Groundwater Quality 2013

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: $\boxed{\mathbf{q = Q/A \quad [L/T]}}$

  Q … water discharge (volume per time)

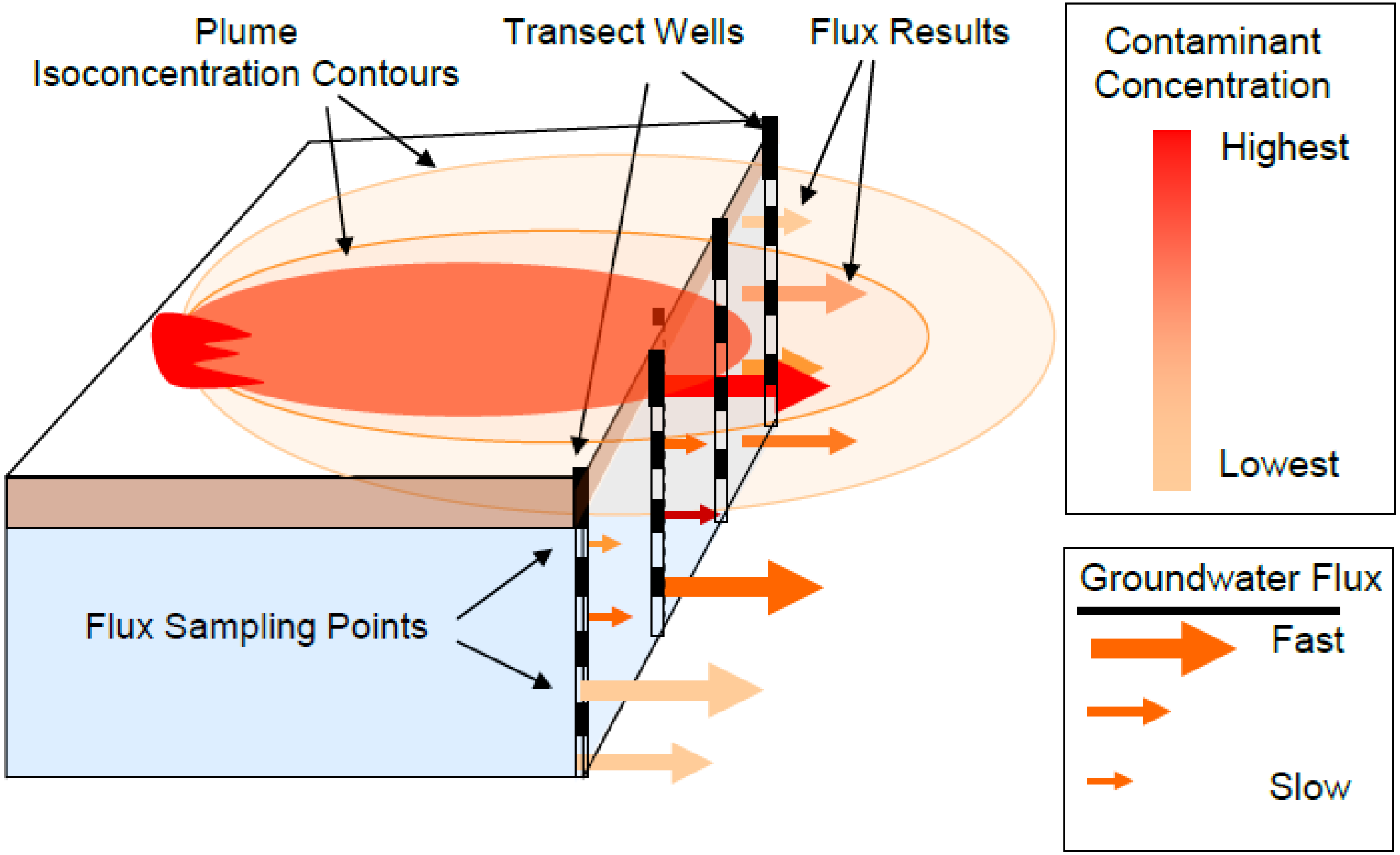
  A … cross-sectional area

- Contaminant mass flux: $\boxed{\mathbf{J = qC \quad [M/(L^2T)]}}$

