Parameter Estimation for Fractional Transport

Chae Young Lim

Department of Statistics and Probability
Michigan State University

Joint work with Paramita Chakraborty, Mark M. Meerschaert

June 2009

fADE model

The space-fractional advection-dispersion equation (fADE):

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{1+\beta}{2}\frac{\partial^\alpha C}{\partial x^\alpha} + D\frac{1-\beta}{2}\frac{\partial^\alpha C}{\partial(-x)^\alpha}, \qquad (1)$$

- $C(x,t)$ is tracer concentration
- v (L/T) is the average plume velocity
- D (L$^\alpha$/T) controls rate of spreading
- β (dimensionless) is the skewness parameter.
- the space-fractional index α (dimensionless) codes the heterogeneity of the porous medium
- When $\alpha = 2$, (1) reduces to the classical ADE with constant parameters.

fADE model

The space-fractional advection-dispersion equation (fADE):

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{1+\beta}{2}\frac{\partial^\alpha C}{\partial x^\alpha} + D\frac{1-\beta}{2}\frac{\partial^\alpha C}{\partial(-x)^\alpha}, \tag{1}$$

- $C(x,t)$ is tracer concentration
- v (L/T) is the average plume velocity
- D (L$^\alpha$/T) controls rate of spreading
- β (dimensionless) is the skewness parameter.
- the space-fractional index α (dimensionless) codes the heterogeneity of the porous medium
- When $\alpha = 2$, (1) reduces to the classical ADE with constant parameters.

fADE model

The space-fractional advection-dispersion equation (fADE):

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{1+\beta}{2}\frac{\partial^\alpha C}{\partial x^\alpha} + D\frac{1-\beta}{2}\frac{\partial^\alpha C}{\partial (-x)^\alpha}, \qquad (1)$$

- $C(x, t)$ is tracer concentration
- v (L/T) is the average plume velocity
- D (L^α/T) controls rate of spreading
- β (dimensionless) is the skewness parameter.
- the space-fractional index α (dimensionless) codes the heterogeneity of the porous medium
- When $\alpha = 2$, (1) reduces to the classical ADE with constant parameters.

fADE model

The space-fractional advection-dispersion equation (fADE):

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{1+\beta}{2}\frac{\partial^\alpha C}{\partial x^\alpha} + D\frac{1-\beta}{2}\frac{\partial^\alpha C}{\partial(-x)^\alpha}, \qquad (1)$$

- $C(x, t)$ is tracer concentration
- v (L/T) is the average plume velocity
- D (L$^\alpha$/T) controls rate of spreading
- β (dimensionless) is the skewness parameter.
- the space-fractional index α (dimensionless) codes the heterogeneity of the porous medium
- When $\alpha = 2$, (1) reduces to the classical ADE with constant parameters.

fADE model

The space-fractional advection-dispersion equation (fADE):

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{1+\beta}{2}\frac{\partial^\alpha C}{\partial x^\alpha} + D\frac{1-\beta}{2}\frac{\partial^\alpha C}{\partial(-x)^\alpha}, \qquad (1)$$

- $C(x, t)$ is tracer concentration
- v (L/T) is the average plume velocity
- D (L$^\alpha$/T) controls rate of spreading
- β (dimensionless) is the skewness parameter.
- the space-fractional index α (dimensionless) codes the heterogeneity of the porous medium
- When $\alpha = 2$, (1) reduces to the classical ADE with constant parameters.

fADE model

The space-fractional advection-dispersion equation (fADE):

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{1+\beta}{2}\frac{\partial^\alpha C}{\partial x^\alpha} + D\frac{1-\beta}{2}\frac{\partial^\alpha C}{\partial(-x)^\alpha}, \qquad (1)$$

- $C(x,t)$ is tracer concentration
- v (L/T) is the average plume velocity
- D (L$^\alpha$/T) controls rate of spreading
- β (dimensionless) is the skewness parameter.
- the space-fractional index α (dimensionless) codes the heterogeneity of the porous medium
- When $\alpha = 2$, (1) reduces to the classical ADE with constant parameters.

fADE model

The space-fractional advection-dispersion equation (fADE):

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{1+\beta}{2}\frac{\partial^\alpha C}{\partial x^\alpha} + D\frac{1-\beta}{2}\frac{\partial^\alpha C}{\partial(-x)^\alpha}, \qquad (1)$$

- $C(x,t)$ is tracer concentration
- v (L/T) is the average plume velocity
- D (L$^\alpha$/T) controls rate of spreading
- β (dimensionless) is the skewness parameter.
- the space-fractional index α (dimensionless) codes the heterogeneity of the porous medium
- When $\alpha = 2$, (1) reduces to the classical ADE with constant parameters.

