

PDF Methods for Uncertainty Quantification in Hyperbolic Conservation Laws

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Hyperbolic Conservation Laws

$$\frac{\partial c}{\partial t} + \nabla \cdot \mathbf{f}(c; \mathbf{x}, t) = r(c; \mathbf{x}, t)$$

Examples:

- Advection-reaction equation

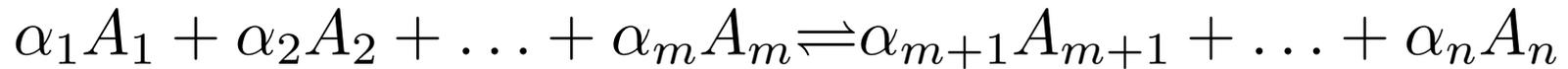
$$\frac{\partial c_i}{\partial t} + \nabla \cdot (\mathbf{u}c_i) = F_i(c_1, c_2, \dots, c_n), \quad i = 1, \dots, n$$

- Kinematic wave (Saint-Venant) equation

$$\frac{\partial c}{\partial t} + \nabla \cdot \mathbf{q}(c) = r(\mathbf{x}, t)$$

Sources of Uncertainty in Reactive Transport

Homogeneous & heterogeneous chemical reactions between n species A_1, A_2, \dots, A_n :



Model: Concentrations $c_i(\mathbf{x}, t) \equiv [A_i]$ satisfy a system of ADR eqs.

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (\mathbf{u}c_i) = \nabla \cdot (\mathbf{D}_i \nabla c_i) + F_i(c_1, c_2, \dots, c_n), \quad i = 1, \dots, n$$

Sources of uncertainty:

- Reaction paths, $F_i(c_1, c_2, \dots, c_n)$
- Flow velocity, $\mathbf{u}(\mathbf{x}, t)$
- Reaction rate constants, $\kappa_i(\mathbf{x})$

Parametric Uncertainty in Chemical Reactions

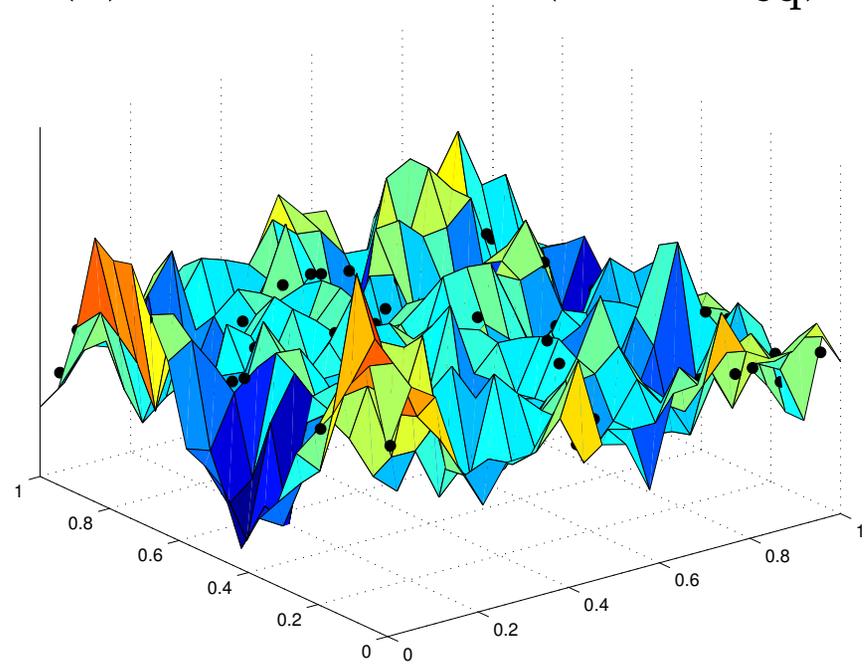
Transport equation for $\alpha A \rightleftharpoons A_{(s)}$:

$$\frac{\partial c}{\partial t} = \nabla \cdot (\mathbf{D} \nabla c) - \nabla \cdot (\mathbf{u}c) + \alpha f_{\alpha}(c), \quad f_{\alpha} = -k(c^{\alpha} - C_{\text{eq}}^{\alpha})$$

- Reaction rate $k(\mathbf{x})$

$$k = k_0 \phi^{-1} A c_{\text{eq}}^{1-\alpha}$$

- Random field $k(\mathbf{x}, \omega)$



- Governing equation becomes **stochastic**
- Solutions are given in terms of PDFs

Stochastic Methods for Parametric UQ

- (Brute-force) Monte Carlo simulations
 - Convergence rate (CR): $1/\sqrt{N}$
- Accelerated Monte Carlo methods
 - Quasi MC (QMC)
 - Markov chain MC (MCMC)
- Numerical methods for SPDEs
 - Stochastic finite elements (polynomial chaos expansions)
 - Stochastic collocation
- **Mode-reduction methods**
 - Fokker-Planck equations & PDF equations
 - Moments equations

