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K-area Fracture Data: Transport Calculations Scaling

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Scaling of Transport

- **Using the K-area fracture data and previous analysis, start to examine the effect of various processes and parameters needed to predict transport at PA time and length scales**
- **Focus here is on diffusion**
  - **Recognized as major process responsible for increased retention in the geosphere**
  - **Sorption sites within the matrix must be accessed by diffusion**

Neretnieks I., (1980) Diffusion in rock matrix: an important factor in radionuclide retardation? *Journal of Geophysical Research* 85(B8): pp. 4379–4397

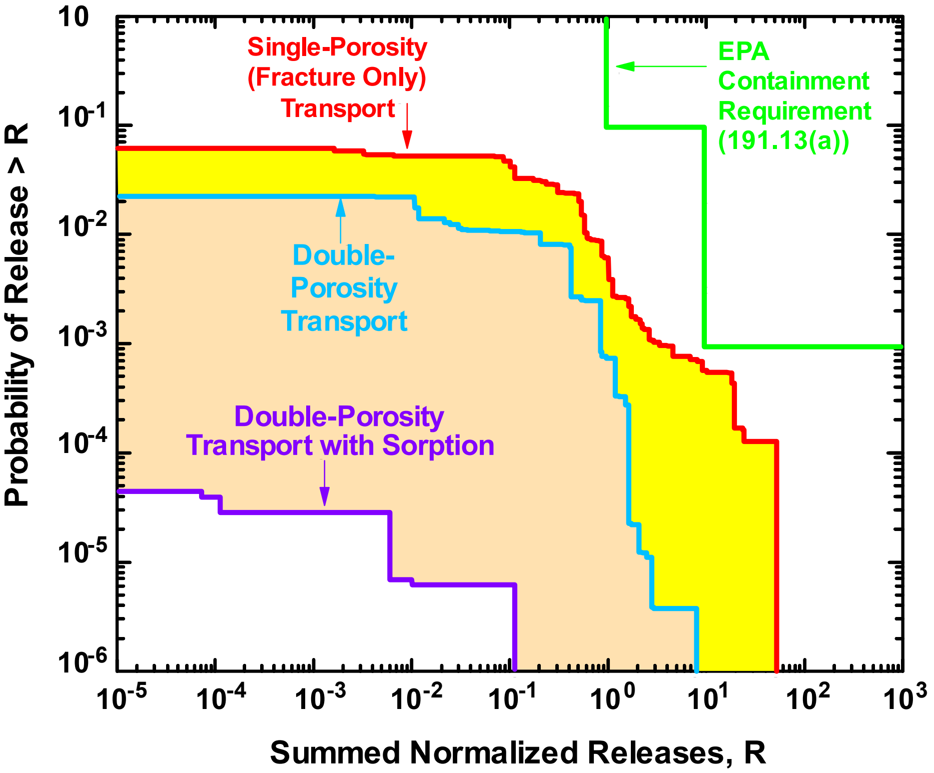
Retention by Diffusion

Probabilistic Systems Analysis is used to predict the future performance of the repository – incorporate uncertainty in multiple processes and parameters

Regulations are written to incorporate uncertainty

Mass transfer processes make a <u>huge difference</u> in predicted repository performance

Other situations: hydrothermal mineralization, partitioning tracer tests for DNAPL, groundwater-surface water coupling with bank storage, etc.



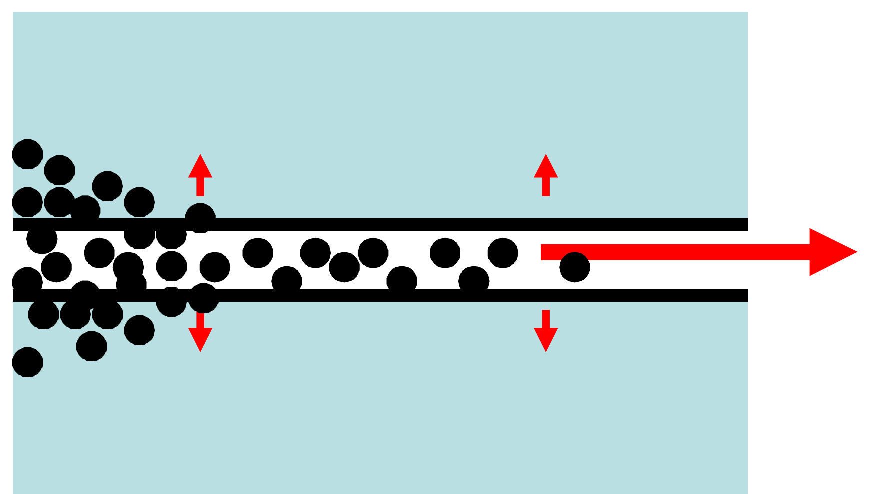
Transport Processes

- **Processes acting in a single fracture:**
  - Dispersion (velocity variation along different flowpaths due to physical heterogeneity in fracture)
  - Diffusion (movement of solute due to concentration gradient – from fracture to matrix and back)
  - Sorption (attachment of solute to fracture walls and matrix pore spaces)

