Prediction of Breakthrough Curves for Conservative and Reactive Transport from the Structural Parameters of Highly Heterogeneous Media

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Motivation

Classical macrodispersion theory derives large-scale dispersivity from structural parameters, but:

1. Limited to unrealistically small heterogeneities, \( \sigma_{\ln K}^2 \ll 1 \)
2. Asymptotic behavior only reached after 10-100 integral scales

CTRW models are suitable for modelling highly heterogeneous advection, are predictive when calibrated, but require ad hoc calibration.

Desirable to determine breakthrough curve shapes from structural parameters without limitation on distance.
Four key ideas

1. Mean arrival time of solute, $\mu_t$, determined by

$$\mu_t = \frac{x}{U},$$

where $U$ is mean velocity, $x$ is distance from injection location.

2. For $\sigma_{\ln K}^2 < 4$, plane breakthrough curves are well described by log-normal distributions, which are defined by mean and variance.

3. All else equal, increasing distance drives increasing BTC symmetry (consequence of central limit theorem).

4. All else equal, increasing heterogeneity drives increasing BTC asymmetry.
Basic approach

1. Generate multiple multi-Gaussian subsurface realizations with different

\[ \sigma_{\ln K}^2. \]

2. Perform particle tracking to find flux-weighted BTCs at uniformly-spaced downgradient planes at

\[ X = \frac{x}{l_{\ln K}}. \] [Integral scale]

3. Perform regression to determine:

\[ \sigma_{\ln t}^2(X, \sigma_{\ln K}^2) \]

Schematic of single particle trajectory breaking through at successive planes.
Particle tracking

*K*-field box generated for each realization, imagined to fill space.

Periodic head BCs applied, with mean flow in \(x\)-direction.

Particles released from grid nodes on upgradient edge of the box.

Streamline tracking, with local-scale dispersion on each realization:
- 200 release points
- 40 particles per point
- 100 planes at which BT recorded
Regression to predict breakthrough curves

Polynomial regression yields $\sigma^2_{\text{ln } t}$, and we know $\mu_t$. For log-normal distribution,

$$\mu_{\text{ln } t} = \ln \mu_{\text{ln } t} + \frac{\sigma^2_{\text{ln } t}}{2}.$$  

Thus, we arrive at BTC expression

$$Uc_f (X, T) = \left[ \frac{U}{l_{\text{ln } K}} \right] \frac{1}{T} \sqrt{\frac{2\pi \sigma^2_{\text{ln } t}}{t}} e^{-\frac{(\ln X - \ln T + \frac{1}{2} \sigma^2_{\text{ln } t})^2}{2\sigma^2_{\text{ln } t}}},$$

where $T \equiv \frac{tU}{l_{\text{ln } K}}$.

3D scatter plot of $\sigma^2_{\text{ln } t}$ as function of $\sigma^2_{\text{ln } K}$ and $X$, with regression surface superimposed.
Robustness of regression

Monte Carlo approach allows assessment of regression reliability.

Two major concerns:

• How informative is ensemble-based regression about a single realization?

• Within a realization, how similar are point-release BTCs to their flux-weighted average?

3D scatter plot of $\sigma^2_{\ln t}$ as function of $\sigma^2_{\ln K}$ and $X$, with regression surface superimposed.
Predictive reliability

\[ X = 4.3 \]

\[ \sigma_{\ln K}^2 = 1 \]

\[ \sigma_{\ln K}^2 = 3.5 \]

Each axes shows a comparison of ten flux-weighted BTCs with corresponding regression prediction.

\[ X = 430 \]
Predictive reliability

All realizations are equally likely.

For regression to be predictive, the flux-weighted breakthrough of any realization must be “close enough” to the regression prediction.

Flux-weighted CDF of each realization \( F_i \) compared with regression CDF \( F_{\text{reg}} \) using log-time of 95\% breakthrough is a metric for this:

\[
\Omega \equiv \frac{1}{N} \sum_{i=1}^{N} \left[ F_{\text{reg}}(X, .95) - F_i(X, .95) \right]^2
\]

Heat map of \( \Omega \) as function of \( \sigma_{\ln K} \) and \( X \).
Point BTC coherence

\[ \sigma_{\ln K}^2 = 1 \quad \text{and} \quad \sigma_{\ln K}^2 = 3.5 \]

Each column is from a single realization.

\[ X = 4.3 \quad \text{and} \quad X = 430 \]
Point BTC coherence

Variance of 95 % breakthrough among point BTCs for each of the 200 release locations within a realization is a proxy for BTC coherence.

Average of this quantity, over all realizations with identical $\sigma_{\ln K}^2$, is a measure of incoherence.

Coherence is necessary condition for regression to be predictive.

Heat map of variance of 95% point breakthrough as function of $\sigma_{\ln K}^2$ and $X$. 
Implied $D_\infty$

We can show that if the solute breakthrough curve at a plane is inverse Gaussian, then:

$$D_\infty = \frac{\sigma_t^2 x^2}{2\mu_t^3}$$

This alternative approach does not require sequential calculation of whole-plume moments.

Once this quantity stabilizes, we have entered the macrodispersion regime. We obtain

- Number of integral scales to macrodispersive limit
- $D_\infty$ as function of $\sigma_{\ln K}^2$. 

Implied $D_\infty$

Heat map of $\ln D_\infty$ as function of $\sigma_{\ln K}^2$ and $X$.

Asymptotic $D_\infty$ from simulation, compared with classical, asymptotic approximation and another recent numerical study.
Key points

1. Approached the problem of linking **breakthrough curve shape** (RP-CTRW transition distribution) to **structural parameters** from a Monte Carlo approach.

2. Monte Carlo analysis allowed empirical error analysis:
   1. Within a realization (point breakthrough curves)
   2. Between realizations

3. BTCs also imply a late-time macrodispersion coefficient.