Historical Reconstruction of Groundwater Contamination at Contaminated Sites and Uncertainty Analysis

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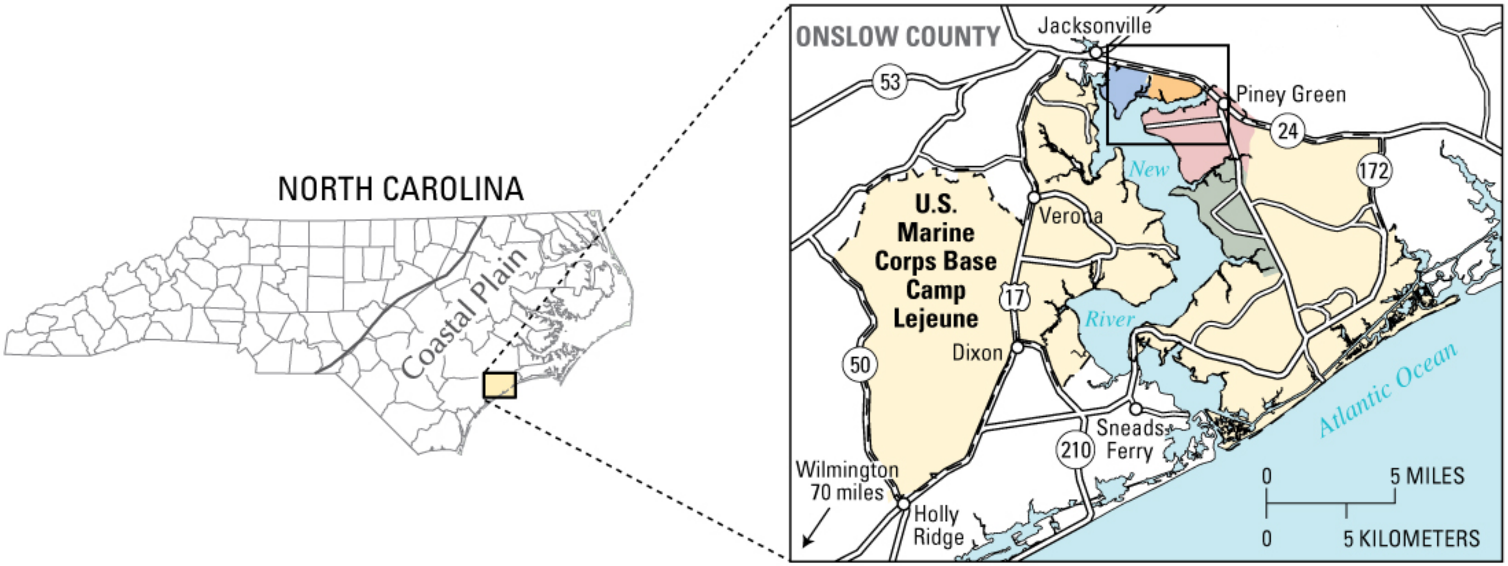
Outline

- Background
- Mathematical Model
- Methodology
- Numerical Applications
- Conclusions

Background

US Marine Corps Base Camp Lejeune, NC



Base from Camp Lejeune GIS Office, June 2003

Background

- Water-distribution systems at the site were contaminated with volatile organic compounds (VOCs)
  - Tarawa Terrace Area was contaminated with PCE.
  - Hadnot Point Area was contaminated with TCE and other chemicals.

- Purpose of the study is to determine if there is an association between exposure to contaminated drinking water and birth defects and childhood cancers in children born to women who were pregnant while living in base house during the period 1968 – 1985.

Background

- ATSDR and Georgia Tech have been involved in water modeling activities to support an epidemiological study conducted by ATSDR at Camp Lejeune Base.

    - Modeling techniques are used to reconstruct historical conditions of groundwater flow, contaminant fate and transport, and the distribution of contaminated drinking water within the water distribution system which may have delivered contaminants to the family housing area.

Background

- Hadnot Point area of the site is the ongoing study area.
- In this presentation the data available at the Tarawa Terrace area is used to test the applicability of the method.
  - Groundwater in the vicinity of the Tarawa Terrace was potentially contaminated by seepage from the dry cleaners;
  - Detailed geohydrologic information on aquifer properties are limited;
  - Limited concentration records are available at some observation sites after 1994; and,
  - Pumping operation schedules for pumping wells at the site are available before 1994.
- The goal is to reconstruct contamination history at several observation sites before 1994.

Background

- Conventional approach to analyze this problem is to develop groundwater flow and contaminant fate and transport models and use them in historical reconstruction.
  - **Advantage:** The concentration distributions can be reconstructed with high accuracy;
  - **Disadvantage:** Computationally expensive and time-consuming.
- The proposed control model as an approximate approach to solve this problem.

