Network modelling of coupled heat transfer and fluid flow at pore-to-mesoscale using MpNM - A Multi-physics Network Model

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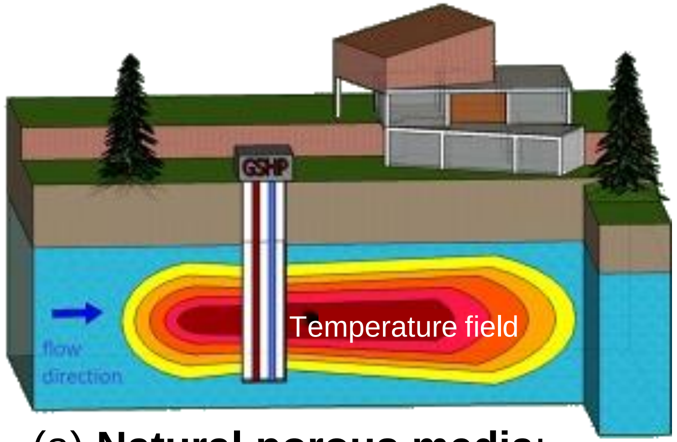
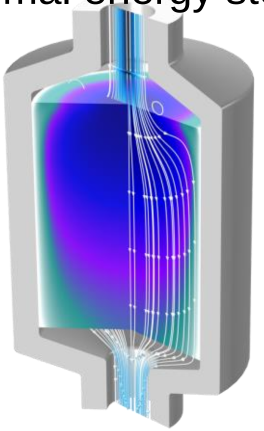
Background

- **Prediction of properties in large systems (cm scale and above) with complex pore structure is important but challenging in many engineering applications**

Large porous media



(a) **Natural porous media**:
e.g. Thermal energy storage



(b) **Engineering porous media**:
e.g. Packed bed reactor, heat exchanger

Challenges

- **Multi-physics processes:**
  - **Coupled heat and mass transfer**
  - **Reaction involved**
- **Pore-scale impacts on large scale:**
  - **Heterogeneity**
  - **Preferential transport path**
- **Large length and time scales**
- **Complex pore structure**
  - **Tortuous**
  - **Irregular**
  - **…**
- **Experimental characterization is difficult**

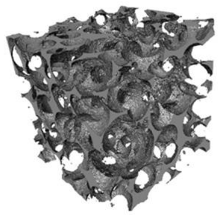
Background

- **Simulations can obtain more detailed information, but how to cross scales remains unresolved.**

Microscopic behaviour

Macroscopic behaviour

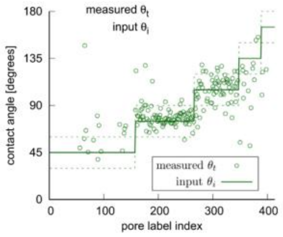
Digital structure



Physical parameters

- Viscosity,
- Density,
- Temperature,
- Conductivity
- …

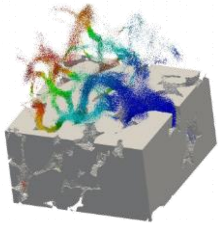
Microscopic mechanism



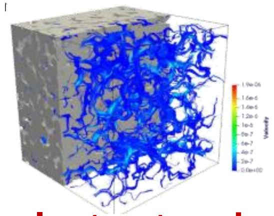
INPUT

DNS

FVM

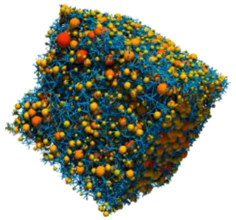


LBM



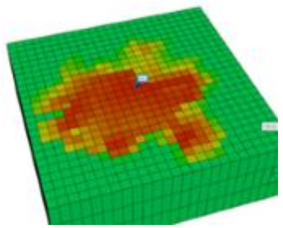
Equivalent network method

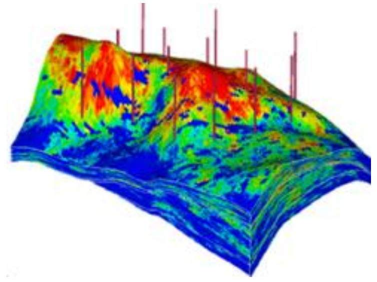
PNM



?

How to connect two scales





Continuum model

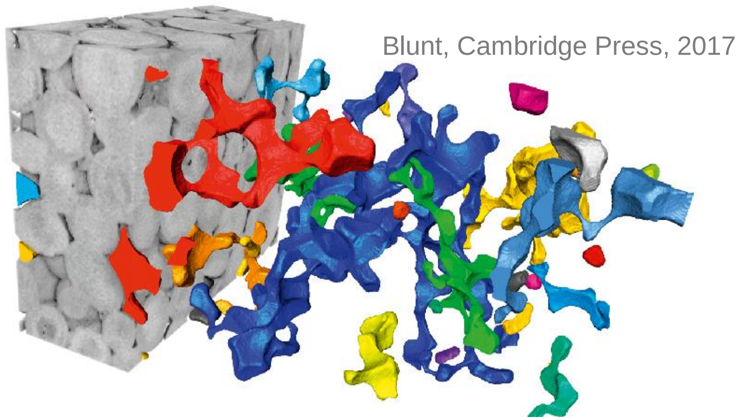
The computational domain is small (nm~μm), difficult to show macroscopic characteristics

The macro scale model can be used to calculate large scale problems (cm~m), but lose pore-scale detail.

It is essential to develop models to consider pore-scale behaviour and reflect the macroscopic characteristics: Pore-to-mesoscale

Requirement for pore-to-mesoscopic model

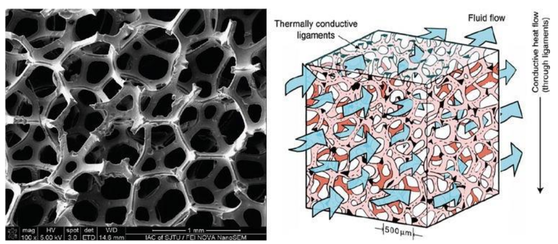
Most pore-scale models are designed for applications in the oil and gas industry where the applications are, to some extent, limited.



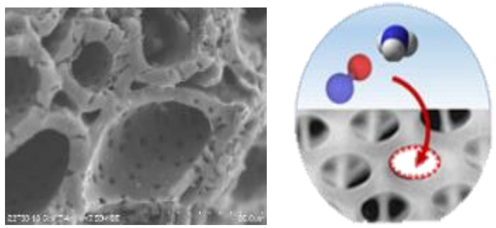
Blunt, Cambridge Press, 2017

Flow and displacement
- ✓ Capillary-controlled flow
- ✓ Often rule-based
- ✓ Emphasis on predicting absolute and relative permeability

Pore-scale models need to be more general to study complex processes in porous media in other fields and make a difference, for example, in applications associated with the energy transition.



Porous foam metal for enhanced heat transfer



Porous catalyst requires optimized transport processes

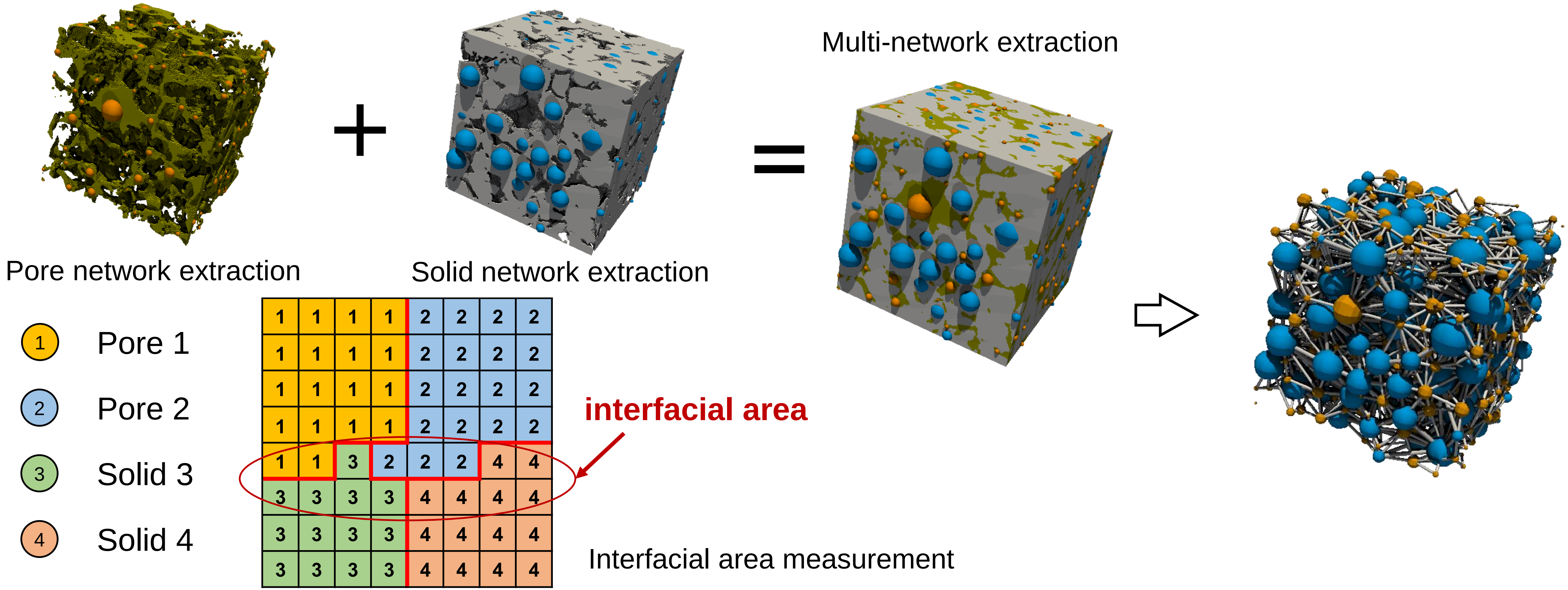
Multi-physics process:
- ✓ Steady-state process
- ✓ Transient process
- ✓ Mass transfer
- ✓ Heat transfer
- ✓ Reactive flow

