The Secret to Successful Solute-Transport Modeling

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ground water

Issue Paper/

The Secret to Successful Solute-Transport Modeling

by Leonard F. Konikow

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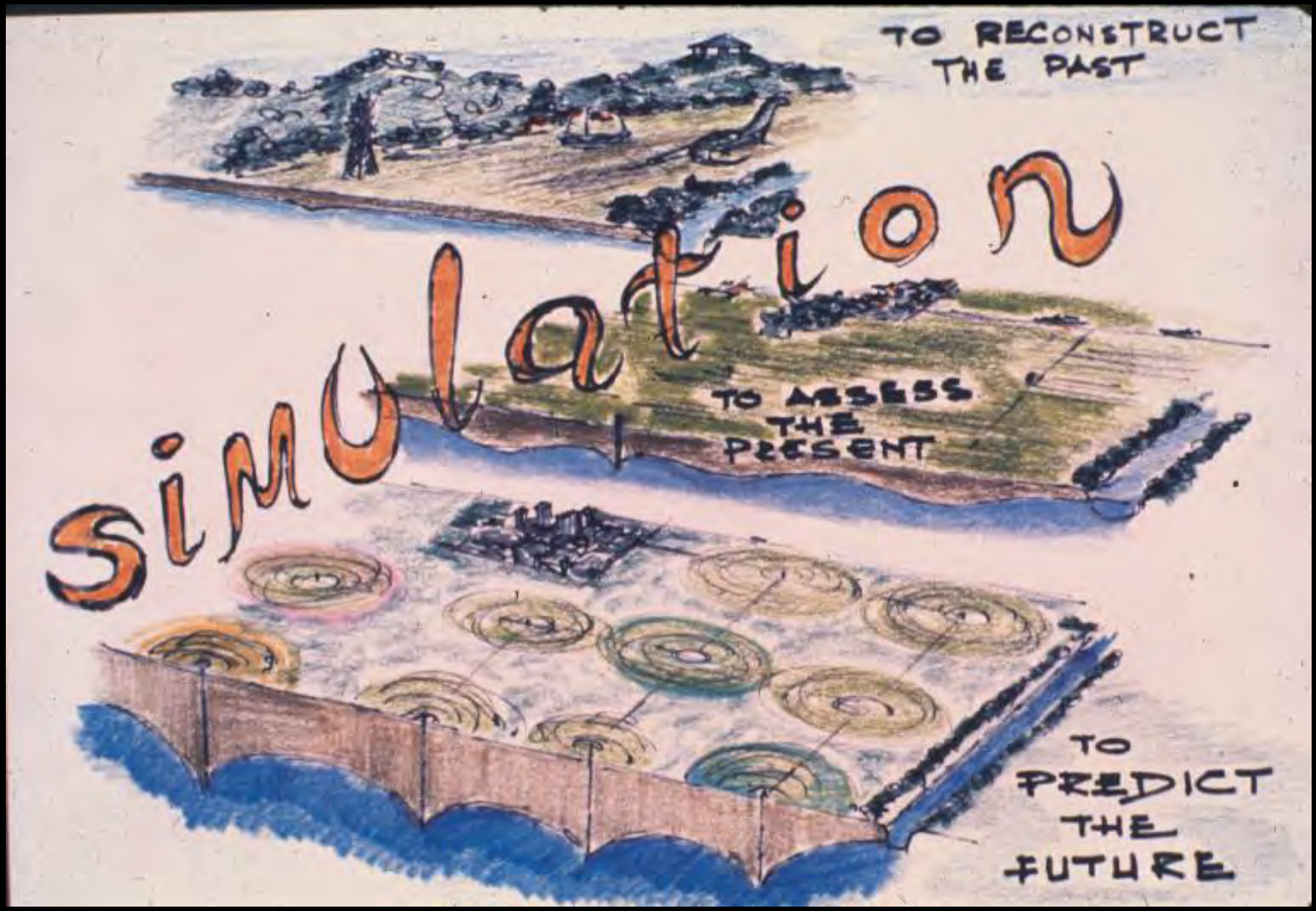
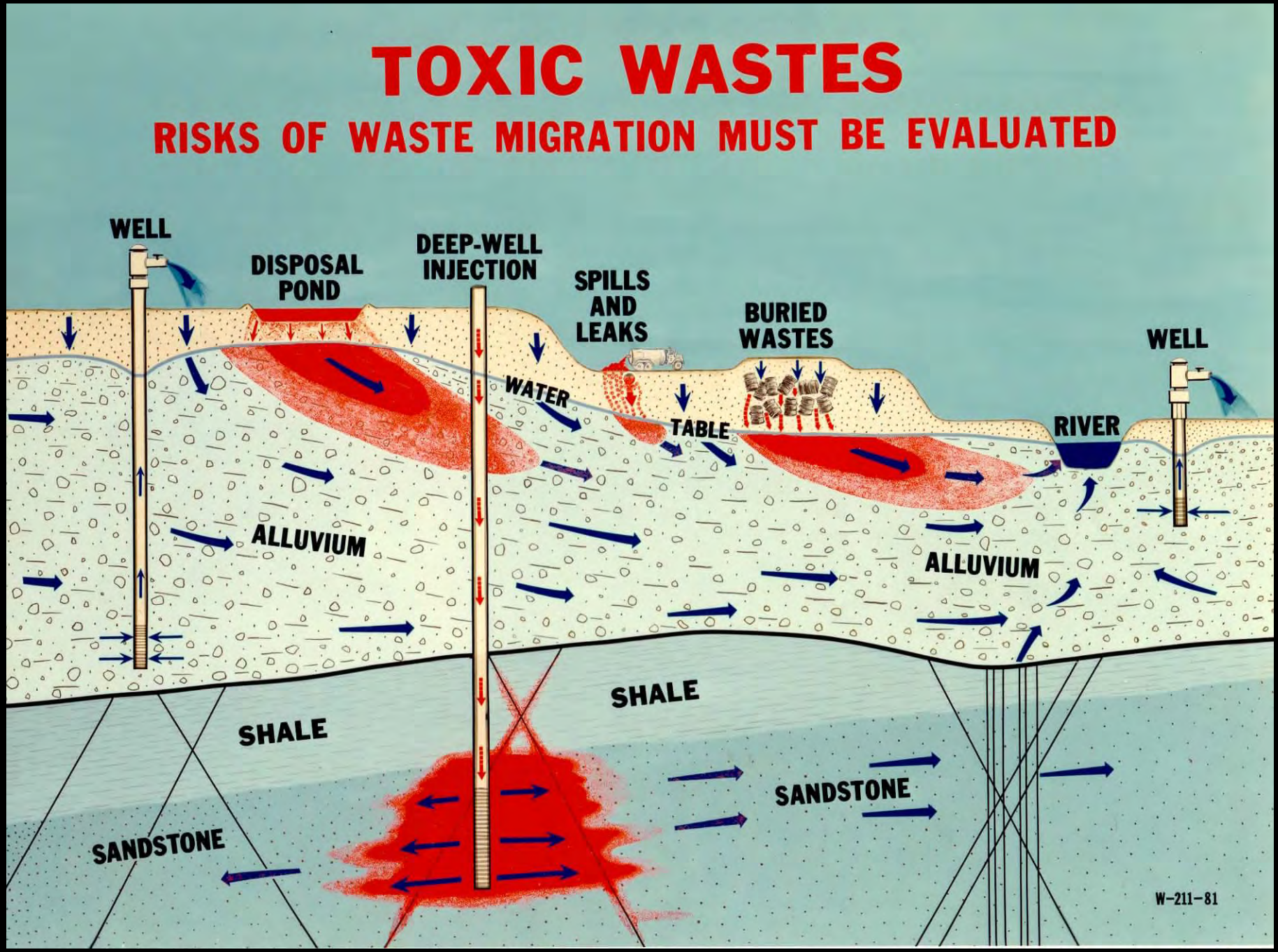