Mathematical Model

- **Forward discrete state equation**

Least square method

System effect

Optimization method

Pumping effect

$$\left.\begin{aligned} \boldsymbol{X}(k+1) &= \mathbf{A}\boldsymbol{X}(k) + \mathbf{B}\boldsymbol{U}(k) \\ \boldsymbol{X}(t_0) &= \boldsymbol{X}_0 \end{aligned}\right\}$$

Mathematical Model

- **Backward discrete state equation**

$$\left.\begin{array}{c} \boldsymbol{X}\left(k\right)=\mathbf{A}_{b}\,\boldsymbol{X}\left(k+1\right)+\mathbf{B}_{b}\boldsymbol{U}\left(k\right) \\ \boldsymbol{X}\left(T_{f}\right)=\boldsymbol{X}_{f} \end{array}\right\}$$

Mathematical Model

- **Forward discrete state equation with errors**
  - **System state equation**

System error

$$\mathbf{X}(k+1) = \mathbf{AX}(k) + \mathbf{BU}(k) + \mathbf{w}(k)$$

  - **Observation equation**

Measurement error

$$\mathbf{Y}(k) = \mathbf{CX}(k) + \mathbf{v}(k)$$

Solution Methodology

- **Kalman filter algorithm**

$$\bar{X}(k+1) = \mathbf{A}\hat{X}(k) + \mathbf{B}U(k)$$

$$\mathbf{M}(k) = \mathbf{A}\mathbf{P}(k)\mathbf{A}^{T} + \mathbf{Q}$$

$$\mathbf{K}(k) = \mathbf{M}(k)\left[\mathbf{M}(k) + \mathbf{R}\right]^{-1}$$

$$\hat{X}(k) = \bar{X}(k) + \mathbf{K}(k)[Y(k) - \bar{X}(k)]$$

$$\mathbf{P}(k) = \left[\mathbf{I} - \mathbf{K}(k)\right]\mathbf{M}(k)$$

where

- **Q(k): covariance matrix of the system noise**
- **R(k): covariance matrix of the measurement error**
- **P(k): covariance matrix of the error of the measurement-updated concentration**
- **M(k): covariance matrix of the error of the time-updated concentration**
- **K(k): Kalman gain matrix**

Solution Methodology

- **Covariance matrix of system errors**

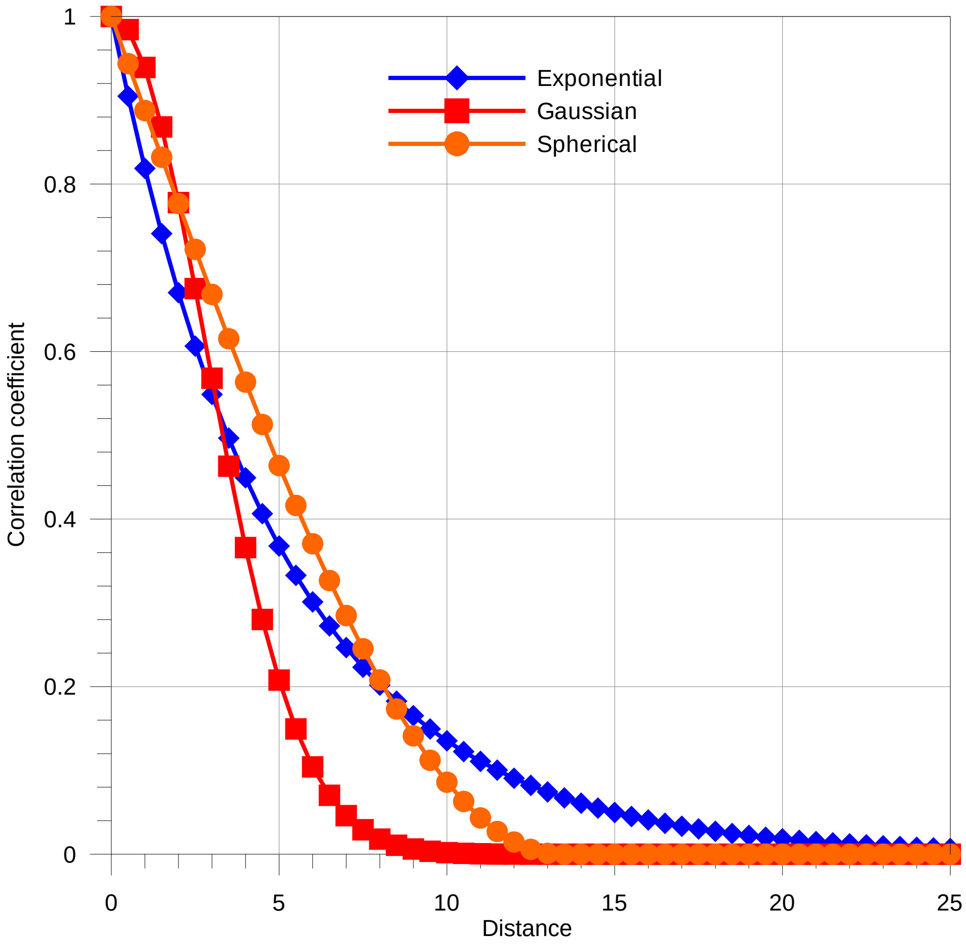
$$\boldsymbol{Q} = [\boldsymbol{q}_{ij}]_{n\times n} = [\sigma_i \sigma_j \rho(\boldsymbol{l})]_{n\times n}$$

where

- σ_i: standard deviations of the system error at observation sites i
- $\rho(l)$: spatial correlation coefficient of the system noise at separation l.