Particle tracking approach

- A tracer plume is represented by a large ensemble of statistically identical particles $[X_t^{(k)} : 1 \leq k \leq n]$.
- Each particle has the same probability density $f_\theta(x,t)$.
- We assume a fixed total mass $K > 0$, so that each particle carries mass K/n.
- The model concentration $C(x,t) = Kf_\theta(x,t)$.
- For the fADE with point source initial condition, $f_\theta(x,t)$ is a stable density.

Particle tracking approach

- A tracer plume is represented by a large ensemble of statistically identical particles $[X_t^{(k)} : 1 \leq k \leq n]$.
- Each particle has the same probability density $f_\theta(x, t)$.
- We assume a fixed total mass $K > 0$, so that each particle carries mass K/n.
- The model concentration $C(x, t) = K f_\theta(x, t)$.
- For the fADE with point source initial condition, $f_\theta(x, t)$ is a stable density.

Particle tracking approach

- A tracer plume is represented by a large ensemble of statistically identical particles $[X_t^{(k)} : 1 \leq k \leq n]$.
- Each particle has the same probability density $f_\theta(x, t)$.
- We assume a fixed total mass $K > 0$, so that each particle carries mass K/n.
- The model concentration $C(x, t) = Kf_\theta(x, t)$.
- For the fADE with point source initial condition, $f_\theta(x, t)$ is a stable density.

Particle tracking approach

- A tracer plume is represented by a large ensemble of statistically identical particles $[X_t^{(k)} : 1 \leq k \leq n]$.
- Each particle has the same probability density $f_\theta(x, t)$.
- We assume a fixed total mass $K > 0$, so that each particle carries mass K/n.
- The model concentration $C(x, t) = Kf_\theta(x, t)$.
- For the fADE with point source initial condition, $f_\theta(x, t)$ is a stable density.

Particle tracking approach

- A tracer plume is represented by a large ensemble of statistically identical particles $[X_t^{(k)} : 1 \leq k \leq n]$.
- Each particle has the same probability density $f_{\boldsymbol{\theta}}(x, t)$.
- We assume a fixed total mass $K > 0$, so that each particle carries mass K/n.
- The model concentration $C(x, t) = Kf_{\boldsymbol{\theta}}(x, t)$.
- For the fADE with point source initial condition, $f_{\boldsymbol{\theta}}(x, t)$ is a stable density.

Particle tracking approach

- A tracer plume is represented by a large ensemble of statistically identical particles $[X_t^{(k)} : 1 \leq k \leq n]$.
- Each particle has the same probability density $f_{\boldsymbol{\theta}}(x, t)$.
- We assume a fixed total mass $K > 0$, so that each particle carries mass K/n.
- The model concentration $C(x, t) = Kf_{\boldsymbol{\theta}}(x, t)$.
- For the fADE with point source initial condition, $f_{\boldsymbol{\theta}}(x, t)$ is a stable density.

- Histogram of a large ensemble of particles

$$\hat{f}_{\boldsymbol{\theta}}(x,t) = \frac{1}{n}\sum_{k=1}^{n} I(x-\Delta < X_t^{(k)} \leq x)$$

- Suppressing t and θ,

$$E[\hat{f}(x)] = \frac{p_\Delta(x)}{\Delta}$$

$$\mathrm{Var}\left[\hat{f}(x)\right] = \frac{1}{n\Delta^2}p_\Delta(x)\left(1-p_\Delta(x)\right)$$

$$\mathrm{Cov}\left[\hat{f}(x),\hat{f}(y)\right] = -\frac{1}{n\Delta^2}p_\Delta(x)p_\Delta(y)$$

$p_\Delta(x) = F(x) - F(x-\Delta)$

- Histogram of a large ensemble of particles

$$\hat{f}_{\theta}(x,t) = \frac{1}{n}\sum_{k=1}^{n} I(x-\Delta < X_t^{(k)} \leq x)$$

- Suppressing t and θ,

$$\begin{aligned} E[\hat{f}(x)] &= \frac{p_\Delta(x)}{\Delta} \\ \mathrm{Var}\left[\hat{f}(x)\right] &= \frac{1}{n\Delta^2} p_\Delta(x)\left(1 - p_\Delta(x)\right) \\ \mathrm{Cov}\left[\hat{f}(x), \hat{f}(y)\right] &= -\frac{1}{n\Delta^2} p_\Delta(x) p_\Delta(y) \end{aligned}$$

$$p_\Delta(x) = F(x) - F(x-\Delta)$$

- It can be shown that

$$\sqrt{n\Delta}\begin{pmatrix} \hat{f}(x) - f(x) \\ \hat{f}(y) - f(y) \end{pmatrix} \rightarrow N\left(0, \begin{pmatrix} f(x) & 0 \\ 0 & f(y) \end{pmatrix}\right).$$

- Observed concentration, $\hat{C}(x,t)$, can be regarded as a scaled histogram bar,

$$\hat{C}(x,t) = \frac{K}{\Delta} \cdot \frac{N_x}{n} = K\hat{f}(x,t)$$

N_x is the number of particles in the bin at location x, and Δ is the bin width.