Source: Giusti & Bennett

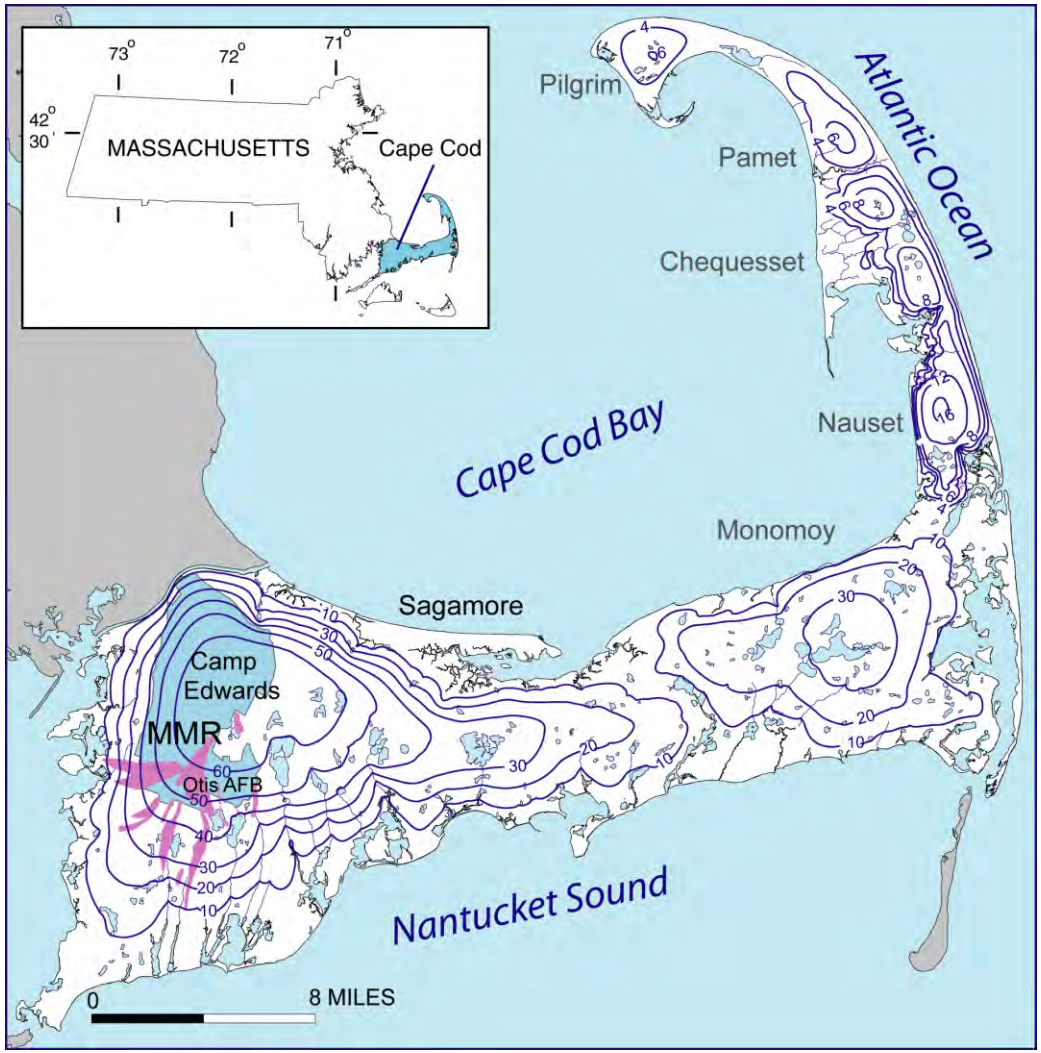
TOXIC WASTES

RISKS OF WASTE MIGRATION MUST BE EVALUATED

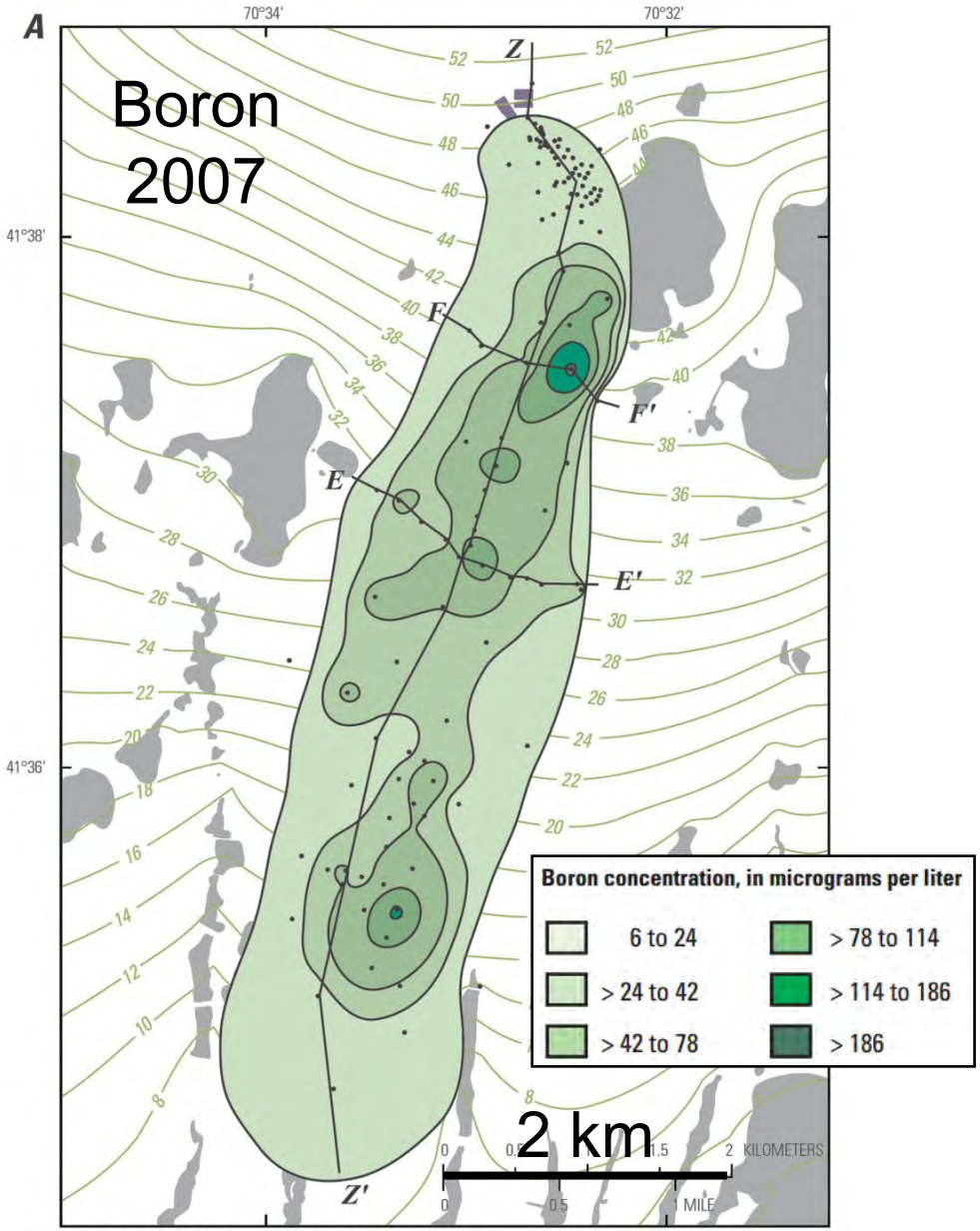


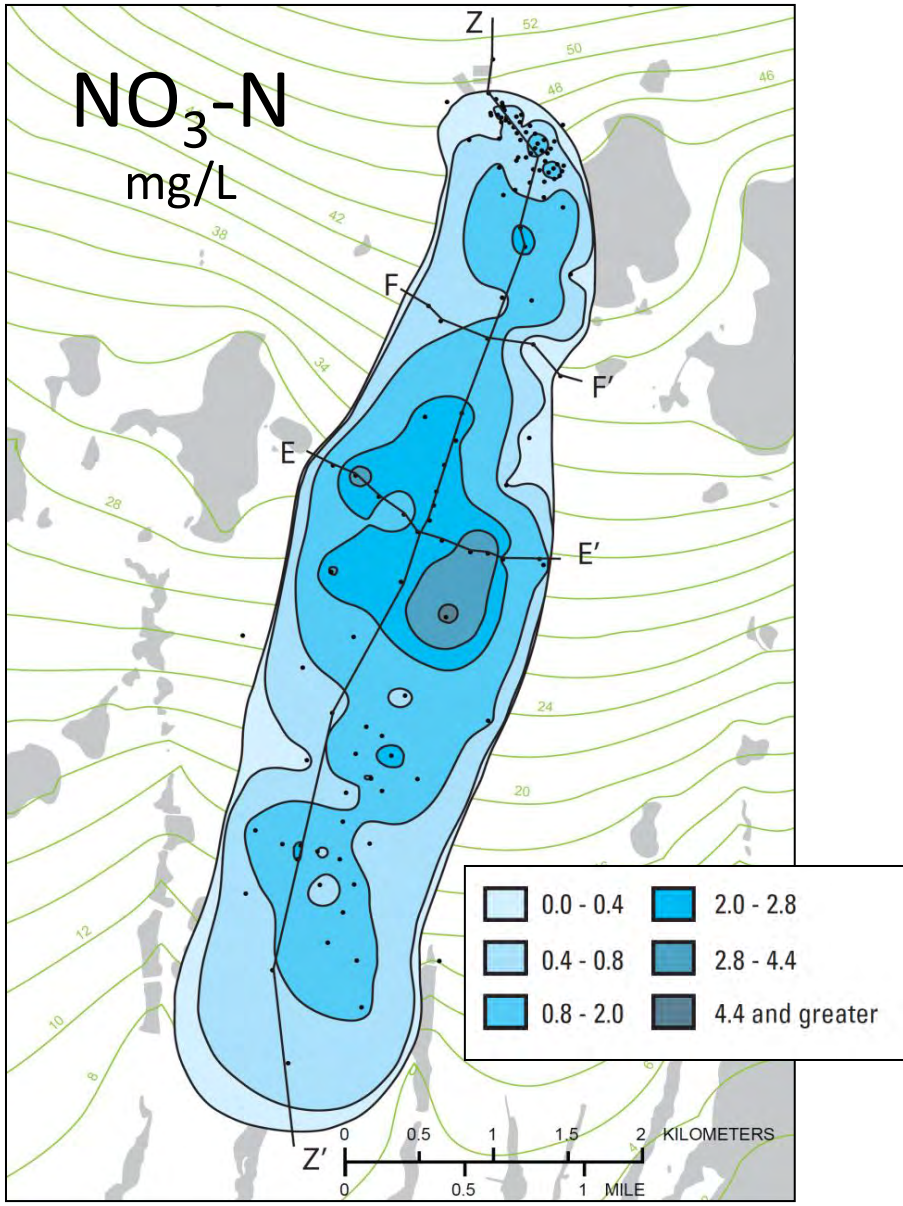
VARIABILITY: HEADS vs CONCENTRATIONS

Example from Cape Cod



From: D. LeBlanc (USGS)





Base from U.S. Geological Survey digital data,