Methodology

- **Spatial correlation models**



Methodology

- **Covariance matrix of measurement errors**

$$R = diag\left\{\sigma_{r_1}^2, \sigma_{r_2}^2, \cdots, \sigma_{r_n}^2\right\}$$

where

- $\sigma_{r_i}^2$ **: the variance of measurement error at site *i*, assumed to be known.**

Methodology

- **Monte Carlo simulation for measurement values**

$$y_i(k) = x_i(k) + \varepsilon_i(k)\beta_i$$

where

- ***$\varepsilon_i(k)$*: random number generated using Monte Carlo simulation**
- ***$\beta_i(t)$*: strength of error at site *i***

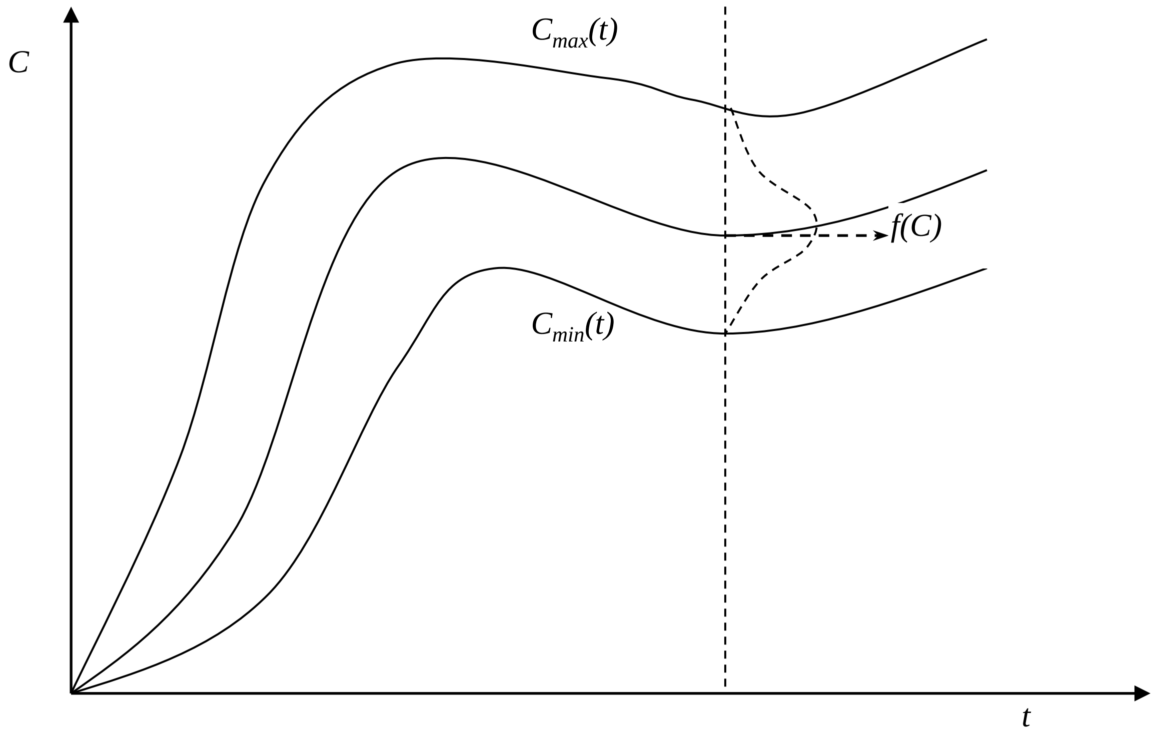
Methodology

- **Monte Carlo simulation procedures**

  - Identify matrices **A** and **B** in the state equation;
  - Generate sets of random series of data using Monte Carlo simulation that is based on the statistical properties of the existing data;
  - Generate measurement values;
  - Calculate smooth solution using Kalman Filter algorithm; and,
  - Implement statistical analyses.