- It can be shown that

$$\sqrt{n\Delta}\begin{pmatrix} \hat{f}(x) - f(x) \\ \hat{f}(y) - f(y) \end{pmatrix} \to N\left(0, \begin{pmatrix} f(x) & 0 \\ 0 & f(y) \end{pmatrix}\right).$$

- Observed concentration, $\hat{C}(x,t)$, can be regarded as a scaled histogram bar,

$$\hat{C}(x,t) = \frac{K}{\Delta} \cdot \frac{N_x}{n} = K\hat{f}(x,t)$$

N_x is the number of particles in the bin at location x, and Δ is the bin width.

What we observe

We don't observe each particle $X_t^{(k)}$ but observe concentration $\hat{C}(x_i, t)$, a scaled histogram bar $K\hat{f}(x, t)$.

- Spatial snapshots: $\{x_i, c_i\}$ for $i = 1, \cdots, N$.
  x_i locations, $c_i = \hat{C}(x_i, t)$ observed concentration at location x_i for fixed time t.
- Temporal breakthrough curves: $\{t_i, c_i\}$ for $i = 1, \cdots, N$.
  t_i times, $c_i = \hat{C}(x, t_i)$ observed concentration at time t_i for fixed location x.

What we observe

We don't observe each particle $X_t^{(k)}$ but observe concentration $\hat{C}(x_i, t)$, a scaled histogram bar $K\hat{f}(x, t)$.

- Spatial snapshots: $\{x_i, c_i\}$ for $i = 1, \cdots, N$.
  x_i locations, $c_i = \hat{C}(x_i, t)$ observed concentration at location x_i for fixed time t.
- Temporal breakthrough curves: $\{t_i, c_i\}$ for $i = 1, \cdots, N$.
  t_i times, $c_i = \hat{C}(x, t_i)$ observed concentration at time t_i for fixed location x.

What we observe

We don't observe each particle $X_t^{(k)}$ but observe concentration $\hat{C}(x_i, t)$, a scaled histogram bar $K\hat{f}(x, t)$.

- Spatial snapshots: $\{x_i, c_i\}$ for $i = 1, \cdots, N$.
  x_i locations, $c_i = \hat{C}(x_i, t)$ observed concentration at location x_i for fixed time t.

- Temporal breakthrough curves: $\{t_i, c_i\}$ for $i = 1, \cdots, N$.
  t_i times, $c_i = \hat{C}(x, t_i)$ observed concentration at time t_i for fixed location x.

Parameter estimation

Since variation of $\hat{f}(x,t)$ is proportional to $f(x,t)$, consider weighted least squares.

- For spatial snapshots, minimize

$$e(\theta, K) = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{Kc_i}\left(c_i - Kf_\theta(x_i,t)\right)^2$$

- Iterative two-step approach
  - Given K minimize θ using $e(\theta, K)$.
  - Given θ,

$$K = \sqrt{\frac{\sum_{i=1}^{n} c_i}{\sum_{i=1}^{n}[f_\theta^2(x_i,t)/c_i]}}$$

- Similar approach for temporal breakthrough curves

Parameter estimation

Since variation of $\hat{f}(x, t)$ is proportional to $f(x, t)$, consider weighted least squares.

- For spatial snapshots, minimize

$$e(\theta, K) = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{Kc_i} \left(c_i - Kf_{\theta}(x_i, t)\right)^2$$

- Iterative two-step approach
  - Given K minimize θ using $e(\theta, K)$.
  - Given θ,

$$K = \sqrt{\frac{\sum_{i=1}^{n} c_i}{\sum_{i=1}^{n} [f_{\theta}^2(x_i, t)/c_i]}}$$

- Similar approach for temporal breakthrough curves

Parameter estimation

Since variation of $\hat{f}(x,t)$ is proportional to $f(x,t)$, consider weighted least squares.

- For spatial snapshots, minimize

$$e(\theta, K) = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{Kc_i}\left(c_i - Kf_{\boldsymbol{\theta}}(x_i,t)\right)^2$$

- Iterative two-step approach
  - Given K minimize θ using $e(\theta, K)$.
  - Given θ,

$$K = \sqrt{\frac{\sum_{i=1}^{n} c_i}{\sum_{i=1}^{n}[f_{\boldsymbol{\theta}}^2(x_i,t)/c_i]}}$$

- Similar approach for temporal breakthrough curves

Parameter estimation

Since variation of $\hat{f}(x,t)$ is proportional to $f(x,t)$, consider weighted least squares.