Conceptually, there are two domains in the rock:

1) *Advective, mobile, fracture*

2) *Diffusive, stagnant, matrix*



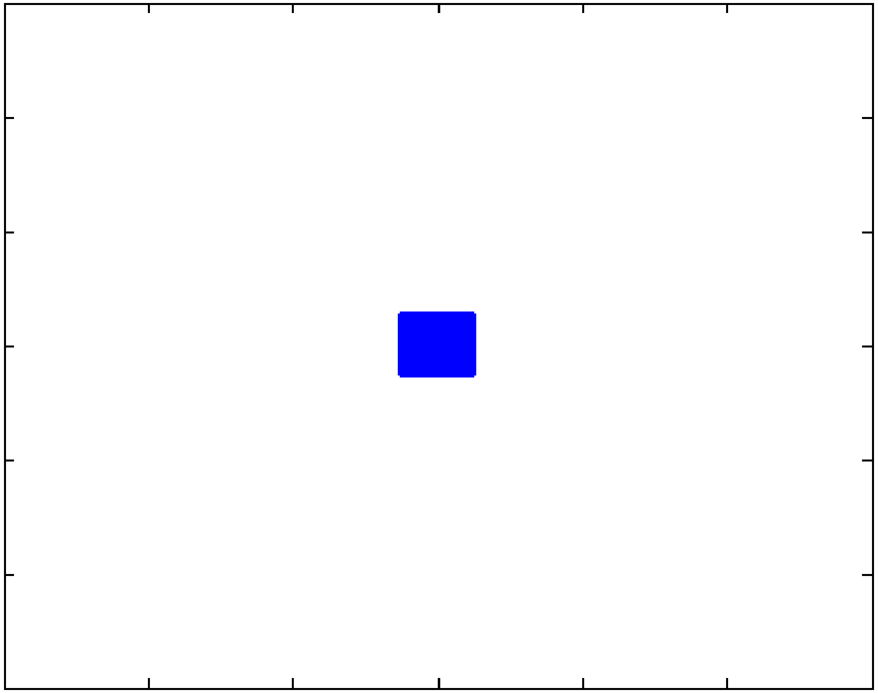
Diffusion

- **Spreading of a solute due to a concentration gradient**

Fick's 1st law: Flux of solute is proportional to concentration gradient

$$F = -D \frac{\partial C}{\partial x}$$

D **is a function of the material(s) through which the solute is diffusing**

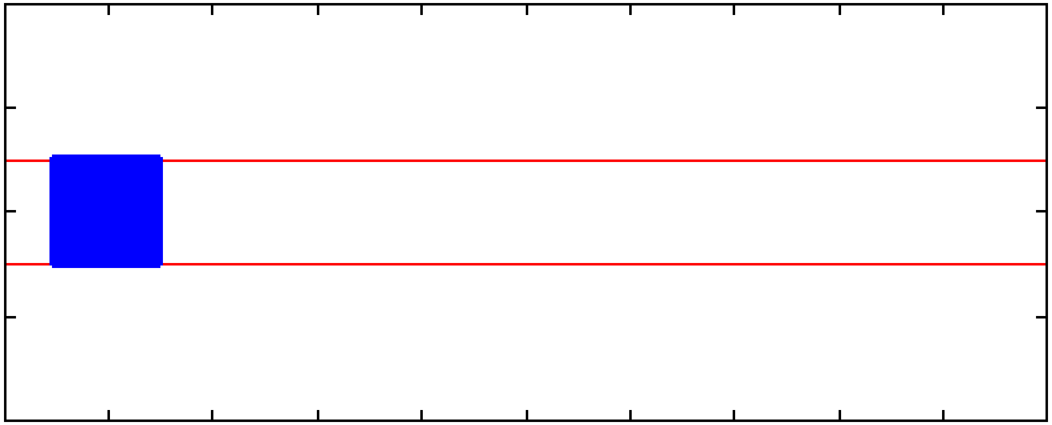


Analogy: Drop of dye in an aquarium

Dispersive Transport

Simple particle tracking model showing solute transport in a single fracture with matrix on top and bottom

