Molecular dynamics simulations of Soret effects and fluid flow in a porous medium

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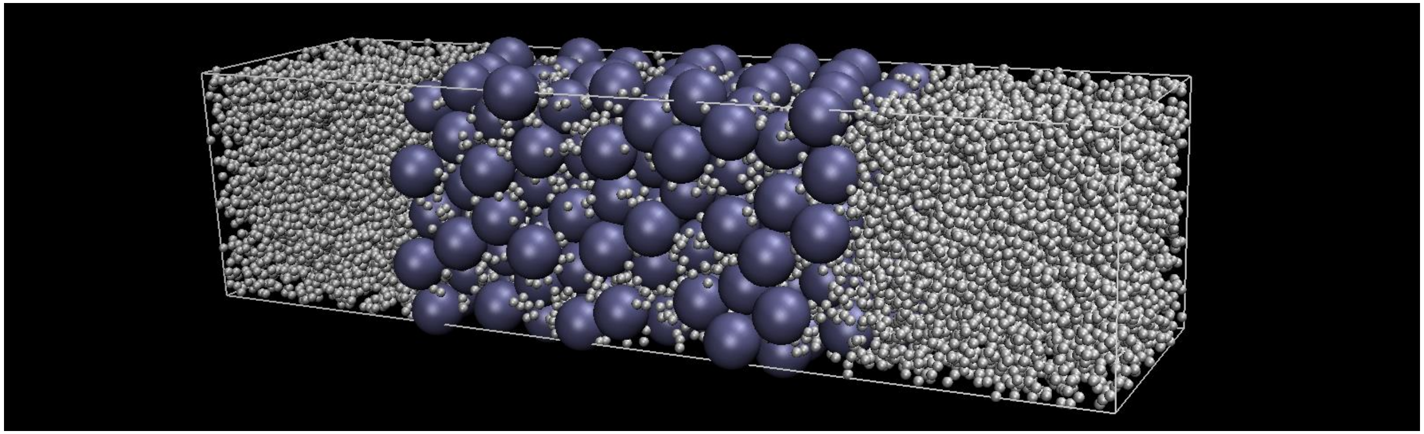
Kunnskap for en bedre verden

Concept

Molecular dynamics: Numerical solution of Newton's equations of motion for N- particle systems ($N \sim 10^3 - 10^6$)
Periodic boundary conditions



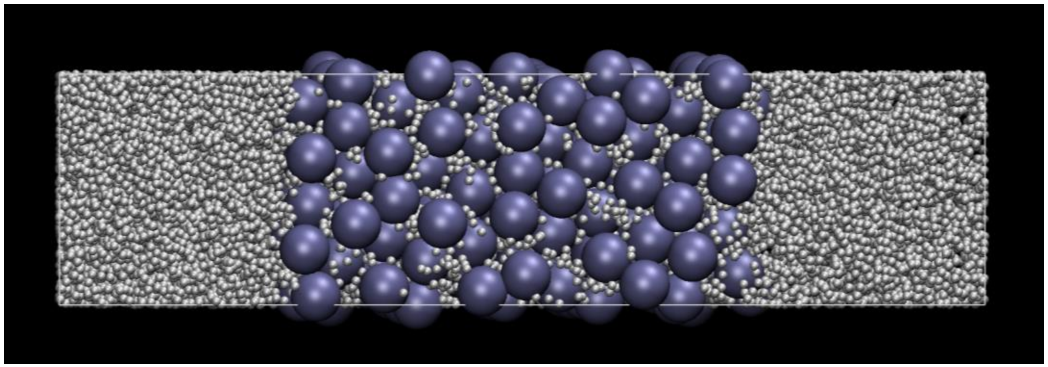
$L \sim 10 - 100$ nm

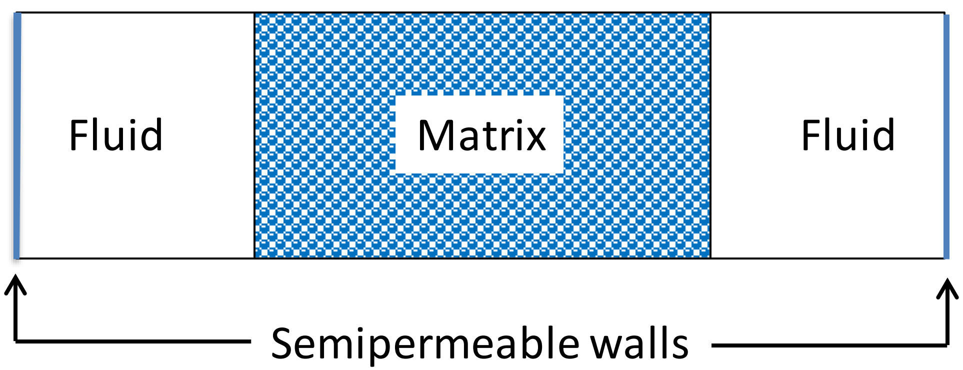
Fluid particle diameter: $\sigma \sim 0.2 - 5$ nm
Simulation time: $\sim 10^{-12} - 10^{-9}$sek
Matrix particle diameter/fluid particle diameter $\sim 5 - 10$

Task

- Illustrate application of Non-Equilibrium Molecular Dynamics (NEMD) to flow in porous media
- Is Darcy's law valid for such small systems?
- Visualize two-phase flow in a porous medium
- How does the porous medium change the Soret effect?
- Connect with theory and experiments

