

Simulation of (Carpet) MOFs

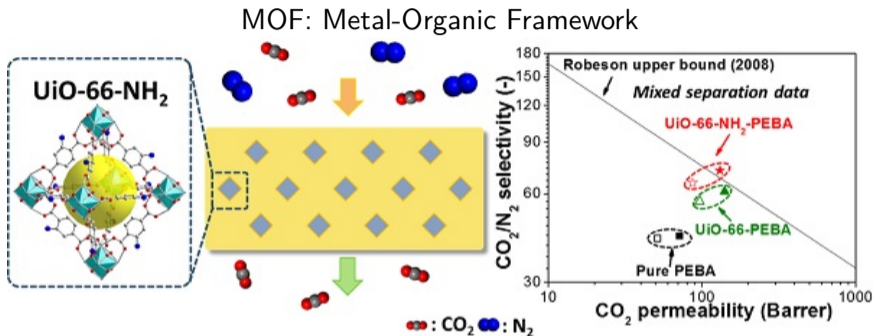
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June 2017

Reminder: Problem



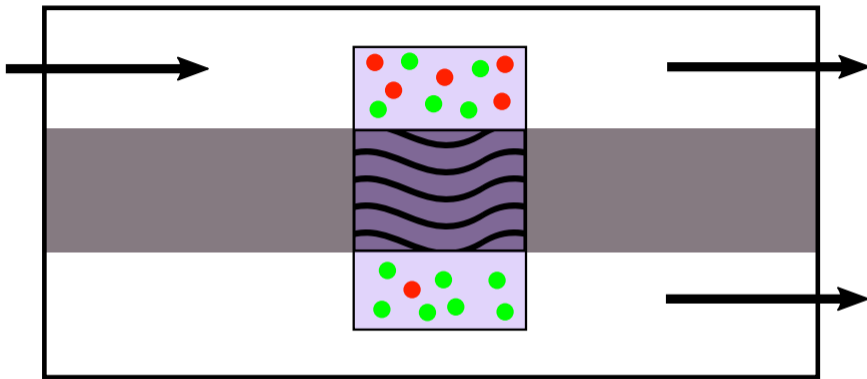
- ▶ mixed gas, want to filter out a species
- ▶ polymer membrane is not selective enough
- ▶ addition of a MOF into polymer improves selectivity
- ▶ multiple timescale simulation

Problem Abstraction



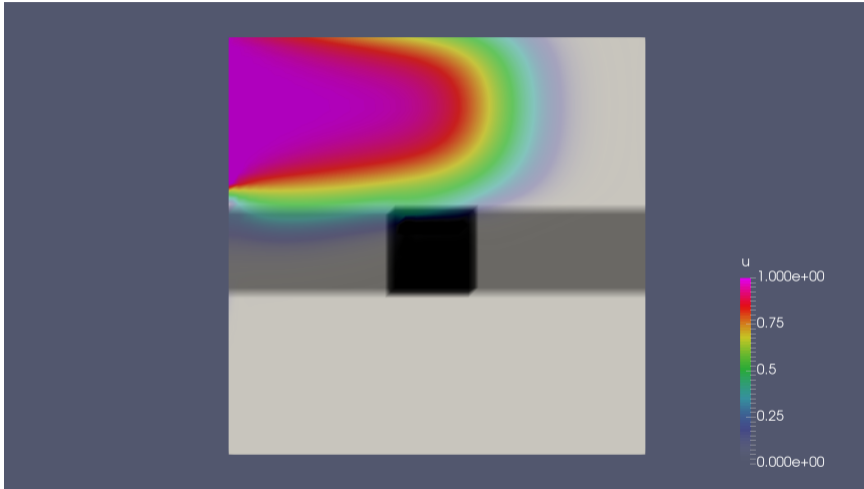
- ▶ top: left-right mixed input gas
- ▶ membrane in middle
- ▶ bottom right-left output flow