We have developed an open-source Multi-physics Network Model (MpNM) in PYTHON.

Contents

Dual-network

- **The network extraction was applied to generate solid and void networks.**
- **The topological and geometric information for the links connecting the two networks was obtained in order to construct the dual-network**



Interfacial areas for heat transfer

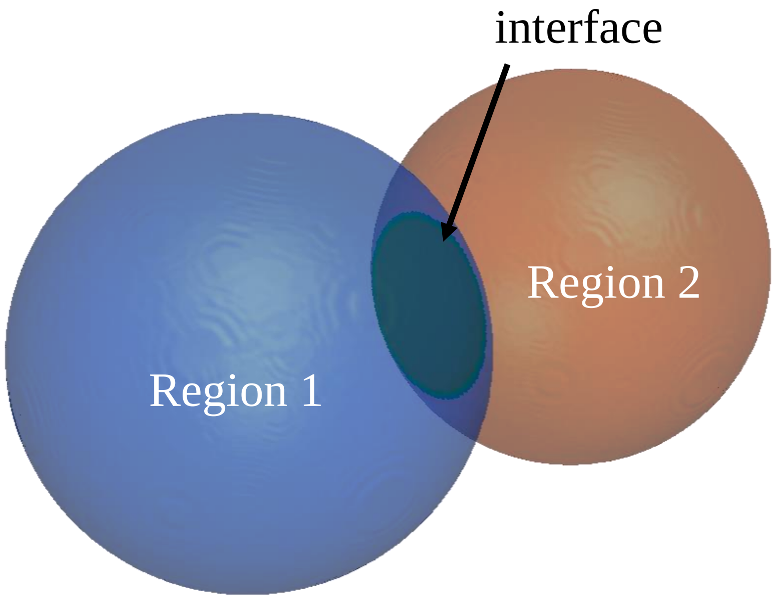


Fig.1 3D schematic

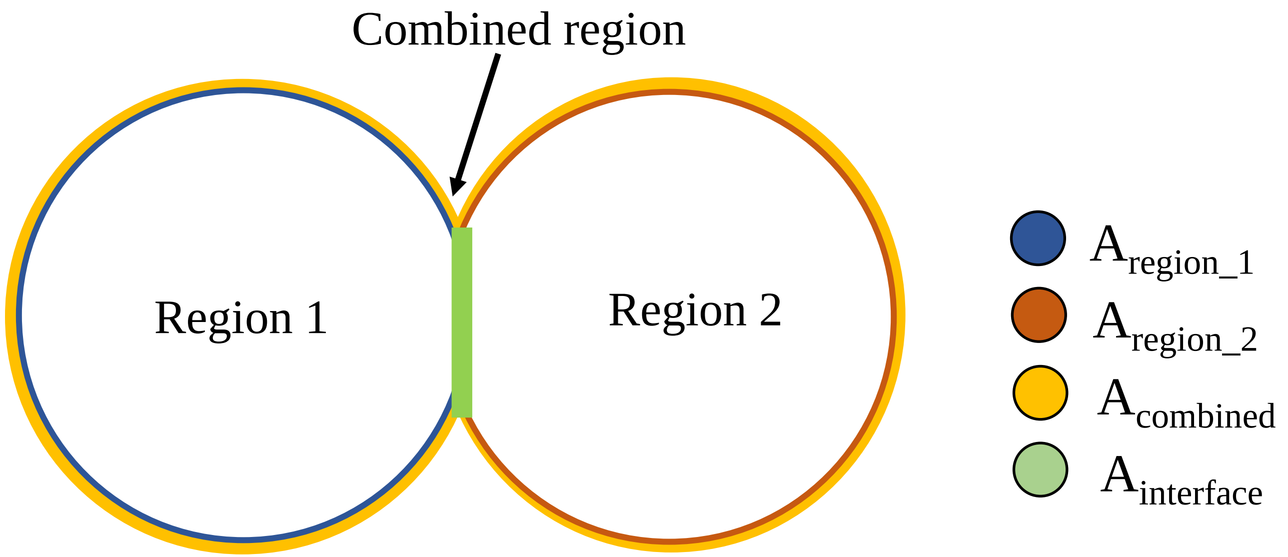


Fig.2 2D schematic

$$A_{interface} = \frac{(A_{region\_1} + A_{region\_2} - A_{overall})}{2}$$

where A_{region_1} and A_{region_2} are individual surface area, the overall surface area excluding the interfacial area is $A_{overall}$.

Governing equations

Mass balance $$\sum_{j=1}^{N_j} g_{ij}\left(P_i - P_j\right) = 0$$

Energy balance $$\sum_{j=1}^{N_{j,void}} g_{ij} c_p \rho\left(P_{i,void} - P_{j,void}\right) T_{i/j,void} - \sum_{j=1}^{N_{j,solid}} A_{ij}\left(T_{i,void} - T_{j,solid}\right) h_{sf} - \sum_{j=1}^{N_{j,void}} \frac{A_{ij}}{L_{ij}}\left(T_{i,void} - T_{j,void}\right)\lambda_f = 0$$

$$\mu = \mu_0 exp\left[aP + \frac{E-bP}{R(T-\theta-cP)}\right]$$ (Likhachev 2003)

$$\begin{cases} Re_{i,void} = \rho v_i d_{i,void}/\mu \\ d_{i,void} = 6V_{i,void}/A_{i,void} \\ Pr = \mu c_p/\lambda_f \end{cases}$$

$$Nu_{sf} = 2 + \left(0.4 Re_{i,void}{}^{1/2} + 0.06 Re_{i,void}{}^{2/3}\right) Pr^{0.4}$$ (Whitaker, 1972)

$$h_{sf} = \frac{1}{\frac{l_{i,void}}{Nu_{sf}\lambda_f} + \frac{l_{i,solid}}{\beta\lambda_{i,solid}}}$$ (Dixon 1979)

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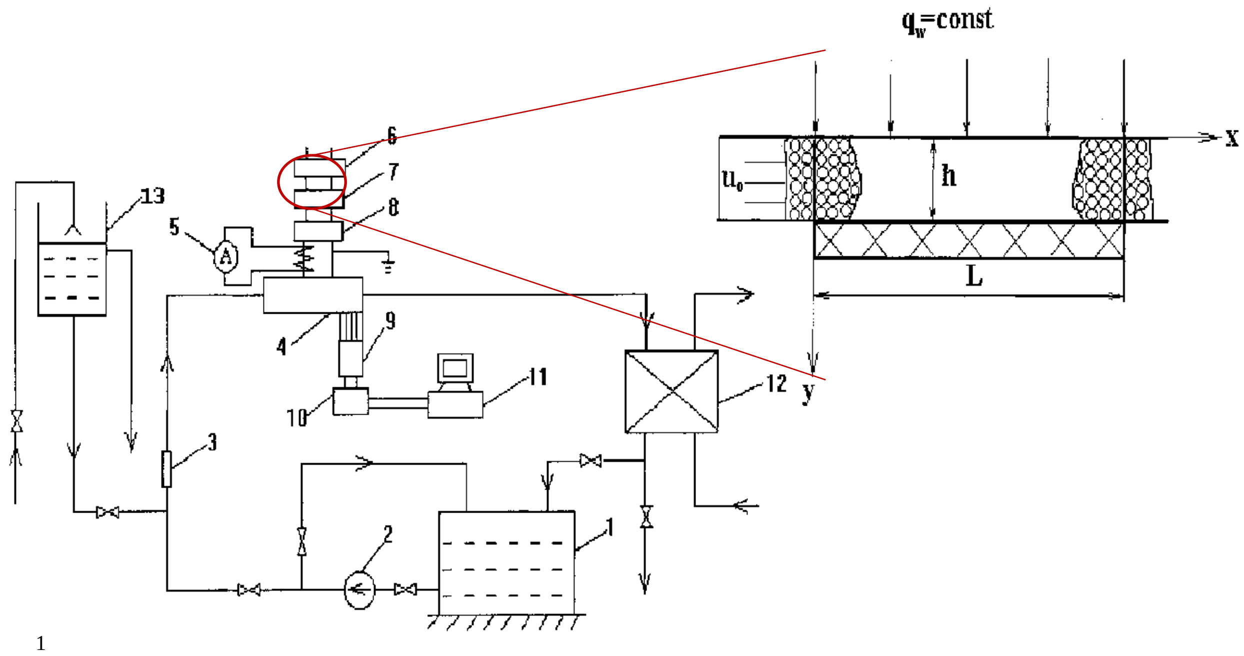
1. In this work, we considered that the viscosity is a function of fluid temperature and pressure.
2. We utilized the local Nusselt number for heat transfer based on local Reynolds number and Prandtl number.
3. The h_{sf} was used to calculate the heat transfer between solid and fluid.