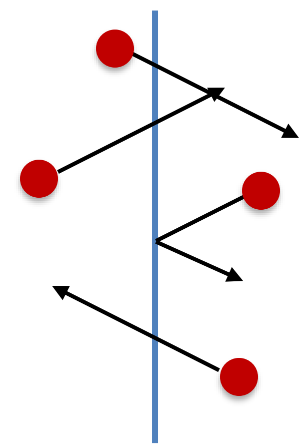
NEMD-method for fluid flow





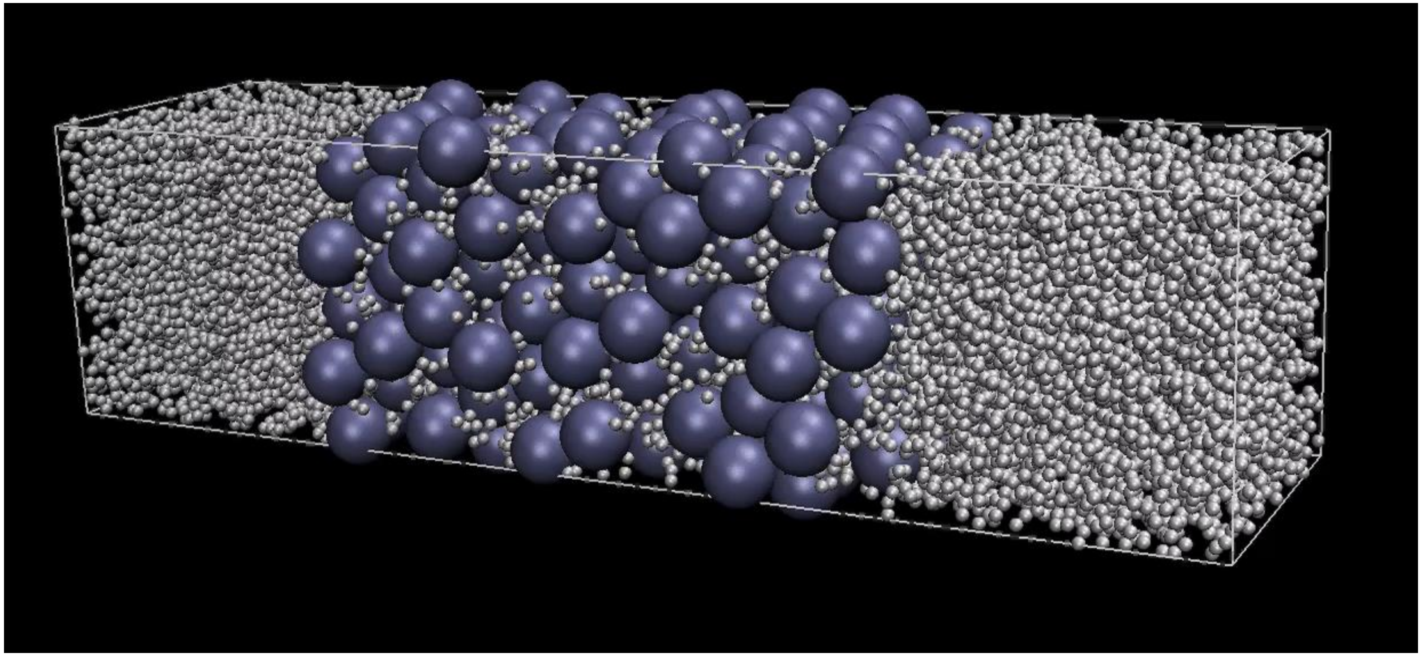
3D periodic boundary conditions

Reflecting Particle Method*): Wall directional permeability is controlled by a probability function

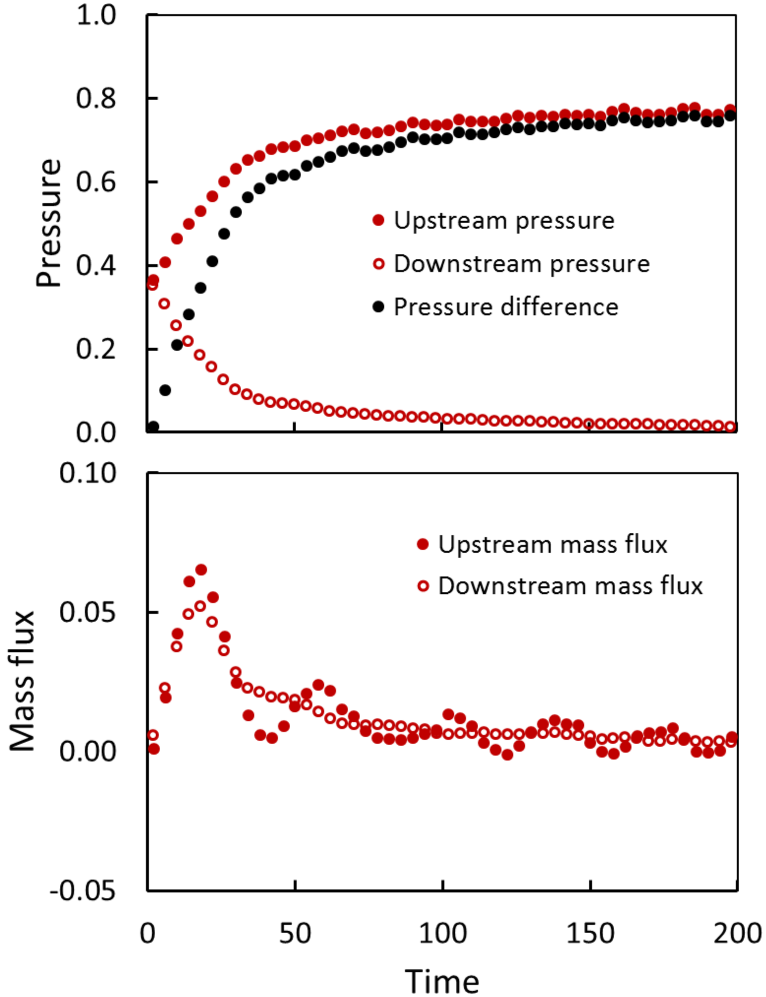


*): J. Li, D, Liao, and S. Yip, Phys. Rev. E, **57**, 7259 – 7267 (1998)