Hydrodynamic dispersion is active, but <u>no mass-transfer</u> with matrix

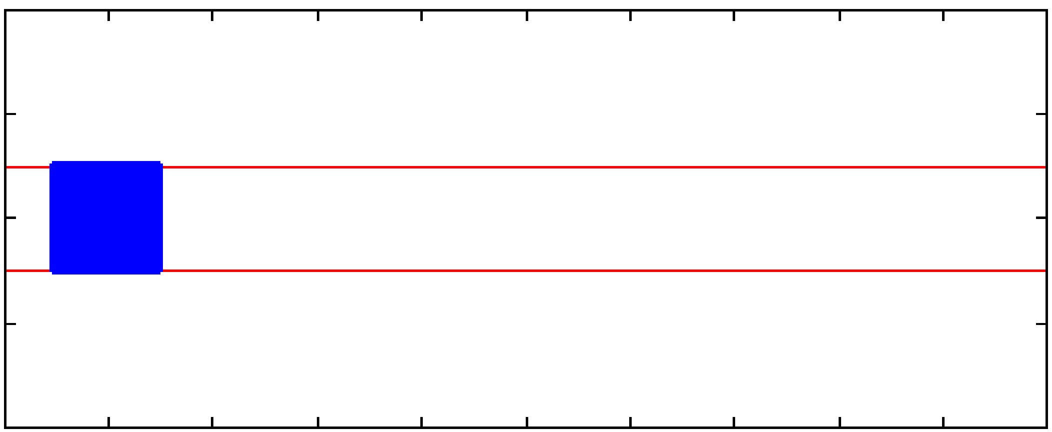


Also referred to as "single-porosity" transport

Dispersion and Diffusion

Simple particle tracking model showing solute transport in a single fracture with matrix on top and bottom

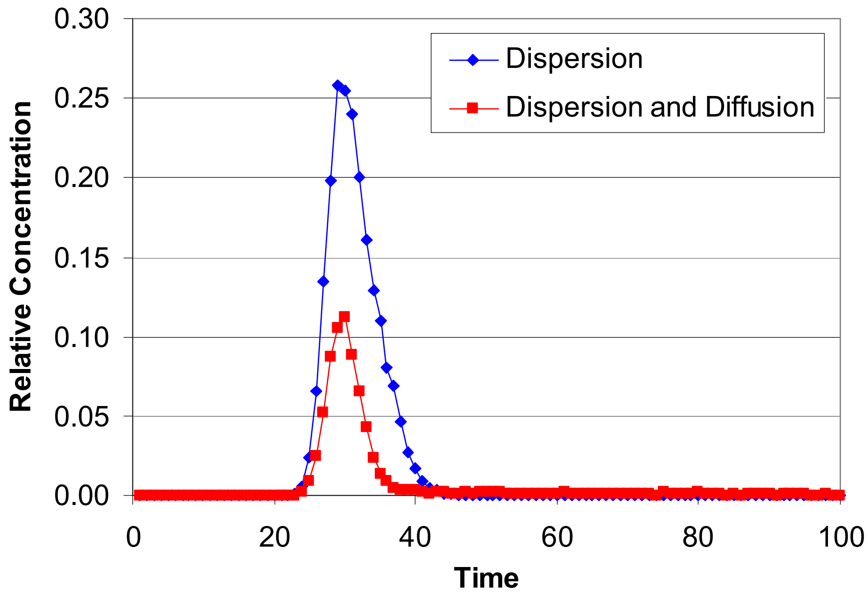
Hydrodynamic dispersion and mass-transfer are active