Contents

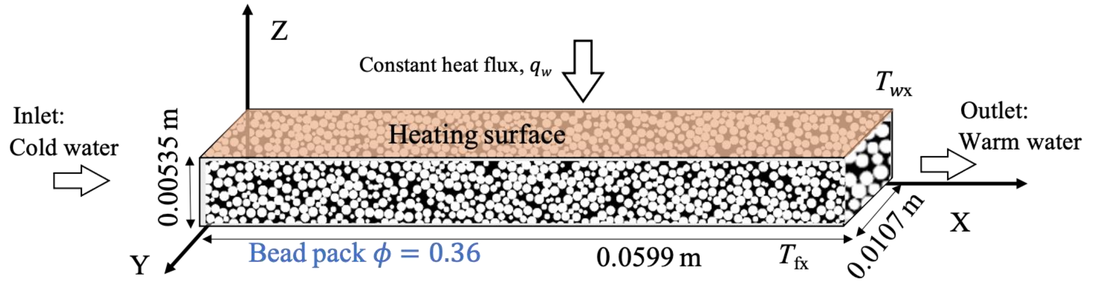
- ➢ Development of MpNM
- ➢ **Model validation**
- ➢ Application 1
  - Mesoscopic insight in heat and mass transfer
- ➢ Application 2
  - Application 2: Simulation driven structure optimization – a demonstration
- ➢ Application 3 (ongoing)
  - Aquifer thermal energy storage

Experimental validation

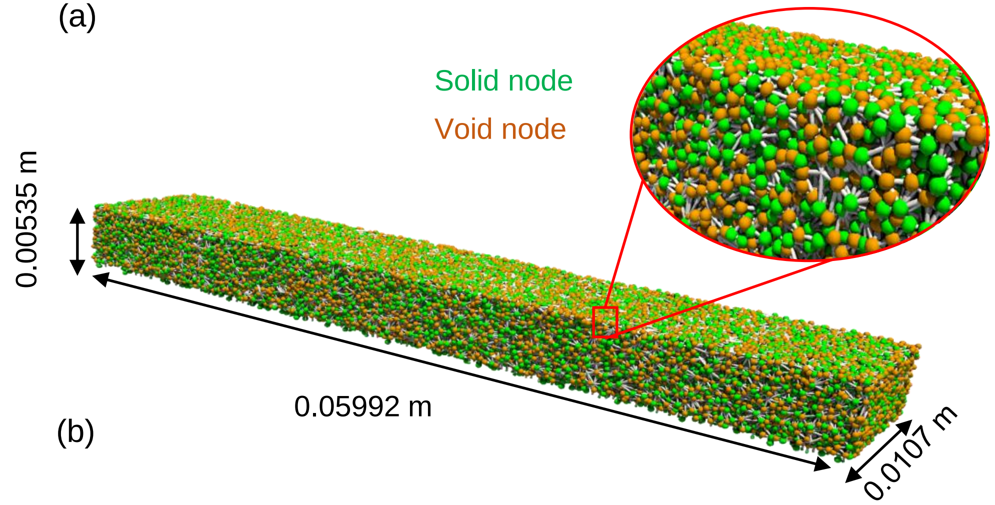
A bead pack structure has been fabricated which is similar as the experiment from Jiang et al 1999. The local heat transfer coefficient based on various Reynolds number has been studied in this case.



- DEM was used to build bead packed structure.
- Image dimension: 2600x500x250 voxels
- **Physical size: 55.64 × 10.70 × 5.35 mm**
- Network: 84,597 nodes & 627,805 links



(a)



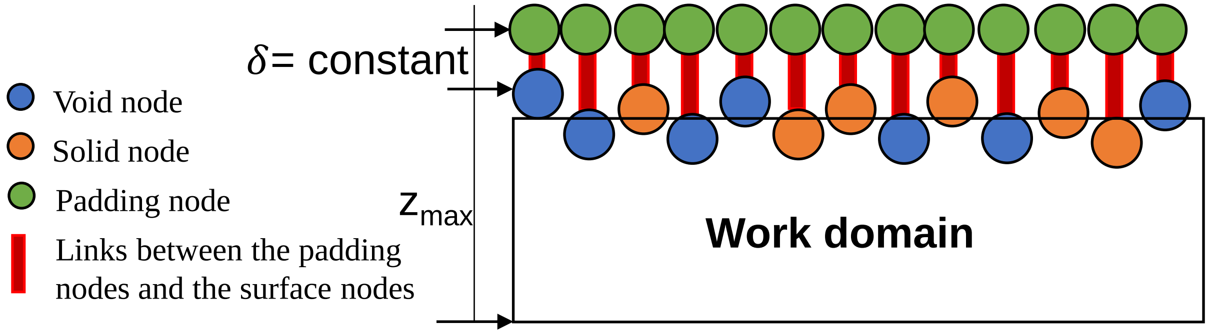
Case description:

- Experimental parameters : 58 x 80 x 5 mm
- Bronze bead diameter: 0.428 mm
- Heat flux: 2 x 10^5 W/m^2
- Entrance temperature: 300 K
- Entrance Reynolds number: 743-4507
- Processes: convection, conduction & single-phase flow

It contains 53,023 beads, which is almost impossible for other pore-scale models.

Boundary conditions for the model

		Boundary condition		values	Initial condition
Heat transfer	Solid	Neumann	Top	2×10^5 W/m^2	300K
		Neumann	others	$\nabla T_s \cdot \mathbf{n} = 0$	
	Fluid	Dirichlet	Left	300K	300K
		Outflow	Right	$\nabla T_f \cdot \mathbf{n} = 0$	
		Neumann	others	$\nabla T_f \cdot \mathbf{n} = 0$	



Heat transfer coefficient

Local heat transfer coefficient:

$$h_x = \frac{q_{heat}}{T_{w,x} - T_{f,x}}$$

Mean heat transfer coefficient:

$$h_m = \frac{q_{heat}}{\left(T_{w,m} - T_{f,m}\right)}$$

$$T_{w,m} = \frac{\sum_{i=1}^{N} T_{w,i}}{N}, \qquad T_{f,m} = \frac{\sum_{i=1}^{N} T_{f,i}}{N}$$

For the constant heat flux boundary condition, we build a padding layer to ensure the sufficient heat flux input and set a ω:

$$\omega = \frac{W \cdot L}{\pi \sum_{i=1}^{N} {r_i}^2}$$

where *W* and *L* are the width and length of the boundary surface, *N* is the number of the padding nodes, and *r* is the radius of original padding nodes.