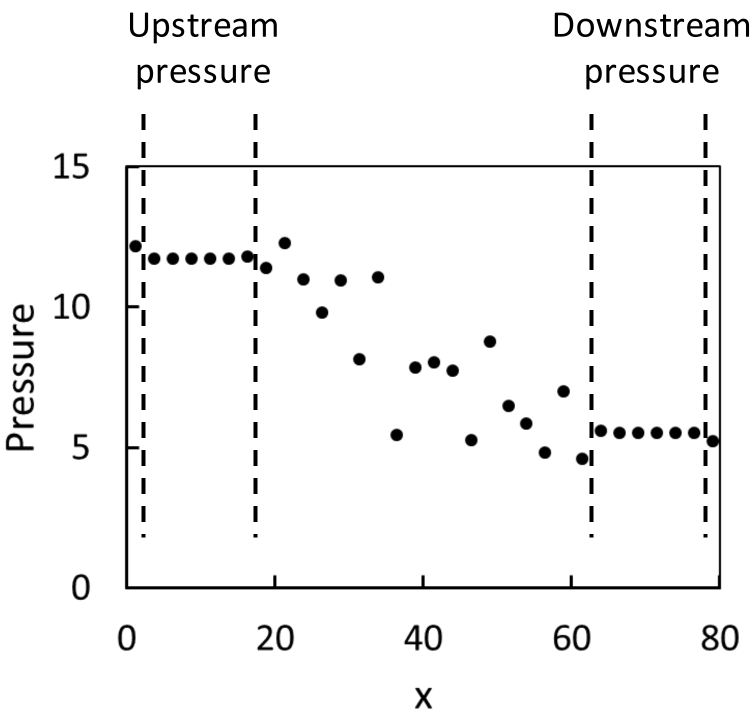
Simulation starts from equilibrium and eventually reaches steady state



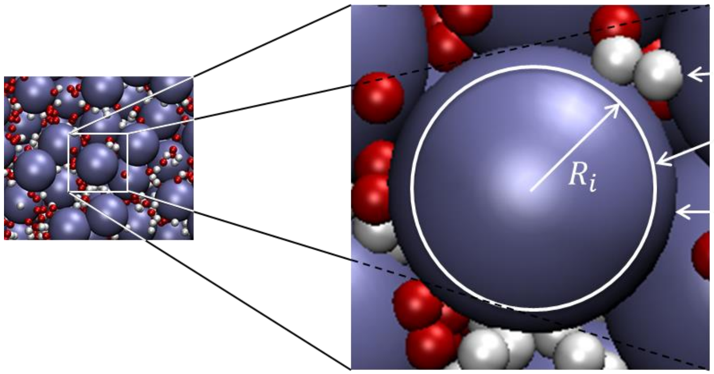
Data acquisition

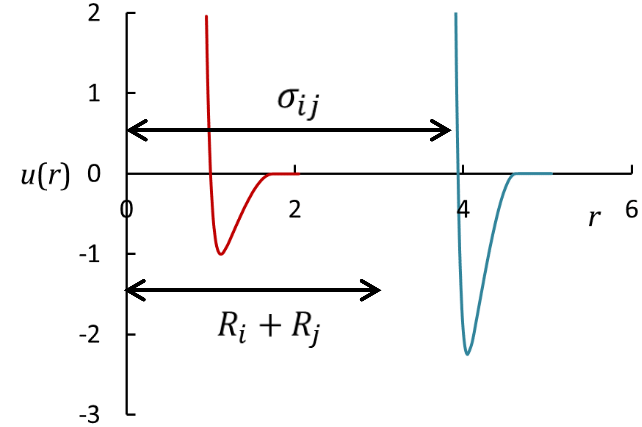


At steady state:



Model



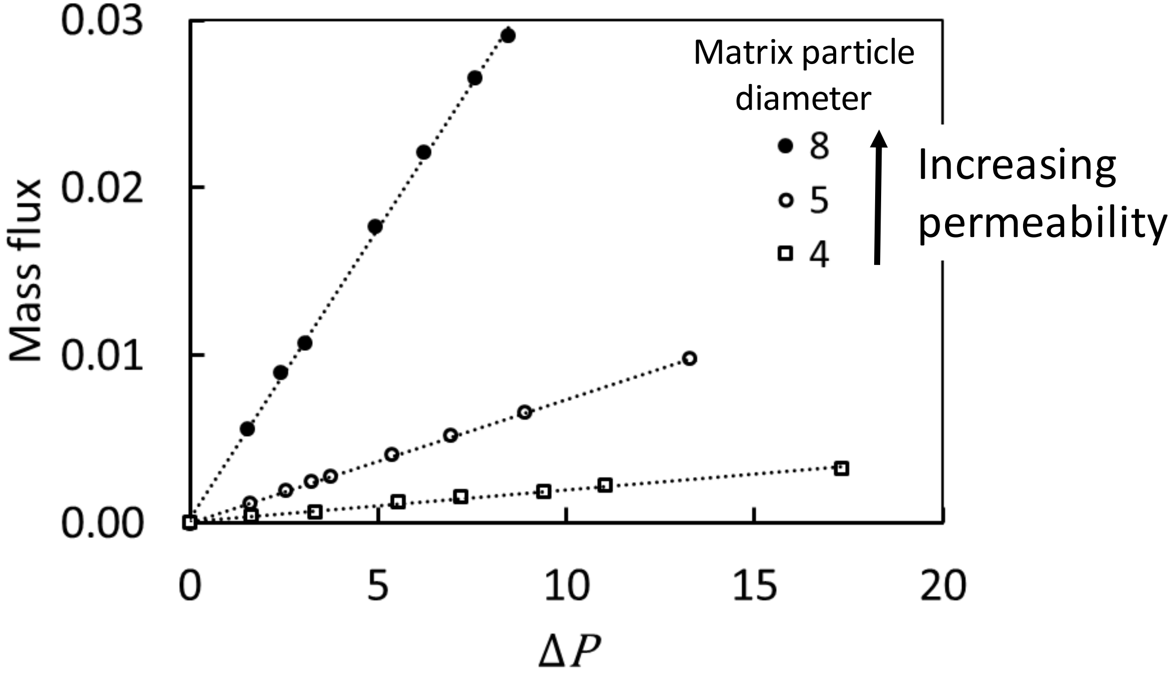


$$u_{ij}(r) = \begin{cases} \infty \quad \text{for } r < (R_i + R_j) \\ 4\varepsilon_{ij}\left[\left(\dfrac{\sigma_{ij} - (R_i + R_j)}{r - (R_i + R_j)}\right)^{12} - \alpha_{ij}\left(\dfrac{\sigma_{ij} - (R_i + R_j)}{r - (R_i + R_j)}\right)^{6}\right] \text{ for } r > (R_i + R_j) \end{cases}$$

Interactions: fluid - fluid, fluid - matrix particle, particle - particle
One or two fluid components, one or two matrix components.
Parameters: Temperature, density, composition, porosity (matrix number density)
permeability (matrix particle size), viscosity ($\alpha_{fluid-fluid}$),
wettability ($\alpha_{fluid-matrix}$), miscibility, one/two phases ($\alpha_{fluid1-fluid2}$)

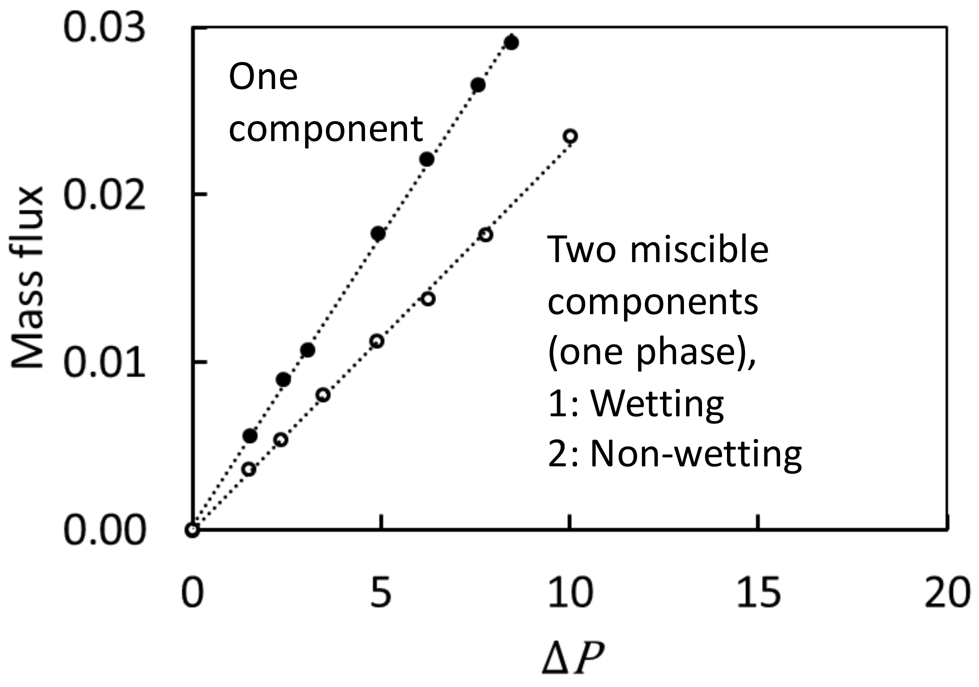
Darcy's law, effect of permeability

Matrix porosity: 40 %
One component
Liquid state, same fluid in all cases



Effect of wettability

Matrix porosity: 40 %
Liquid state
Matrix particle diameter: 8



Effect of fluid viscosity

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One component
Liquid state
Matrix particle diameter: 8

