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, $\sigma^2_{\ln K} \ll 1$
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, μ_t, determined by

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

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

2. For $\sigma^2_{\ln K} < 4$, 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

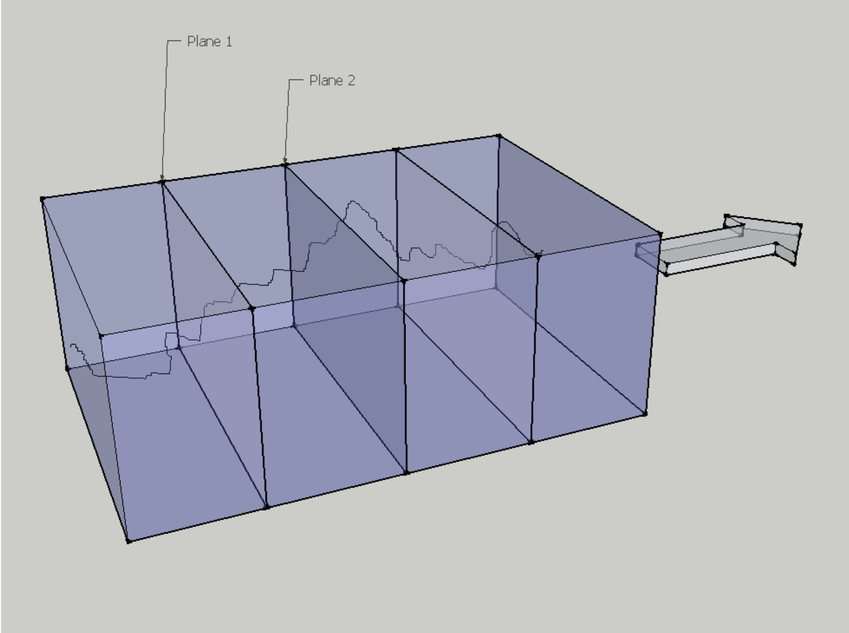
$$\sigma^2_{\ln K}.$$

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

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

3. Perform regression to determine:

$$\sigma^2_{\ln t}(X, \sigma^2_{\ln K})$$



Schematic of single particle trajectory breaking through at successive planes.

Particle tracking

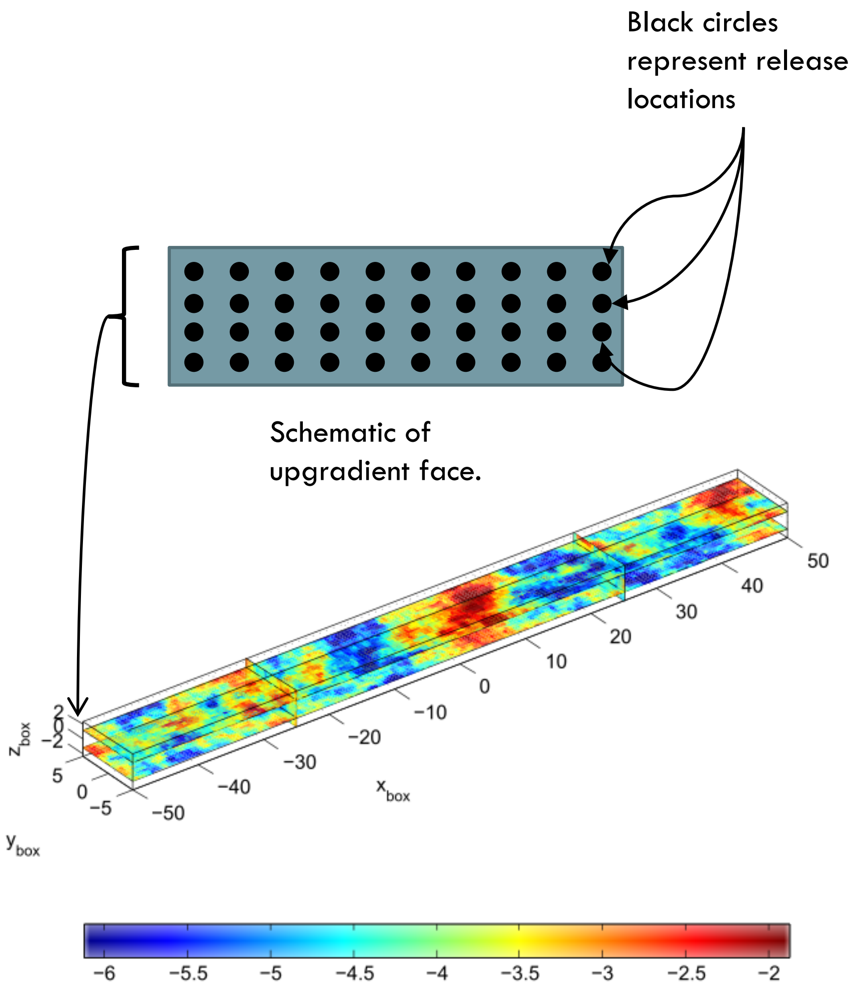
K-field box generated for each realization, imagined to fill space.