Massachusetts State Plane Coordinate System,
North American Datum of 1927,
National Geodetic Vertical Datum of 1929

Modified from: Barbaro, Walter, and LeBlanc (2013) USGS Sci. Inv. Report 2013-5061

COMPUTER SIMULATION: SOLVE SET OF GOVERNING MATHEMATICAL EQUATIONS

1. GROUNDWATER FLOW EQUATION

2. SOLUTE-TRANSPORT EQUATION

CLASSICAL SIMPLIFIED FORM OF SOLUTE-TRANSPORT EQUATION

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i}\left(C V_i \right)$$

DISPERSION **ADVECTION**

COEFFICIENT OF HYDRODYNAMIC DISPERSION (L^2/T)

$$D_{ij} = \alpha_{ijmn} \frac{V_m V_n}{|V|} + D_m$$

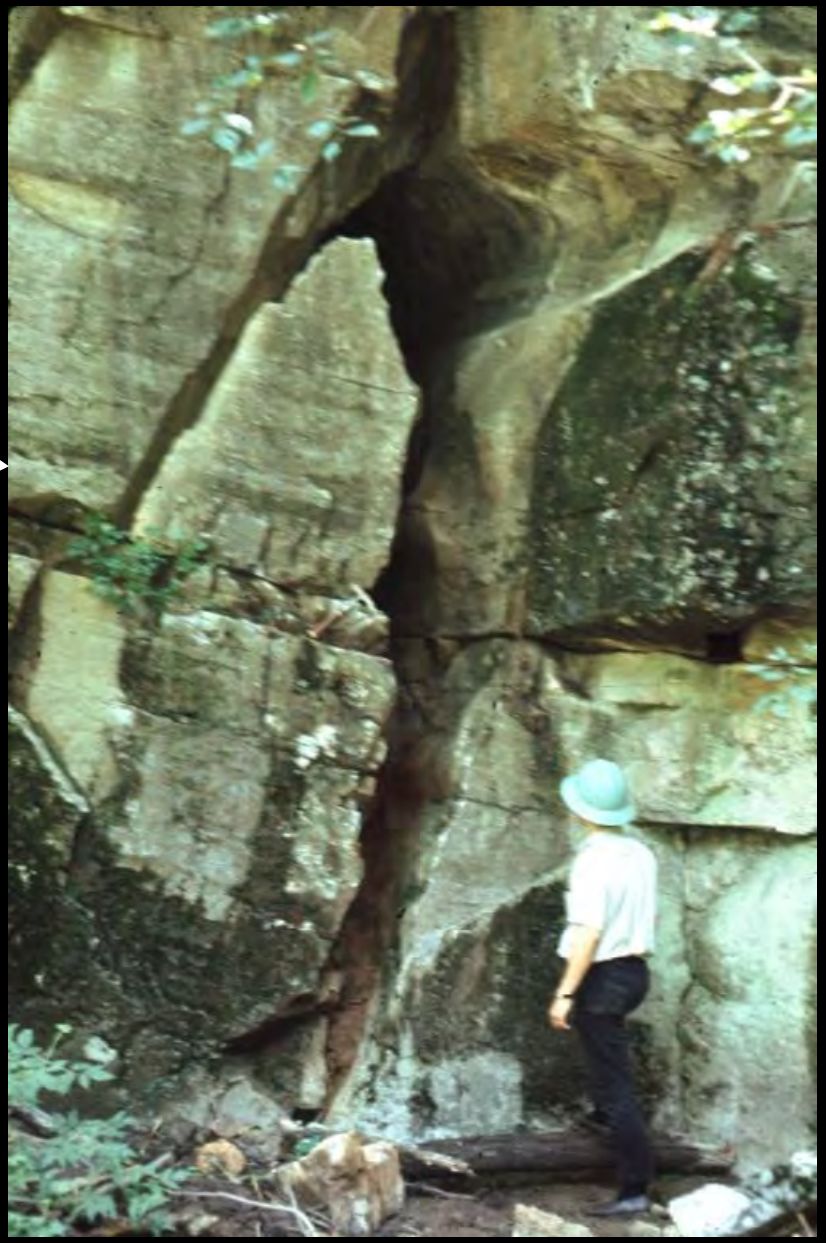
where: D_m is the effective coefficient of molecular diffusion (L^2/T), and
α is the dispersivity tensor (L)