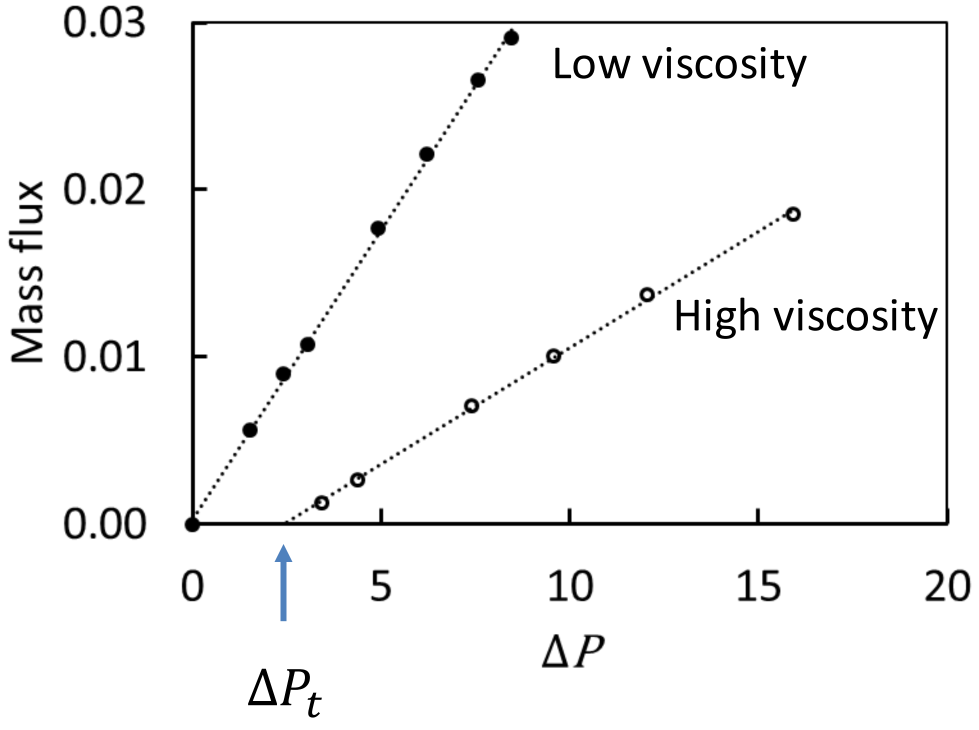
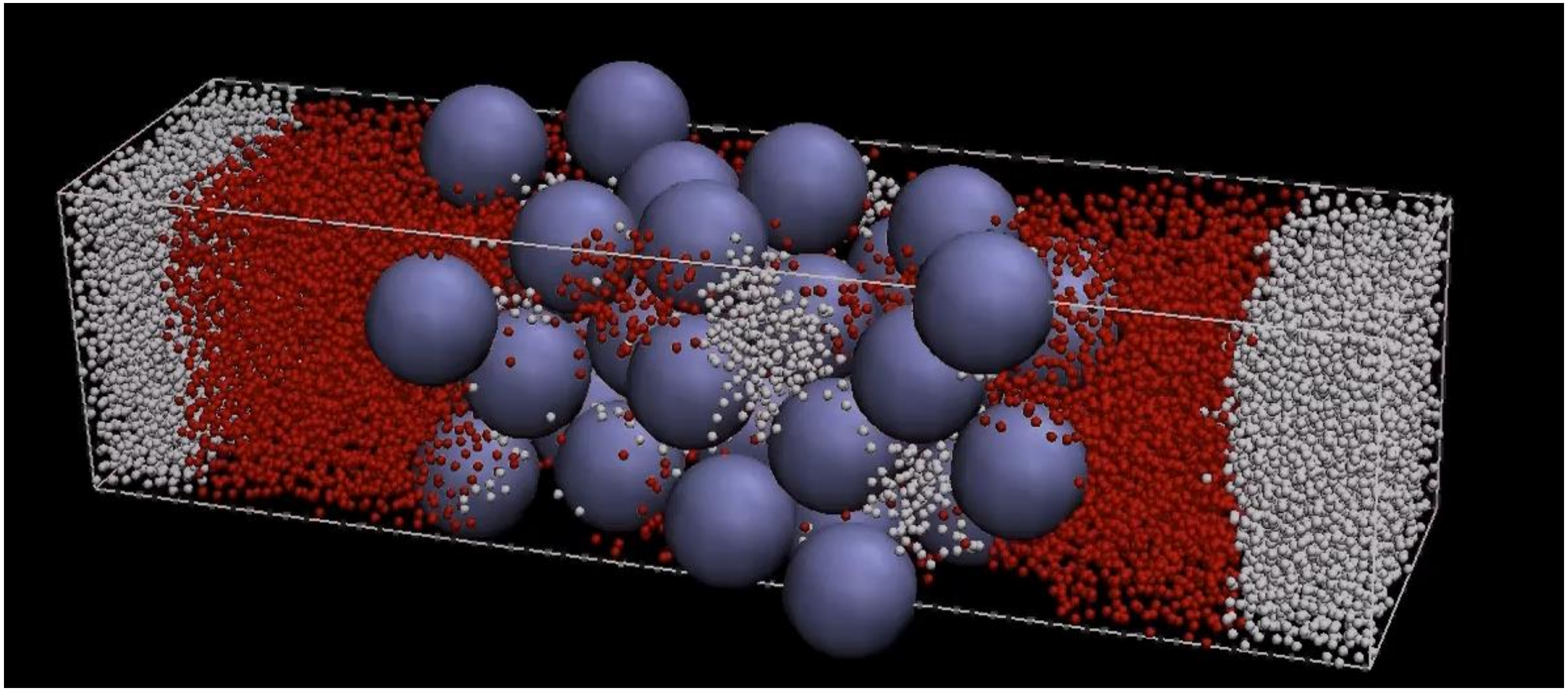