PDF Methods

- Motivation
 - To avoid the linearization of $f_\alpha(c)$
 - To obtain complete statistics
 - To develop an efficient & accurate tool for UQ
- Raw distribution:

$$\Pi(c, C; \mathbf{x}, t) \equiv \delta[c(\mathbf{x}, t) - C]$$

- Probability density function (PDF):

$$p_c(C; \mathbf{x}, t) = \langle \Pi(c, C; \mathbf{x}, t) \rangle$$

Indelman and Shvidler (1985); Pope (1981)

Advective-Reactive Transport

Start with advective transport for $\alpha\mathcal{A} \rightleftharpoons \mathcal{A}_{(s)}$,

$$\frac{\partial c}{\partial t} = -\nabla \cdot (\mathbf{u}c) + \alpha f_{\alpha}(c), \quad f_{\alpha} = -k(c^{\alpha} - C_{\text{eq}}^{\alpha})$$

Deal with diffusion later,

$$\frac{\partial c}{\partial t} = D\nabla^2 c - \nabla \cdot (\mathbf{u}c) + \alpha f_{\alpha}(c), \quad f_{\alpha} = -k(c^{\alpha} - C_{\text{eq}}^{\alpha})$$

Sources of uncertainty / random fields, $\mathbf{u} = \mathbf{u}(\mathbf{x}, t; \omega)$ & $k = k(\mathbf{x}; \omega)$

Reactive Transport in “Homogeneous” Media

Physical homogeneity: \mathbf{u} is deterministic (certain)

Chemical heterogeneity:

$$p_k(k) = \frac{1}{k\sqrt{2\pi\sigma^2}} \exp \left[-\frac{(\ln k + \sigma_\kappa^2/2)^2}{2\sigma^2} \right]$$

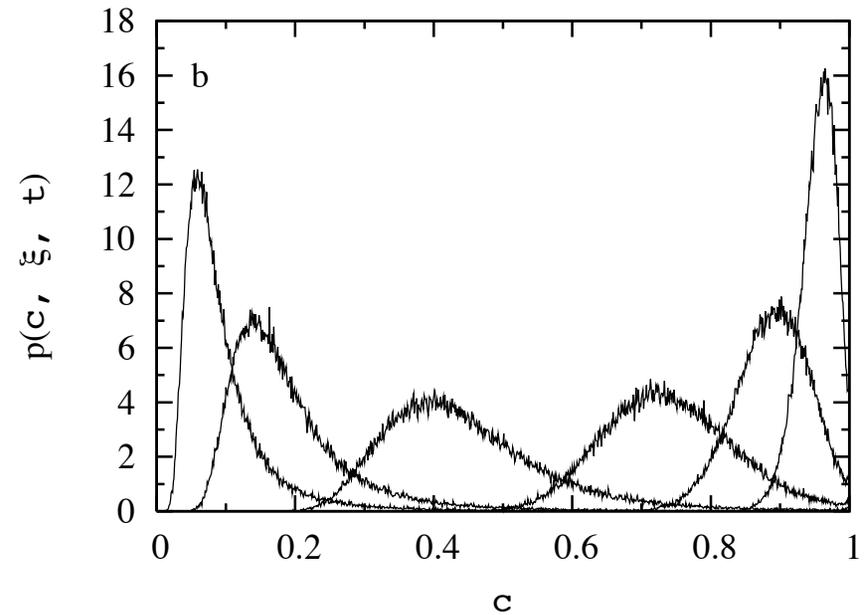
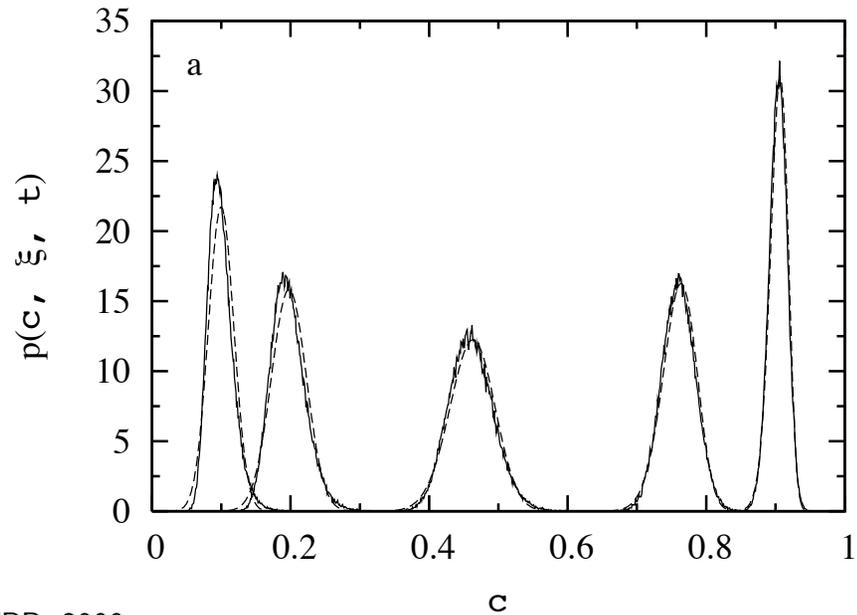
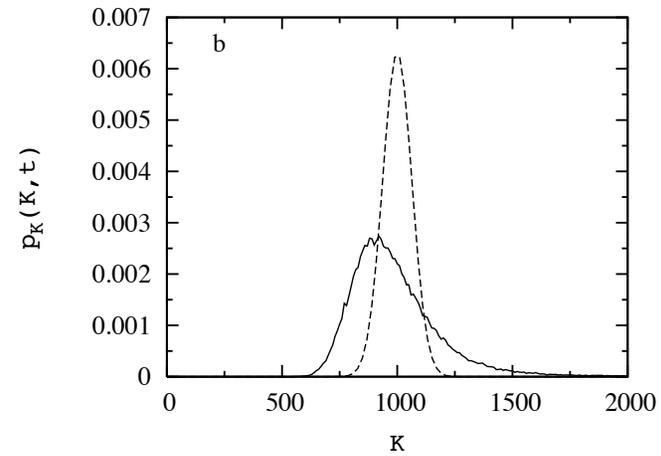
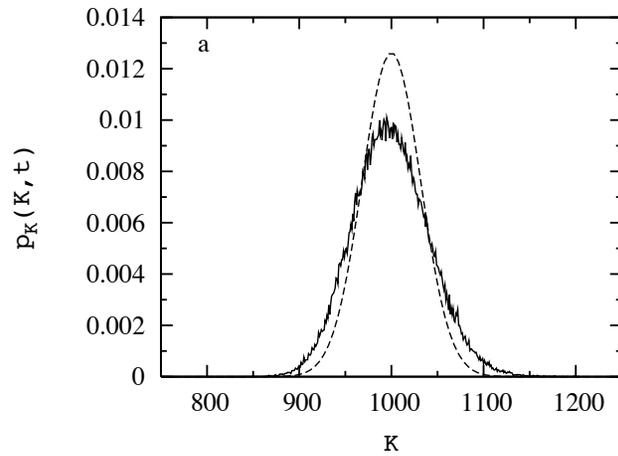
Reynolds decomposition