  C … contaminant concentration

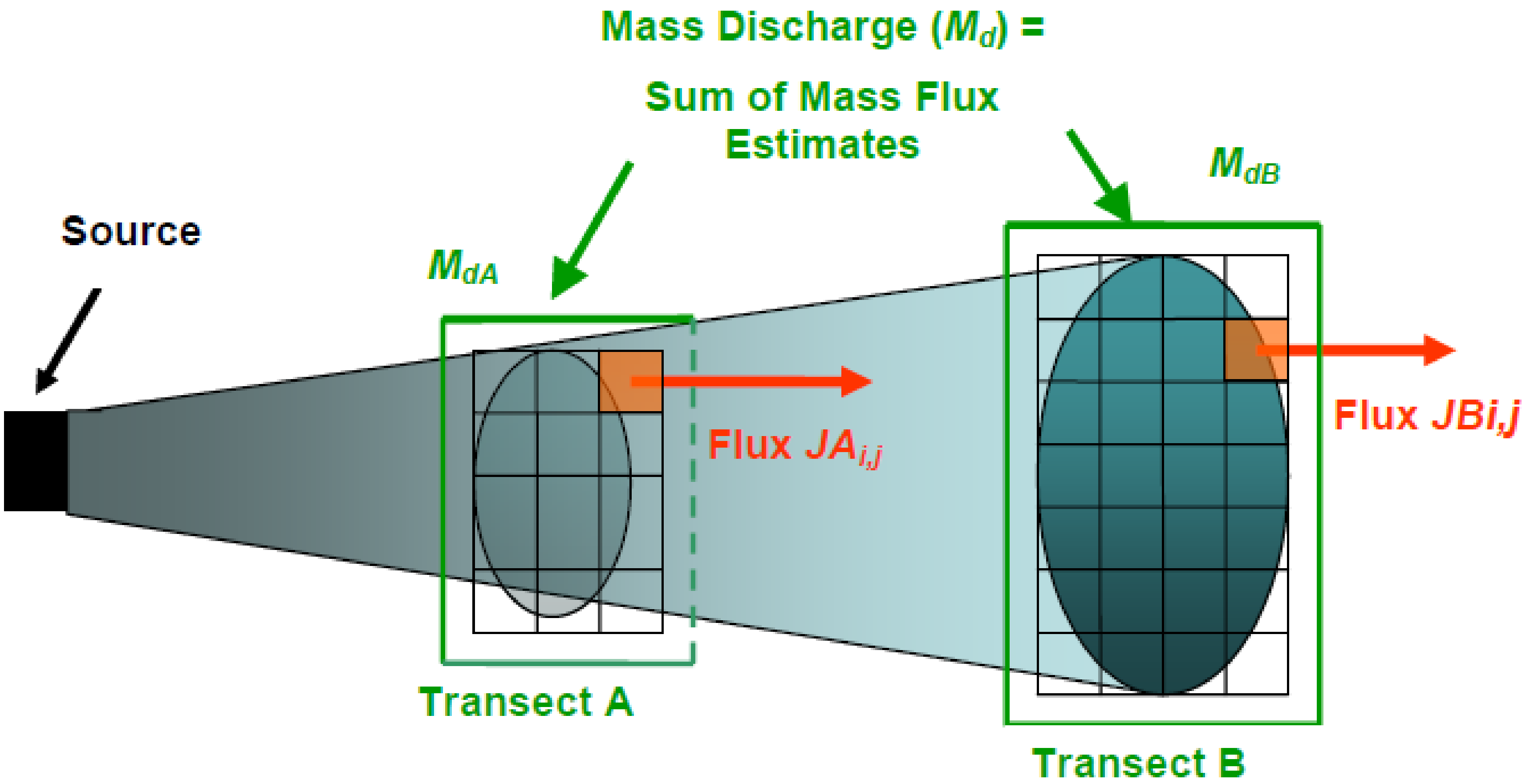
- **J is the mass of a contaminant passing a unit cross sectional area per unit time interval**

What is Flux?



From ITRC (2010) “Use and Measurement of Mass Flux and Mass Discharge”.

What is Discharge?



