Post-doc
Common Discussion

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Why

- Geo materials characterization
  - are Time consuming
  - require specific and costly equipment
  - not always possible
- Need agile tools for
  - Law carbon materials design such as CO_2 friendly concrete
  - Carbon storage materials design
- Traditional simulations tools
  - are time consuming
  - may include empirical formulas
  - are difficult to resolve at pore scale

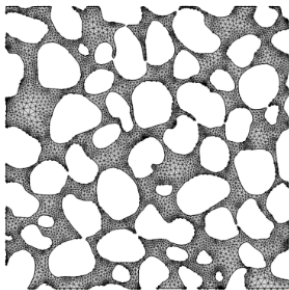## Potential of the method

Potential applications of pore network modeling

- Material characterization
    - Relative diffusivity and permeability
    - Absolute permeability
    - Effective diffusivity and tortuosity
    - Desorption isotherm
- Geo materials design
    - concrete
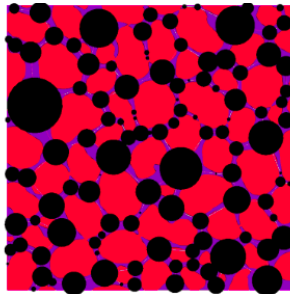   - ceramics
    - fibers composites

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Continum vs. PNM modeling

(a) FEM mesh   (b) Equivalent PNM

Figure: FEM vs. PNM

Continum vs. PNM modeling

Continum modeling

- Mathematically rigorous, but practical limitations
- Requires experimentally measured constitutive relationships
- Discrete pore-scale phenomena not resolved
- Distribution of phases within the continuum not often well predicted
- Not appropriate for thin materials

Pore Network modeling

- Transport inside the network is modeled using finite difference schemes to solve 1D analytical solutions of the relevant transport equations.
- PNMs can predict constitutive relationships for experimentally inaccessible multiphase parameters.
- PNMs Include interaction between the structure and flow characteristics included

PNM concept

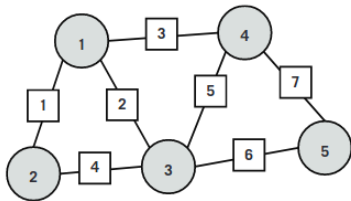- Sizes and connectivity of the pores and throats are chosen to match the known physical structure

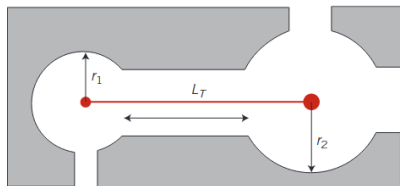Figure: Network of pores and throats Gostick et al. (2016)

Figure: PNM unit Gostick et al. (2016)

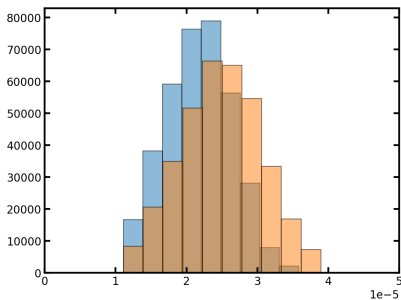- Structural properties of the porous material can be readily obtained from various imaging techniques

How the network properties can be obtained ?

- Key structural properties are
  - Size of throats and pores
  - Pores and throat connectivity
- Can be obtained :
  - from imaging techniques
  - from computer generated structures
  - by adjusting pores and throat size to allow the model to reproduce experimental known properties
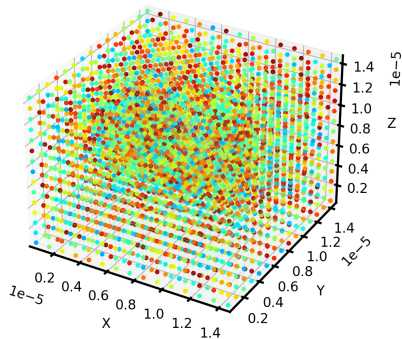
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Artificially generated material

Figure: Desired statistical properties:
pore and throat size

Figure: Generated pore network
model

Relative transport properties

Challenges

Well known methods need:

- Empirical formulas to account for dependence of diffusivity and permeability to saturation
- A lot of parameters to calibrate, not always easy
- Require experimental data not always available

Relative transport properties

Opportunities

PNMs allows:

- Direct simulation of transport properties :
  - absolute permeability
  - effective diffusivity and and tortuosity
  - relative permeability
  - relatve diffusivity
- sensitivity study:
  - fluid temperature
  - fluid viscosity
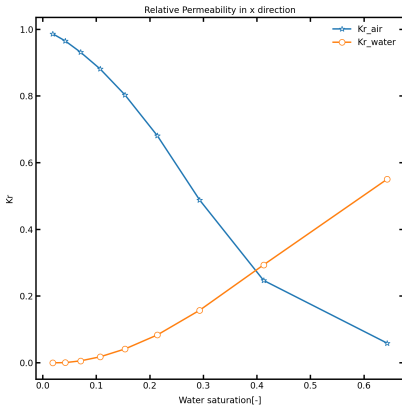 - material porosity

Relative transport properties
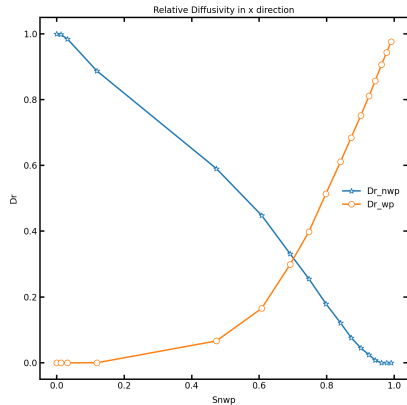

Figure: Relative permeability
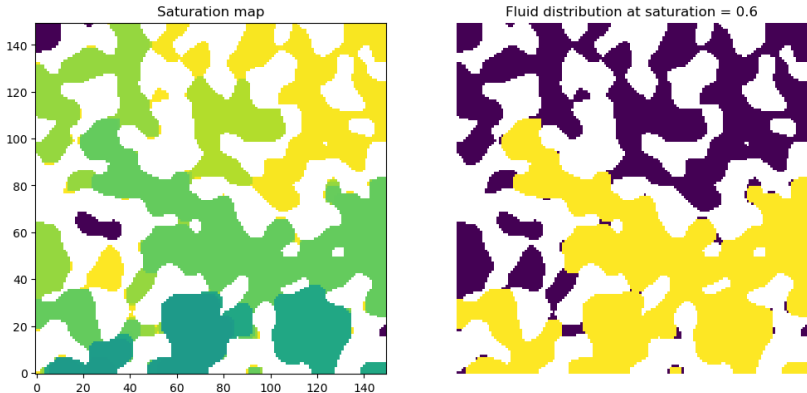

Figure: Relative diffusivity

Transport simulations

Figure: Fluid distribution within the network during injection
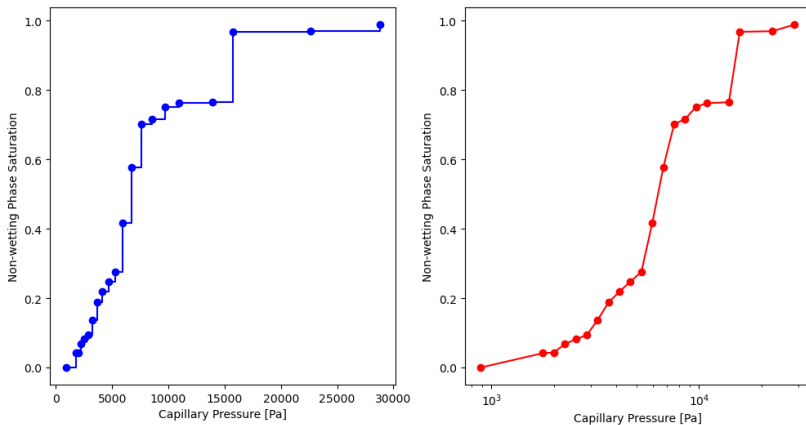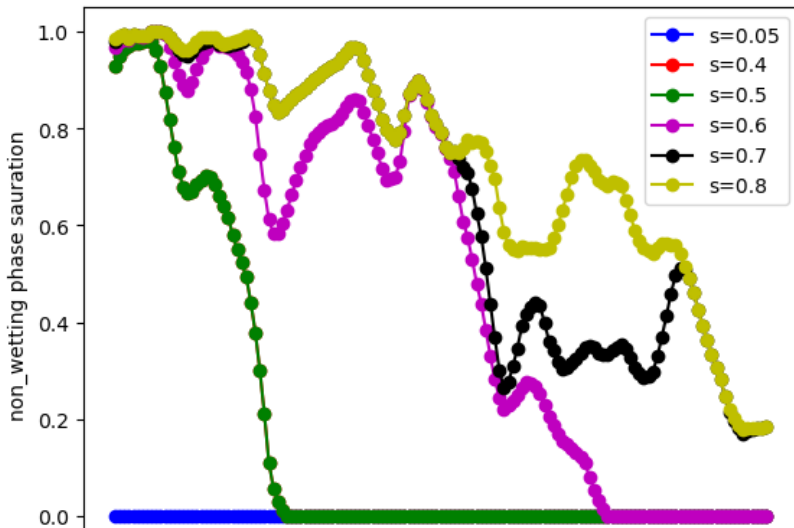
Transport simulations