Illustration: Two-phase flow

Red fluid: Low viscosity, nonwetting
White fluid: High viscosity, wetting



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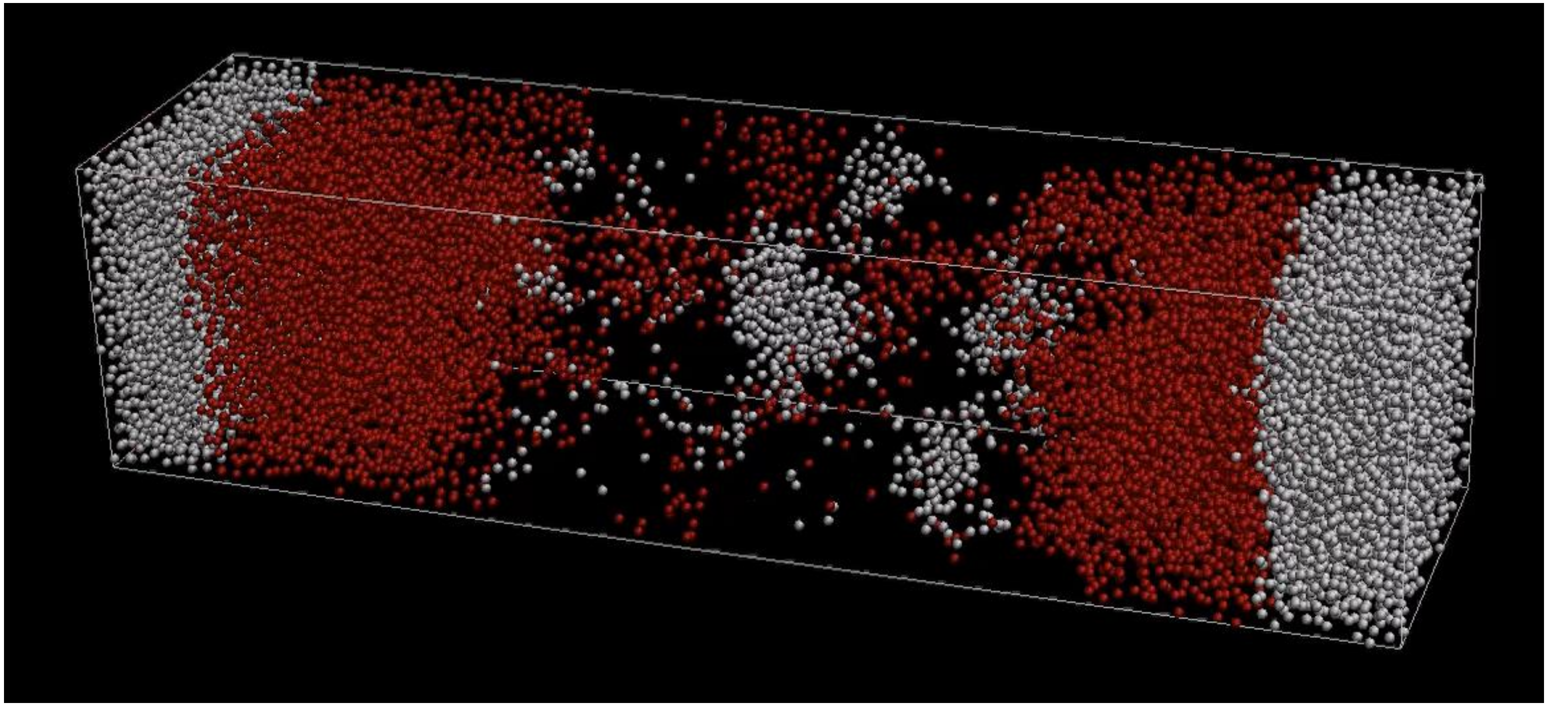
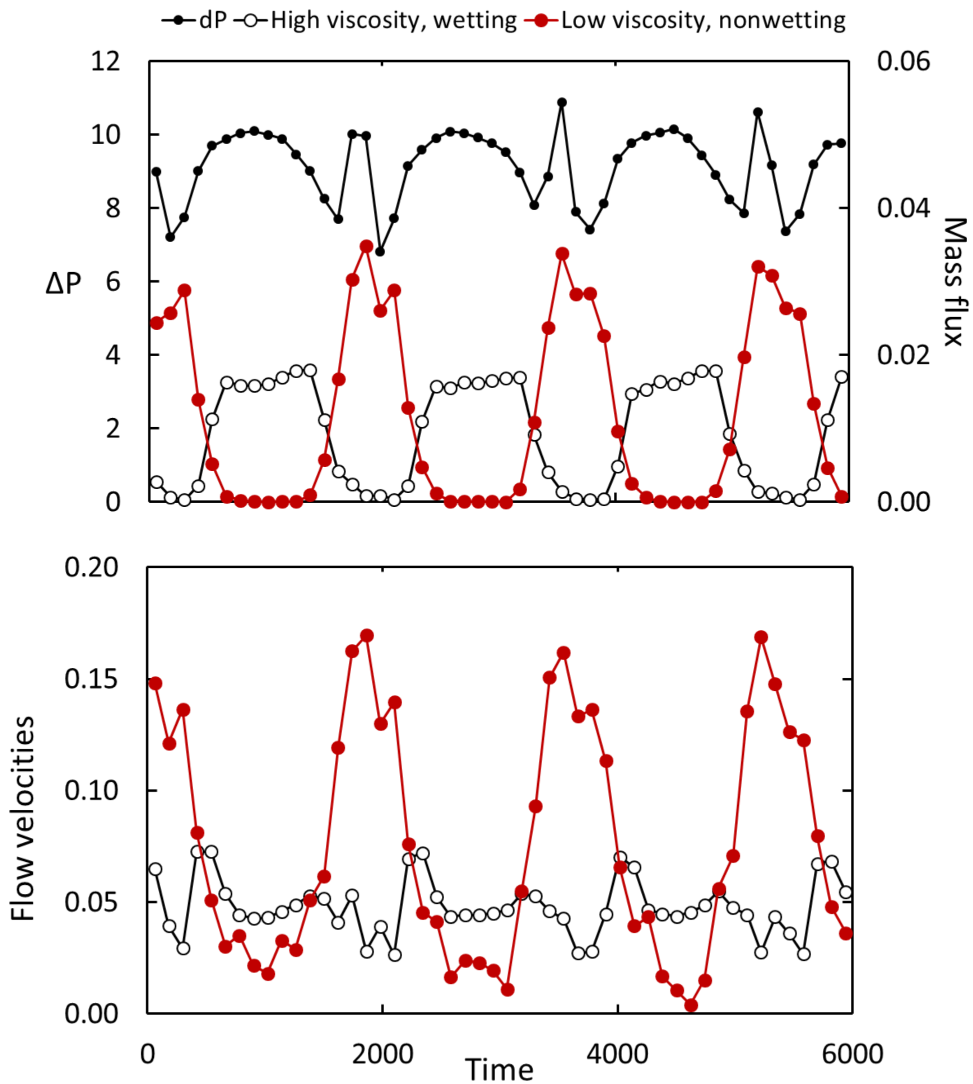
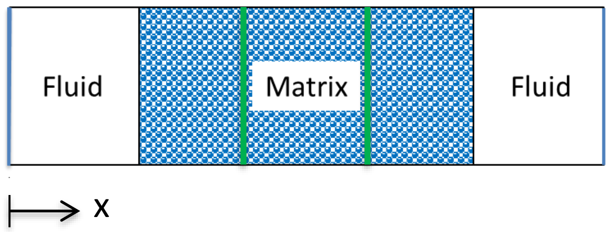
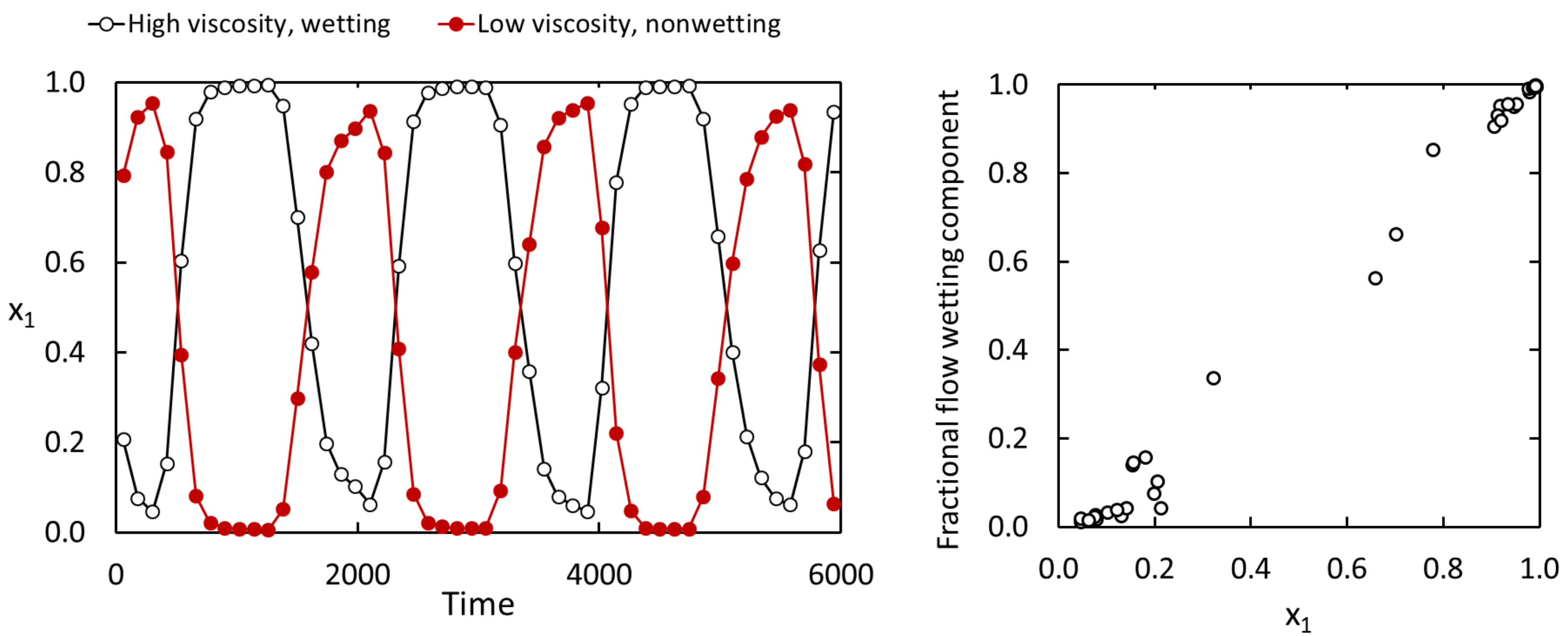