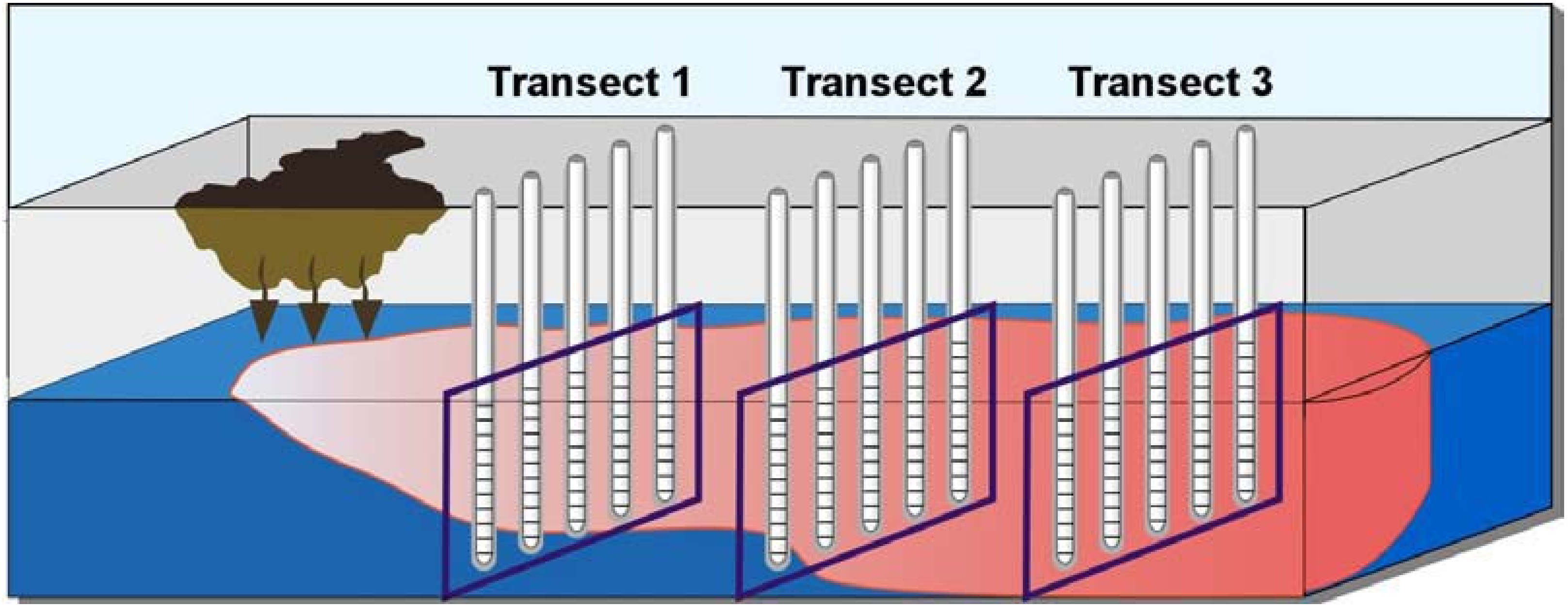
$JA_{i,j}$ = Individual mass flux measurement at Transect A

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

From ITRC (2010) “Use and Measurement of Mass Flux and Mass Discharge”.

Why Discharge?

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



From ITRC (2010) “Use and Measurement of Mass Flux and Mass Discharge”.

Estimating Discharge

(from point measurements)

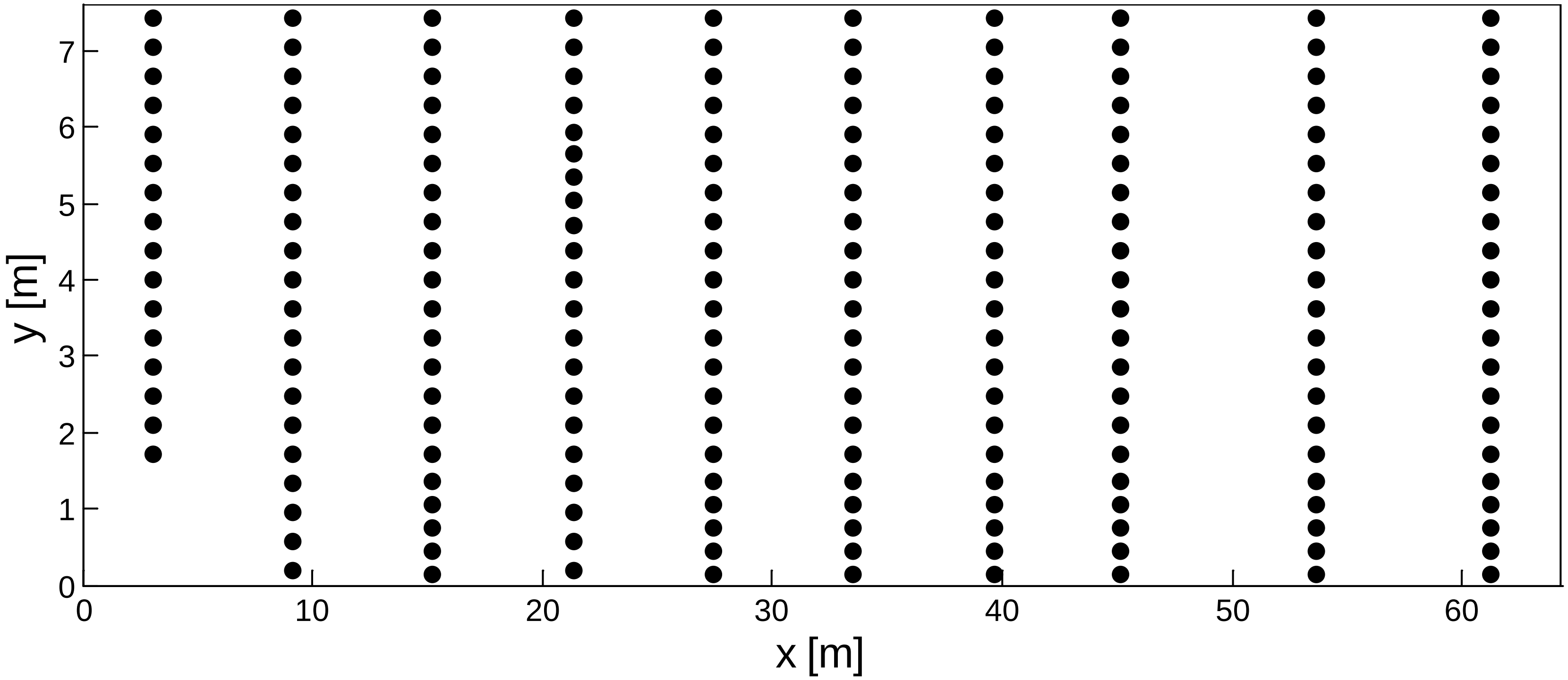
- Complex methods incorporating different types of site information:
    - Heads, conductivities, fluxes, concentrations, etc.
- **FLUXES** are most “direct” information, because simple summation gives discharge
- Fluxes are only known at a **LIMITED NUMBER OF SAMPLING POINTS** in the control plane
- 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

