M^5

Mixed Matrix Membrane Multiscale Modelling

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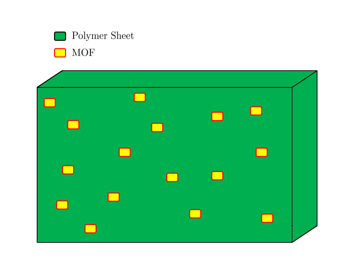
Friday 9th June 2017

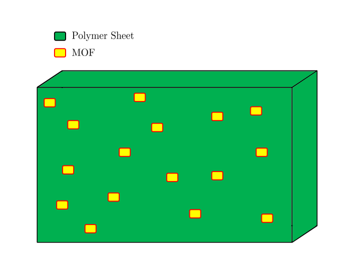
ITT6

What is a mixed matrix membrane?



Schematic for a MMM

What is a mixed matrix membrane?



Schematic for a MMM

Different scales:

Polymer sheet depth $\sim cm$

MOF size $\sim 100\mu m$

Polymer sheet pores $nm \sim mm$

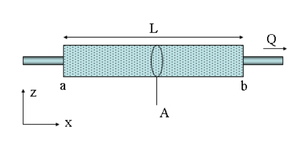
MOF pores $\sim nm$

Question: How to characterise the flow through the MMM?

Question: Global adsorption?

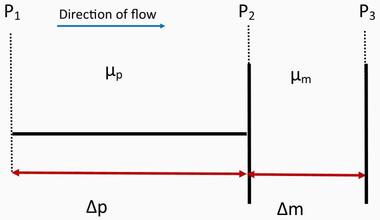
Approach 1: Darcy's law

- Looked at one and two dimensions
- MOF permeability μ_m and polymer sheet permeability μ_p
- Control the density of MOFs
- Continuum method in the polymer sheet: Darcy's law



Darcy flow experiment

Approach 1: Darcy's law



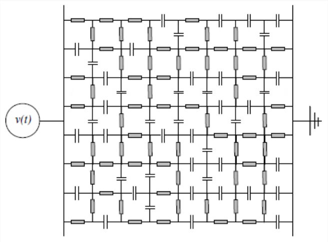
One-dimensional section with MOF

Permeabilities related according to weighted harmonic mean[1]:

$$\frac{1}{\mu^*} = \frac{\Delta_p}{\mu_p} + \frac{\Delta_m}{\mu_m} \Leftrightarrow \mu^* = \frac{\mu_p \mu_m}{\Delta_p \mu_m + \Delta_m \mu_p}.$$

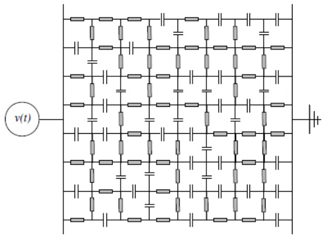
[1] Zimmerman *et al.*, *Journal of Membrane Science* 1997

Approach 1: Towards a solution



Resistor-capacitor circuit. Taken from Almond *et al.*, *Physica A* (2012).

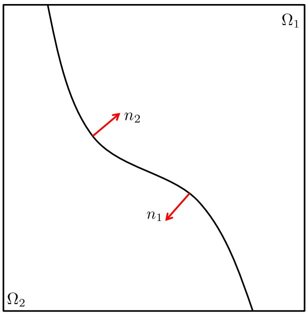
Approach 1: Towards a solution



Resistor-capacitor circuit. Taken from Almond *et al.*, *Physica A* (2012).

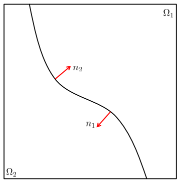
- Kirchoff's laws give equations for current (and voltage)
- We may "view" currents as fluid flow, conductances as permeabilities, voltages as pressures
- We would model MMM using randomly distributed components
- Emergent behaviour of large networks is known in literature
- Used to find global permeability of large MMM

Approach 1a: PDE modelling

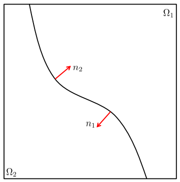


Two materials with different permeabilities

Approach 1a: PDE modelling



Approach 1a: PDE modelling



PDE for permeability:

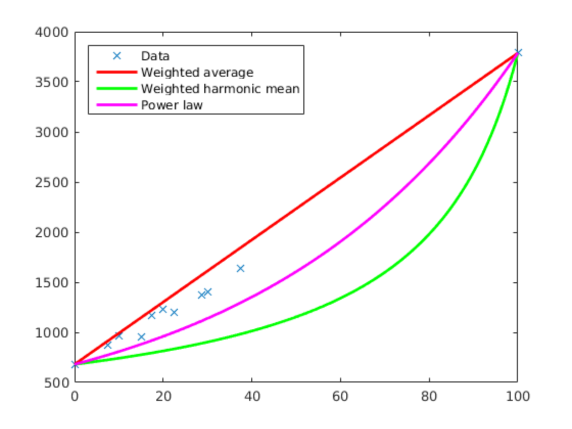
$$\nabla \cdot (\mu(x)\nabla P) = 0$$

Solving over the entire domain (in one dimension) with

$$\mu(x) = \begin{cases} \mu_1 & x \in \Omega_1 \\ \mu_2 & x \in \Omega_2 \end{cases}$$

and over individual domains gives the same harmonic mean result.

Approach 2: Hybrid modelling



Effective surface area of a mixture of two polymers

x-axis: Percentage of one of the polymers

y-axis: Effective surface area

Approach 2: Hybrid modelling

Observations:

Unknown interface between two polymers affects the effective surface area

Conjecture:

Model interface as third "material": $ESA = \mu_1^{f_1(\Delta_1)} \mu_2^{f_2(\Delta_2)} \mu_i^{f_i(\Delta_i)}$

Approach 2: Hybrid modelling

How do we model the interface? Hybrid modelling

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Possible hybrid method. Taken from Plapp *et al.*, *Physical Review Letters* (2000)

Thank you

Thank you for your attention. HasselMOF asks if you have any questions?