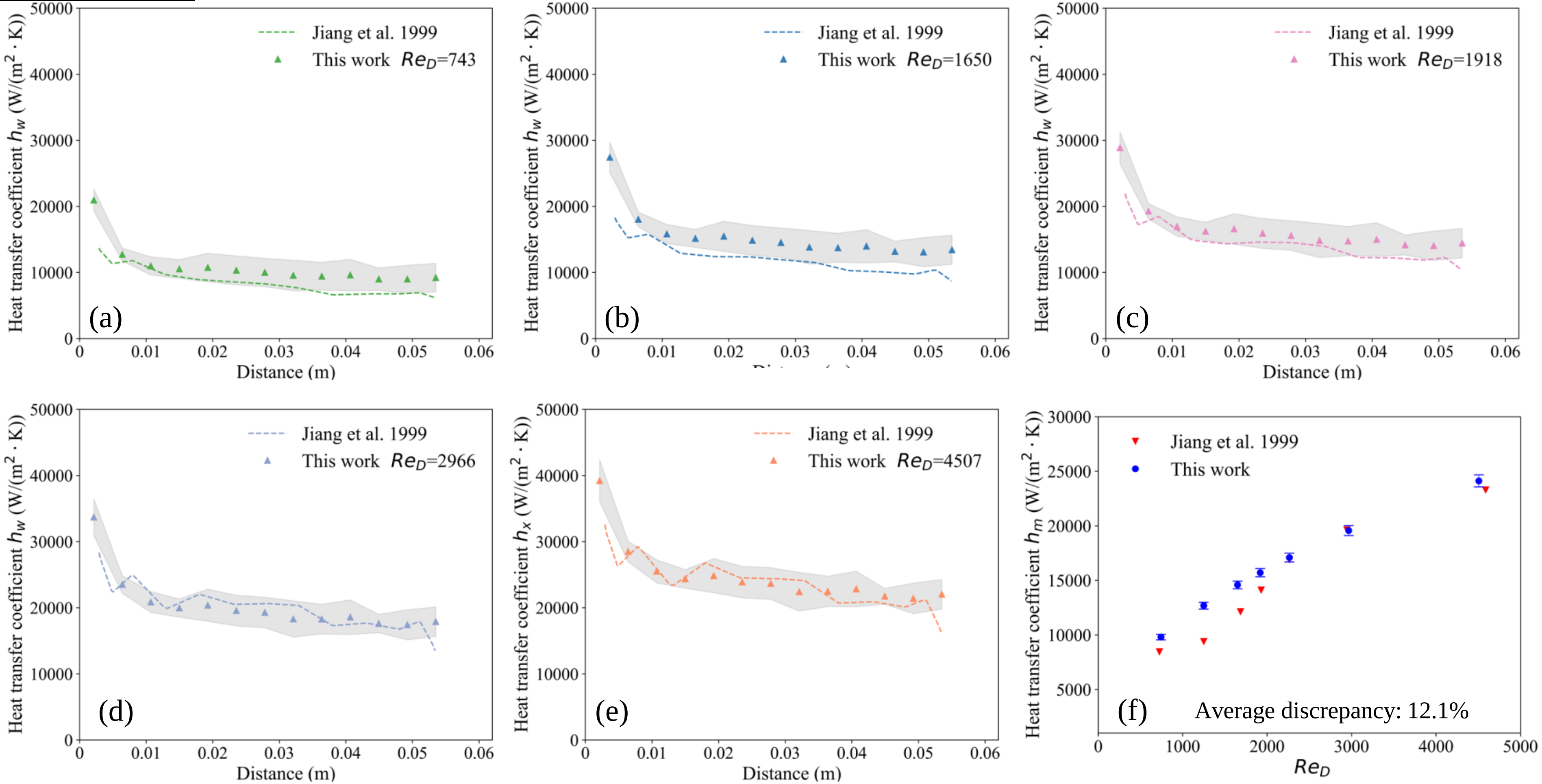
Simulation results against experimental measurements

Local heat transfer coefficient:

$$h_x = \frac{q_{heat}}{T_{w,x} - T_{f,x}}$$

Mean heat transfer coefficient:

$$h_m = \frac{q_{heat}}{(T_{w,m} - T_{f,m})}$$



According to the results, we can see:

1. The local heat transfer coefficients of our model match experimental results well.
2. The average deviation between mean heat transfer coefficients and experimental results is 12%.

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- Application 2
  - Simulation driven structure optimization – a demonstration
- Application 3 (ongoing)
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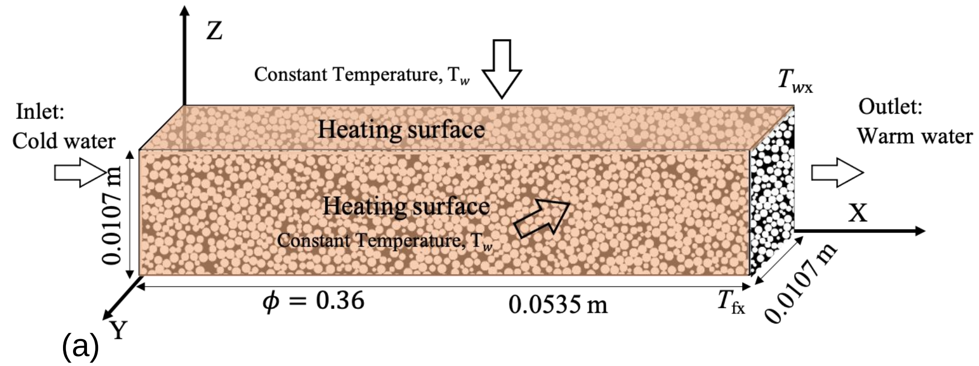
Application 1: Mesoscopic insights into heat and mass transfer

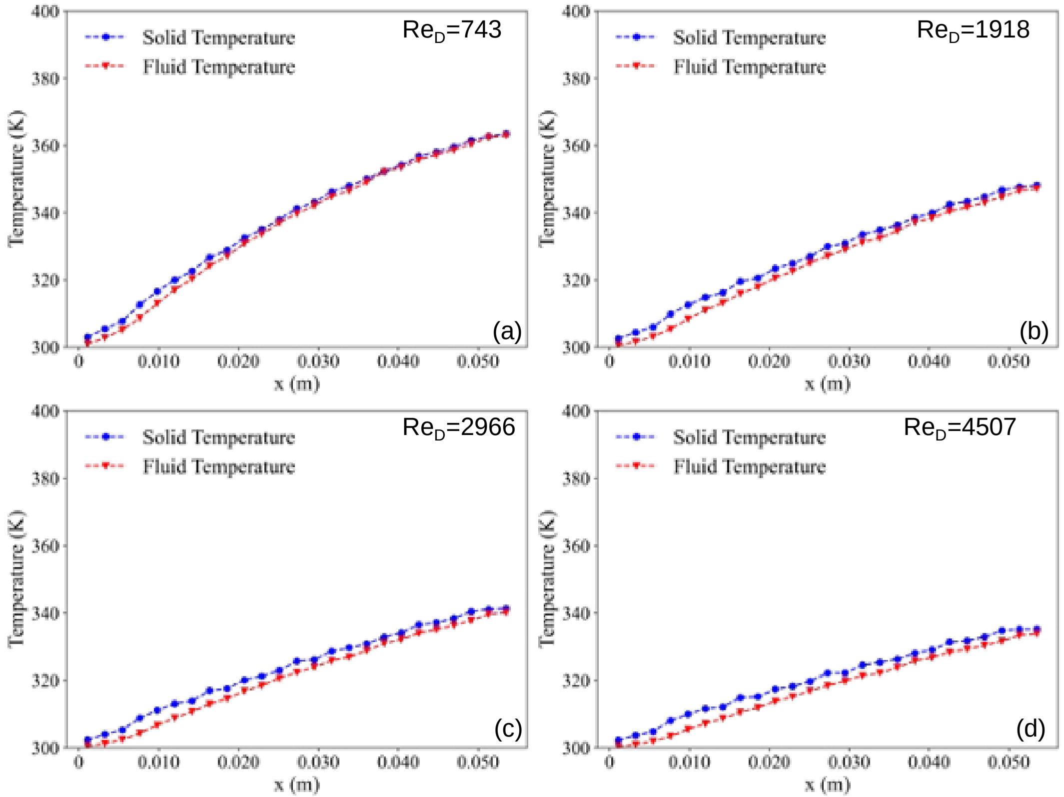


In this case, we studied a typical constant temperature scenario.

Case description:

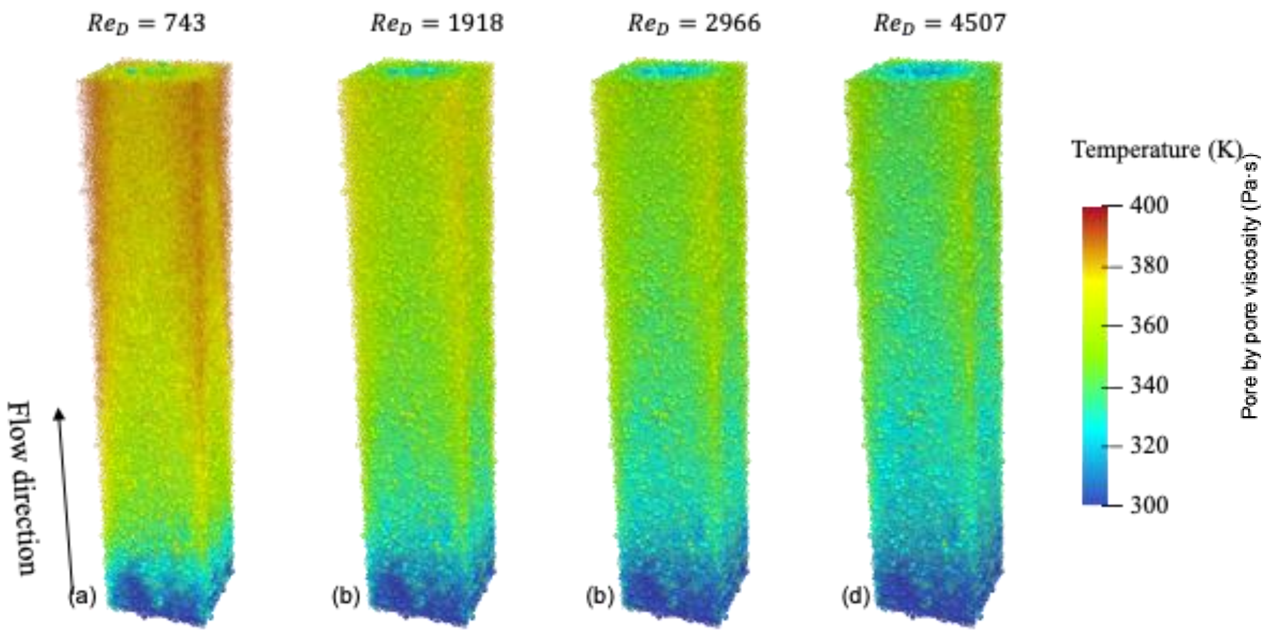
- Image dimension: 2500 x 500 x 500 voxels (containing 108,213 beads)
- Physical size: 55.64 × 10.70 × 5.35 mm
- Network: 158,592 nodes & 1,164,579 links
- Processes: steady-state, convection, conduction & single-phase flow

		Boundary condition		values	Initial condition
Heat transfer	Solid	Dirichlet	Bottom, Top, Front, Back	400K	300K
		Neumann	others	$\nabla T_s \cdot \mathbf{n} = 0$	
	Fluid	Dirichlet	Left	300K	300K
		Outflow	Right	$\nabla T_f \cdot \mathbf{n} = 0$	
		Neumann	others	$\nabla T_f \cdot \mathbf{n} = 0$	

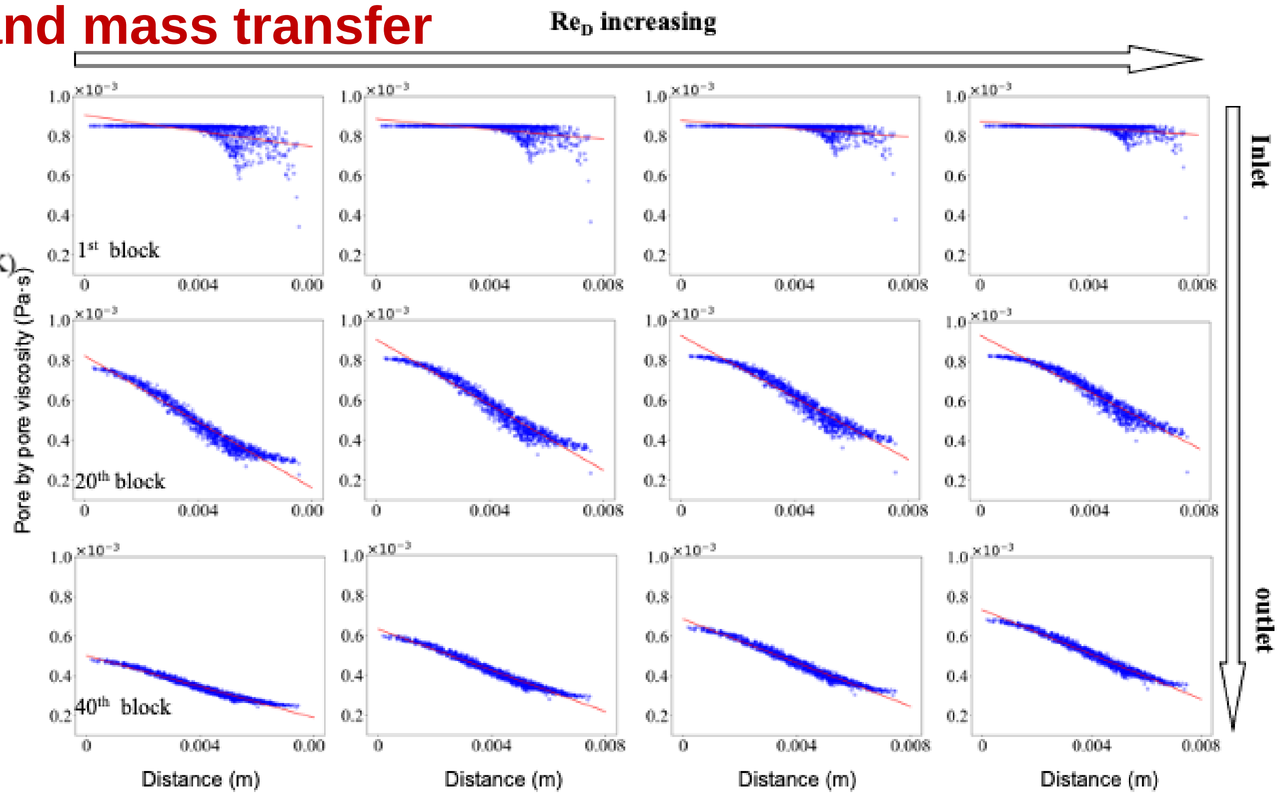


- **We calculated the average temperature profile of the solid and the fluid phase along the flow direction.**
- **The low ReD has a higher fluid temperature out than the high ReD.**
- **The maximum difference in temperature between solid and fluid for high ReD rises with increasing ReD.**

