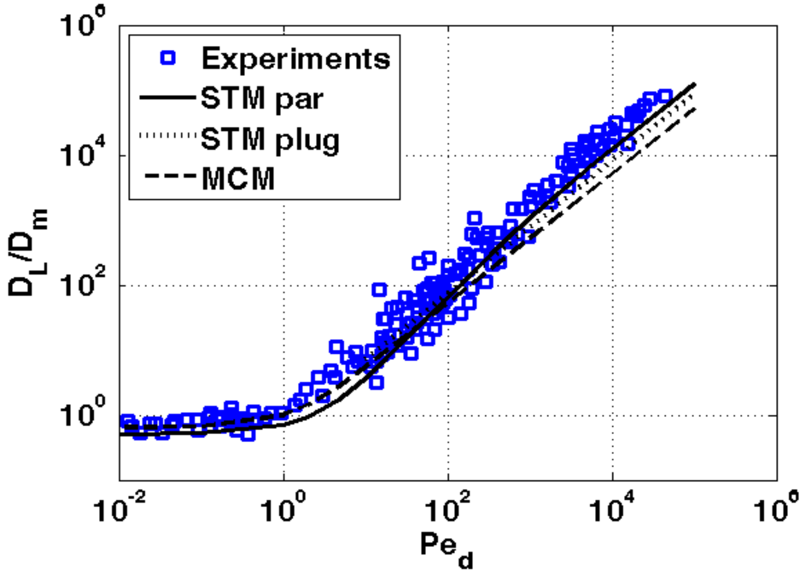
Eulerian Network Modeling of Longitudinal Dispersion



Normalized longitudinal dispersion coefficient vs. Pe_d for STM_{par}, STM_{plug}, and MCM against experimental data [Jha et al., 2011

Scientific Achievement

Developed novel Eulerian network model (Superposing Transport Method; STM) that accounts for shear dispersion

Significance and Impact

Pore-level model is able to accurately predict mixing and dispersion in CO2 sequestration

Research Details

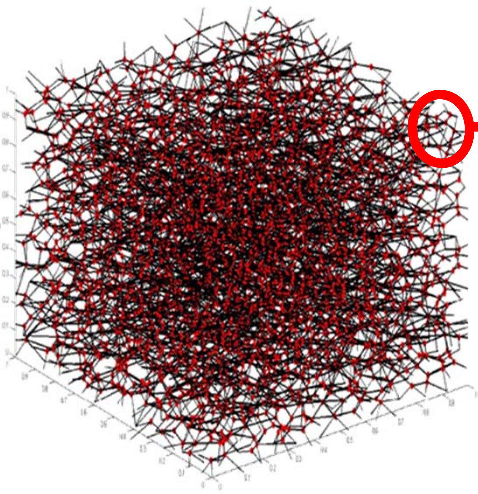
- **STM is non-local in time and is equivalent to performing network-wide time-convolutions of “elementary throat response functions”.**
- **Predicted macroscopic longitudinal dispersion coefficients for disordered sphere packs are in good agreement with published experimental data.**

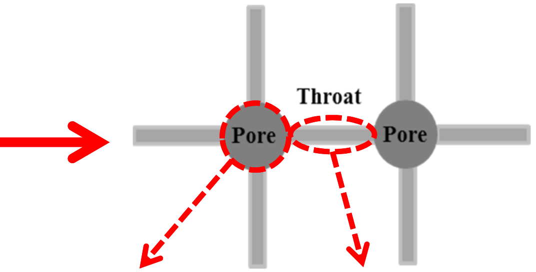
References

- Mehmani, Y., Balhoff, M. “Eulerian Network Modeling of Longitudinal Dispersion”, *Water Resources Research*, in review
- Mehmani, Y., Balhoff, M. “Chapter 13. Pore-Scale and Cross-Scale Modeling of Fluid Flow and Solute Transport”, *Reviews in Mineralogy & Geochemistry*, Volume 80, pages 433-459, August 2015

Work was performed at UT-Austin

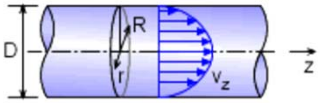
Traditional (Mixed Cell Method) Network Modeling





Mass Balance:

$$\sum_{j=1}^{n} \dot{m}_{ij} = 0$$



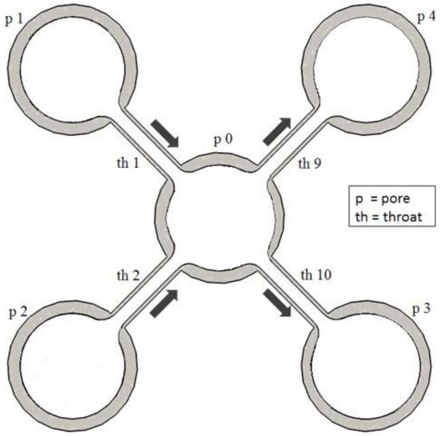
$$\dot{m}_{ij} = \frac{\rho \pi R^4}{8 \mu L}(p_j - p_i)$$

Flow Problem

- Mass conserved in pores
- Throats have all resistance; pores all volume

Flow Problem

- Species mass conserved in pores
- Perfect mixing assumed
- Throats have all resistance, so no shear dispersion



“perfect mixing” implicitly assumed!