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

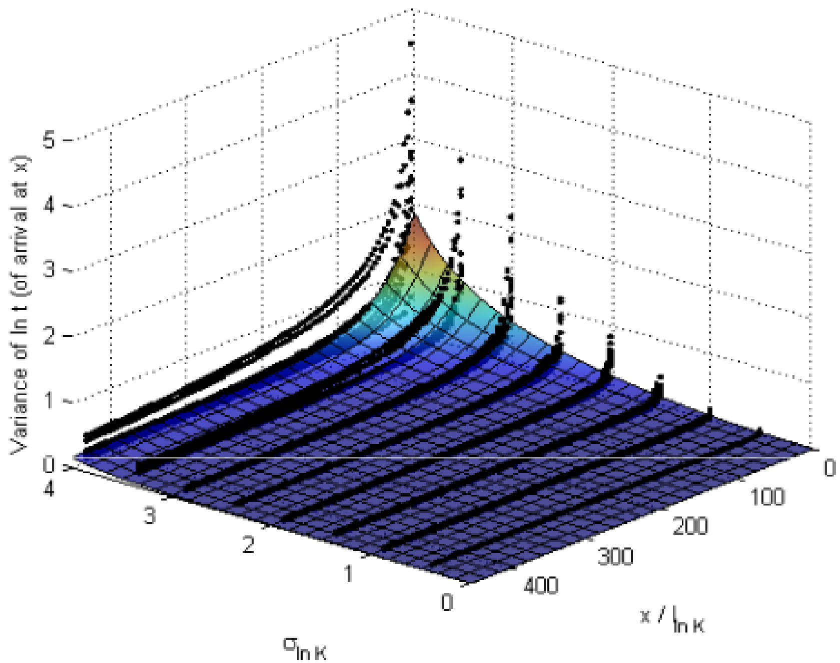
Polynomial regression yields $\sigma^2_{\ln t}$, and we know μ_t. For log-normal distribution,

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

Thus, we arrive at BTC expression

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

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



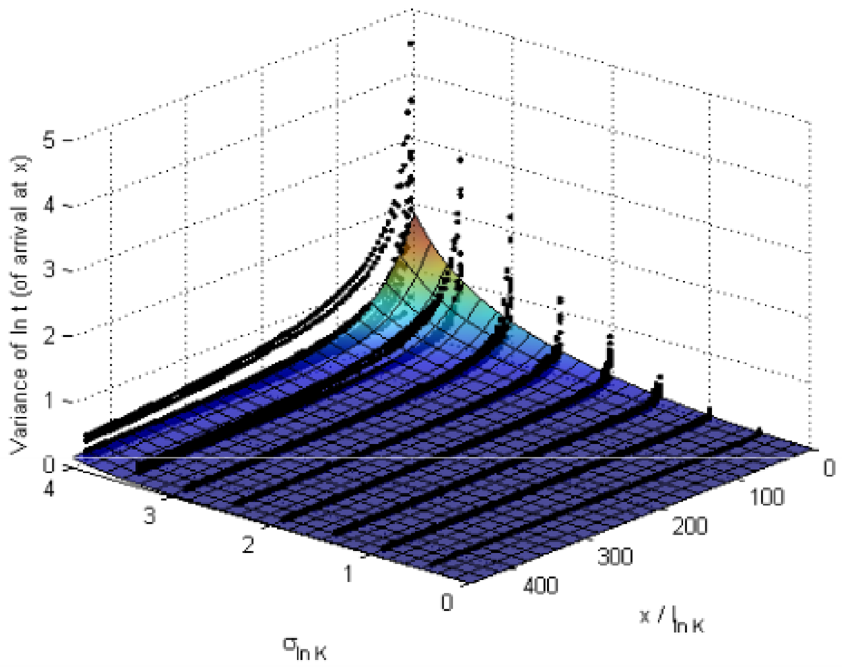
3D scatter plot of $\sigma^2_{\ln t}$ as function of $\sigma^2_{\ln K}$ and X, with regression surface superimposed.

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?



