Impact of Compound-Specific Transverse Mixing on Steady-State Reactive Plumes

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1. Overview
We study the effect that transverse dispersion has on mixing-limited reactive transport in porous media, focusing on steady-state reactive plumes.

Mixing is critical and \( D_t \) is used to characterize it.

Our research objectives are to:
1) Evaluate the appropriateness of a nonlinear compound-specific description of \( D_t \) and its direct application to reactive transport
2) Assess the performance of such a parameterization of \( D_t \) in predicting mixing-limited reactive transport across a range of relevant groundwater flow velocities
3) Compare the predictive capability of the proposed nonlinear parameterization of \( D_t \) to that of the classical linear model

2. Problem Setup and Approach
Flow:
\[-\rho \frac{Dp}{Dt} + \rho \frac{Du}{Dt} = 0\]
Transport:
\[\nabla \cdot (\nabla D_t \nabla c) = R\]

\( D_t \) is used to characterize it.

Transverse dispersion (a) and dispersivities (b) as a function of velocity. Lines indicate nonlinear parameterization of \( D_t \).

3. Conservative Results
- Conservative tracers:
  - 2 compounds: fluorescein (\( D_{t,\text{fl}} = 4.8 \times 10^{-10} \text{ m}^2/\text{s} \)), oxygen (\( D_{t,\text{o}} = 1.97 \times 10^{-9} \text{ m}^2/\text{s} \)).
  - 8 flow velocities in the range: 0.1-10 m/d
- Determine \( D_t \) for each simulation
- Use for 2 parameterization approaches
  - Nonlinear, compound-specific: \( D_t = D_{t,\text{fl}} + D_{t,\text{o}} \) (parameterized)
    - \( \delta = 5:7 \): ratio length-hydraulic radius of pore channel
    - \( \beta = 0.47 \): captures extent of incomplete mixing
  - Linear: \( D_t = D_{t,\text{fl}} + a_t u \)
- Compute\( \alpha_t \) for each simulation

4. Reactive Results
- \( A + B \rightarrow C \)
  - \( R_t = \pm k_t c_A c_B \), \( k = 2 \times 10^5 \text{ M}^{-1} \text{ s}^{-1} \) (effectively instantaneous)
  - \( D_{t,\text{fl}} \) and \( D_{t,\text{o}} \) are set equal to that of fluorescein and oxygen, respectively.
  - \( D_{t,\text{fl}} \) and \( D_{t,\text{o}} \) with 4 different \( \alpha_t \) from 4 different tracer tests (red points above)

5. Conclusions
- Nonlinear parameterization captures the effect of incomplete mixing in the pore channels
- Critical in determining amount of reactions
- Linear parameterization cannot account for this
- Transverse dispersivity is not constant for a given porous medium but depends on both flow conditions and diffusive properties of the species
- Nonlinear \( D_t \) improves accuracy of continuum reactive transport predictions
- Steady-state reactive plume length increases with the square root of the flow velocity
- Molecular diffusion important
  - Micro process \( \rightarrow \) macro impact

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