SOLUTE-TRANSPORT MODELING ISSUES

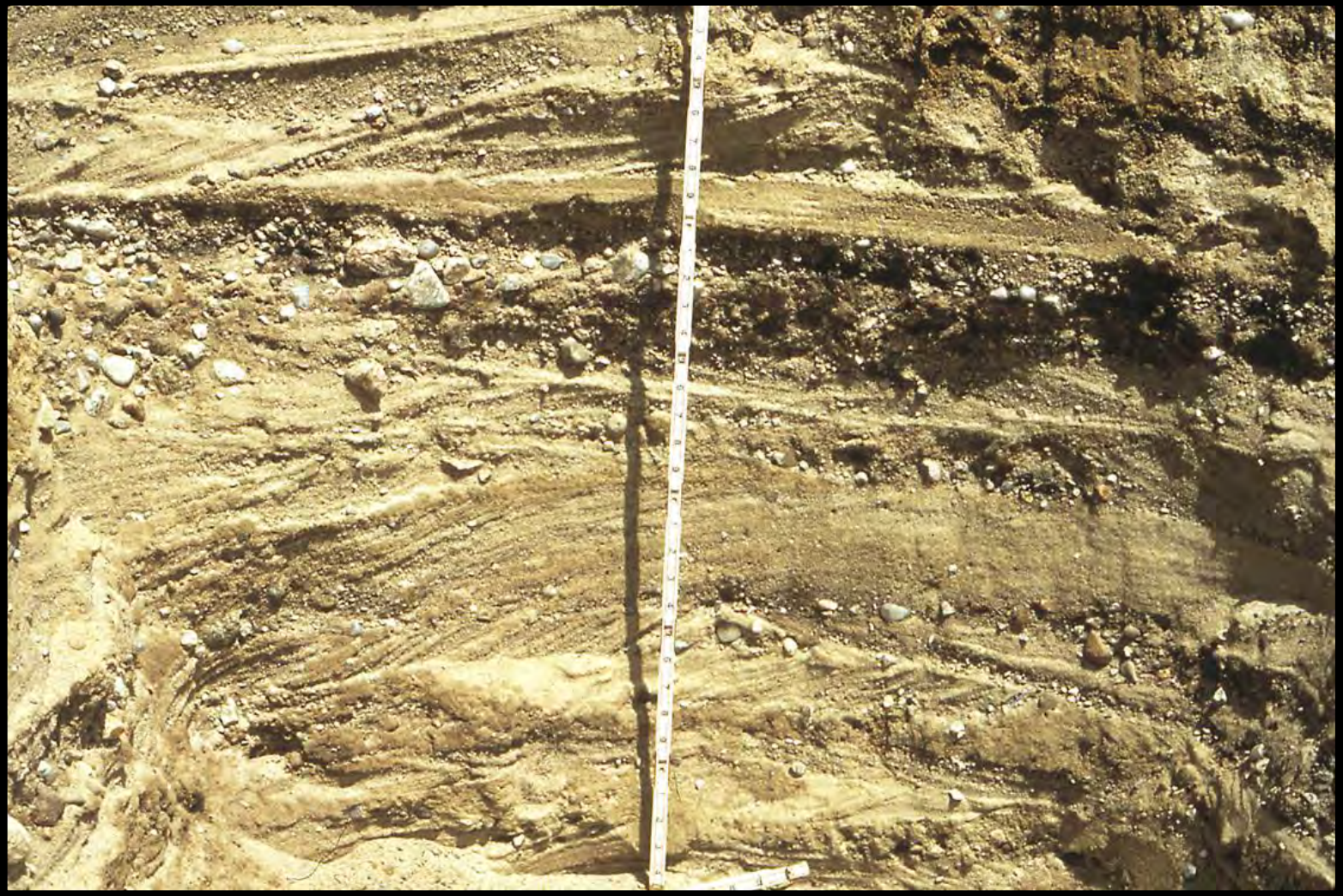
- CONCEPTUAL ACCURACY OF GOVERNING EQUATION
- ACCURACY OF NUMERICAL SOLUTION TO GOVERNING EQUATION
- PARAMETER ESTIMATION
- MODEL COMPLEXITY