Application 1 Mesoscopic insights into heat and mass transfer



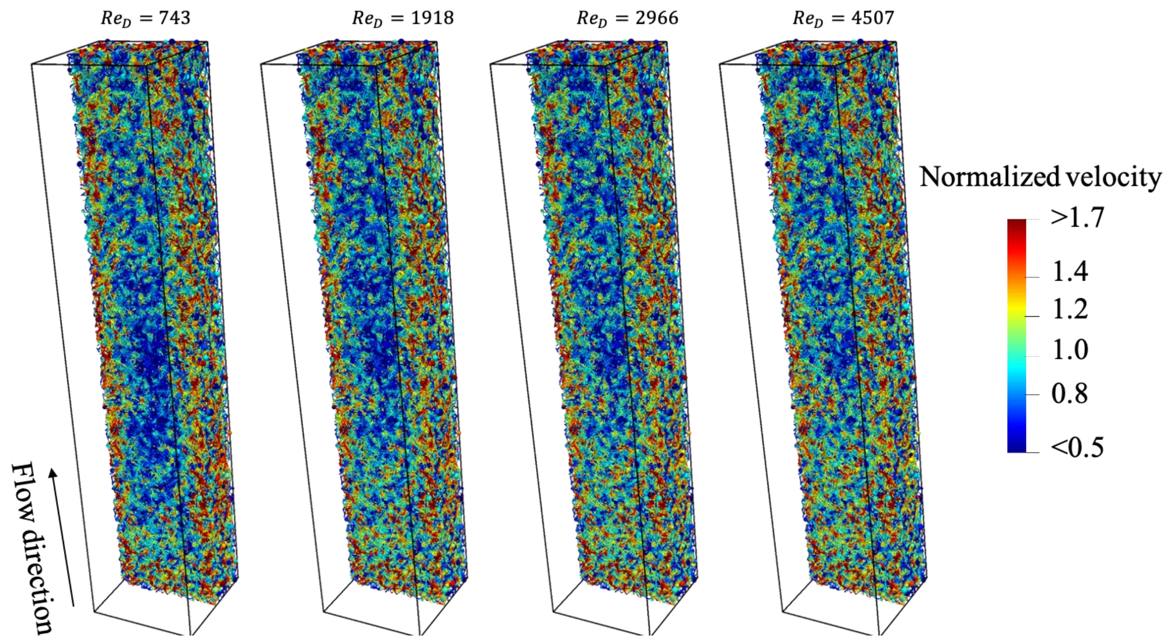
Temperature fields



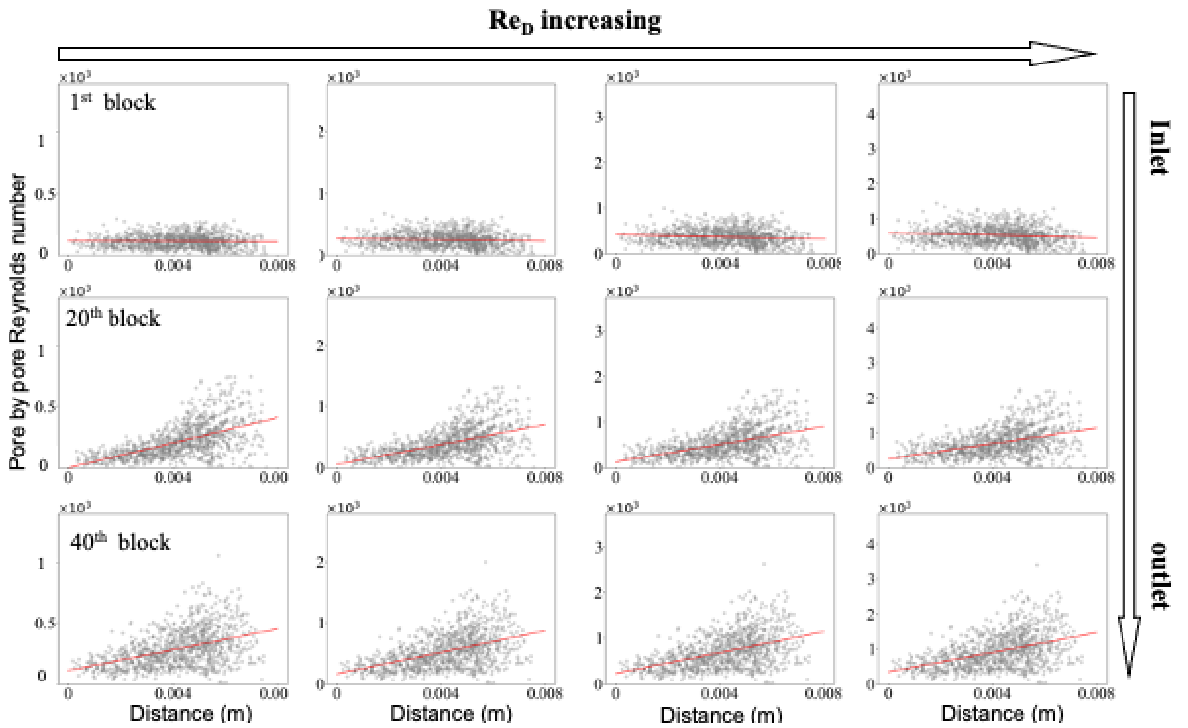
Local viscosity distribution along the flow direction

- **The temperature fields show the node temperature including solid and void.**
- **The work domain can be divided into 50 blocks along the flow direction.**
- **We computed the viscosity in each void node as a function of shortest distance to the centre axis along the flow direction on a pore-by-pore basis.**
- **The viscosity near the inlet and along the centre-line is larger, where the fluid is cooler.**

Application 1 Mesoscopic insights into heat and mass transfer



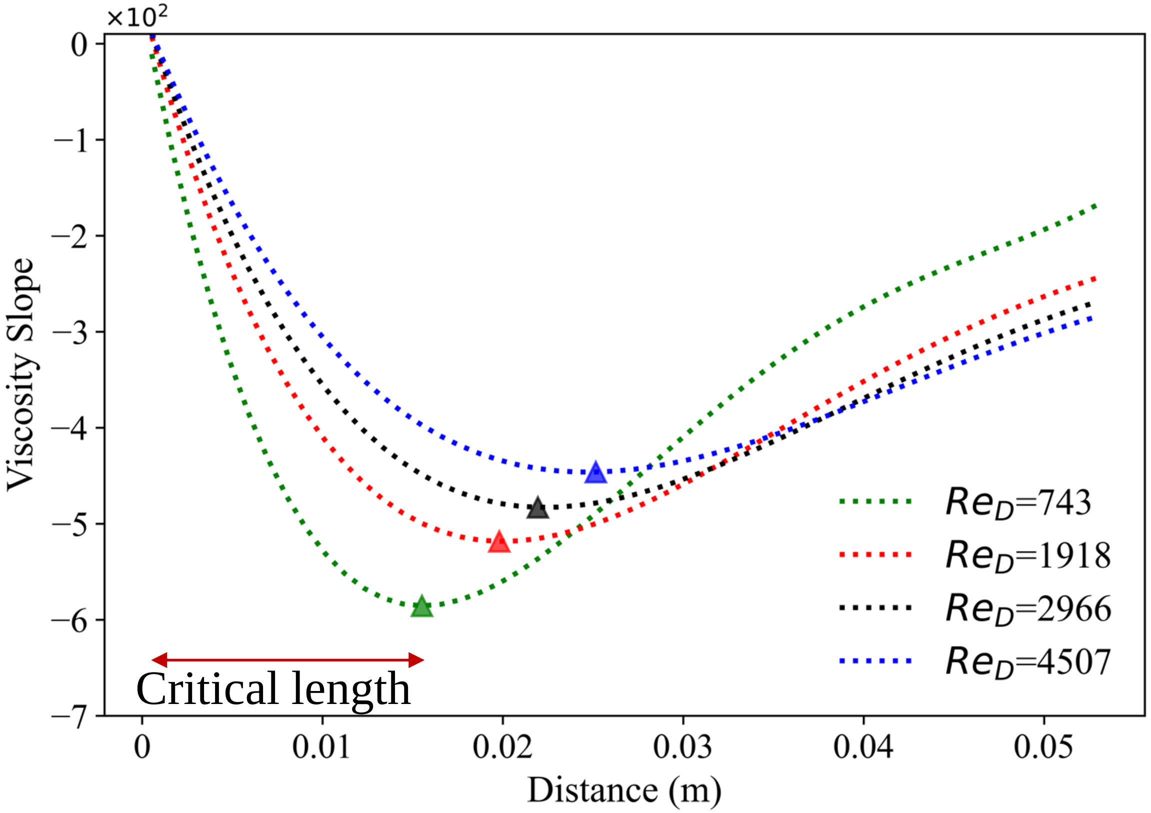
Normalized velocity fields

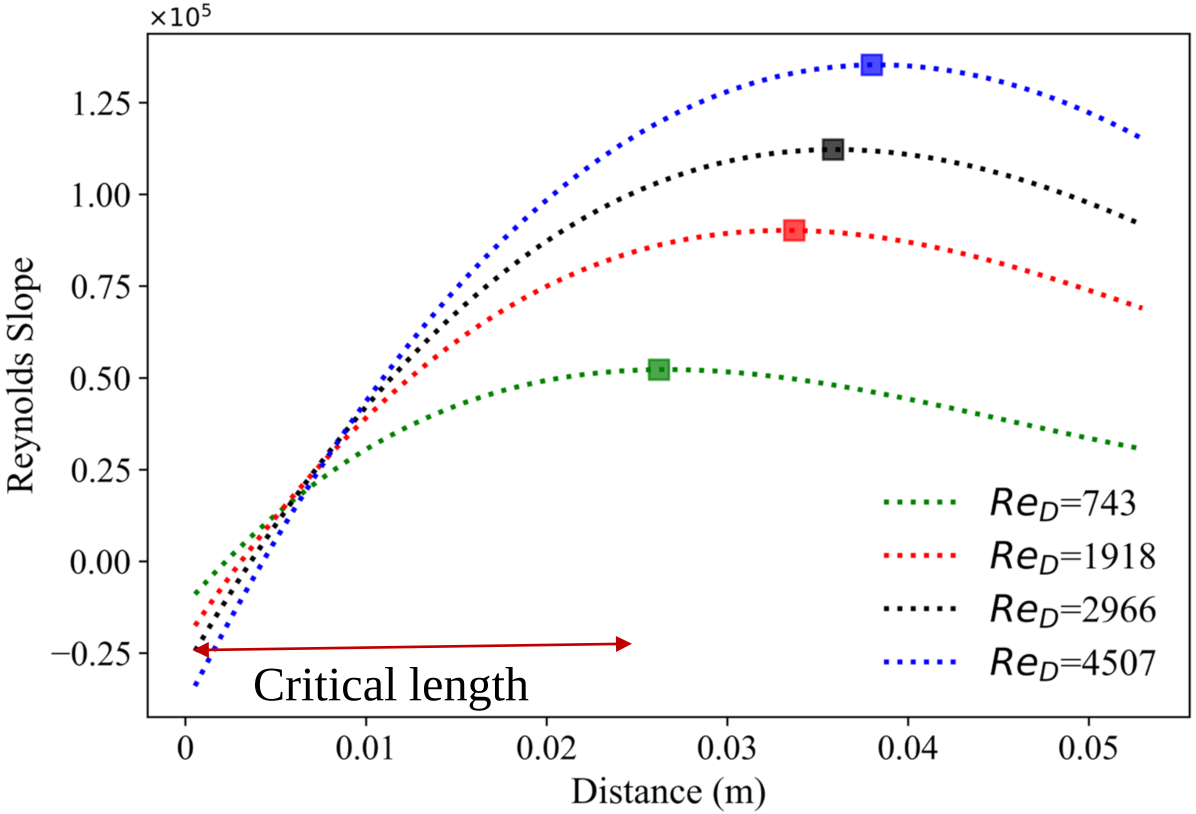


Local Reynolds number distribution along the flow direction

- **The figure shows the normalized velocity fields with various Re_D.**
- **With an increase in Re_D, the velocity fields become more uniform.**
- **We computed the Reynolds number in each void node as a function of shortest distance to the centre axis along the flow direction on a pore-by-pore basis.**