Mass fluxes and flow velocities in central matrix





Saturations in central matrix



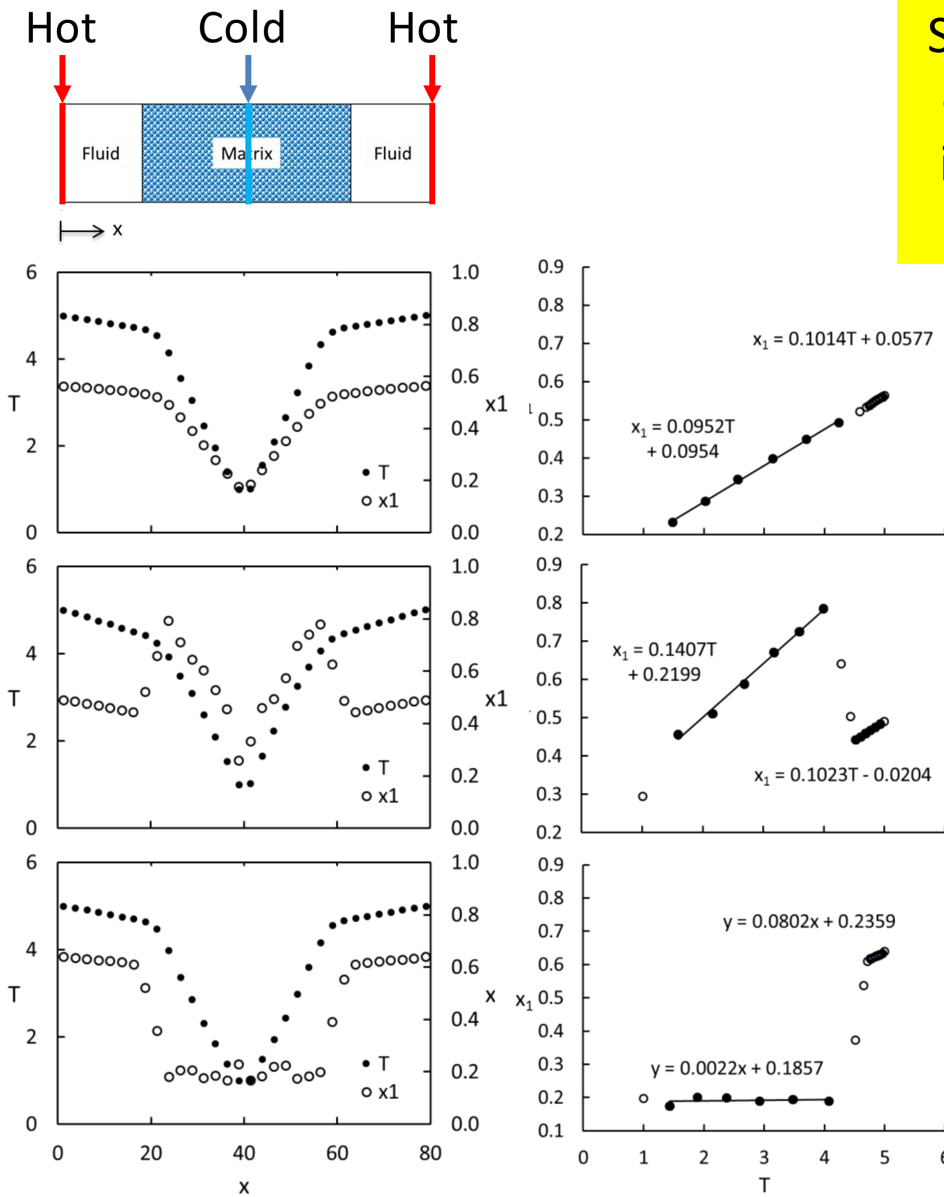
Soret effect, two components

Mass ratio $m_1 : m_2 = 1:10$
All other fluid parameters are equal
Overall composition: $x_1 = 0.5$
Matrix particle diameter: 5

Equal wettabilities:

Lighter component wetting:

Heavier component wetting:



Separation efficiency in matrix, $\Delta x_1/\Delta T$

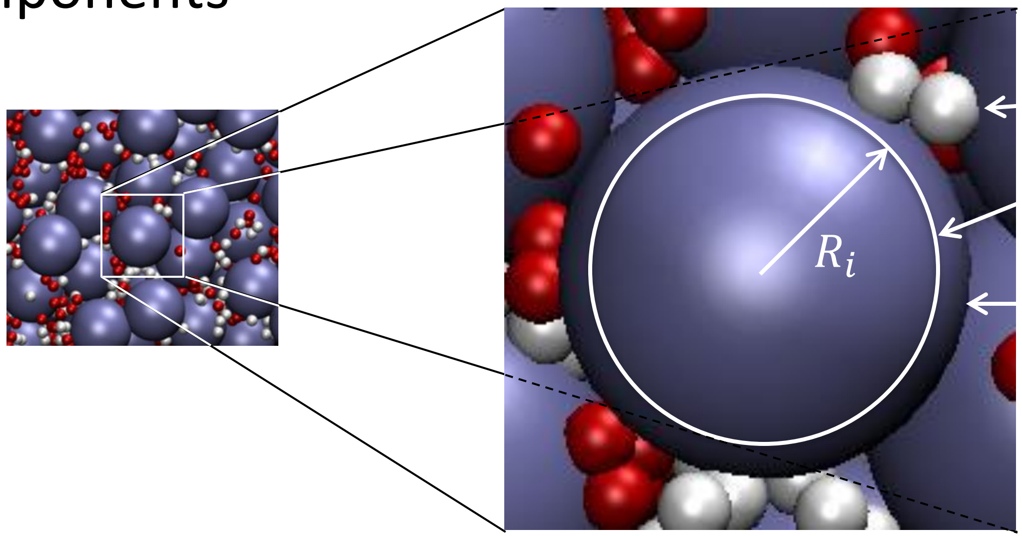
0.10

0.14

0.00

Questions?

Model



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