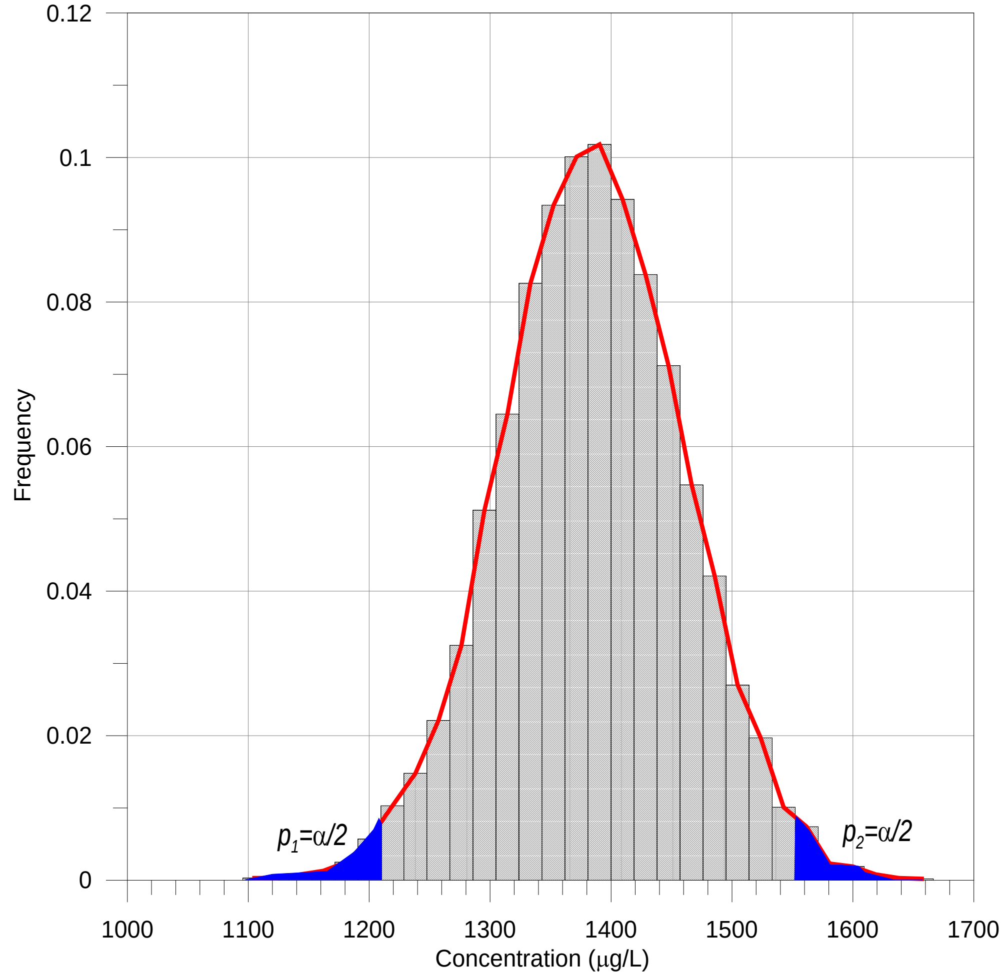
Methodology

- **Results of Monte Carlo simulation**



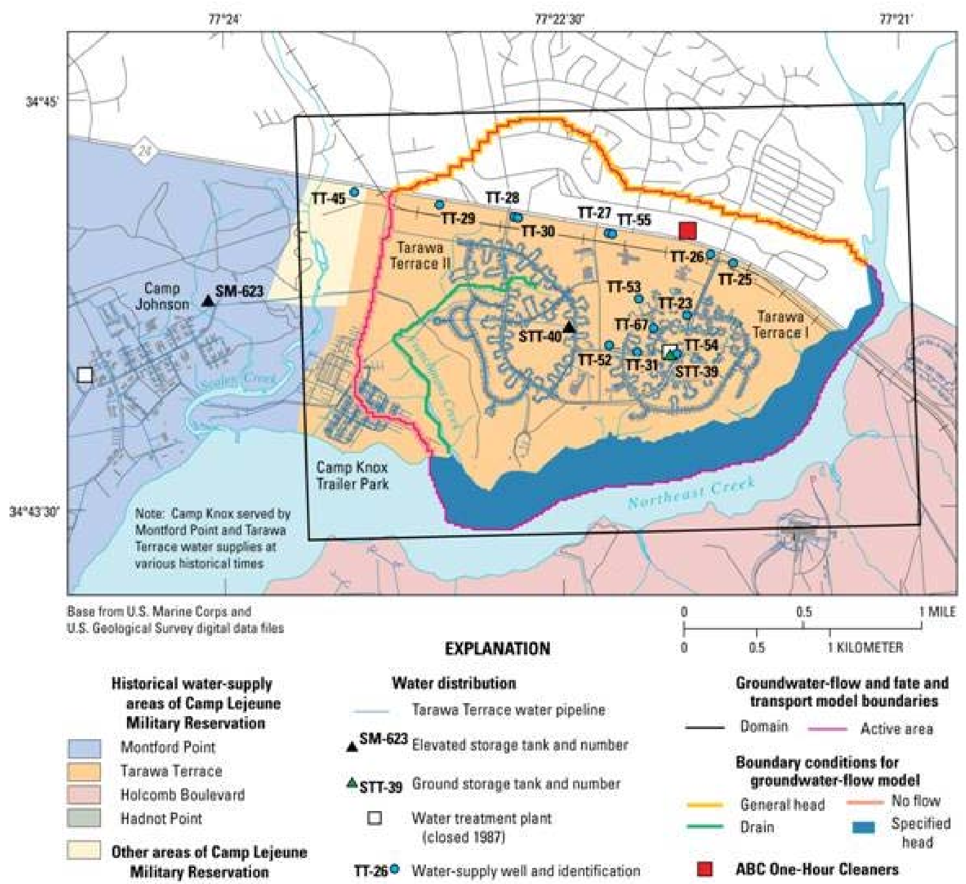
Methodology

- Estimation of the confidence corridor



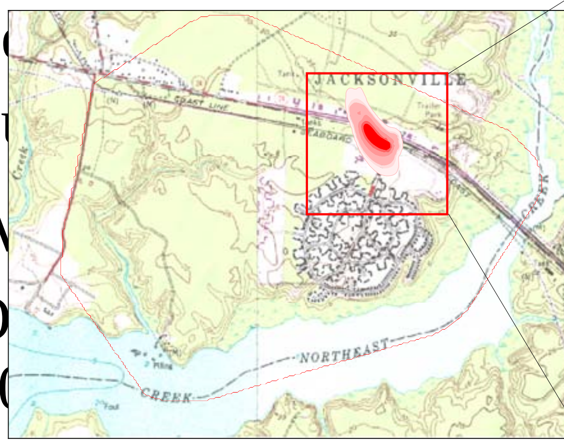
