside the void space needs to be considered.



$$C_{\mathrm{L}} = HC_{\mathrm{g}}$$

$$D_g \frac{\partial C_g}{\partial n_g} = \lambda_{\mathrm{s}} \frac{\partial C_L}{\partial n_L}$$



The non-continuous concentration across the phase interface poses additional challenge for numerical simulations.

同舟共济
渡彼岸！