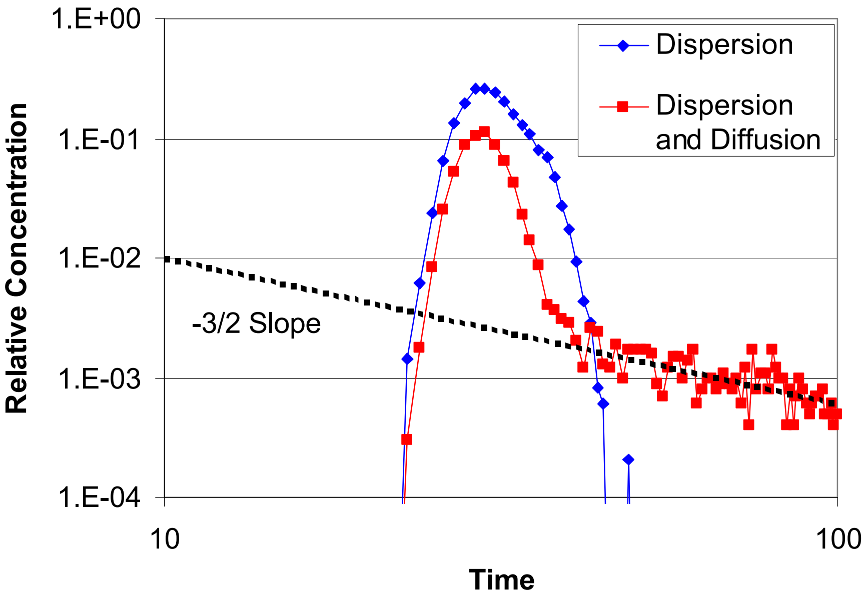


Also referred to as "dual-porosity" transport

Breakthrough Curves

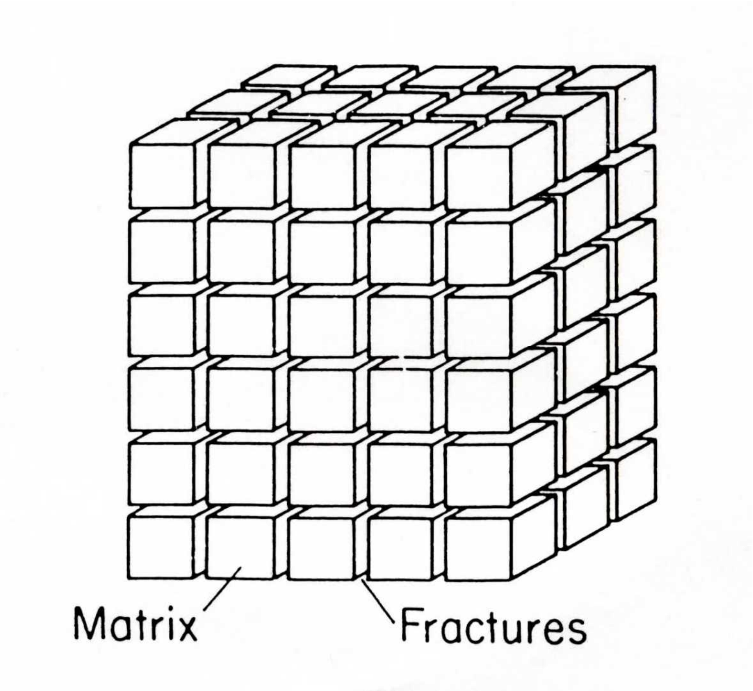
The breakthrough curve is the plot of the concentration as a function of time at a downgradient location (e.g., pumping well).





- ***To characterize tailing behavior, examine results in log-log space***
- ***-3/2 slope is characteristic of diffusion into an infinite medium***

Traditional Dual Porosity Model



The classic dual-porosity representation of a fractured medium is the "sugar-cube" model

To match an observed breakthrough curve that does not have a –3/2 slope, the amount of dispersion and the matrix block size are adjusted

The Real World

Large blocks: bigger capacity, less surface area per aquifer volume, slower diffusion rate

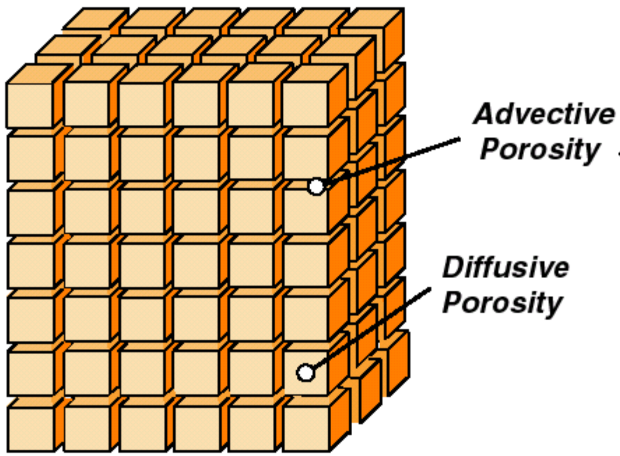
Small blocks: small capacity, more surface area per aquifer volume, faster diffusion rate

Solute accesses all blocks simultaneously

Cemented breccia zone at Yucca Mountain, Nevada

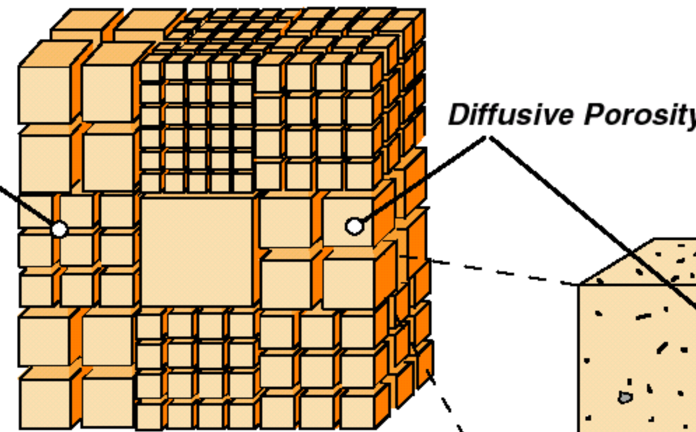
Multi-Porosity Model

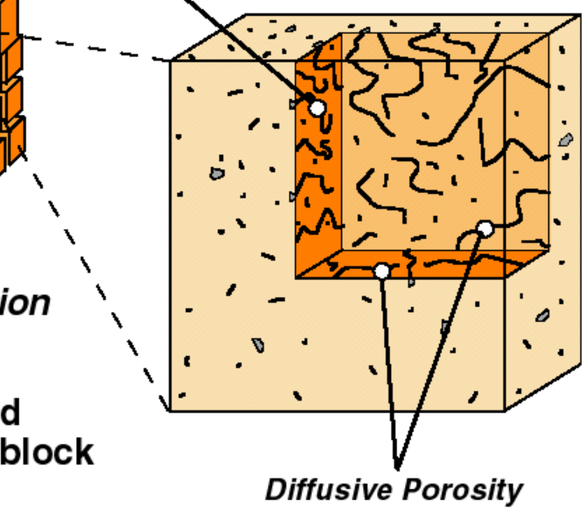
Conventional Single Rate Diffusion



- ***Constant Matrix Block Size***
  Surface area for diffusion and diffusion distance
- ***Constant tortuosity***
  Tortuous nature of "matrix" pores