$$k(x) = \bar{k} [1 + \kappa(x)], \quad \bar{\kappa} = 0, \quad \overline{\kappa(x)\kappa(x')} = \sigma_\kappa^2 \rho_\kappa(x - x')$$

PDF solution

$$p_c(c; x, t) \sim p_\kappa(\mathcal{K}; t), \quad \mathcal{K}(t) = \int_0^t k(t') dt'$$

PDF for Concentration



WRR, 2009

Reactive Transport in Uncertain Velocity Field

Uncertain velocity $\mathbf{u}(\mathbf{x}; \omega)$ and reaction rate constant $\kappa(\mathbf{x}; \omega)$

- Transport equation for $\alpha\mathcal{A} \rightleftharpoons \mathcal{A}_{(s)}$:

$$\frac{\partial c}{\partial t} = -\mathbf{u} \cdot \nabla c + \alpha f_\alpha(c), \quad f_\alpha = -k(c^\alpha - C_{\text{eq}}^\alpha)$$

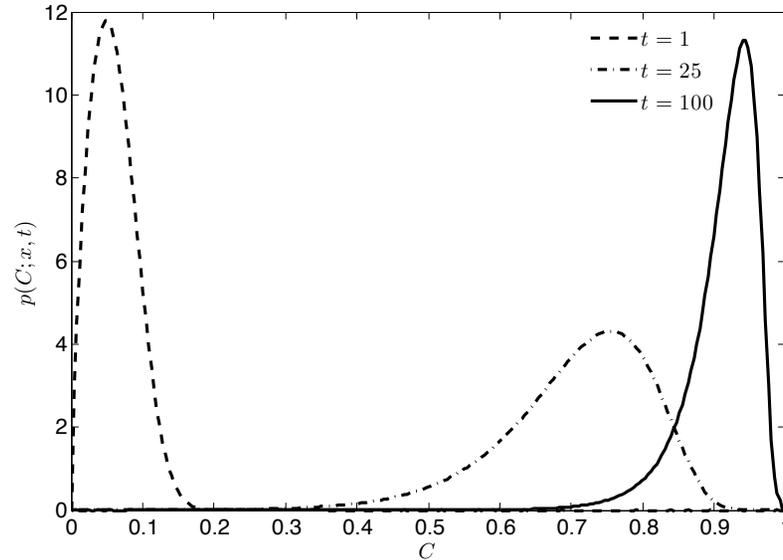
- Stochastic PDE for the raw distribution in \mathcal{R}^4 : $\tilde{\mathbf{x}} = (x_1, x_2, x_3, C)^T$

$$\frac{\partial \Pi}{\partial t} = -\tilde{\nabla} \cdot (\tilde{\mathbf{u}}\Pi) \quad \tilde{\mathbf{u}} = (u_1, u_2, u_3, f_\alpha)^T$$