Application 1 Mesoscopic insights into heat and mass transfer

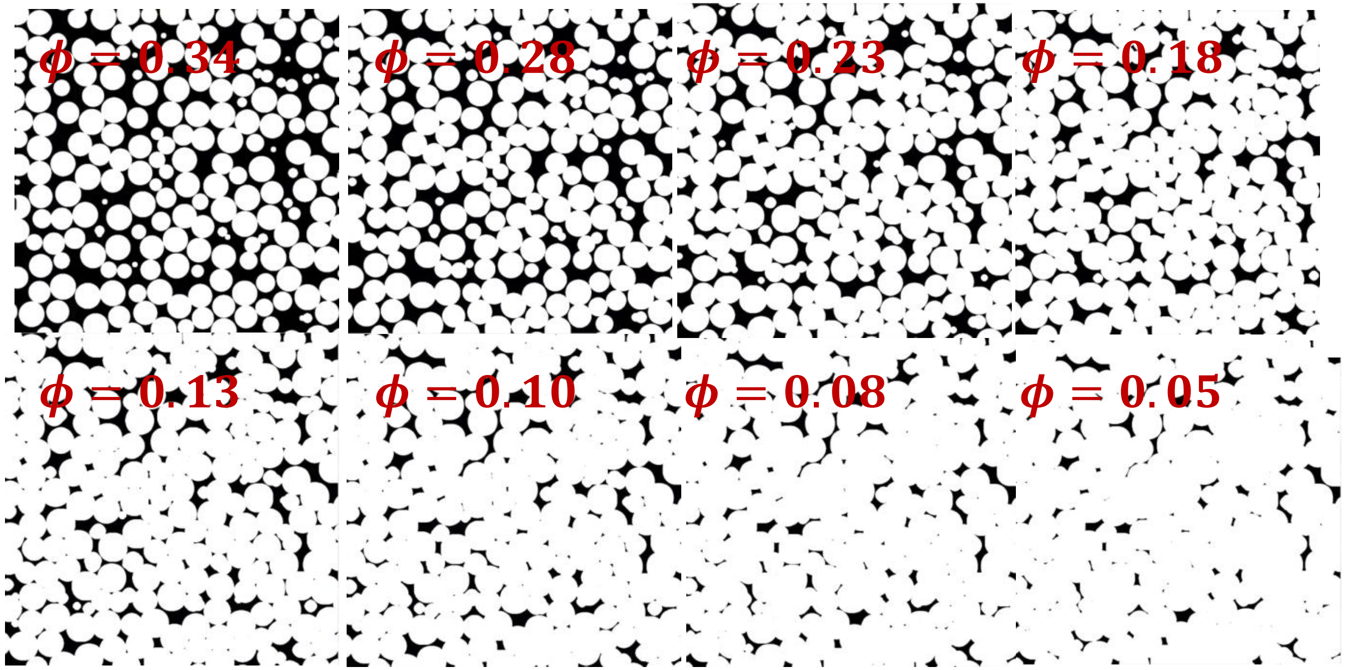


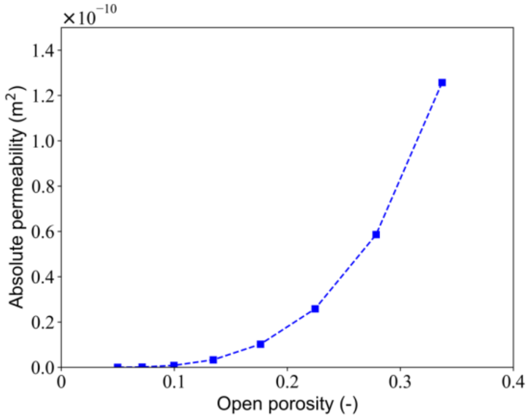


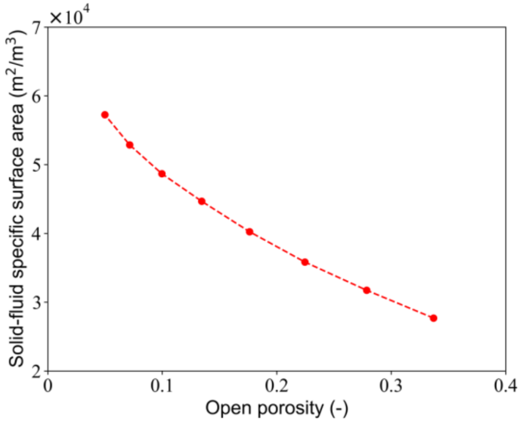
- **There are existing maximum or minimum values for viscosity slope and Reynolds number slope.**
- **The viscosity and Re are uniform at the inlet.**
- **The location of maximum/minimum value for those curves increase with increased Re_D .**

