Slip Flows of Gases through Nanopores

Combined view from nanofluidics, rocks, and DSMC

Nanofluid experiments
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Rock experiments
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DSMC simulations
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Introduction on DSMC method

- DSMC = Direct Simulation Monte-Carlo
- Gas molecules are simplified as point particles
- A common method to simulate nano-scale gas flows

- **Range of applicability**
  Kn = mean free path of gas molecules / pore size
  Flow with Kn << 1 obeys Darcy's law
  When Kn > 0.1, gas flow through nanopores develops non-negligible slip – the Klinkenberg effect
  DSMC is applicable for most flows with Kn > 0.1

- **Benefit and limitation**
  Interactions at high densities and with walls are not as realistic as molecular dynamics but computational cost is much lower

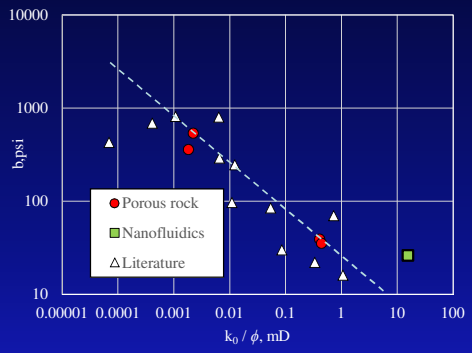
Motivation for carrying out DSMC simulations

- The Klinkenberg factors obtained from nanofluidic experiments and rocks indicate that there may exist a **scaling relation** that can be used to estimate the Klinkenberg coefficient of nanoporous rocks and thereby the degree of slip at various pressures

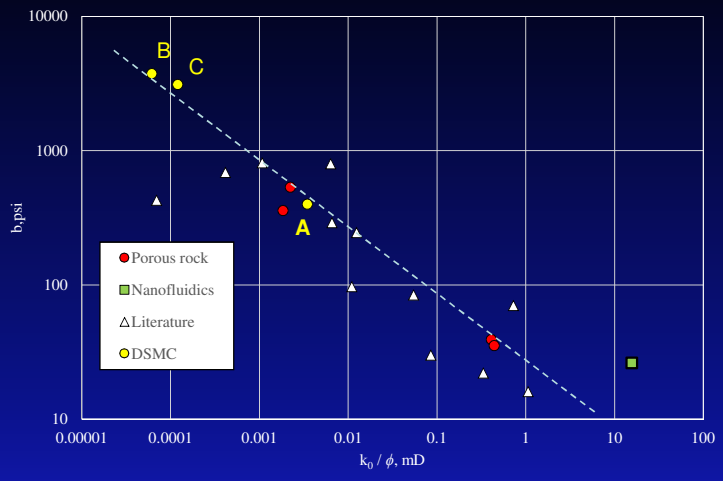
$$\frac{k}{k_0} = 1 + \frac{b}{P}$$

$$b \propto (k_0/\phi)^{-1/2}$$

Will DSMC simulations support this finding?



Answer = Rather Well

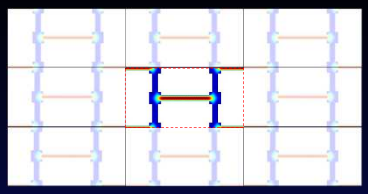


Information on the DSMC models

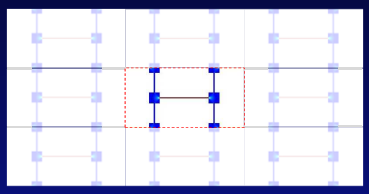
- **A** is a geometry model with a high porosity (**22%**) and inter-pore connections are **10 nm**
- Permeability (Klinkenberg corrected) = **770 Nanodarcy**
- Porosity of large pores (**20 nm**) = **8%**

- **B** is a geometry model with a good porosity (**9.4%**) but poor inter-pore connections of **2 nm**
- Permeability (Klinkenberg corrected) = **5.8 Nanodarcy**
- Porosity of large pores (**18 nm**) = **6.5%**

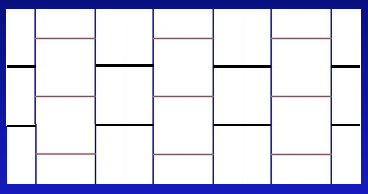
- **C** is a geometry model with a poor porosity (**4.0%**) and dimension of pores is **2 nm**
- Permeability (Klinkenberg corrected) = **4.8 Nanodarcy**
- There are no large pores



Geometry A



Geometry B



Geometry C