- Deterministic PDE for PDF

$$\frac{\partial p}{\partial t} = -\frac{\partial \tilde{u}_i p}{\partial \tilde{x}_i} + \frac{\partial}{\partial \tilde{x}_j} \left[\tilde{D}_{ij} \frac{\partial p}{\partial \tilde{x}_i} \right]$$

Concentration PDF



| | Relative error, \mathcal{E} |
|------------|-------------------------------|
| $t = 250$ | 0.0008 |
| $t = 500$ | 0.0011 |
| $t = 750$ | 0.0023 |
| $t = 1000$ | 0.0077 |

Advective-Diffusive Transport

$$\frac{\partial c}{\partial t} = D\nabla^2 c - \nabla \cdot (\mathbf{u}c)$$

Random velocity field, $\mathbf{u} = \mathbf{u}(\mathbf{x}, t; \omega)$

$$\begin{aligned}\langle \mathbf{u}(\mathbf{x}, t) \rangle &= \bar{\mathbf{u}}, & \sigma_u^2 &= \langle \mathbf{u}'(\mathbf{x}, t)^2 \rangle, \\ C_{ij}(\mathbf{x} - \mathbf{x}', t - t') &= \langle u'_i(\mathbf{x}, t) u'_j(\mathbf{x}', t') \rangle\end{aligned}$$

Correlation length and time scales l_{ij} and τ_{ij}

Advection time-scale: $\tau_u = \ell_u / |\bar{\mathbf{u}}|$

Diffusion time-scale: $\tau_D = \ell_D / D$

Péclet number: $Pe = \tau_D / \tau_u$

General Approach

Map $p_c(\psi; \mathbf{x}, t)$ onto two observables:

- center of mass of the plume, $\mathbf{m}(t)$
- width of the plume, $\kappa(t)$

Particle trajectories $\mathbf{x}(t)$ satisfy a Langevin equation

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{u}[\mathbf{x}(t), t] + \boldsymbol{\xi}(t), \quad \langle \xi_i(t) \xi_j(t') \rangle_{\xi} = 2D_{ij} \delta(t - t')$$

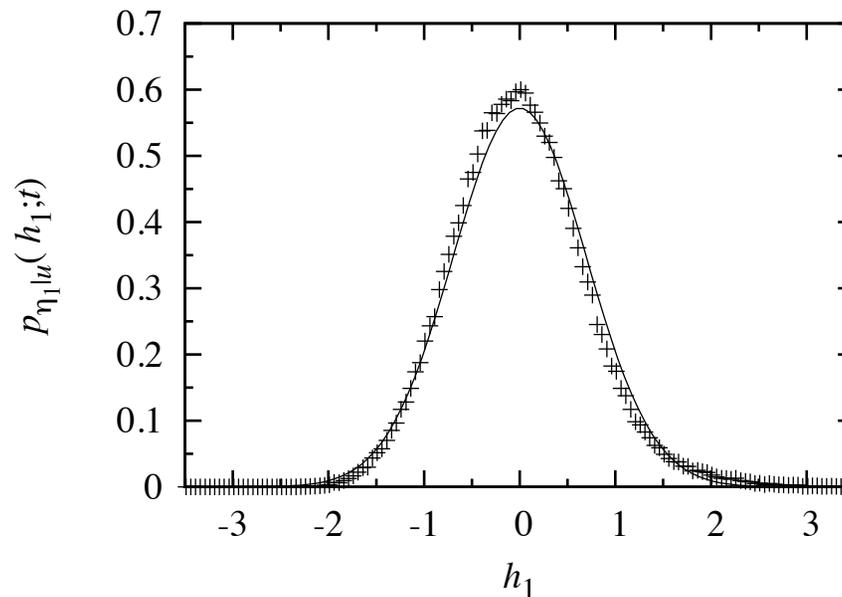
Note that $\mathbf{m}(t) = \langle \mathbf{x}(t) \rangle_{\xi}$

Stochastic Mapping

An alternative form of the Langevin equation

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{v}(t) + \boldsymbol{\eta}(t), \quad \mathbf{v}(t) = \frac{d\mathbf{m}(t)}{dt}, \quad \boldsymbol{\eta}(t) = \delta\mathbf{u}(t) + \boldsymbol{\xi}(t)$$

Assumption: $\boldsymbol{\eta}(t)$ is Gaussian



Statistics of Velocity Fluctuations $\boldsymbol{\eta}(t)$

For a given realization of $\mathbf{u}(\mathbf{x}, t)$,

- Mean: $\langle \boldsymbol{\eta}(t) \rangle_{\xi} = \mathbf{0}$
- Covariance: $C_{ij}^{\eta}(t, t') = 2D_{ij}\delta_{ij}\delta(t - t') + \langle \delta u_i(t)\delta u_j(t') \rangle_{\xi}$