GEOLOGIC MATERIALS ARE HETEROGENEOUS

Carbonate rocks in central Pennsylvania →

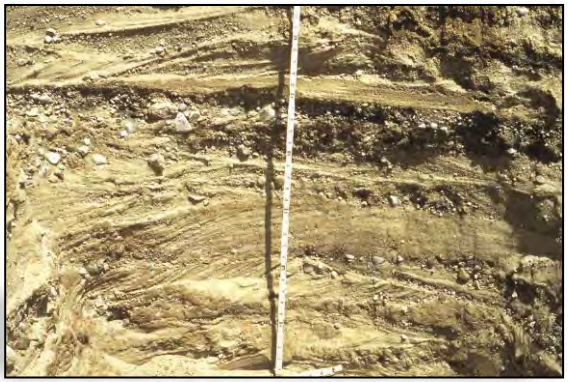


Sand and Gravel Aquifer, Cape Cod, MA

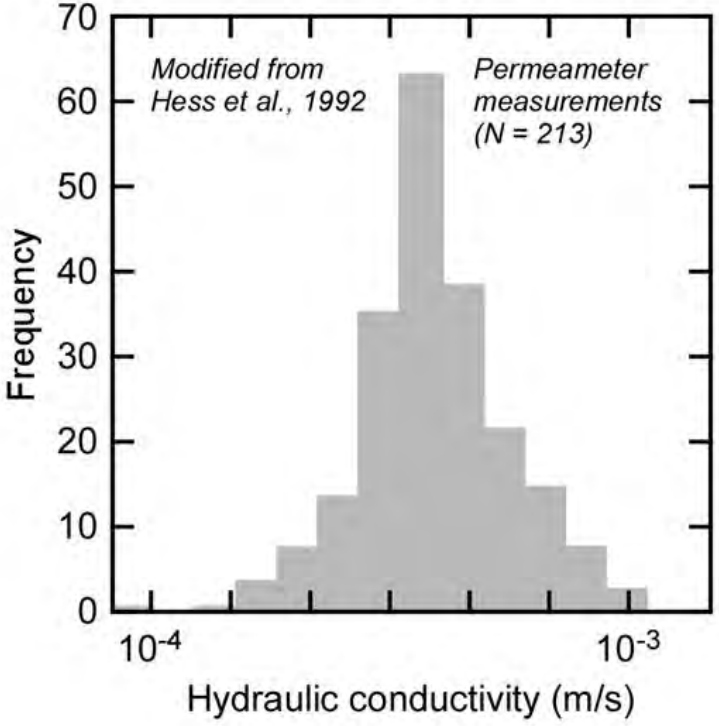


Source: D. LeBlanc, USGS

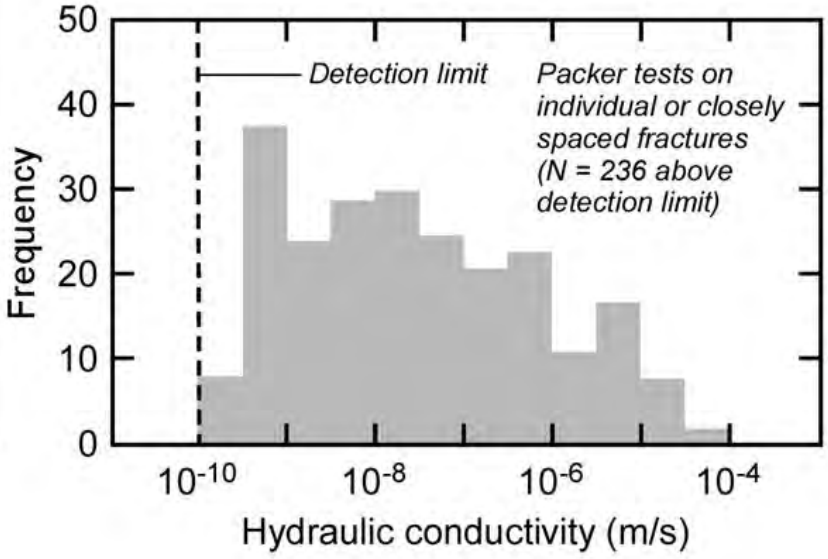
Large variability in hydraulic properties. . .



Sand and Gravel Glacial Outwash
Cape Cod, MA



Fractured Granite and Schist
Mirror Lake Watershed, NH



Source: Al Shapiro, USGS

CLASSICAL SIMPLIFIED FORM OF SOLUTE-TRANSPORT EQUATION

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i}\left(C V_i \right)$$

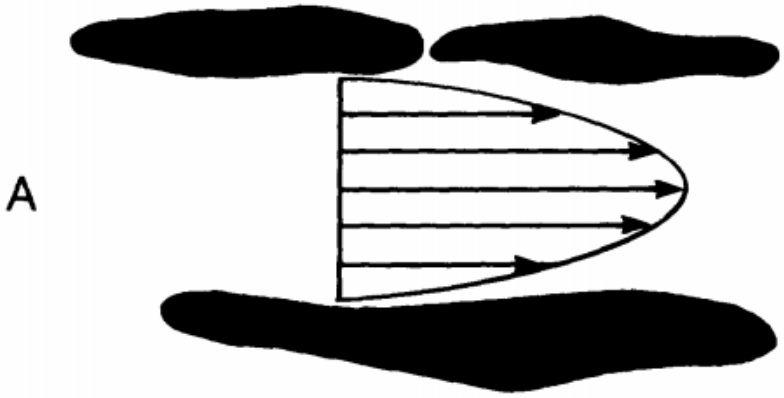
DISPERSION **ADVECTION**

MAJOR PROBLEM IN ANALYSIS OF GROUNDWATER SYSTEMS:

GEOLOGY → HETEROGENEITY

HETEROGENEITY → UNCERTAINTY

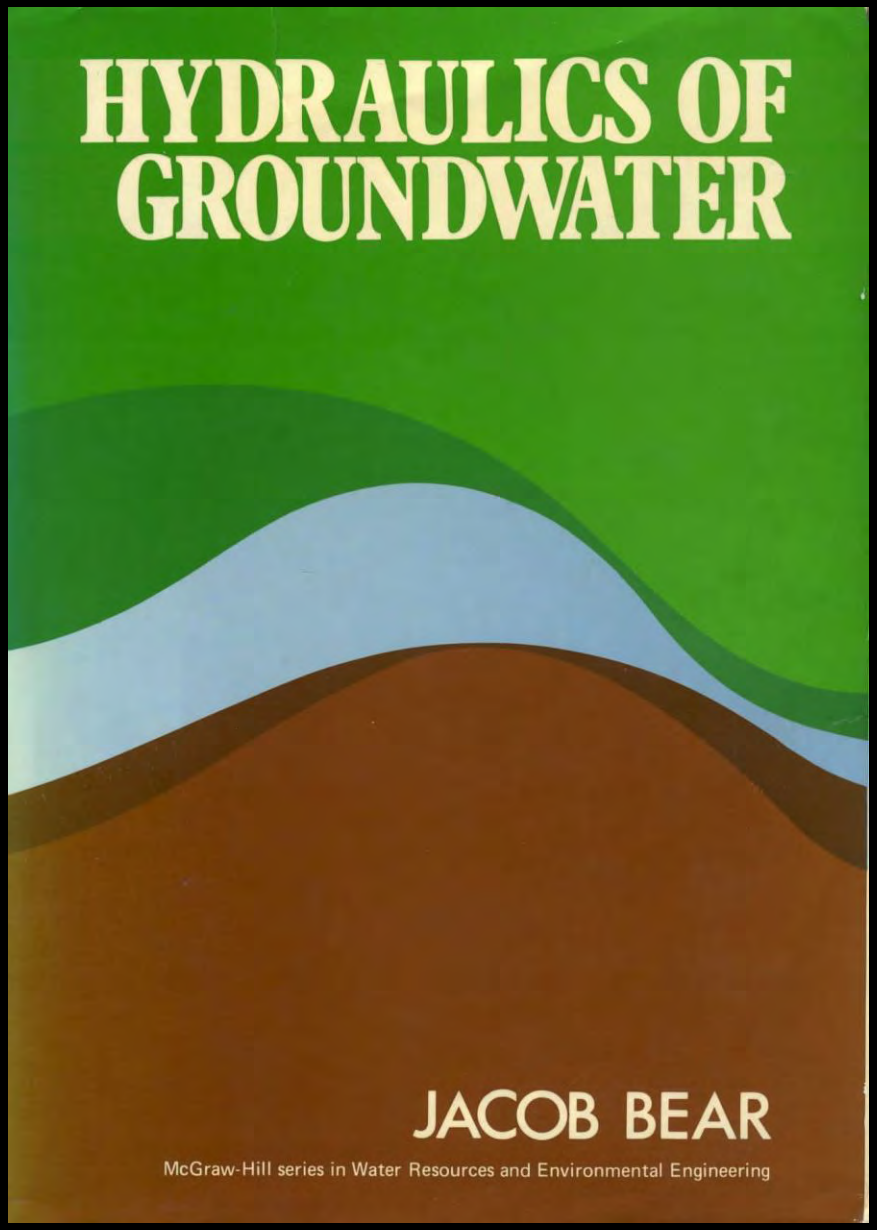
UNCERTAINTY → NONUNIQUENESS



Approximate fluid velocity distribution in a single pore

Tortuous paths of fluid movement at intergranular scale

From: Reilly, Franke, Buxton, and Bennett (1987), USGS WRI Report 87-4191



1979

"As a working hypothesis, we shall assume that the dispersive flux can be expressed as a Fickian type law"

in order to obtain a macroscopic description of them (see, for example, de Josselin de Jong, 1958; Saffman, 1959, 1960; Wilson and Gelhar, 1974).

The partial differential equation itself can be obtained by averaging over a Representative Elementary Volume (REV) around a point (Sec. 7-4 and App. A4). However, in order to obtain an insight of the structure of the coefficients, models of the types mentioned above have to be employed. In what follows, a summary is presented of the coefficients and their structure. For the detailed development, the reader is referred to the literature or to the summaries mentioned above.

The average product $\overline{c_\alpha \mathbf{V}_\alpha}$ expresses the mass flux of a solute at a point in a porous medium. By the definition of the average, we have (App. A-3)

$$\overline{c_\alpha \mathbf{V}_\alpha} \equiv \overline{(\bar{c}_\alpha + \mathring{c}_\alpha)(\overline{\mathbf{V}}_\alpha + \mathring{\mathbf{V}}_\alpha)} = \bar{c}_\alpha \overline{\mathbf{V}}_\alpha + \overline{\mathring{c}_\alpha \mathring{\mathbf{V}}_\alpha} \tag{7-1}$$

This is a flux through the α phase only. In (7-1) c_α is mass of a solute, γ, per unit volume of α phase. The term $\bar{c}_\alpha \overline{\mathbf{V}}_\alpha$ expresses the transport by convection. The second term $\overline{\mathring{c}_\alpha \mathring{\mathbf{V}}_\alpha} \equiv \overline{c_\alpha \mathbf{V}_\alpha}$ is an additional flux at the macroscopic scale—the dispersive flux—introduced by the process of averaging. It is a flux of γ carried by the fluctuating velocity. This new phenomenon at the macroscopic scale (as it does not exist at the microscopic one) represents the loss of information by the passage from one scale of description to another, larger, one.

