Multiscale modelling of MMMs

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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?

Approach 1: Darcy flows

- Start in one or two dimensions
- Randomly allocate MOFs using Poisson process in \mathbb{R} , \mathbb{R}^2
- MOF permeability μ_1 and polymer sheet permeability μ_2
- How do we find these?
- Control the density of MOFs
- Continuum method in the polymer sheet: Darcy flow?



Darcy flow experiment

Approach 2: Hybrid modelling



Sample hybrid method

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Sample hybrid method

Question: Can we use hybrid techniques to characterise MMM flow?

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Sample hybrid method

Question: Can we use hybrid techniques to characterise MMM flow? **Question:** How does this method compare to the Darcy law flow?