- For spatial snapshots, minimize

$$e(\theta, K) = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{Kc_i}\left(c_i - Kf_{\theta}(x_i,t)\right)^2$$

- Iterative two-step approach
  - Given K minimize θ using $e(\theta, K)$.
  - Given θ,

$$K = \sqrt{\frac{\sum_{i=1}^{n} c_i}{\sum_{i=1}^{n}[f_{\theta}^2(x_i,t)/c_i]}}$$

- Similar approach for temporal breakthrough curves

Stable density $f_\theta(x, t)$

Recall $f_\theta(x, t)$ for fADE is a stable density

- No closed form
- It can be characterized by Fourier transform:

$$\int e^{ikx} f_\theta(x, t)\, dx = \exp\left(i\mu k - \sigma^\alpha \omega_{\alpha,\beta}(k)\right), \qquad (2)$$

where

$$\omega_{\alpha,\beta}(k) = \begin{cases} |k|^\alpha[1 + i\beta \mathrm{sign}(k) \tan(\pi\alpha/2)] & \text{for } \alpha \neq 1, \\ |k|[1 + i\beta(2/\pi)\mathrm{sign}(k) \log|k|] & \text{for } \alpha = 1 \end{cases}$$

- $0 < \alpha \leq 2$ is the tail index
- $-1 \leq \beta \leq 1$ controls skewness
- $-\infty < \mu < \infty$ controls center
- $\sigma \geq 0$ controls scale.

Stable density $f_{\theta}(x, t)$

Recall $f_{\theta}(x, t)$ for fADE is a stable density

- No closed form
- It can be characterized by Fourier transform:

$$\int e^{ikx} f_{\theta}(x, t)\, dx = \exp\left(i\mu k - \sigma^{\alpha}\omega_{\alpha,\beta}(k)\right), \qquad (2)$$

where

$$\omega_{\alpha,\beta}(k) = \begin{cases} |k|^{\alpha}[1 + i\beta \operatorname{sign}(k)\tan(\pi\alpha/2)] & \text{for } \alpha \neq 1, \\ |k|[1 + i\beta(2/\pi)\operatorname{sign}(k)\log|k|] & \text{for } \alpha = 1 \end{cases}$$

- $0 < \alpha \leq 2$ is the tail index
- $-1 \leq \beta \leq 1$ controls skewness
- $-\infty < \mu < \infty$ controls center
- $\sigma \geq 0$ controls scale.

Stable density $f_{\boldsymbol{\theta}}(x, t)$

Recall $f_{\boldsymbol{\theta}}(x, t)$ for fADE is a stable density

- No closed form
- It can be characterized by Fourier transform:

$$\int e^{ikx} f_{\boldsymbol{\theta}}(x, t)\, dx = \exp\left(i\mu k - \sigma^{\alpha}\omega_{\alpha,\beta}(k)\right), \qquad (2)$$

where

$$\omega_{\alpha,\beta}(k) = \begin{cases} |k|^{\alpha}[1 + i\beta \text{sign}(k) \tan(\pi\alpha/2)] & \text{for } \alpha \neq 1, \\ |k|[1 + i\beta(2/\pi)\text{sign}(k) \log|k|] & \text{for } \alpha = 1 \end{cases}$$

- $0 < \alpha \leq 2$ is the tail index
- $-1 \leq \beta \leq 1$ controls skewness
- $-\infty < \mu < \infty$ controls center
- $\sigma \geq 0$ controls scale.

Asymptotics of estimated parameters

- It can be shown that the estimated parameters are asymptotically normal.

$$(\hat{\theta} - \theta_0) \approx \frac{1}{\sqrt{n\,dx_n}} A \mathcal{N}(0, I) \quad \text{where}$$

$$A = \left[\frac{\partial f_{\theta_0}(\mathbf{x}, t)}{\partial \theta}^T \mathrm{diag}\left[f_{\theta_0}(\mathbf{x}, t) \right]^{-1} \frac{\partial f_{\theta_0}(\mathbf{x}, t)}{\partial \theta} \right]^{-1} \times \frac{\partial f_{\theta_0}(\mathbf{x}, t)}{\partial \theta}^T \left[\mathrm{diag}(f_{\theta_0}(\mathbf{x})) \right]^{-1/2}$$

- The matrix A can be evaluated numerically.