Numerical Applications

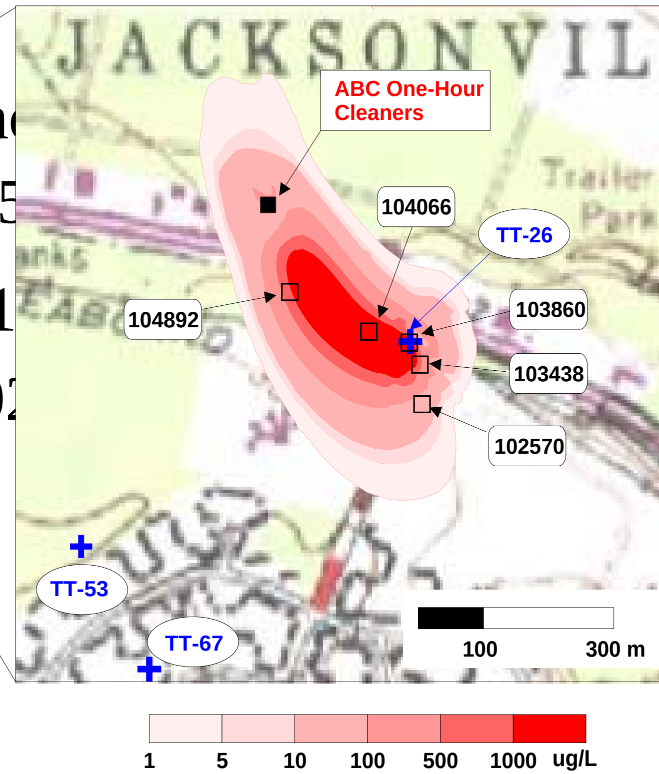
- Tarawa Terrace Area



Numerical Applications

- **Simulation conditions**
  - P 28 m
  - P TT-5
  - W 1951
  - O s 102 T-26), 10
  - Source: ABC Cleaner