Multirate Diffusion

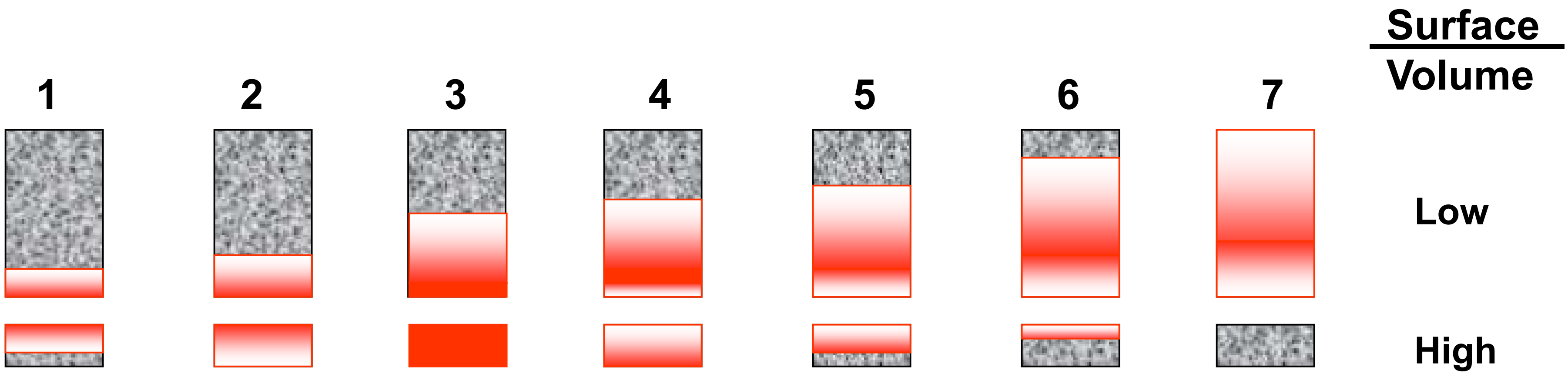


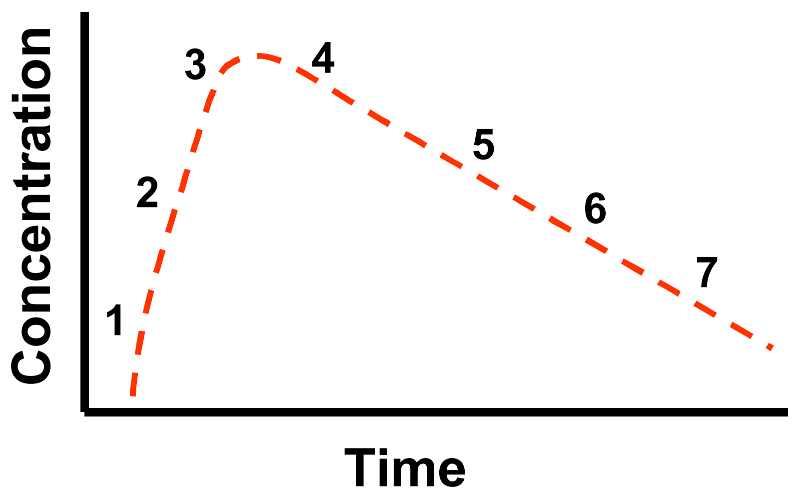


- ***Multiple Rates of Diffusion***

  Distribution of mass transfer rates attributed to variations in matrix block size and tortuosity