Asymptotics of estimated parameters

- It can be shown that the estimated parameters are asymptotically normal.

$$(\hat{\theta} - \theta_0) \approx \frac{1}{\sqrt{n\, dx_n}} A \mathcal{N}(0, I) \quad \text{where}$$

$$A = \left[\frac{\partial f_{\boldsymbol{\theta}_0}(\mathbf{x}, t)}{\partial \boldsymbol{\theta}}^T \operatorname{diag}\left[f_{\boldsymbol{\theta}_0}(\mathbf{x}, t) \right]^{-1} \frac{\partial f_{\boldsymbol{\theta}_0}(\mathbf{x}, t)}{\partial \boldsymbol{\theta}} \right]^{-1} \times \frac{\partial f_{\boldsymbol{\theta}_0}(\mathbf{x}, t)}{\partial \boldsymbol{\theta}}^T \left[\operatorname{diag}(f_{\boldsymbol{\theta}_0}(\mathbf{x})) \right]^{-1/2}$$

- The matrix A can be evaluated numerically.

Asymptotics of estimated parameters

- It can be shown that the estimated parameters are asymptotically normal.

$$(\hat{\theta} - \theta_0) \approx \frac{1}{\sqrt{n\,dx_n}} A \mathcal{N}(0, I) \quad \text{where}$$

$$A = \left[\frac{\partial f_{\boldsymbol{\theta}_0}(\mathbf{x}, t)}{\partial \boldsymbol{\theta}}^T \operatorname{diag}\left[f_{\boldsymbol{\theta}_0}(\mathbf{x}, t) \right]^{-1} \frac{\partial f_{\boldsymbol{\theta}_0}(\mathbf{x}, t)}{\partial \boldsymbol{\theta}} \right]^{-1} \times \frac{\partial f_{\boldsymbol{\theta}_0}(\mathbf{x}, t)}{\partial \boldsymbol{\theta}}^T \left[\operatorname{diag}(f_{\boldsymbol{\theta}_0}(\mathbf{x})) \right]^{-1/2}$$

- The matrix A can be evaluated numerically.

Stable parameters v.s. fADE parameters

- $\boldsymbol{\theta} = (\alpha, \beta, \mu, \sigma)$
- The plume center of mass $\mu = vt$
- The scale σ is given by $\sigma^\alpha = Dt|\cos(\pi\alpha/2)|$.

Computing stable density

- Analytical inversion of the Fourier transform and numerical integration of the resulting formula
- Programs are widely available [e.g. see *Nolan*, 1999]

Stable parameters v.s. fADE parameters

- $\boldsymbol{\theta} = (\alpha, \beta, \mu, \sigma)$
- The plume center of mass $\mu = vt$
- The scale σ is given by $\sigma^\alpha = Dt|\cos(\pi\alpha/2)|$.

Computing stable density

- Analytical inversion of the Fourier transform and numerical integration of the resulting formula
- Programs are widely available [e.g. see *Nolan*, 1999]

Stable parameters v.s. fADE parameters

- $\boldsymbol{\theta} = (\alpha, \beta, \mu, \sigma)$
- The plume center of mass $\mu = vt$
- The scale σ is given by $\sigma^\alpha = Dt|\cos(\pi\alpha/2)|$.

Computing stable density

- Analytical inversion of the Fourier transform and numerical integration of the resulting formula
- Programs are widely available [e.g. see *Nolan*, 1999]

Spatial snapshots from a MADE tracer test

- Natural-gradient tracer tests at the MAcroDispersion Experimental (MADE) site at Columbus Air Force Base in northeastern Missisipi.
- The MADE-2 tritium plume data was considered [*Boggs et al.*, 1993]
- The data represent the maximum concentration measured in vertical slices perpendicular to the direction of plume travel
- Four spatial snapshots at day 27, day 132, day 224, and day 328 days after injection

Spatial snapshots from a MADE tracer test

- Natural-gradient tracer tests at the MAcroDispersion Experimental (MADE) site at Columbus Air Force Base in northeastern Missisipi.
- The MADE-2 tritium plume data was considered [*Boggs et al.*, 1993]
- The data represent the maximum concentration measured in vertical slices perpendicular to the direction of plume travel
- Four spatial snapshots at day 27, day 132, day 224, and day 328 days after injection

Spatial snapshots from a MADE tracer test

- Natural-gradient tracer tests at the MAcroDispersion Experimental (MADE) site at Columbus Air Force Base in northeastern Missisipi.
- The MADE-2 tritium plume data was considered [*Boggs et al.*, 1993]
- The data represent the maximum concentration measured in vertical slices perpendicular to the direction of plume travel
- Four spatial snapshots at day 27, day 132, day 224, and day 328 days after injection

Spatial snapshots from a MADE tracer test

- Natural-gradient tracer tests at the MAcroDispersion Experimental (MADE) site at Columbus Air Force Base in northeastern Missisipi.
- The MADE-2 tritium plume data was considered [*Boggs et al.*, 1993]
- The data represent the maximum concentration measured in vertical slices perpendicular to the direction of plume travel
- Four spatial snapshots at day 27, day 132, day 224, and day 328 days after injection