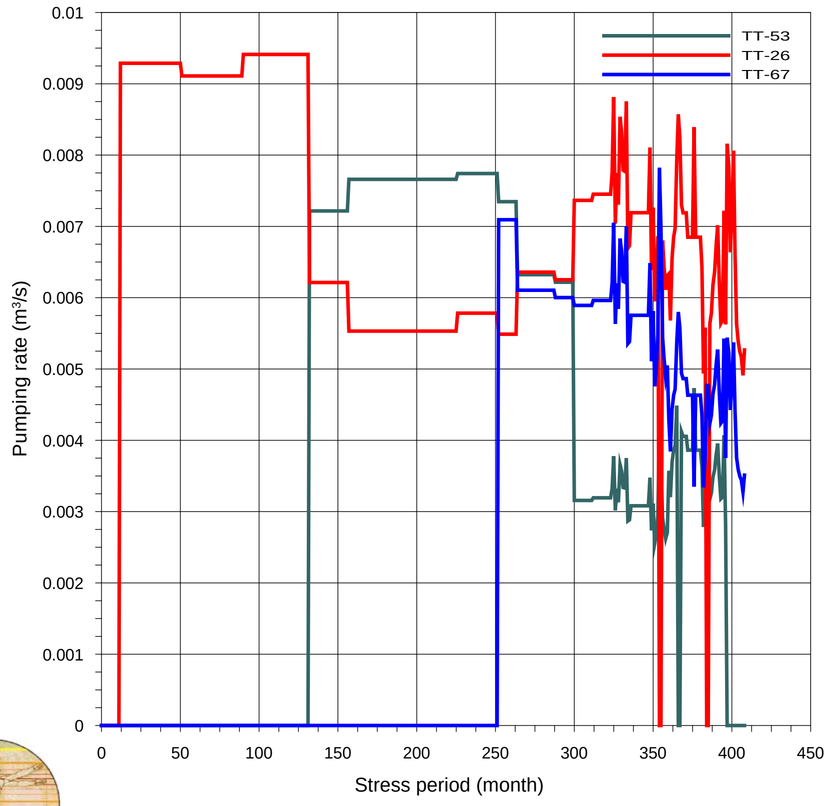


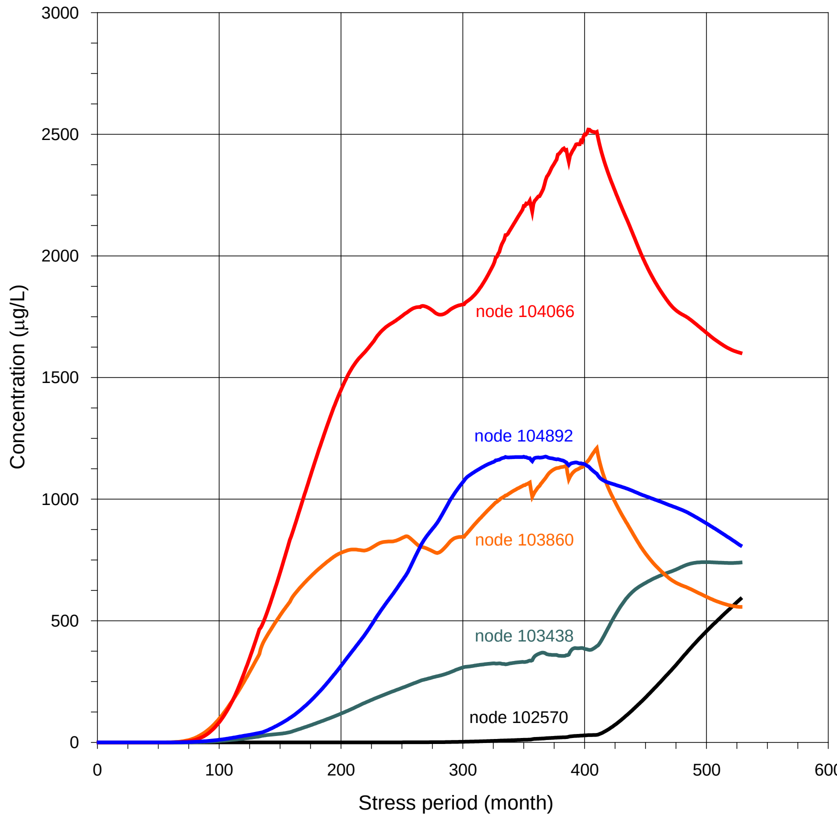
- Three pumping wells: TT-26, TT-53, and TT-67
- Five monitoring points.

PCE concentration distribution in December 1984 (stress period=408) at z = -24 m.

Numerical Applications

- Pumping schedules and simulation results



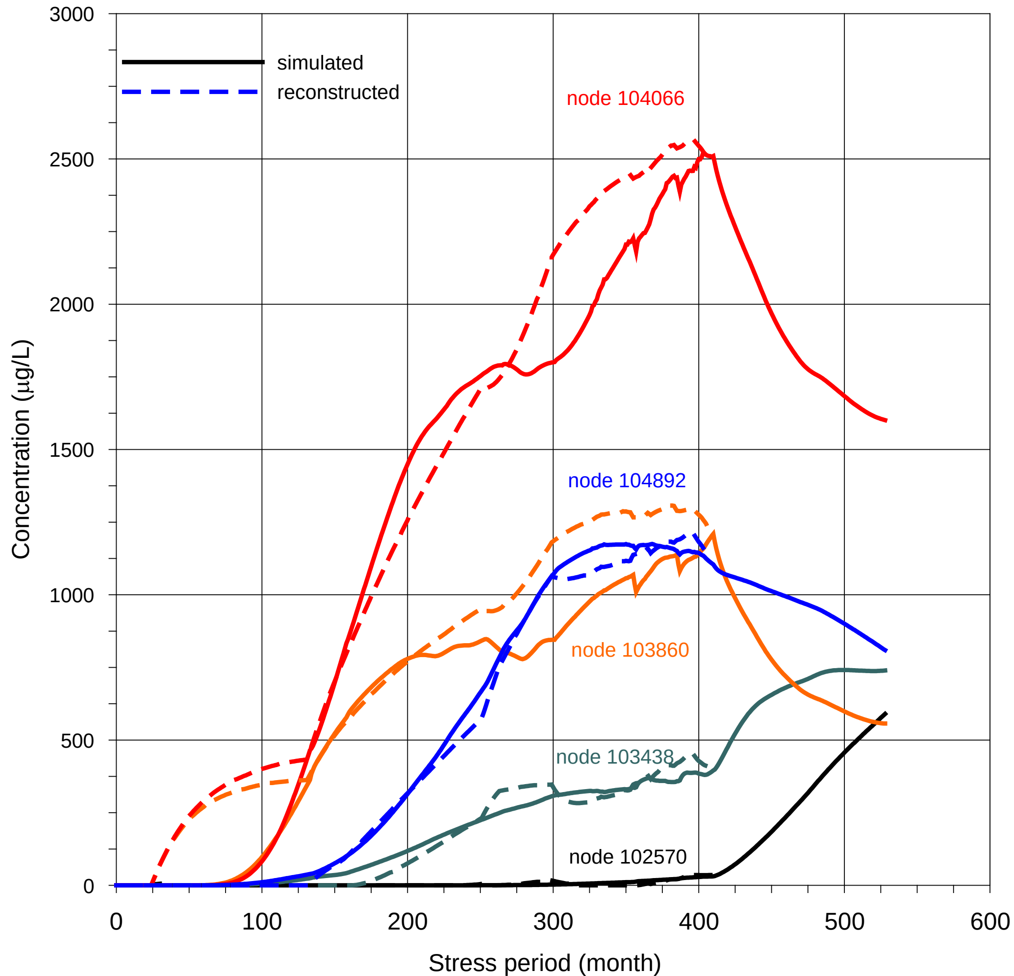


Numerical Applications

- **Data used in system recognition**
  - Concentration data within stress period 408 – 528 are used to identify system matrix **A**; and,
  - Concentration data at stress period 408 and pumping rate data before stress period 408 is used to search pumping effects matrix **B** optimally.