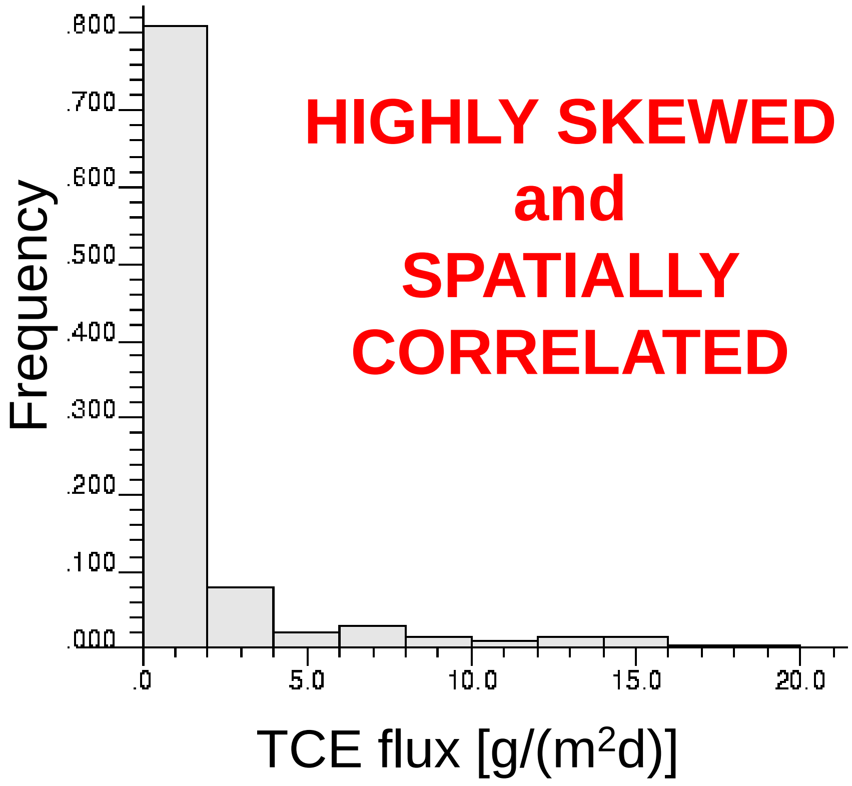
- Control plane with measured flux locations (possibly irregular)



