Estimation of Contaminant Mass Discharges at Plume Control Planes

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Overview

- Concept of mass flux and discharge
- Problem of estimating discharges from point measurements → **UNCERTAINTY**
- Geostatistical approach for **POROUS AQUIFERS**
  - Spatial correlation (variogram)
  - Data skewness (non-Gaussian)
- Alternative approach for **FRACTURED ROCK**
  - Object oriented (linear fracture traces)
What is Flux?

• Water (Darcy) flux: \[ q = \frac{Q}{A} \text{ [L/T]} \]
  
  \( Q \) … water discharge (volume per time)

  \( A \) … cross-sectional area

• Contaminant mass flux: \[ J = qC \text{ [M/(L}^2\text{T)}]] \]

  \( C \) … contaminant concentration

• \( J \) is the mass of a contaminant passing a unit cross-sectional area per unit time interval
What is Flux?


What is Discharge?

Mass Discharge ($M_d$) =
Sum of Mass Flux Estimates

$J_{A_{i,j}} =$ Individual mass flux measurement at Transect A

$M_{dA} =$ Mass discharge at Transect A (total of all $J_{A_{i,j}}$ estimates)

Why Discharge?

- Quantify source strengths and plume attenuation rates
- Assess impact on potential receptors (e.g., supply well)
- Evaluate remediation performance or legal compliance

Estimating Discharge
(from point measurements)

• Complex methods incorporating different types of site information:
  • Heads, conductivities, fluxes, concentrations, etc.

• **FLUXES** are most “direct” information, because simple summation gives discharge

• Fluxes are only known at a **LIMITED NUMBER OF SAMPLING POINTS** in the control plane

• This requires **INTERPOLATION OF FLUXES** at unsampled locations before integration

• Interpolation introduces **UNCERTAINTY** due to random spatial variability of fluxes
Porous Aquifers

• Fluxes may be regarded as a continuous spatially random variable (GEOSTATISTICS)

• Spatial variability may be described by a VARIOGRAM

• CONDITIONAL STOCHASTIC SIMULATION can generate a large number of possible scenarios of flux distributions (discharges) across a control plane

• PROBABILITY DISTRIBUTION OF DISCHARGE to define confidence limits

• Simpler approximate methods have been developed based on an EFFECTIVE NUMBER OF INDEPENDENT DATA
TCE plume, Ft. Lewis, WA

- Control plane with measured flux locations (possibly irregular)

(WRR, 2012, Contaminant discharge and uncertainty estimates from passive flux meter measurements)
TCE plume, Ft. Lewis, WA

- Flux histogram and variogram

HIGHLY SKEWED and SPATIALLY CORRELATED
TCE plume, Ft. Lewis, WA

- Three examples of simulated flux distributions (log-scale) and discharges
**TCE plume, Ft. Lewis, WA**

- Cumulative distribution functions of TCE discharge
Fractured Rock

• Flow occurs along fractures (predominantly)
• Fluxes are measured only where a borehole intersects a flowing fracture (assumed here to be plane)

Sources of UNCERTAINTY:
• Unknown fracture density
• Random fracture locations, sizes and orientations
• Random flux variability between fractures
• Random flux variability within fractures
• Random flux measurement errors
Sampling Transect

- Control plane with observation wells intersecting flow and transport through fracture planes

TRACES:
Intersections of fractures with control plane
Conceptual Model

• Trace locations are assumed to follow Poisson process (complete randomness for a given density)

(WRR, 2013, A stochastic model for estimating groundwater and contaminant discharges from fractured rock passive flux meter measurements)
Observed Data

• Number of intersections $N$

• For each intersection:
  • Trace location and orientation
  • Flux per unit trace length

• Trace density $\lambda$ and trace length distribution $pdf(\tau)$ remain $UNKNOWN$

• HOWEVER, both $N$ and discharge $Q$ are proportional to the product $\lambda \mu_{\tau}$ ($\mu_{\tau}$ … mean trace length)

• Trace density and length properties do not have to be explicitly known for discharge estimation !!!
Discharge Estimator $Q^*$

\[ Q^* = A_T \sum_{k=1}^{N_{\text{well}}} \frac{\omega_k}{L_k} \sum_{j=1}^{N_k} \frac{q^*_j}{\cos \theta_j} \]

- $A_T$ … Area of control plane
- $N_{\text{well}}$ … Number of borings in control plane
- $N_k$ … Number of intersections on the k-th boring
- $L_k$ … Lengths of k-th boring
- $\omega_k$ … Weight of k-th boring (for irregular separation distances)
- $\theta_j$ … Orientation angle of j-th intersection with k-th boring
- $q^*_j$ … Measured flux at j-th intersection with k-th boring
Upper Uncertainty Bound

\[ CV_e^2 \leq \frac{1 + CV_{\rho^*}^2 + CV_{\rho^*}^4}{N_{total}} \]

\( CV_e \) … Error coefficient of variation

\( N_{total} \) … Total number of intersections over all borings

\( CV_{\rho^*} \) … CV of measured fluxes after simple transformation

• Ex.: For \( CV_{\rho^*} \approx 1 \) and \( N_{total} \approx 50 \) we get \( CV_e \leq 0.21 \)

• Device for measuring fracture fluxes is currently being field tested → presentation **TOMORROW AFTERNOON**
Summary

• Contaminant mass discharges are useful parameters in site characterization and decision making, **IF** uncertainty is quantified

• Local flux measurements heavily simplify and improve discharge and uncertainty estimation (no flow and transport modeling required)

• Approaches presented for porous and fractured rock aquifers

• Both require sufficient data to reliably represent flux heterogeneity across control plane
Thank you!

QUESTIONS ?