Numerical Applications

- **Concentration distributions reconstructed**



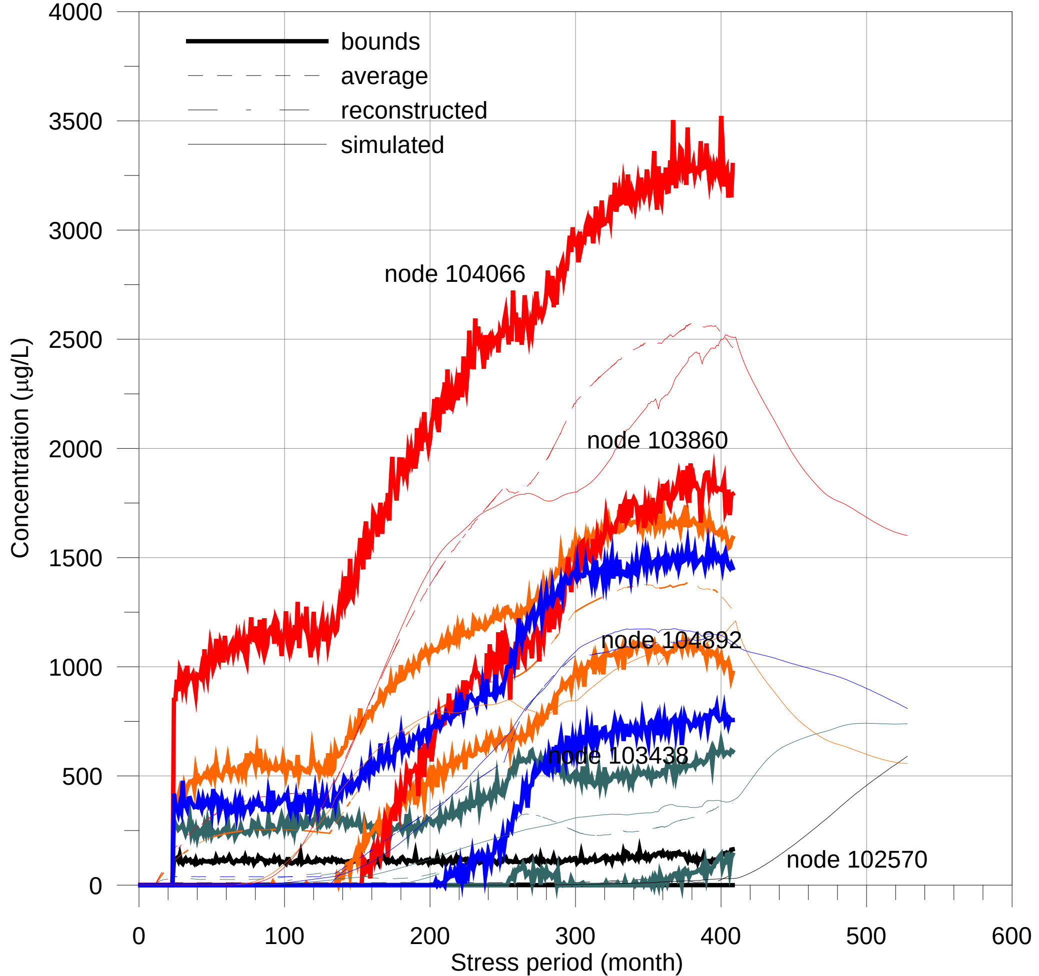
Numerical Applications

Uncertainty analysis conditions

- Mean and variance of measurement error are given as 0.0 and 0.1;
- Gaussian spatial correlation model is used;
- β_i takes the average value of input concentration data at each observation site ;
- 10,000 sets of random numbers is generated for Monte Carlo simulation and Kalman filtering algorithm; and,
- Confidence level is 80%.