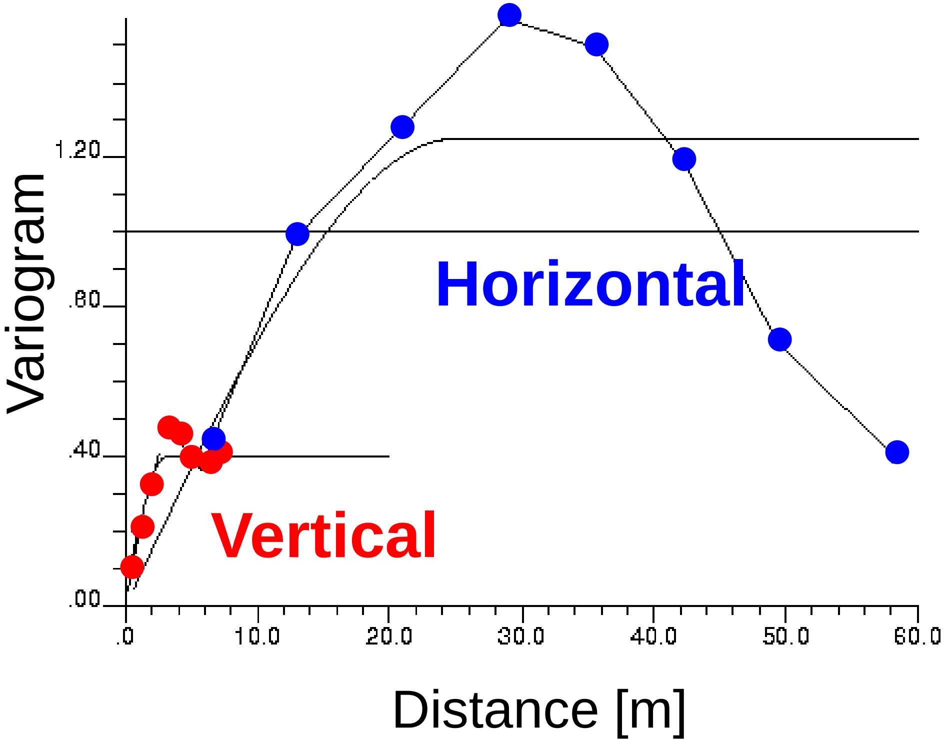
(WRR, 2012, Contaminant discharge and uncertainty estimates from passive flux meter measurements)

