Eulerian Network Modeling of Longitudinal Dispersion

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.

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

References
- Mehmani, Y., Balhoff, M. “Eulerian Network Modeling of Longitudinal Dispersion”, Water Resources Research, in review

Work was performed at UT-Austin
Traditional (Mixed Cell Method) Network Modeling

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

Mass Balance:
\[ \sum_{j=1}^{n} \dot{m}_{ij} = 0 \]
\[ \dot{m}_j = \frac{\rho \pi R^4}{8 \mu L} (p_j - p_i) \]

Solute Balance:
\[ V \frac{dc_0}{dt} = \left( \text{accumulation} \right) \]
\[ \sum_{j=1}^{N_{th}} c_j^p q_{0j} + \left( \text{convection} \right) \]
\[ \sum_{j=1}^{N_p} D_m \Delta c_j \frac{\Delta c_{0j}}{L_{0j}} + \left( \text{diffusion} \right) \]
\[ R(c_0) \left( \text{reaction} \right) \]

"perfect mixing" implicitly assumed!
Shear Dispersion and Superposing Transport Method (STM)

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

(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.

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

• $\text{STM}_{\text{par}}$ 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.