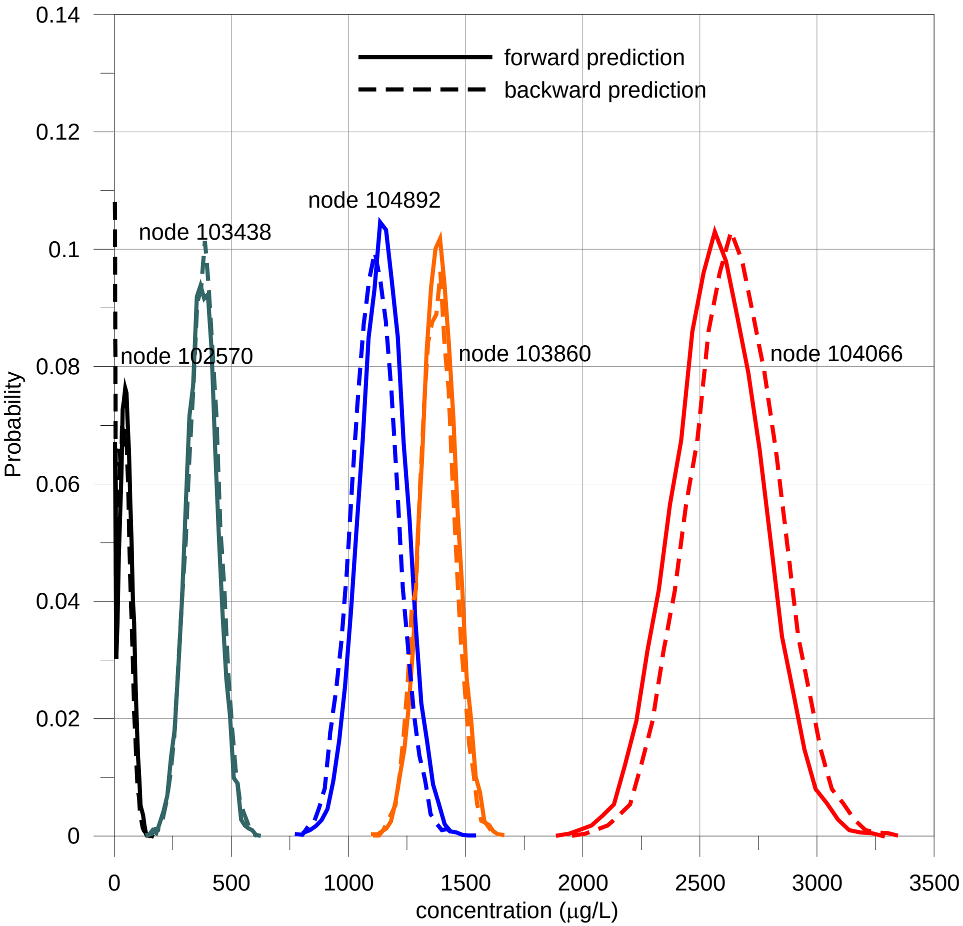
Numerical Applications

- Concentration distributions reconstructed



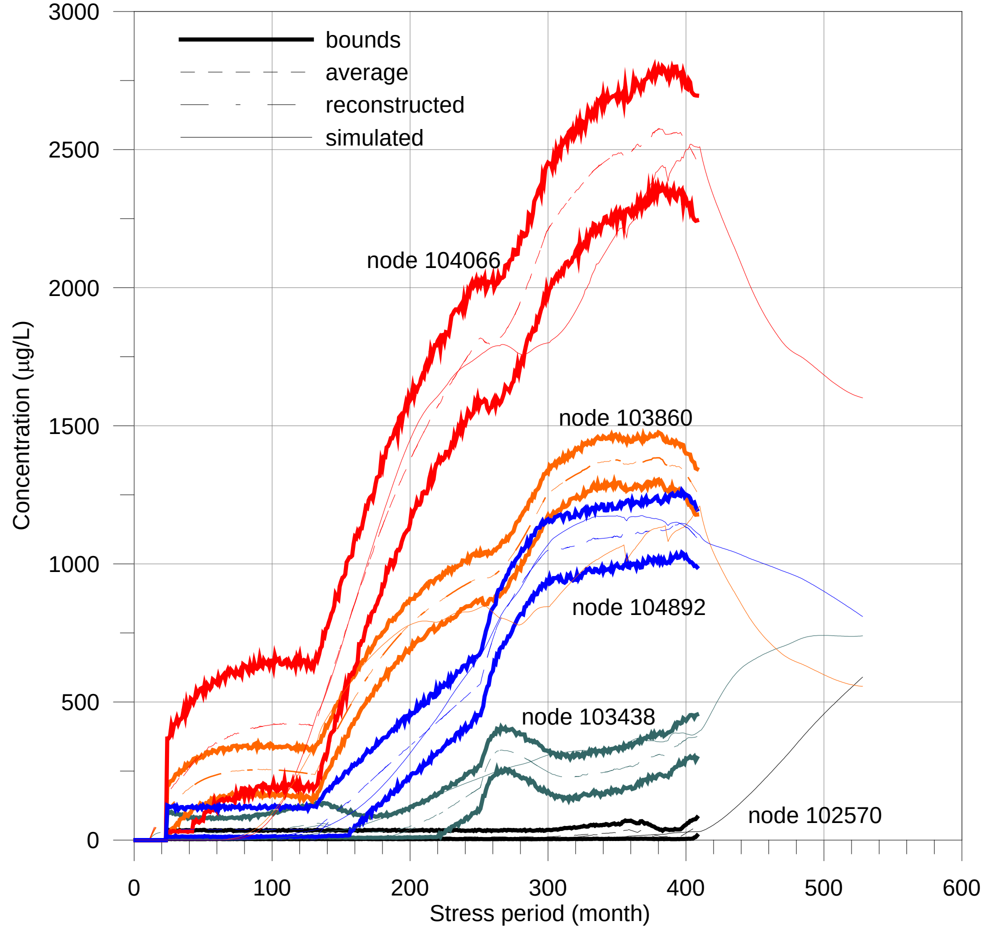
Numerical Applications

- Probability distributions at maximum concentrations



Numerical Applications

- Confidence corridors at 80% level



Conclusions

- Monte Carlo simulation method coupled with Kalman filter algorithm can be used to implement uncertainty analyses in case of limited data available;

- Methodology may obtain the bounds of concentration distributions, probability distributions of concentrations at any stress period and confidence corridors for a given confidence level; and,

- Results obtained using proposed methodology may be sufficient for health risk assessment at the site..

Thank You!

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