Spatial snapshots from a MADE tracer test

- Natural-gradient tracer tests at the MAcroDispersion Experimental (MADE) site at Columbus Air Force Base in northeastern Missisipi.
- The MADE-2 tritium plume data was considered [*Boggs et al.*, 1993]
- The data represent the maximum concentration measured in vertical slices perpendicular to the direction of plume travel
- Four spatial snapshots at day 27, day 132, day 224, and day 328 days after injection

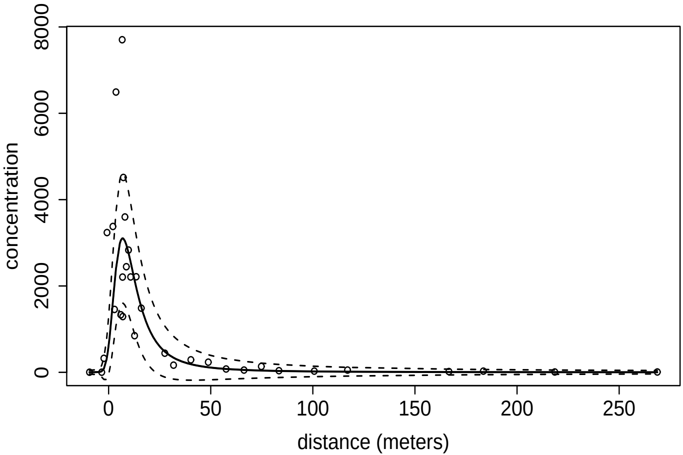


Figure: Day 224, $\alpha = 1.0915$, $\beta = 0.99$, $v = 0.196$ m/day, $D = 0.186$ m^{α}/day, and $K = 56,778$ mg/L
95% CI for α: $[1.08, 1.11]$, 95% CI for v: $[0.15, 0.23]$

Breakthrough curve for the Red Cedar river

- From a tracer test reported in *Phanikumar et al.* [2007]
- A fourth-order stream in south central Michigan, United States
- Four slug additions of Flourescein dye were released in the middle 75% of the channel
- The distances to the three sampling locations from the point of release: 1.4 km, 3.1 km and 5.08 km from the injection site

Breakthrough curve for the Red Cedar river

- From a tracer test reported in *Phanikumar et al.* [2007]
- A fourth-order stream in south central Michigan, United States
- Four slug additions of Flourescein dye were released in the middle 75% of the channel
- The distances to the three sampling locations from the point of release: 1.4 km, 3.1 km and 5.08 km from the injection site

Breakthrough curve for the Red Cedar river

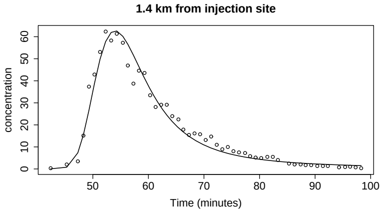
- From a tracer test reported in *Phanikumar et al.* [2007]
- A fourth-order stream in south central Michigan, United States
- Four slug additions of Flourescein dye were released in the middle 75% of the channel
- The distances to the three sampling locations from the point of release: 1.4 km, 3.1 km and 5.08 km from the injection site

Breakthrough curve for the Red Cedar river

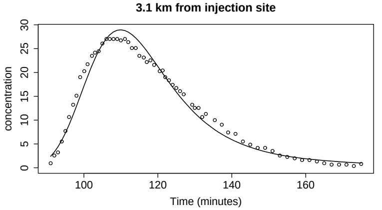
- From a tracer test reported in *Phanikumar et al.* [2007]
- A fourth-order stream in south central Michigan, United States
- Four slug additions of Flourescein dye were released in the middle 75% of the channel
- The distances to the three sampling locations from the point of release: 1.4 km, 3.1 km and 5.08 km from the injection site

Breakthrough curve for the Red Cedar river

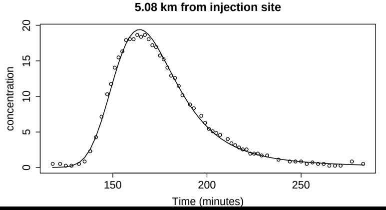
- From a tracer test reported in *Phanikumar et al.* [2007]
- A fourth-order stream in south central Michigan, United States
- Four slug additions of Flourescein dye were released in the middle 75% of the channel
- The distances to the three sampling locations from the point of release: 1.4 km, 3.1 km and 5.08 km from the injection site



- 1.4 km: $\alpha = 1.32$, $\beta = -0.99$, $v = 0.022$ km/min, $D = 0.00181$ km$^\alpha$/min, and $K = 22.64$ μg/L.



- 3.1 km: $\alpha = 1.56$, $\beta = -0.99$, $v = 0.026$ km/min, $D = 0.00131$ km$^\alpha$/min, and $K = 25.48$ μg/L.