Spread of the plume is given by

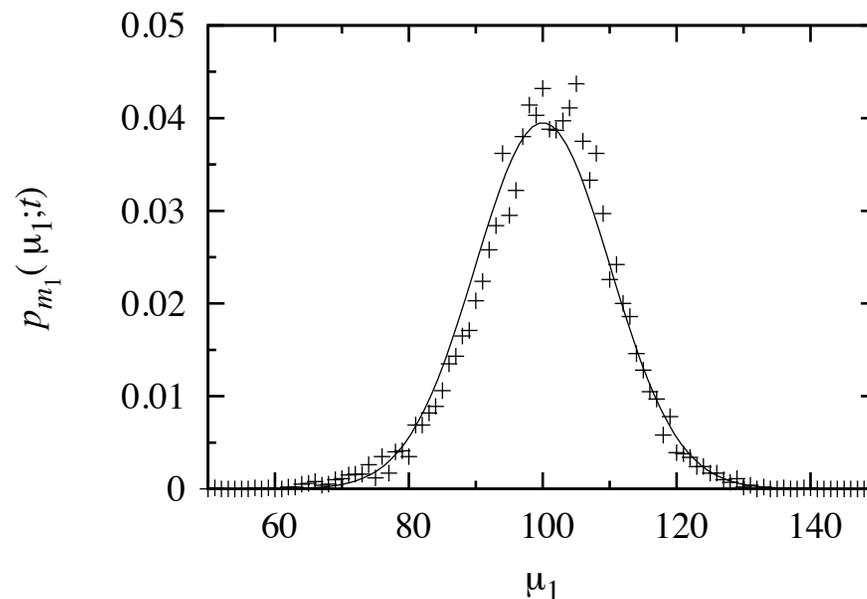
$$\kappa_{ij}(t) = \int_0^t dt' \int_0^t dt'' C_{ij}^{\eta}(t', t'')$$

Concentration mapping

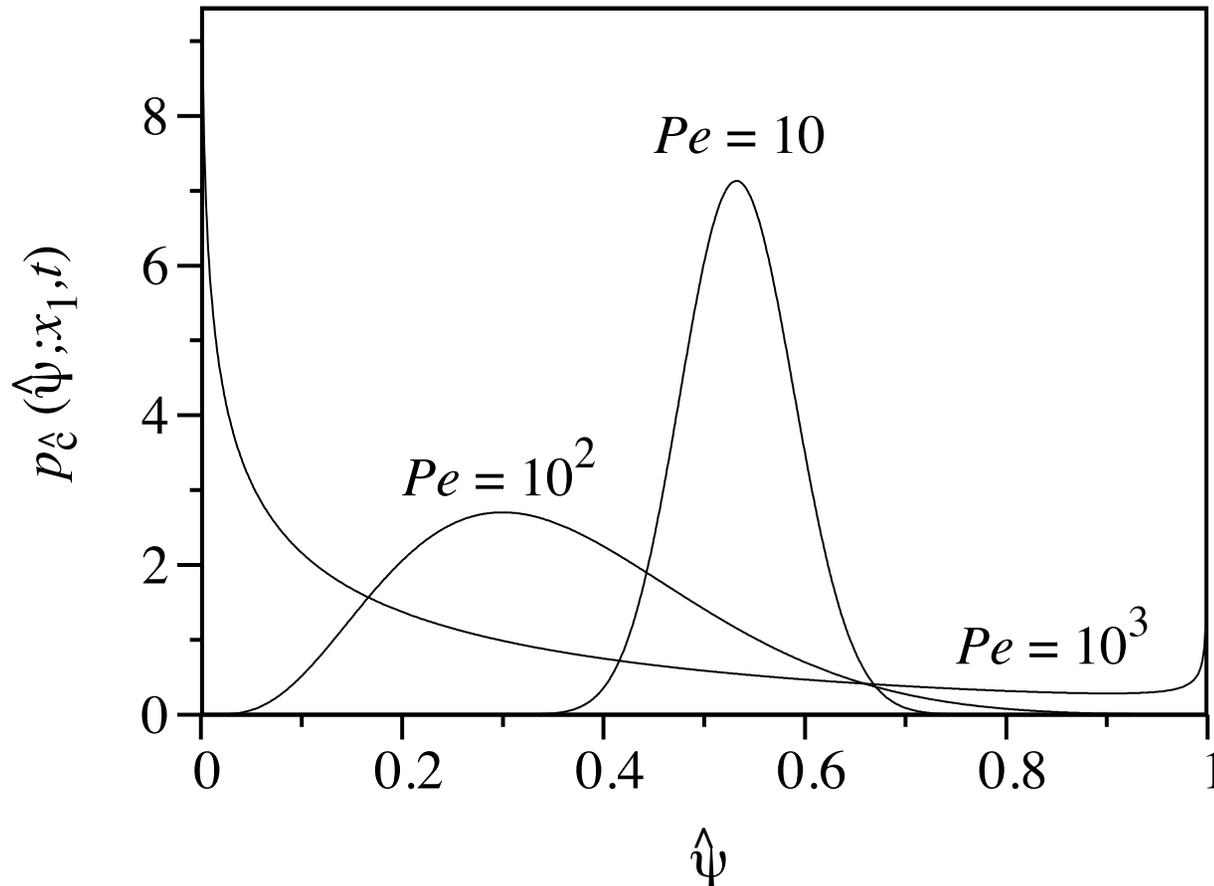
$$c(\mathbf{x}, t) = \frac{\exp \left\{ -\frac{1}{2} [\mathbf{x} - \mathbf{m}(t)] \boldsymbol{\kappa}(t)^{-1} [\mathbf{x} - \mathbf{m}(t)] \right\}}{\sqrt{(2\pi)^d \det \boldsymbol{\kappa}(t)}}$$