Solute Balance:

$$V_{p0}\frac{dc_0}{dt} =$$ (accumulation)

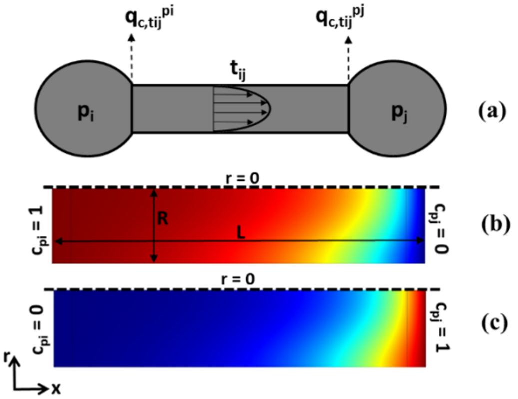
$$\sum_{j=1}^{N_{th}} c_j^{up} q_{0j} +$$ (convection)

$$\sum_{j=1}^{N_{th}} D_m a_{0j} \frac{\Delta c_{0j}}{l_{0j}} +$$ (diffusion)

$$R(c_0)$$ (reaction)

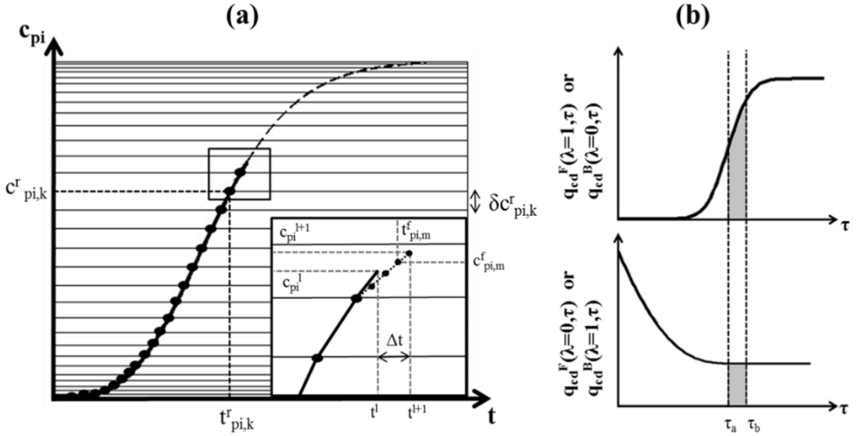
Shear Dispersion and Superposing Transport Method (STM)

$$\frac{\partial c}{\partial \tau} + (1-\xi^2)\frac{\partial c}{\partial \lambda} = \frac{\kappa^2}{Pe_L}\frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi \frac{\partial c}{\partial \xi}\right) + \frac{1}{Pe_L}\frac{\partial^2 c}{\partial \lambda^2}$$

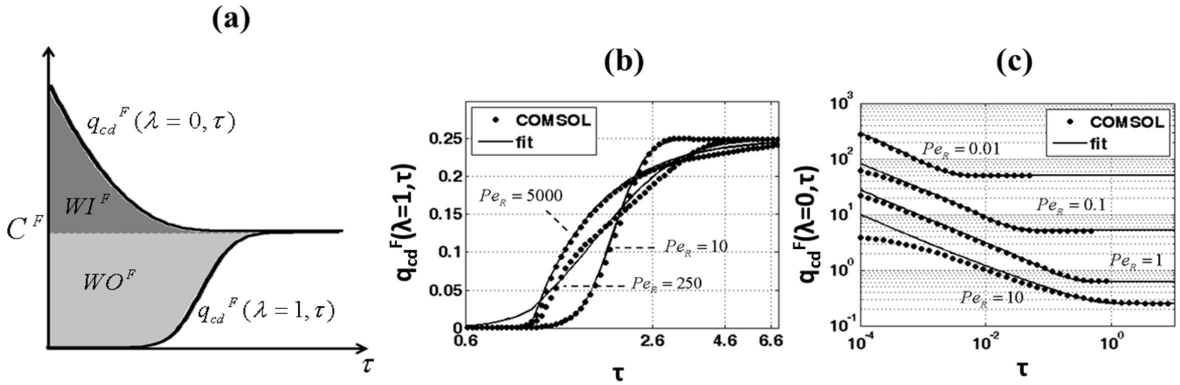


(a) Schematic of throat, t_{ij}, connected to two adjacent pores p_i and p_j. The parabolic velocity profile is responsible for shear dispersion. Axisymmetric representation of throat t_{ij} undergoing (b) forward transport, and (c) backward transport

$$V_{p_i}(c_{p_i}^{l+1} - c_{p_i}^{l}) = \sum_{j=1}^{N_{p_i}^{t}} \int_{t^l}^{t^{l+1}} q_{c,t_{ij}}^{p_i}\, dt$$