- 5.08 km: $\alpha = 1.58$, $\beta = -0.96$, $v = 0.029$ km/min, $D = 0.00181$ km$^\alpha$/min, $K = 27.75$ μg/L.

Breakthrough curve for the Grand river

- From a tracer test reported in *Shen et al.* [2008]
- Test on a 40 km stretch of the Grand River, a 420km long tributary to Lake Michigan, traveling through the city of Grand Rapids and extending to Coopersville, Michigan, United States
- Rodamine WT 20% (weight) solution was used in the study.
- The distances to the four sampling locations from the point of release: 4558 m (Bridge 1), 13,687 m (Bridge 2), 28,375 m (Bridge 3) and 37,608 m (Bridge 4).

Breakthrough curve for the Grand river

- From a tracer test reported in *Shen et al.* [2008]
- Test on a 40 km stretch of the Grand River, a 420km long tributary to Lake Michigan, traveling through the city of Grand Rapids and extending to Coopersville, Michigan, United States
- Rodamine WT 20% (weight) solution was used in the study.
- The distances to the four sampling locations from the point of release: 4558 m (Bridge 1), 13,687 m (Bridge 2), 28,375 m (Bridge 3) and 37,608 m (Bridge 4).

Breakthrough curve for the Grand river

- From a tracer test reported in *Shen et al.* [2008]
- Test on a 40 km stretch of the Grand River, a 420km long tributary to Lake Michigan, traveling through the city of Grand Rapids and extending to Coopersville, Michigan, United States
- Rodamine WT 20% (weight) solution was used in the study.
- The distances to the four sampling locations from the point of release: 4558 m (Bridge 1), 13,687 m (Bridge 2), 28,375 m (Bridge 3) and 37,608 m (Bridge 4).

Breakthrough curve for the Grand river

- From a tracer test reported in *Shen et al.* [2008]
- Test on a 40 km stretch of the Grand River, a 420km long tributary to Lake Michigan, traveling through the city of Grand Rapids and extending to Coopersville, Michigan, United States
- Rodamine WT 20% (weight) solution was used in the study.
- The distances to the four sampling locations from the point of release: 4558 m (Bridge 1), 13,687 m (Bridge 2), 28,375 m (Bridge 3) and 37,608 m (Bridge 4).

Breakthrough curve for the Grand river

- From a tracer test reported in *Shen et al.* [2008]
- Test on a 40 km stretch of the Grand River, a 420km long tributary to Lake Michigan, traveling through the city of Grand Rapids and extending to Coopersville, Michigan, United States
- Rodamine WT 20% (weight) solution was used in the study.
- The distances to the four sampling locations from the point of release: 4558 m (Bridge 1), 13,687 m (Bridge 2), 28,375 m (Bridge 3) and 37,608 m (Bridge 4).

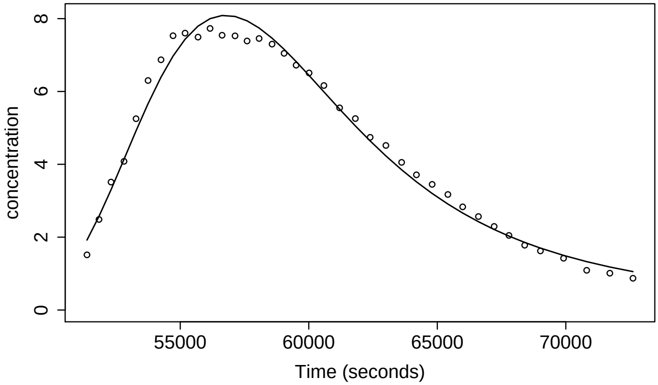


Figure: Bridge 3: $\alpha = 1.38$, $\beta = -1.0$, $v = 0.446$ m/sec, $D = 0.887$ m$^\alpha$/sec, and $K = 50,179$ ppb

Interactive Ground Water simulation (IGW)

- Provide unified deterministic, stochastic, and multi-scale groundwater modeling [*Li and Liu*, 2006; *Li et al.*, 2006]
- Fit fADE (1) to an ensemble average plume simulated in IGW using a multiscale hydraulic conductivity field on a model domain of 500 m $\times$ 125 m.
- An ensemble mean of 100 simulated plumes was averaged along the axis transverse to the flow to produce one dimensional concentration.