Simplifying assumptions:

- Fluctuations of $\boldsymbol{\kappa}(t) \ll$ fluctuations of $\mathbf{m}(t)$, s.t., $\boldsymbol{\kappa}(t) \approx \bar{\boldsymbol{\kappa}}(t)$
- $\mathbf{m}(t)$ is Gaussian



Concentration PDF



$x_1 = 10^3 l$ and $t = 1025 \tau_u$, for $\sigma_u^2 = 10^{-1}$

Parametric Uncertainty in Kinematic Wave Eq.

Kinematic wave (Saint-Venant) equation

$$\frac{\partial c}{\partial t} + \frac{\partial q}{\partial x} = r(x, t), \quad q = \alpha c^{1/\beta}$$

Sources of uncertainty

- surface slope and resistance, $\alpha = \alpha(x)$
- measure of turbulence, β
- sources, $r(x, t)$
- initial and boundary conditions

CDF Equations

Cumulative density function (CDF),

$$\Pi(Q; x, t) = \mathcal{H}[Q - q(x, t)], \quad \bar{\Pi}(Q; x, t) = F_q(Q; x, t)$$

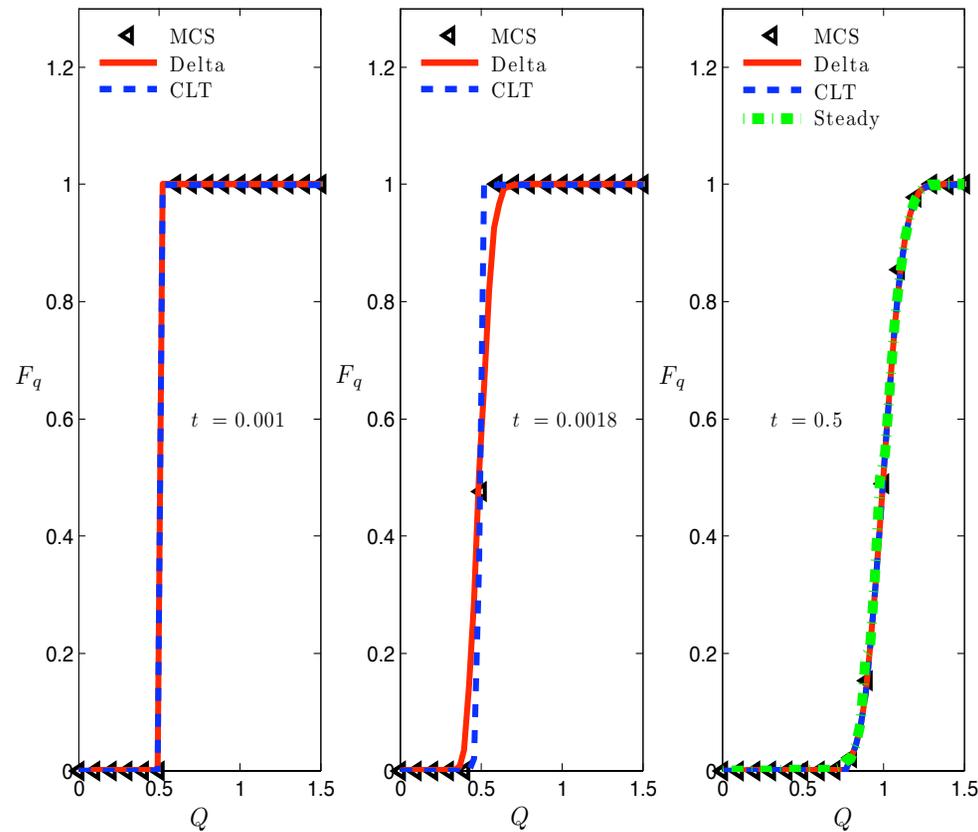
A raw CDF equation,

$$\beta\gamma(x)Q^{\beta-1}\frac{\partial\Pi}{\partial t} + \frac{\partial\Pi}{\partial x} + r(x, t)\frac{\partial\Pi}{\partial Q} = 0$$

An effective CDF equation,

$$\frac{\partial F_q}{\partial t} + \mathbf{v}_{\text{eff}} \cdot \nabla_{\mathbf{x}} F_q = \nabla_{\mathbf{x}} \cdot (\mathbf{D} \nabla_{\mathbf{x}} F_q)$$

CDF Solutions



Flow rate CDF computed with MCS, the white noise γ approximation (Delta), and the CLT-based approximation (CLT).