Figure: Capillary pressure curve

Transport simulations
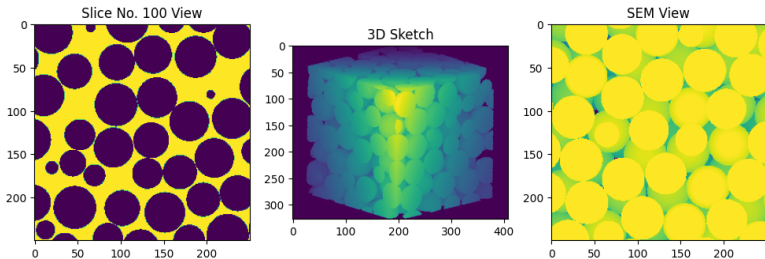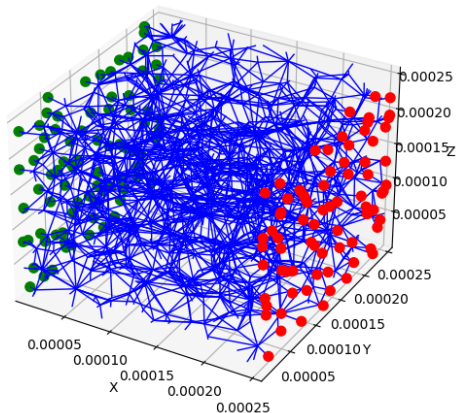
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Material: Berea sandstone

Figure: Material obtained from tomography imaging

Pore network modeling: network extraction

Figure: Network extracted form tomography images with boundary pores highlighted
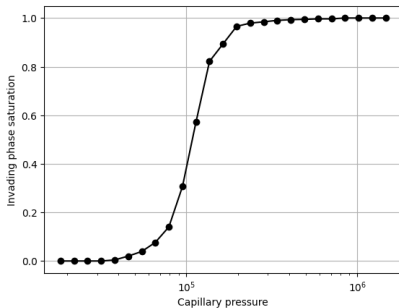
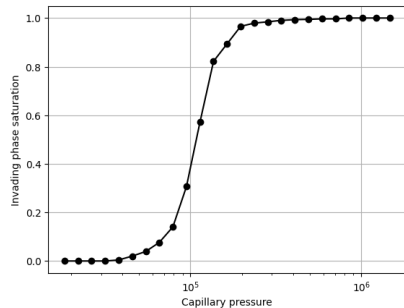## Mercury intrusion test

Figure: Mercury intrusion

Figure: Water intrusion

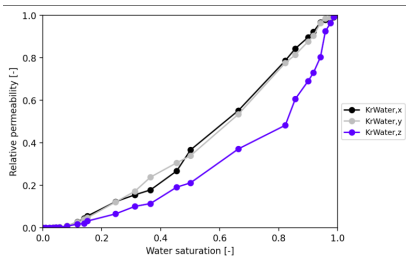# Pore network modeling: computed relative permeability
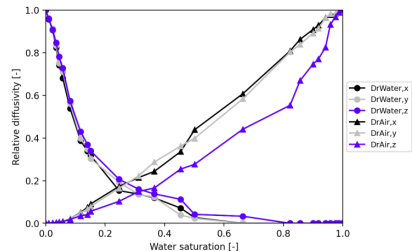

Figure: Relative permeability for water

Figure: Relative diffusivity for water and gas (air)

J. Gostick, M. Aghighi, J. Hinebaugh, T. Tranter, M. A. Hoeh,
H. Day, B. Spellacy, M. H. Sharqawy, A. Bazylak, A. Burns,
et al. Openpnm: a pore network modeling package. *Computing
in Science & Engineering*, 18(4):60–74, 2016.