Interactive Ground Water simulation (IGW)

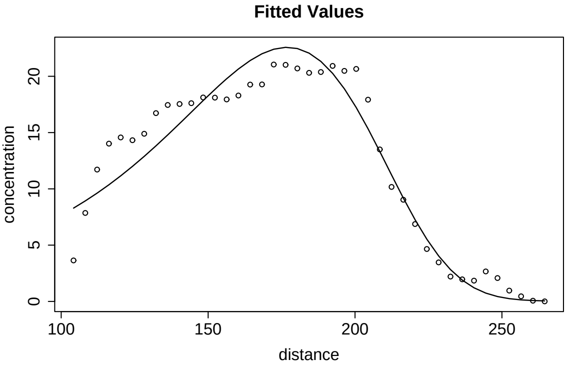
- Provide unified deterministic, stochastic, and multi-scale groundwater modeling [*Li and Liu*, 2006; *Li et al.*, 2006]
- Fit fADE (1) to an ensemble average plume simulated in IGW using a multiscale hydraulic conductivity field on a model domain of 500 m $\times$ 125 m.
- An ensemble mean of 100 simulated plumes was averaged along the axis transverse to the flow to produce one dimensional concentration.

Interactive Ground Water simulation (IGW)

- Provide unified deterministic, stochastic, and multi-scale groundwater modeling [*Li and Liu*, 2006; *Li et al.*, 2006]
- Fit fADE (1) to an ensemble average plume simulated in IGW using a multiscale hydraulic conductivity field on a model domain of 500 m $\times$ 125 m.
- An ensemble mean of 100 simulated plumes was averaged along the axis transverse to the flow to produce one dimensional concentration.

Interactive Ground Water simulation (IGW)

- Provide unified deterministic, stochastic, and multi-scale groundwater modeling [*Li and Liu*, 2006; *Li et al.*, 2006]
- Fit fADE (1) to an ensemble average plume simulated in IGW using a multiscale hydraulic conductivity field on a model domain of 500 m $\times$ 125 m.
- An ensemble mean of 100 simulated plumes was averaged along the axis transverse to the flow to produce one dimensional concentration.



- $\alpha = 1.25$, $\beta = -1.0$, $\mu = 93.4$, $\sigma = 31.8$, $K = 2578$

Conclusion

- Parameter estimation based on a particle tracking approach, where concentration measurements are interpreted as a random histogram.
- Can also be used for any other transport model that admits a particle tracking solution.
- The particle tracking model implies that concentration variance is proportional to concentration.
- The method is effective for both spatial snapshots and temporal breakthrough data.

Conclusion

- Parameter estimation based on a particle tracking approach, where concentration measurements are interpreted as a random histogram.
- Can also be used for any other transport model that admits a particle tracking solution.
- The particle tracking model implies that concentration variance is proportional to concentration.
- The method is effective for both spatial snapshots and temporal breakthrough data.

Conclusion

- Parameter estimation based on a particle tracking approach, where concentration measurements are interpreted as a random histogram.
- Can also be used for any other transport model that admits a particle tracking solution.
- The particle tracking model implies that concentration variance is proportional to concentration.
- The method is effective for both spatial snapshots and temporal breakthrough data.

Conclusion

- Parameter estimation based on a particle tracking approach, where concentration measurements are interpreted as a random histogram.
- Can also be used for any other transport model that admits a particle tracking solution.
- The particle tracking model implies that concentration variance is proportional to concentration.
- The method is effective for both spatial snapshots and temporal breakthrough data.

Conclusion

- Parameter estimation based on a particle tracking approach, where concentration measurements are interpreted as a random histogram.
- Can also be used for any other transport model that admits a particle tracking solution.
- The particle tracking model implies that concentration variance is proportional to concentration.
- The method is effective for both spatial snapshots and temporal breakthrough data.

Thank You!

References

1. Nolan, J.P (1999), An Algorithm for Evaluating Stable Densities in Zolotarev's (M) Parameterization, *Mathematical and Computer Modeling, 29*, 229–233.
2. Boggs, J. M., L. M. Beard , S. E. Long, and M. P. McGee, (1993): Database for the second macro dispersion experiment (MADE-2), *EPRI report TR-102072*, Electric Power Res. Inst., Palo Alto, CA.
3. Phanikumar M. S., I. Aslam, C. Shen, D.T. Long and T.C. Voice (2007), Separating Surface Storage from Hyporheic Retention in Natural Streams Using Wavelet Decomposition of Acoustic Doppler Current Profiles, *Water Resour. Res., 43*(5), W05406.
4. Shen, C., M.S. Phanikumar, T.T. Fong, I. Aslam, S.L. Molloy and J.B. Rose (2008), Evaluating Bacteriophage P22 as a Tracer in a Complex Surface Water System: The Grand River, Michigan,*Environ. Sci. Tech., 42*(7), 2426–2431.
5. Li, S.G. and Q. Liu (2006), A Real-time, Computational Steering Environment for Integrated Groundwater Modeling, *J. Ground Water., 44*(5), 758–763.
6. Li, S. G., Q. Liu, and S. Afshari (2006), An object-oriented hierarchical patch dynamics paradigm (HPDP) for modeling complex groundwater systems across multiple-scales, *Environmental Modeling and Software, 21*(5), 744–749.