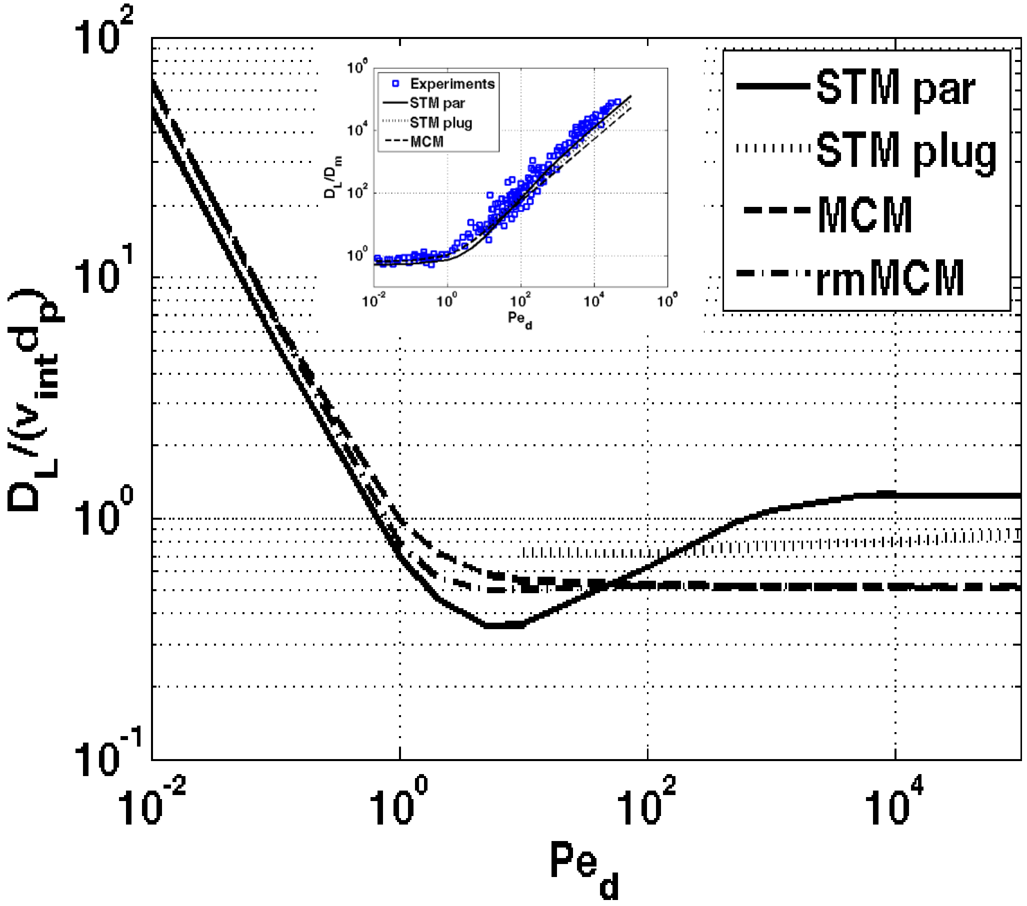


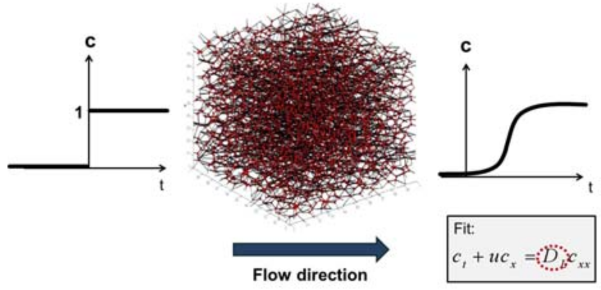
Evolving concentration of pore p_i. Horizontal lines mark where pore concentrations are recorded; shown by solid dots. Inset shows M=4 forecast points, and variables involved in eq. 14-16. (b) Schematic of typical profiles of q_{cd}^F and q_{cd}^B evaluated at $\lambda = 0$ and $\lambda = 1$.



(a) Shaded areas correspond to integrals i.e., WI^F and WO^F. Comparison between CFD and the fit by eq. 20 for (b) $q_{cd}^F(\lambda=1,\tau)$ and $\kappa = 15$, and (c) $q_{cd}^F(\lambda=0,\tau)$ and $\kappa = 1$, for various Pe_R.

Computed Dispersion Coefficients





- Dispersion coefficients back-calculated from network model
- STM (parabolic profile) matches experimental data well
- STM also predicts minimum in curve to the left. Accounting for shear dispersion is only way to predict boundary-layer dispersion

Conclusions

- STM captures shear dispersion within throats, which is not possible by any other Eulerian network model

- STM verified against convolution expressions, making it equivalent to performing network-wide convolutions of elementary throat response functions

- STM_{par} was validated against published experimental data for D_L in disordered bead/sand packs.

- Mixing assumptions within pores seem to have negligible impact on D_L predictions i.e., MCM and SSM results are indistinguishable.