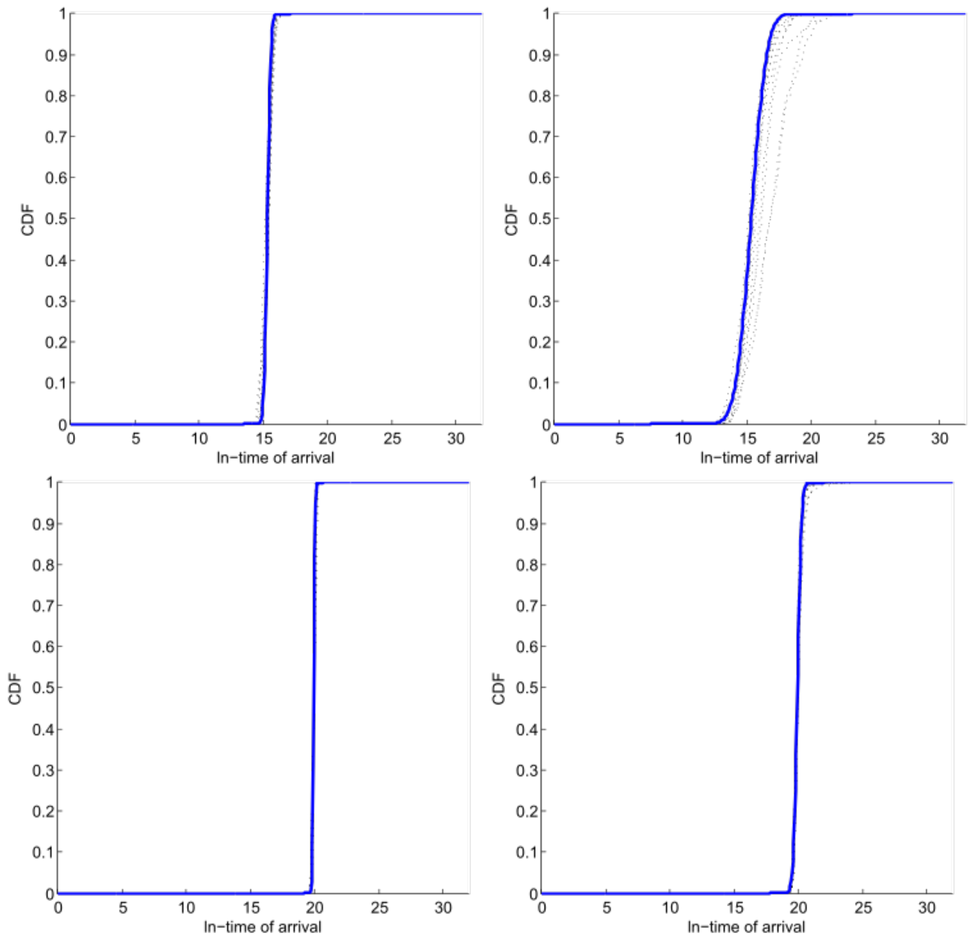
3D scatter plot of $\sigma^2_{\ln t}$ as function of $\sigma^2_{\ln K}$ and X, with regression surface superimposed.

Predictive reliability

$\sigma^2_{\ln K} = 1$ $\sigma^2_{\ln K} = 3.5$

$X = 4.3$

$X = 430$



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

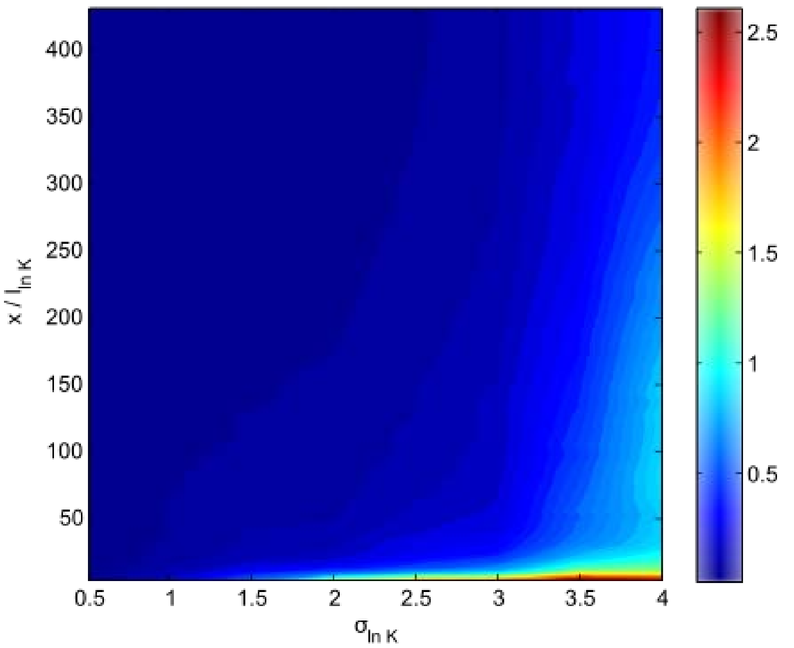
Predictive reliability

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_{reg}) using log-time of 95% breakthrough is a metric for this:

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



Heat map of Ω as function of $\sigma^2_{\ln K}$ and X.