Conclusions

- While standard techniques for uncertainty quantification typically yield only concentration's mean and variance, the proposed approach leads to its full probabilistic description.
- The shape of the PDF changes with time, varying between the known initial and steady-state distributions. This makes reliance on assumed PDFs problematic.
- PDF methods provide a computationally efficient means for uncertainty quantification.

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Quantification of Model Uncertainty

Master equation: PDF of collisions between the molecules of A_i

Modified Gillespie algorithm: PDF $P(\tau, \mu)$ for reaction μ to occur in time interval $[t + \tau, t + \tau + \Delta\tau]$ given a certain state at time t .

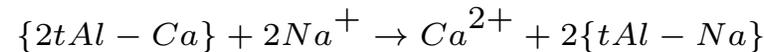
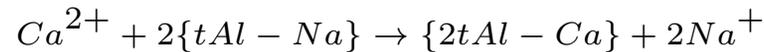
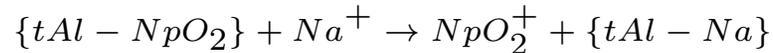
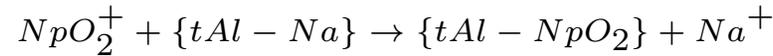
Residence time τ , during which no reactions occur, depends upon the total molecular population of all reacting species and reflects the randomness of collisions.

A constant deterministic τ corresponds to standard reaction rate equations

$$\frac{dC_i}{dt} = F_i(C_1, C_2, \dots, C_n), \quad i = 1, \dots, n$$

Example: Neptunium Ion Exchange

Reacting system:



Standard deterministic model (rate equations):

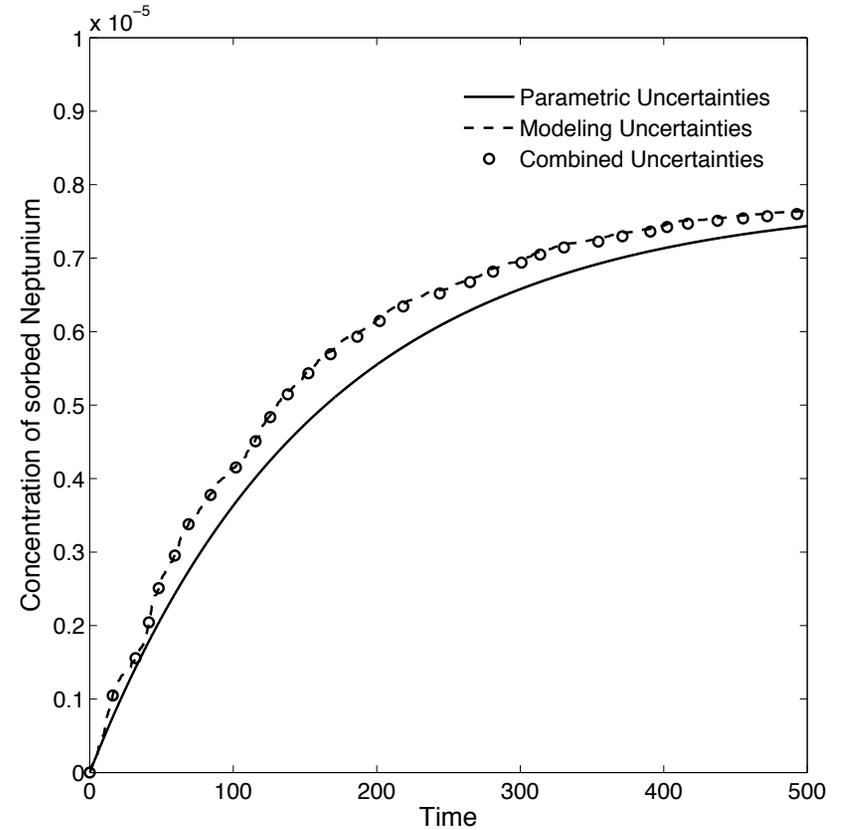
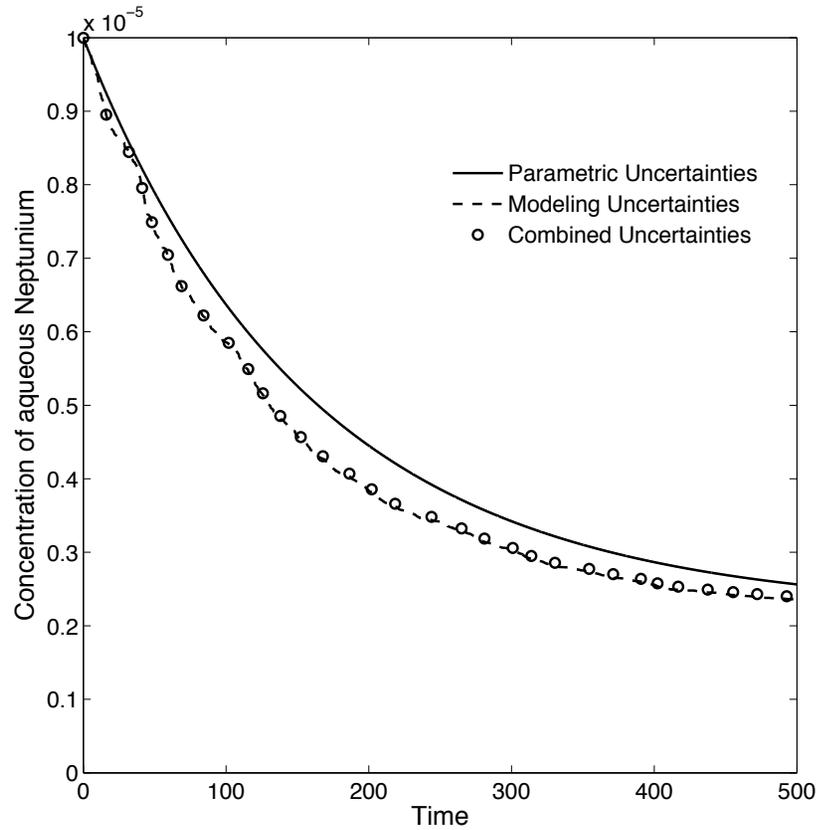
$$\frac{dC_1}{dt} = -k_1 C_1 C_4 + k_2 C_2 C_3 - 2k_3 C_1^2 C_6 + 2k_4 C_2^2 C_5,$$