Reminder: Our Idea



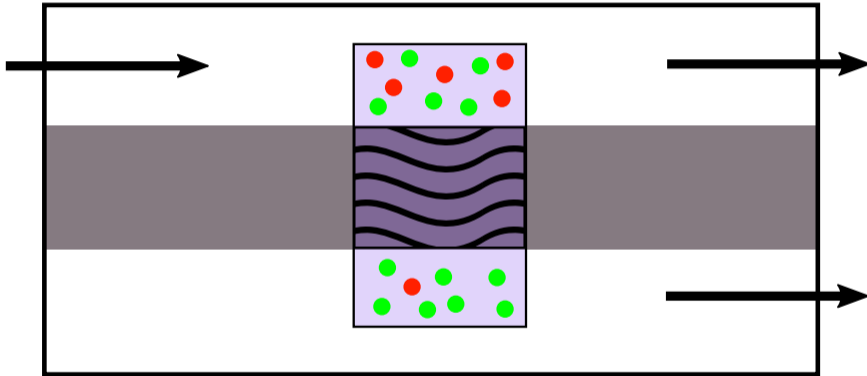
- ▶ PDE model for fluid
- ▶ Molecular Dynamics model for MOF
- ▶ Coupled by brute force and ignorance (for these last two days)

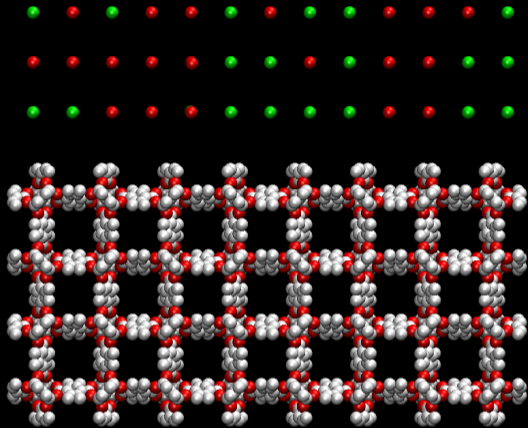
PDE

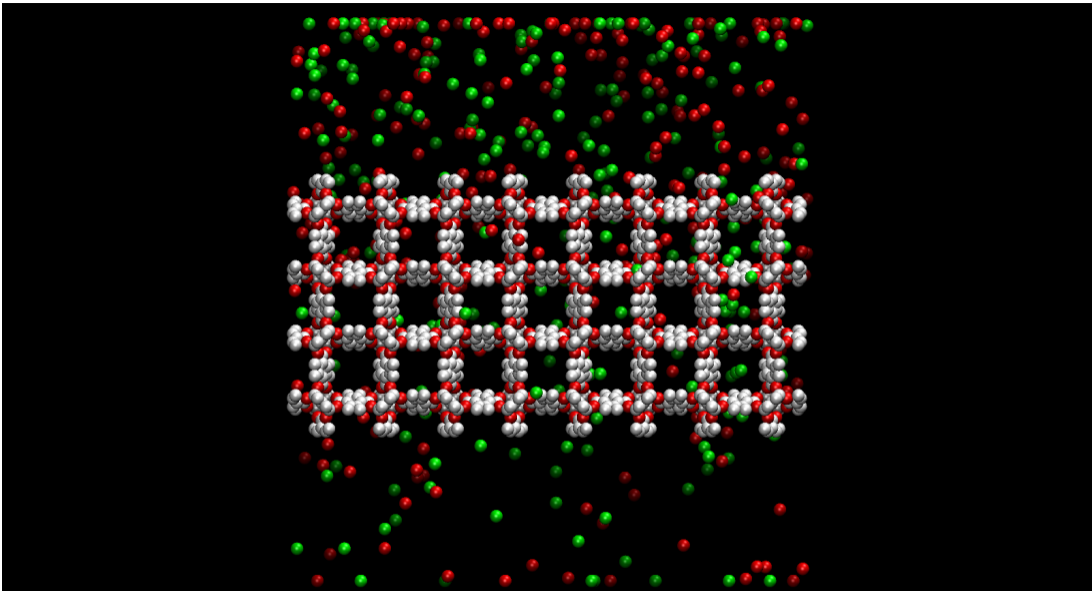


$$\frac{\partial u}{\partial t} = \nabla \cdot (D \nabla u - \beta u)$$