TCE plume, Ft. Lewis, WA

- Flux histogram and variogam

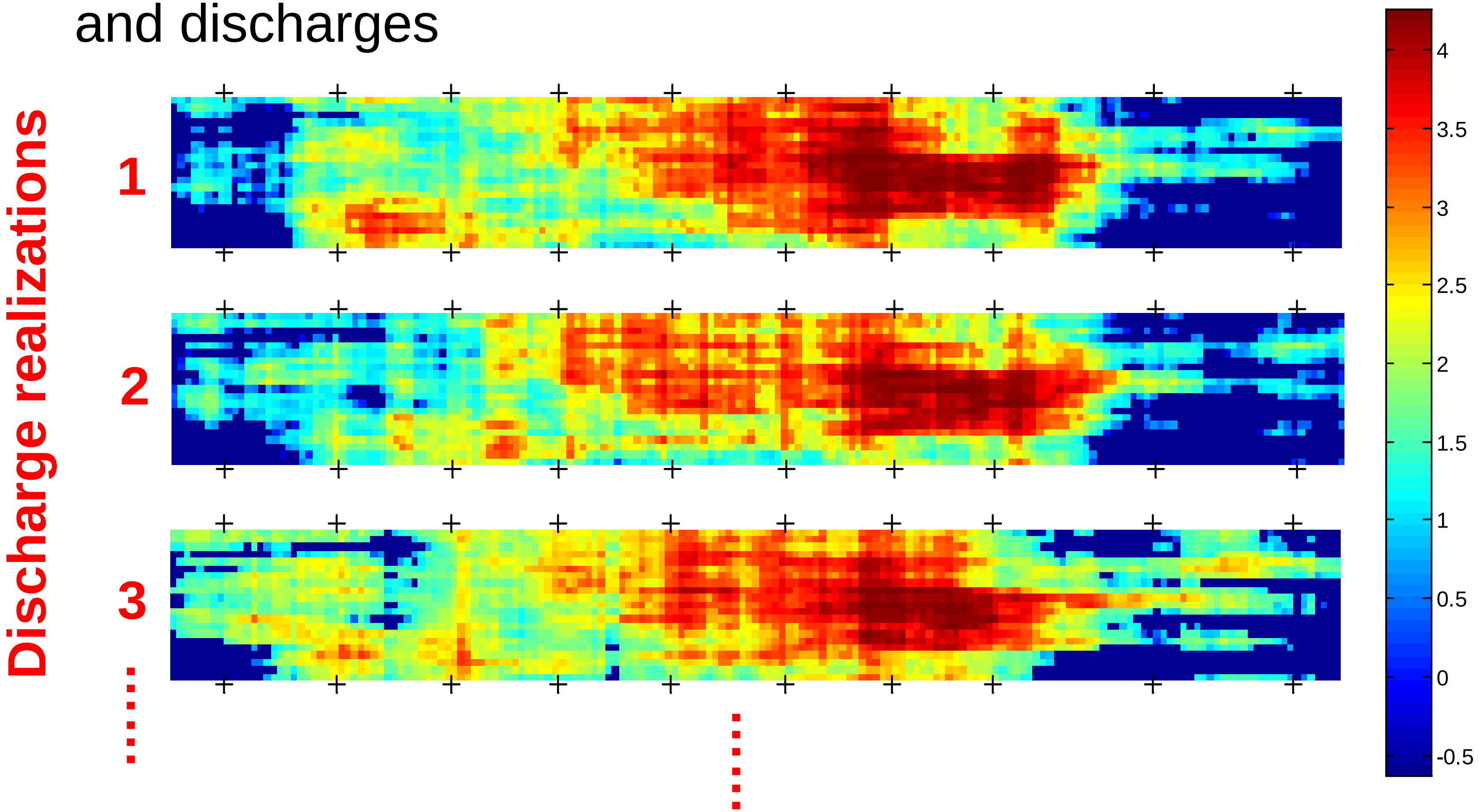


HIGHLY SKEWED and SPATIALLY CORRELATED



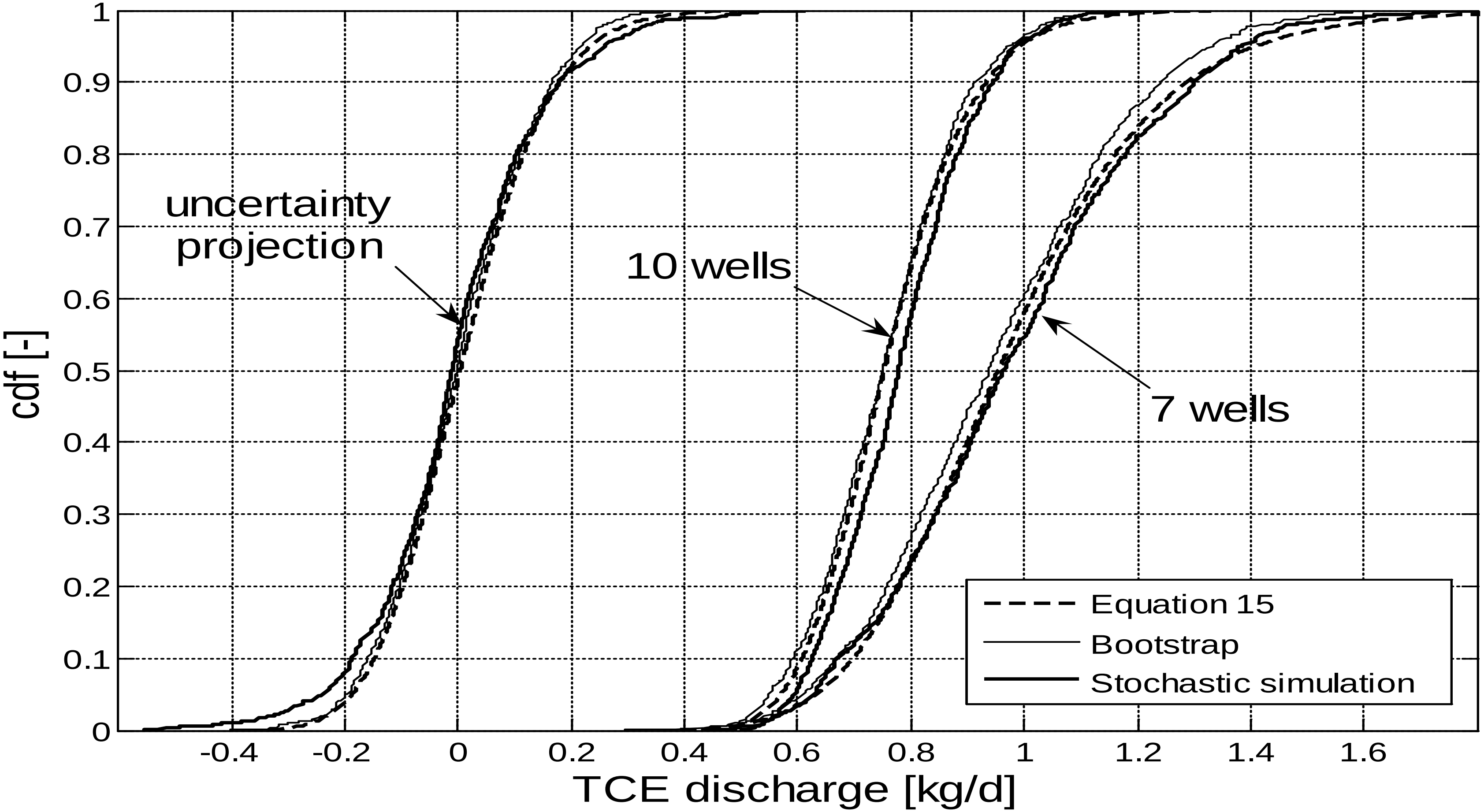
TCE plume, Ft. Lewis, WA

- Three examples of simulated flux distributions (log-scale) and discharges



TCE plume, Ft. Lewis, WA

- Cumulative distribution functions of TCE discharge

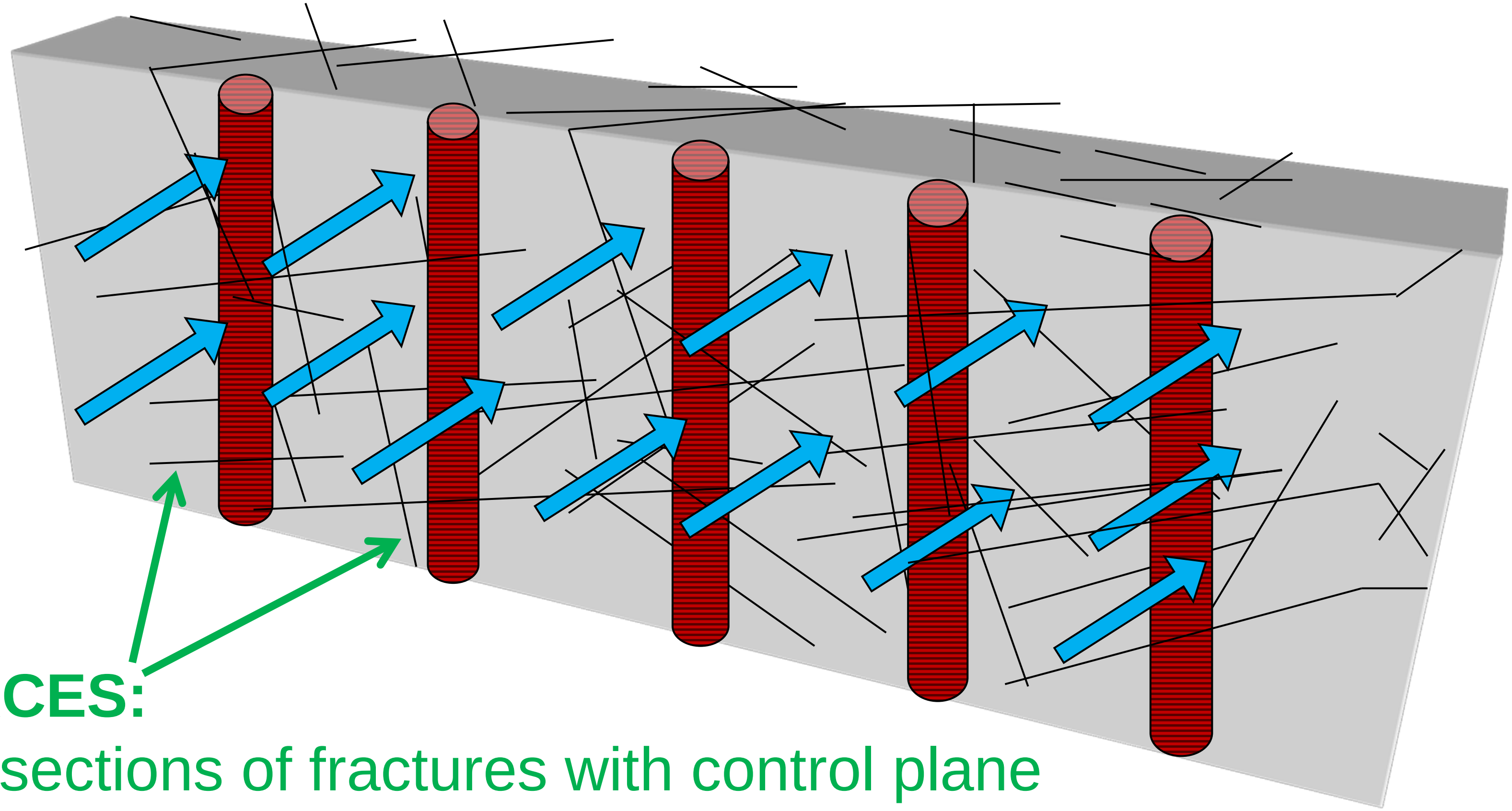


Fractured Rock

- 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

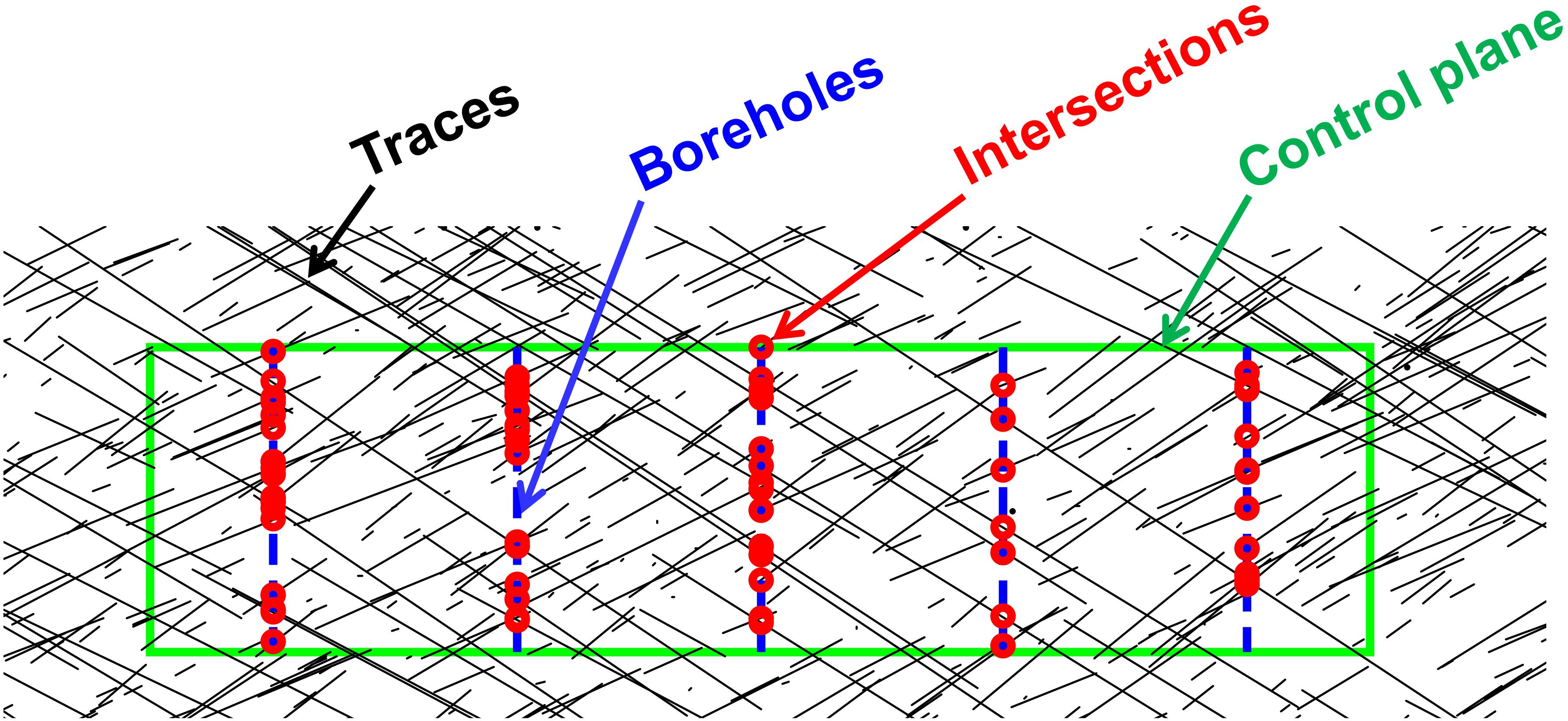
- Control plane with observation wells intersecting flow and transport through fracture planes



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 $\boldsymbol{\lambda}$ and trace length distribution **pdf($\boldsymbol{\tau}$)** remain **UNKNOWN**
- **HOWEVER**, both **N** and discharge **Q** are proportional to the product $\boldsymbol{\lambda\mu_\tau}$ ($\boldsymbol{\mu_\tau}$ … mean trace length)
- **Trace density and length properties do not have to be explicitly known for discharge estimation !!!**

Discharge Estimator Q*

$$Q^* = A_T \sum_{k=1}^{N_{well}} \frac{\omega_k}{L_k} \sum_{j=1}^{N_k} \frac{q_j^*}{\cos\theta_j}$$

A_T … Area of control plane

N_{well} … Number of borings in control plane

N_k … Number of intersections on the k-th boring

L_k … Lengths of k-th boring

ω_k … Weight of k-th boring (for irregular separation distances)

θ_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

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

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 ?