$$\frac{dC_2}{dt} = k_1 C_1 C_4 - k_2 C_2 C_3 + 2k_3 C_1^2 C_6 - 2k_4 C_2^2 C_5,$$

$$\frac{dC_3}{dt} = k_1 C_1 C_4 - k_2 C_2 C_3, \quad \frac{dC_4}{dt} = -k_1 C_1 C_4 + k_2 C_2 C_3,$$

$$\frac{dC_5}{dt} = k_3 C_1^2 C_6 - k_4 C_2^2 C_5, \quad \frac{dC_6}{dt} = -k_3 C_1^2 C_6 + k_4 C_2^2 C_5$$

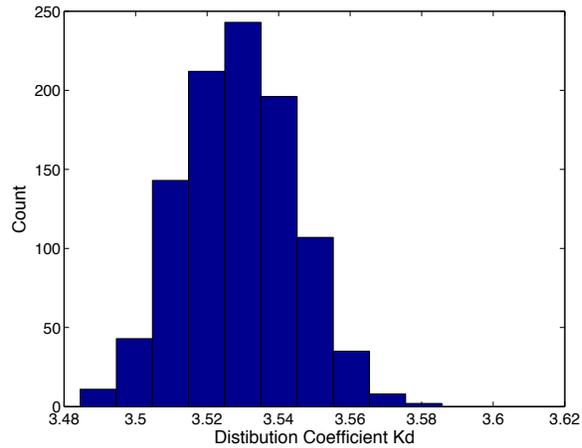
Neptunium Ion Exchange: UQ



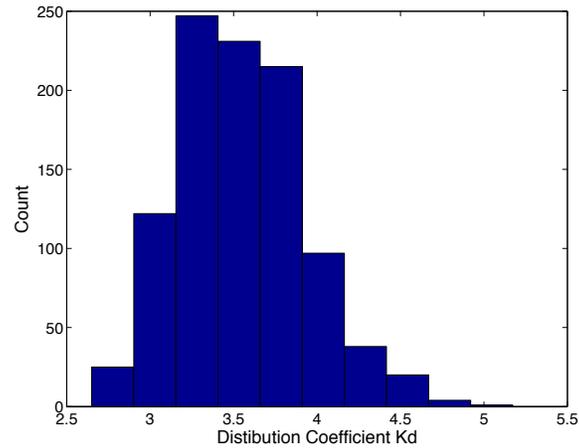
WRR, 2007

Neptunium Ion Exchange: UQ

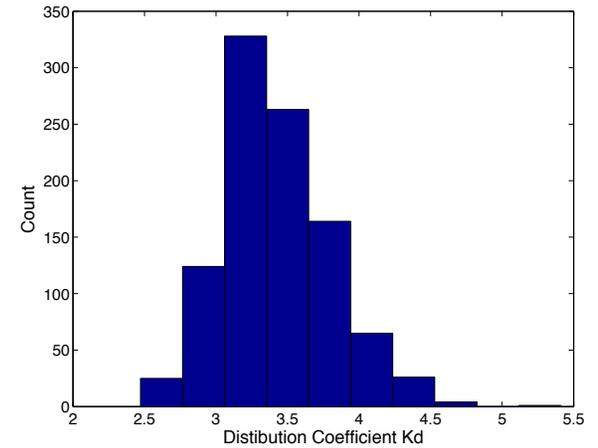
Distribution coefficient $K_d = C_3/C_4$:



Parametric U



Model U



Joint U

Reactive transport (*instantaneous* adsorption):

$$\omega R \frac{\partial C}{\partial t} = \nabla \cdot (\tilde{\mathbf{D}} \nabla C) - \nabla \cdot (\mathbf{v}C), \quad R_c = 1 + \frac{1 - \omega}{\omega} \rho_s K_d$$