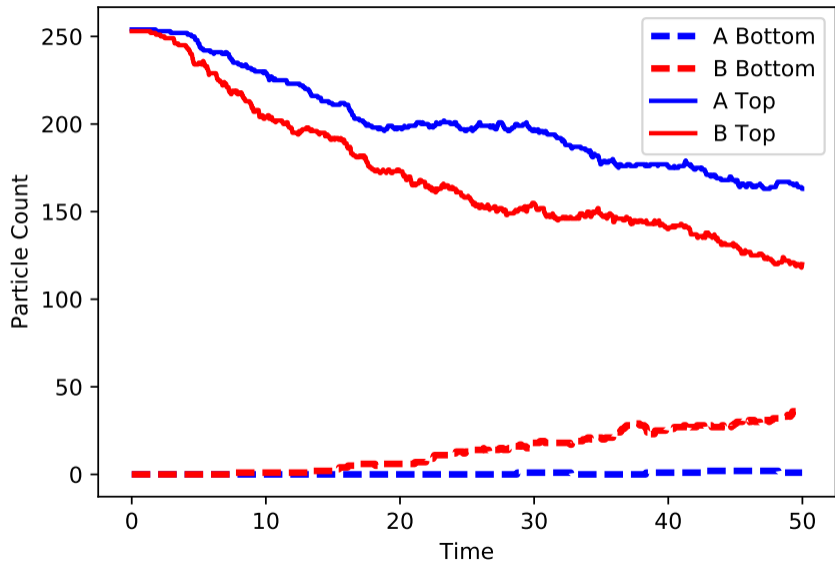
Reminder: Our Idea



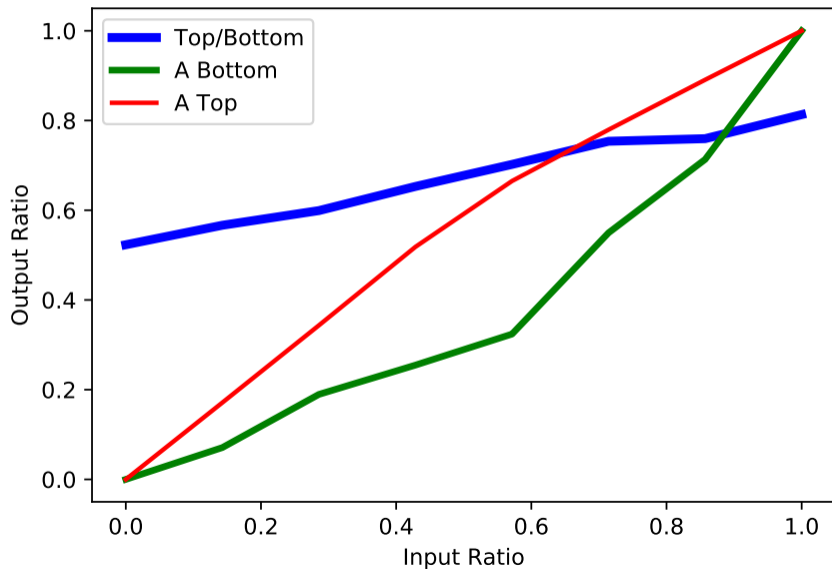




Concentration over time



Coupling between MD and PDE



Future Directions

- ▶ More sophisticated MD-PDE coupling
- ▶ pre-computing MD simulations and interpolating

Movie Time