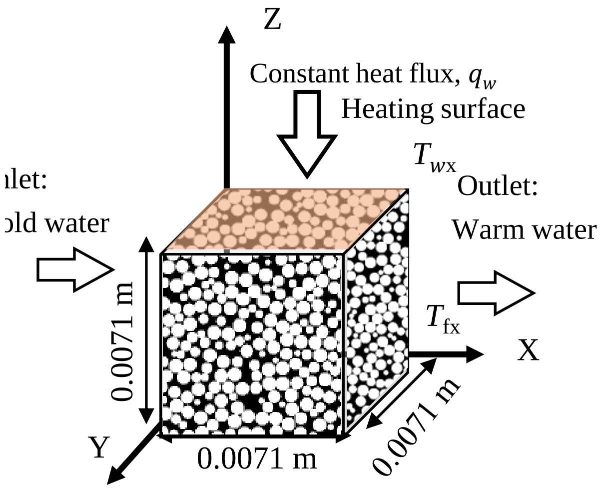
Contents

Application 2: Simulation driven structure design – a demonstration



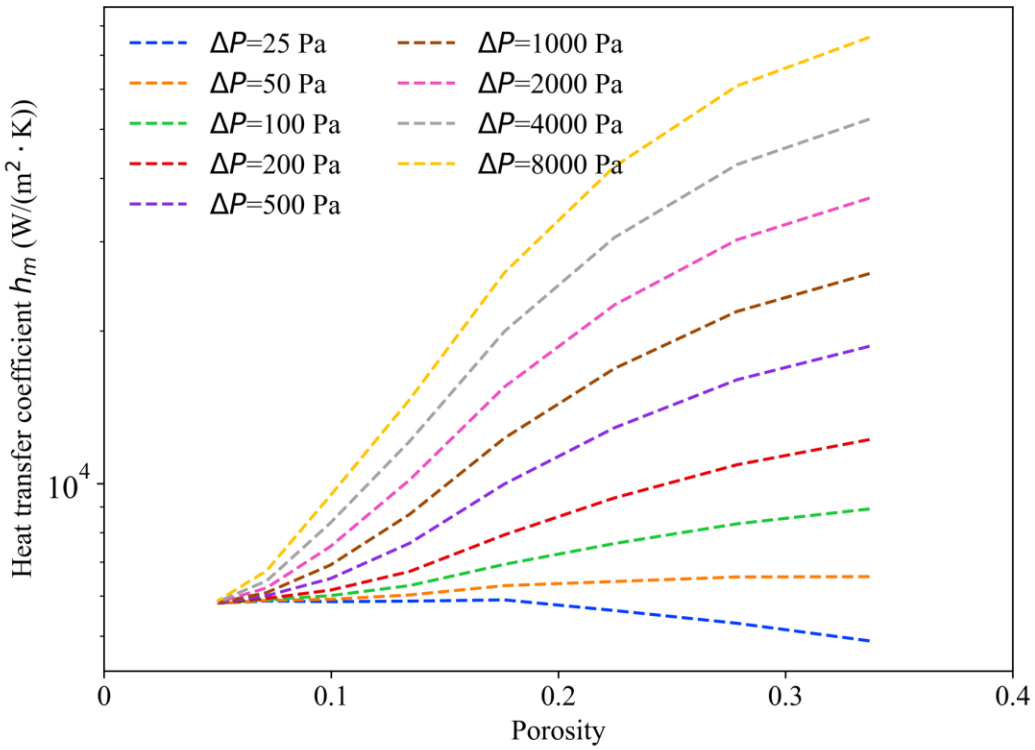


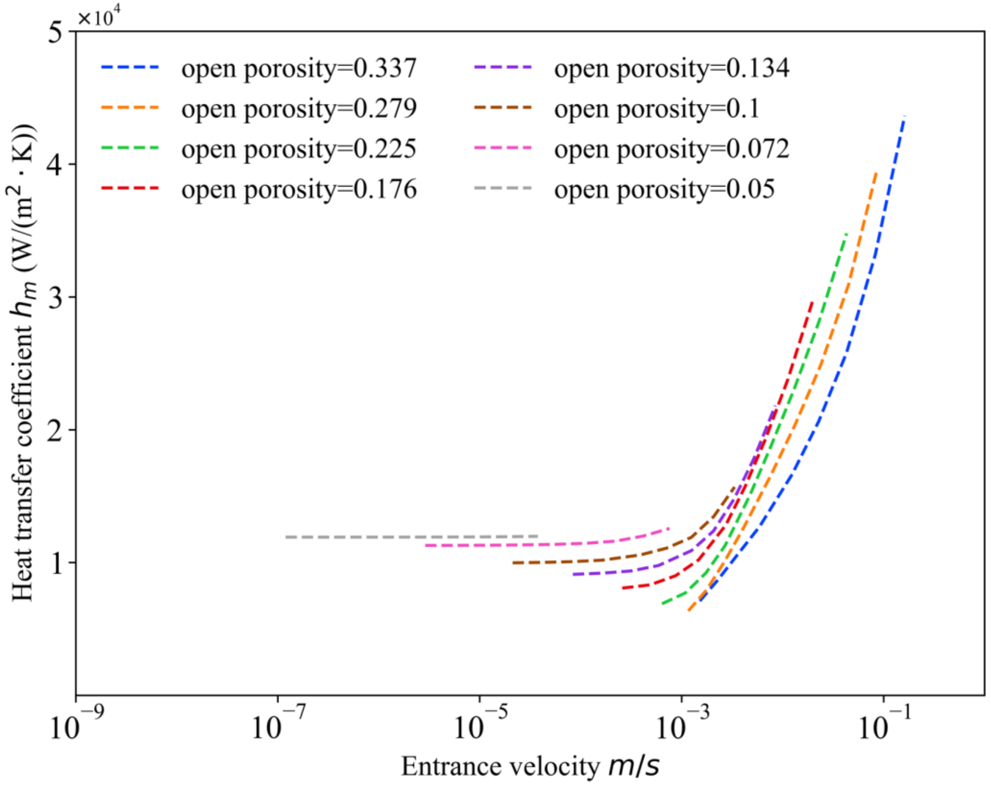




- **We apply a dilation algorithm to the original image (we dilate the spheres and allow them to overlap).**
- **The porosity and permeability decrease, but the solid-fluid interfacial areas increase. Both curves are non-linear.**

Application 2 Simulation driving structure design





- **Various constant pressure drops (25-8000 Pa) were set as the boundary conditions to simulate the mass and heat transfer processes and compute the associated mean heat transfer coefficients.**
- **When entrance velocity is lower than 1×10^{-4} m/s, the thermal conduction is dominant.**
- **When entrance velocity is higher than 1×10^{-4} m/s, the thermal convection is dominant.**

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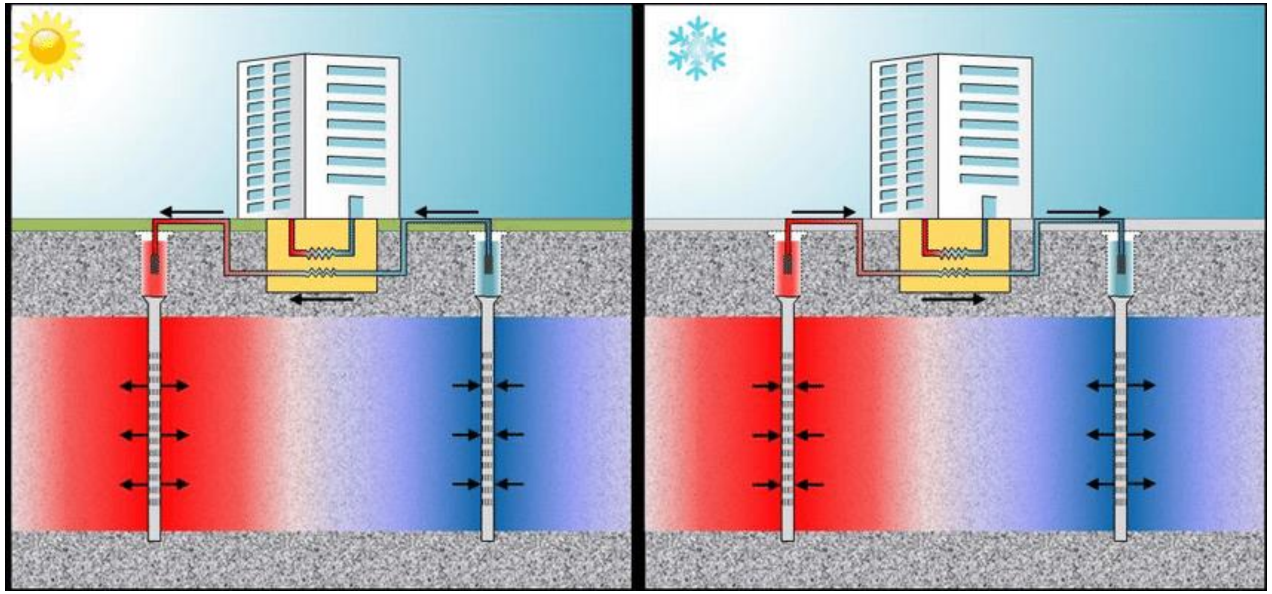
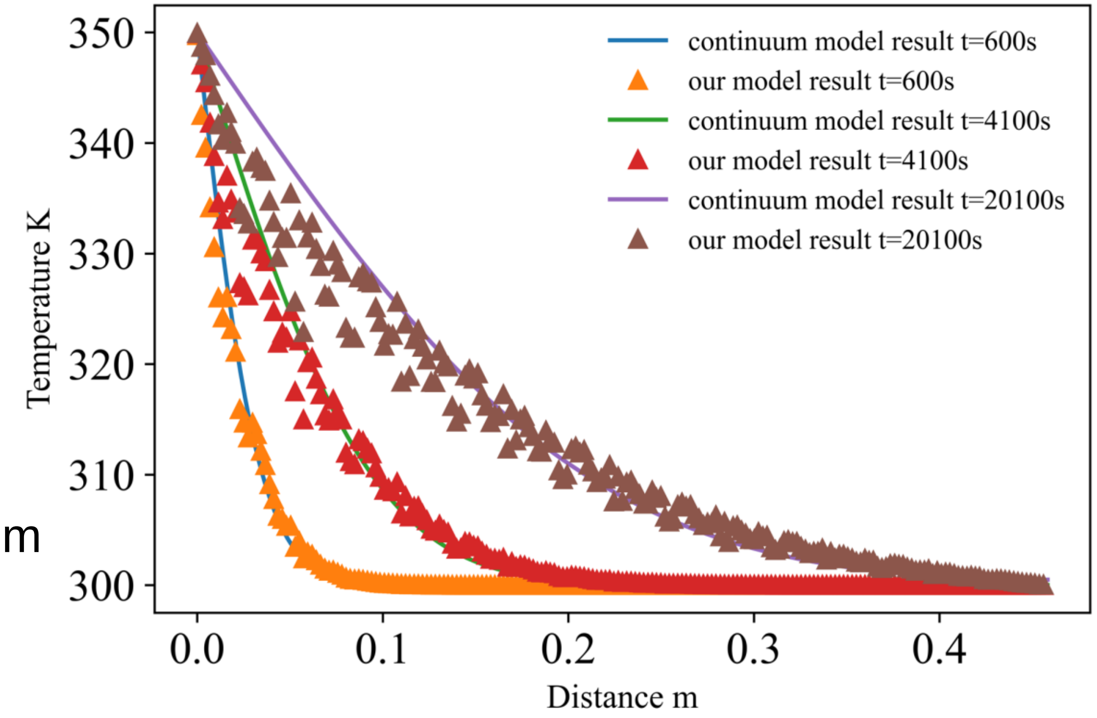
Application 3: Aquifer thermal energy storage (ongoing)



MpNM model:

Based on real-structure, we fabricated a thermal conduction case with length of ~0.4 m and time range ~3 h.



Common assumptions:

- Homogeneous system
- Same phase temperature
- Constant fluid parameters

Reality:

- Heterogeneous system
- Local thermal nonequilibrium
- Varying fluid parameters

Conclusions

- **We developed an approach for fabricating a multi-physics dual-network model.**
- **A validation for this model has been made by matching experimental results.**
- **According to MpNM, we can obtain the temperature and velocity fields node by node.**
- **The model shows the capacity for guiding structure design.**
- **This model is a potential tool in simulating underground thermal energy storage system.**
- **Future work will extend the model to study reaction, phase change and multiphase flow.**

Thank you for listening!

Questions and comments