Point BTC coherence

$\sigma^2_{\ln K} = 1$ $\sigma^2_{\ln K} = 3.5$

$X = 4.3$

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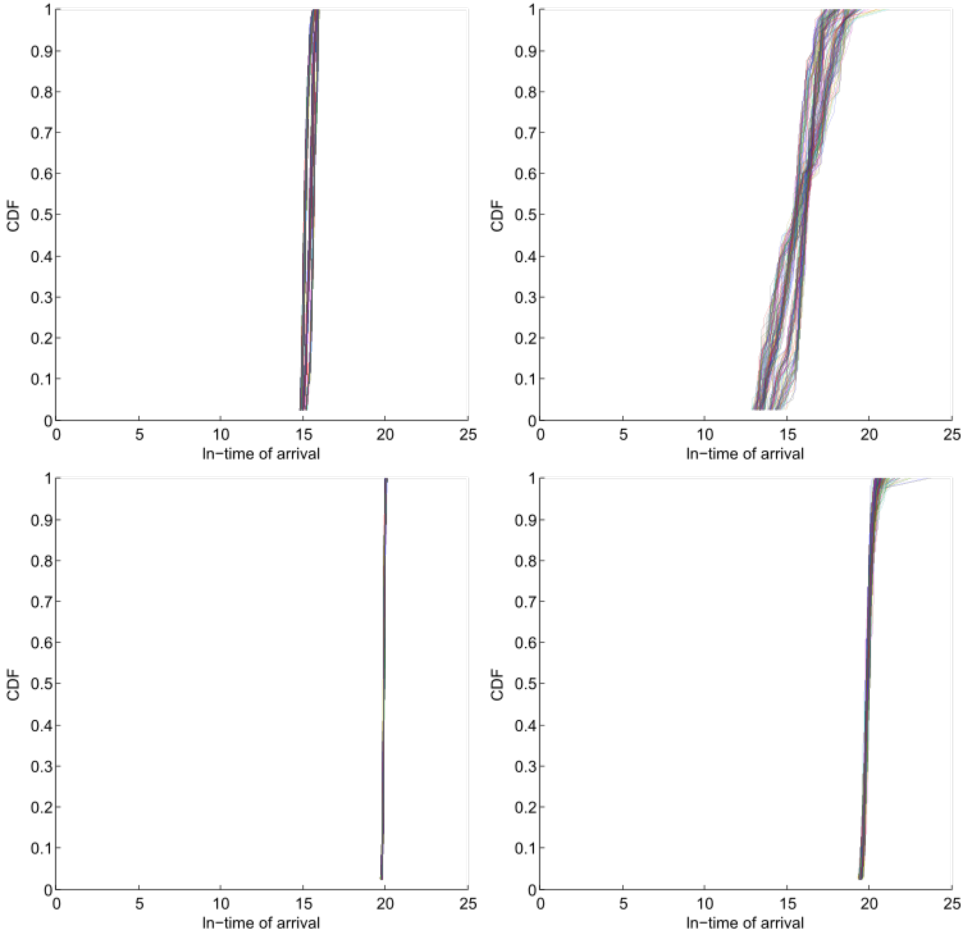


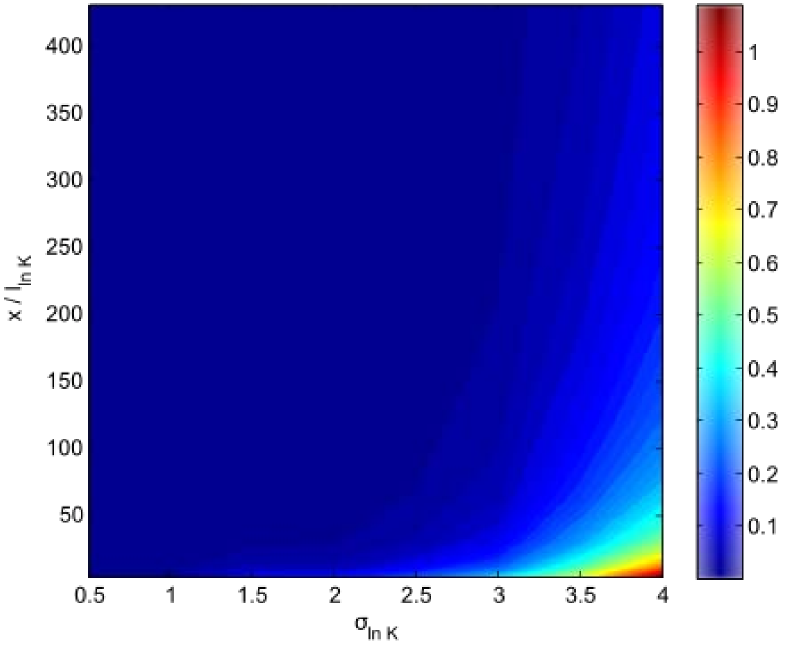
Each column is from a single realization