Matrix Block Size



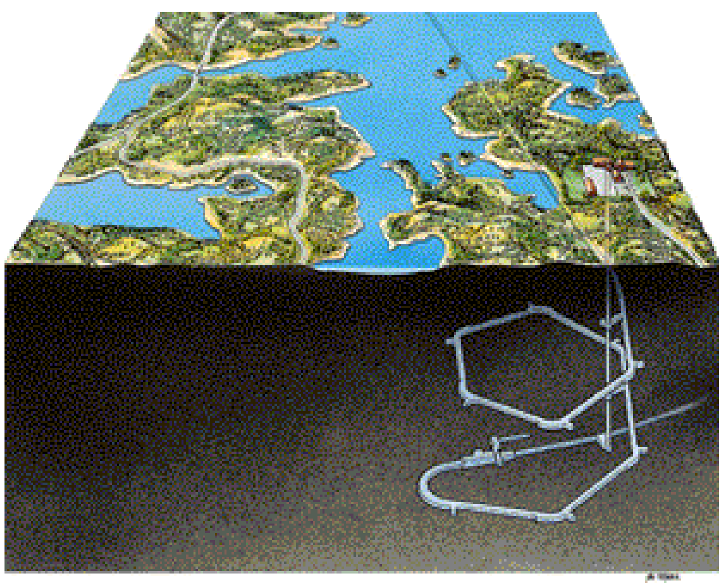


Slower mass transfer from matrix results in shallower (longer) tail

Different rates of mass transfer create different slopes in late time tail

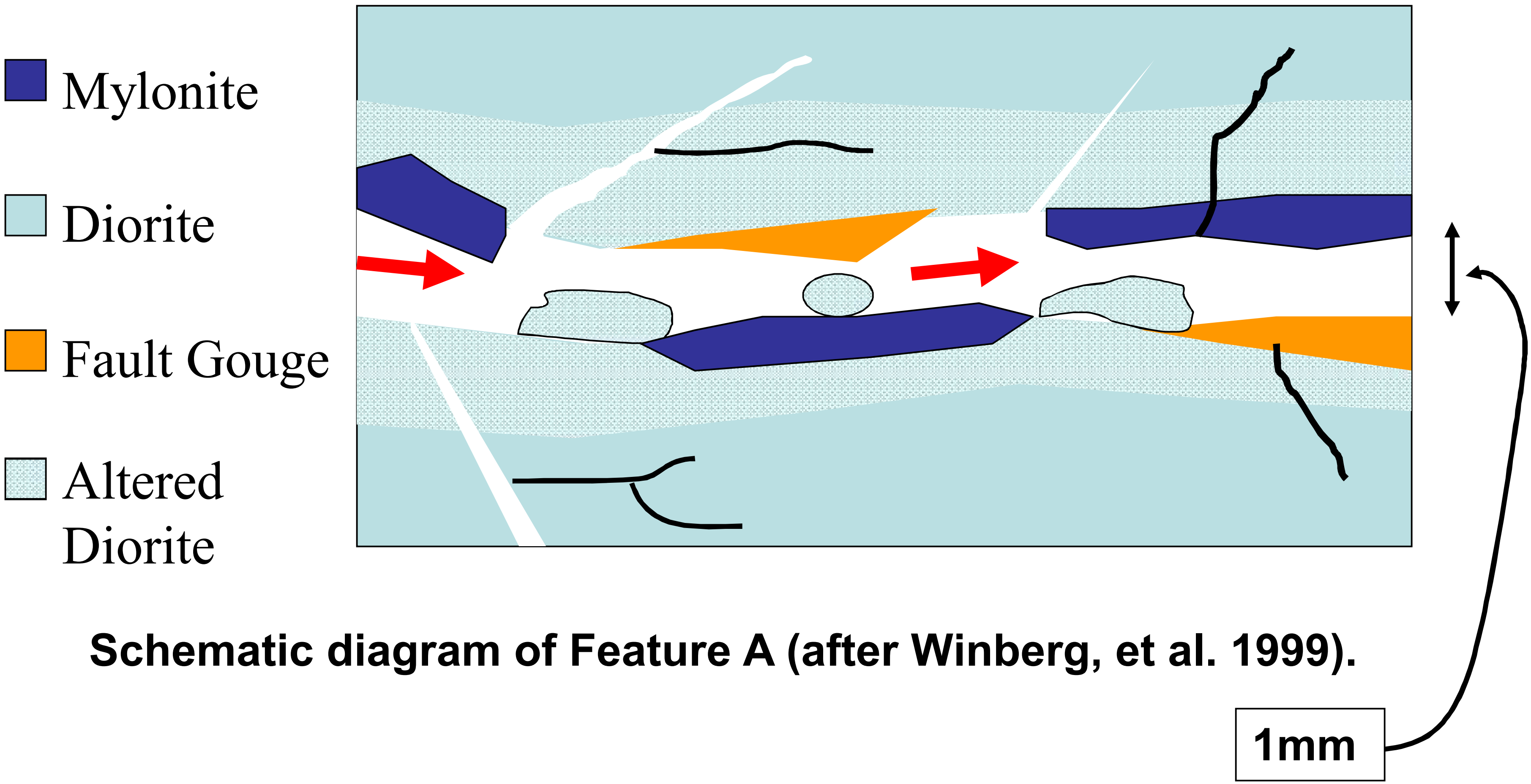
Application to Granitic Rocks

- **Aspo Task Force**
  - 10 nuclear waste organizations from 8 countries
  - Tracer experiments conducted at Aspo underground research laboratory in Sweden



The Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes

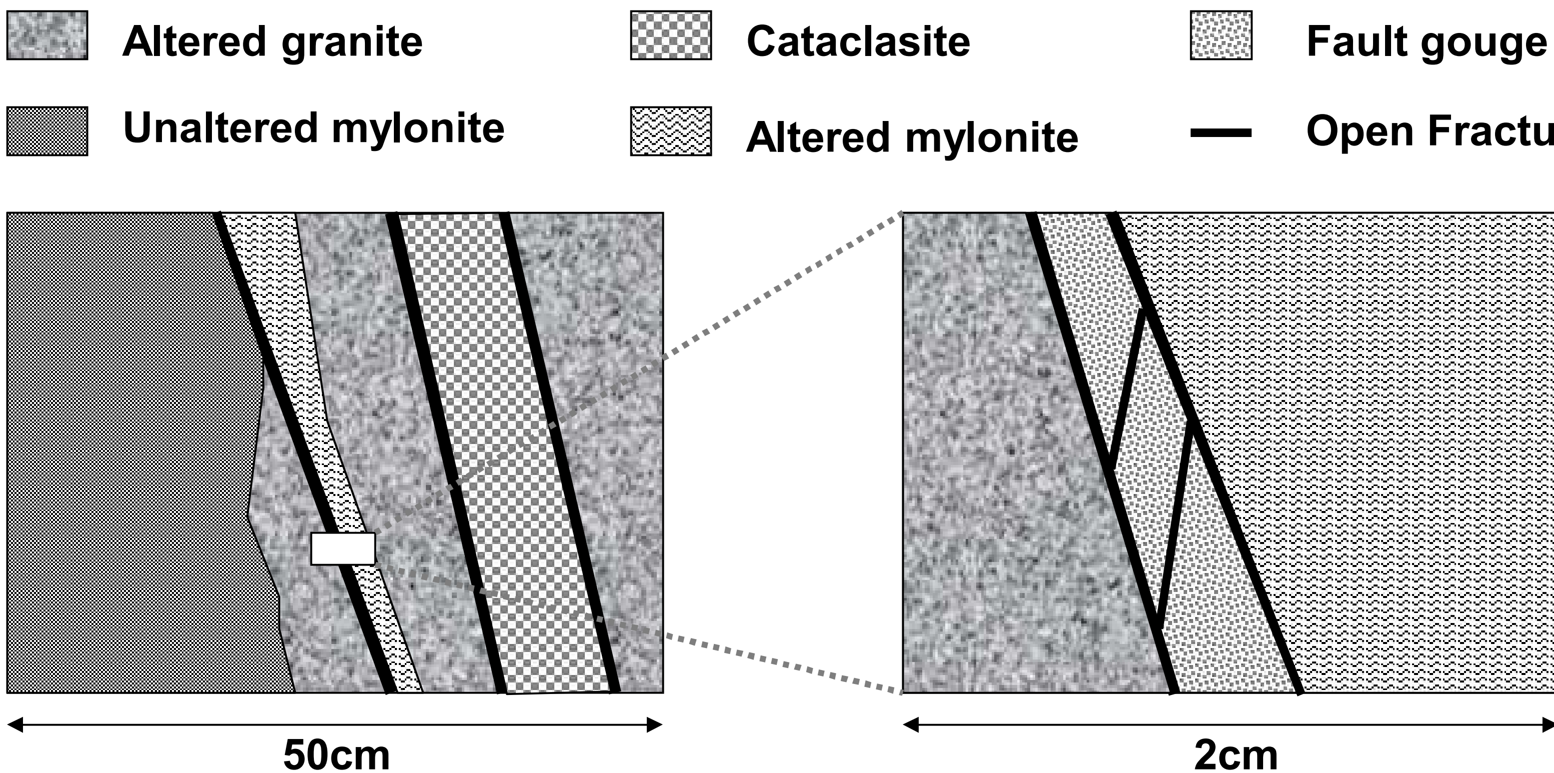
Conceptual Model: Fractured Granite



Schematic diagram of Feature A (after Winberg, et al. 1999).

Conceptual Model: Feature A

- **Precambrian granites experienced episodic ductile and brittle deformation with hydrothermal mineralization**



After Mazurek, et al., 2003, Jour. Contaminant Hydrology

Transport: Analytical Solution

- **Transport in a single fracture with infinite matrix (immobile zone) capacity, continuous source**

$$\frac{C_m}{C_0} = \begin{cases} erfc\left[\dfrac{(\phi_m D^*/Vb)x + z}{2\left[D^*(t - x/V)\right]^{1/2}}\right], & t > V/x \\ 0, & t < V/x \end{cases}$$

$$\frac{C_f}{C_0} = \begin{cases} erfc\left[\dfrac{(\phi_m D^*/Vb)x}{2\left[D^*(t - x/V)\right]^{1/2}}\right], & t > V/x \\ 0, & t < V/x \end{cases}$$

After Pickens and Grisak, 1981, *Journal of Hydrology*

Transport: Analytical Solution

- Parameters for analytical solution
  - b aperture half-width
  - C_f concentration in fracture
  - C_m concentration in matrix
  - C_0 input concentration
  - D* effective molecular diffusion coefficient of solute in matrix
  - erfc complimentary error function
  - t time
  - V ground water velocity in the fracture
  - x distance along the fracture
  - z distance into the matrix normal to the fracture
  - ϕ_m matrix porosity