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 $\boldsymbol{\sigma^2_{ln\ K}}$**, 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 $\sigma^2_{\ln K}$ and X.

Implied D_∞

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

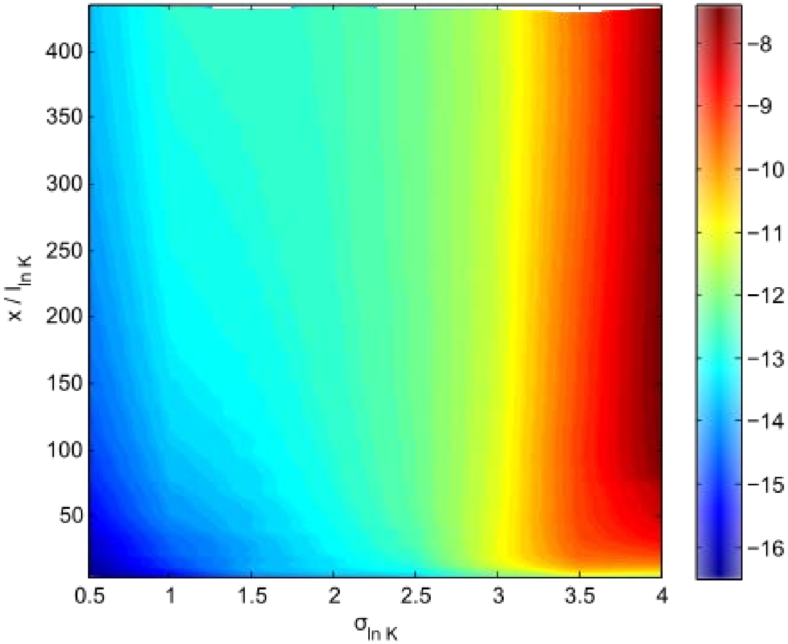
$$D_\infty = \frac{\sigma_t^2 x^2}{2\mu_t^3}$$

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

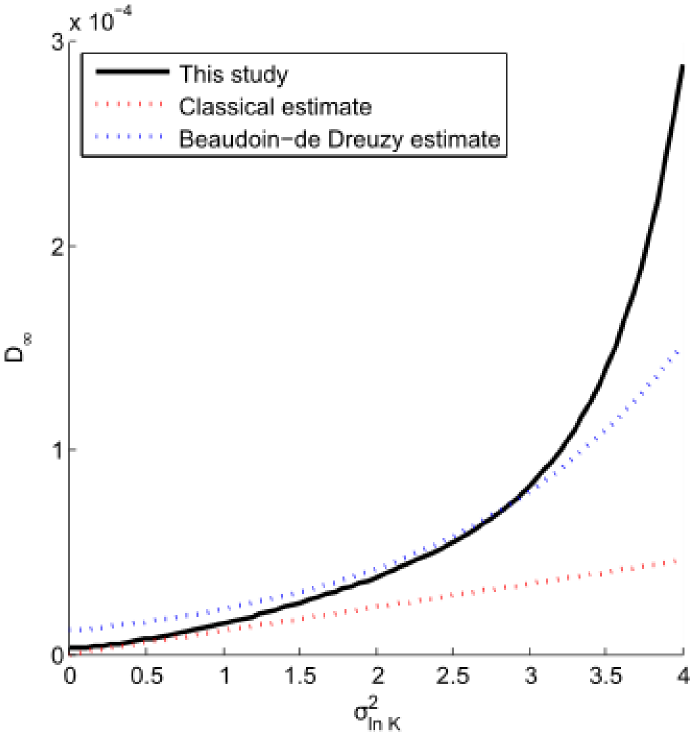
Once this quantity stabilizes, we have entered the macrodispersion regime. We obtain

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

Implied D_∞



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



Asymptotic D_∞ 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.