Approximation

- **Relative concentration at the center of a matrix block (approximate)**

$$\frac{C_m}{C_0} = erfc\left[\frac{z}{2(D_p t)^{1/2}}\right]$$

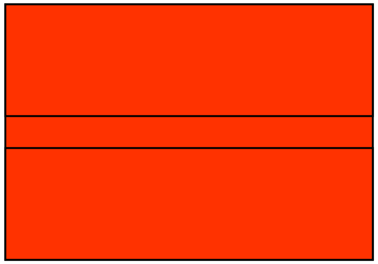
- **"early time" solution for diffusion into a semi-infinte slab (Crank, 1975)**

What Can the Test See?

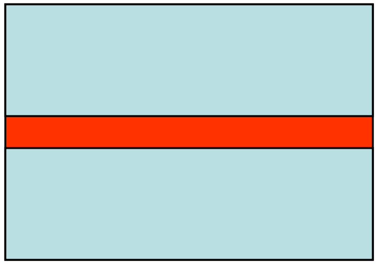
Damkohler number provides ratio of mass-transfer rate to advective rate

$$DaI = 3\alpha_i (1 + \beta_i) \frac{LR_m}{V}$$

DaI **>> 1.0 indicates local equilibrium behavior**



DaI **<< 1.0 indicates single porosity transport**

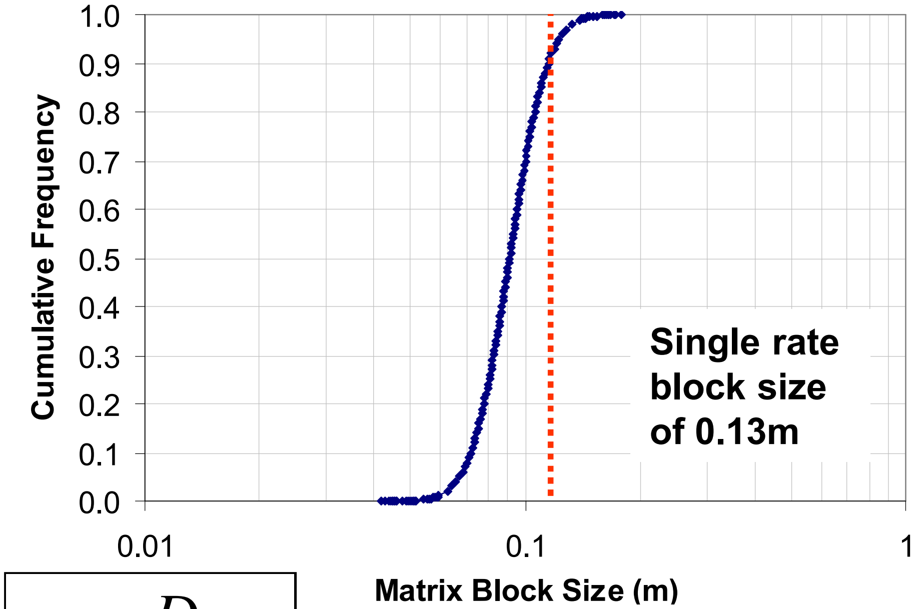


Transport Scaling: K-area

- Excel Exercise

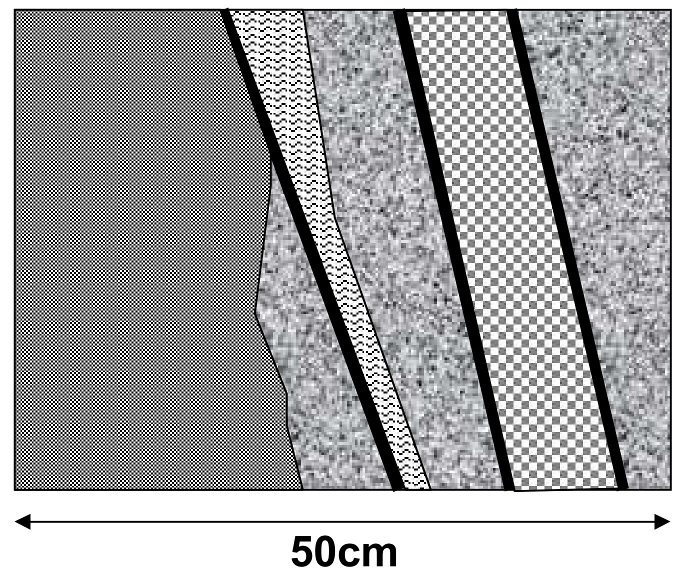
Fit to Conceptual Model

Distribution of mass-transfer rates can be converted to matrix block size distributions



$$\alpha_i = \frac{D_{aq}\tau}{l^2 R_{im}}$$

Block size distribution fits conceptual model of materials within Feature A



Beyond the Tracer Test Scale