As a working hypothesis, we shall assume that the dispersive flux can be expressed as a Fickian type law

$$\overline{\mathring{c}_\alpha \mathring{\mathbf{V}}_\alpha} = -\boldsymbol{D} \cdot \operatorname{grad} \bar{c}_\alpha; \qquad \overline{\mathring{c}_\alpha \mathring{V}_{i\alpha}} = -D_{ij}\, \partial \bar{c}_\alpha / \partial x_j \tag{7-2}$$

or, for $\rho_\alpha = \text{const.}$, and a concentration $C = \bar{c}_\alpha / \rho_\alpha =$ mass of γ per unit mass of α phase

$$\overline{\mathring{C}\mathring{\mathbf{V}}} = -\boldsymbol{D} \cdot \operatorname{grad} C; \qquad \overline{\mathring{C}\mathring{V}_i} = -D_{ij}\, \partial C / \partial x_j \tag{7-3}$$

where $\boldsymbol{D}$, a second rank symmetric tensor, is the coefficient of mechanical (or convective) dispersion, and we have omitted the subscript α in $\mathbf{V}$.

Henceforth to the end of this section, we shall use $\overline{\mathbf{V}}$ to indicate average α phase velocity; in the following sections $\mathbf{V}$ will be used.

Bear and Bachmat (1967), who employed a model composed of a network

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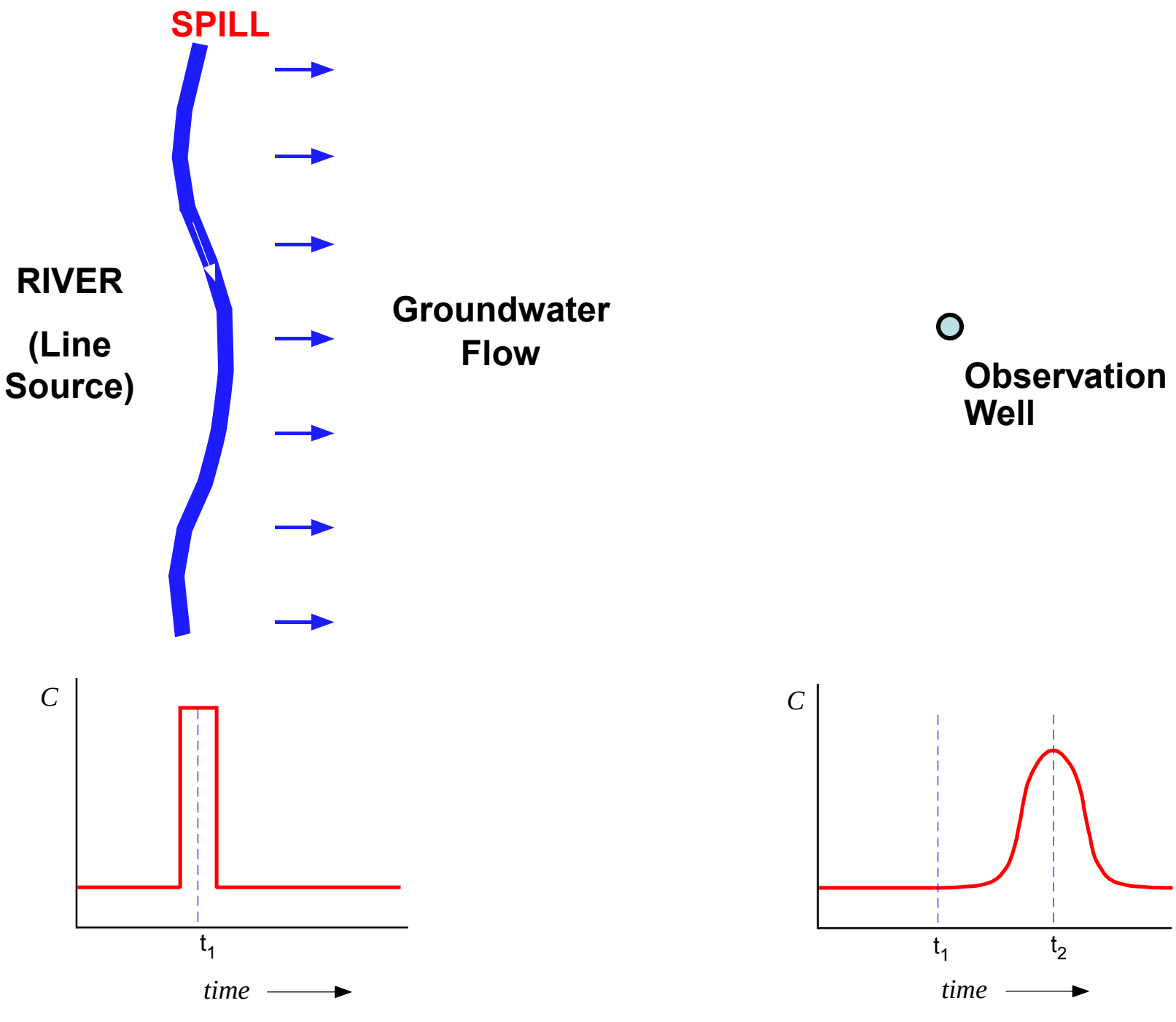
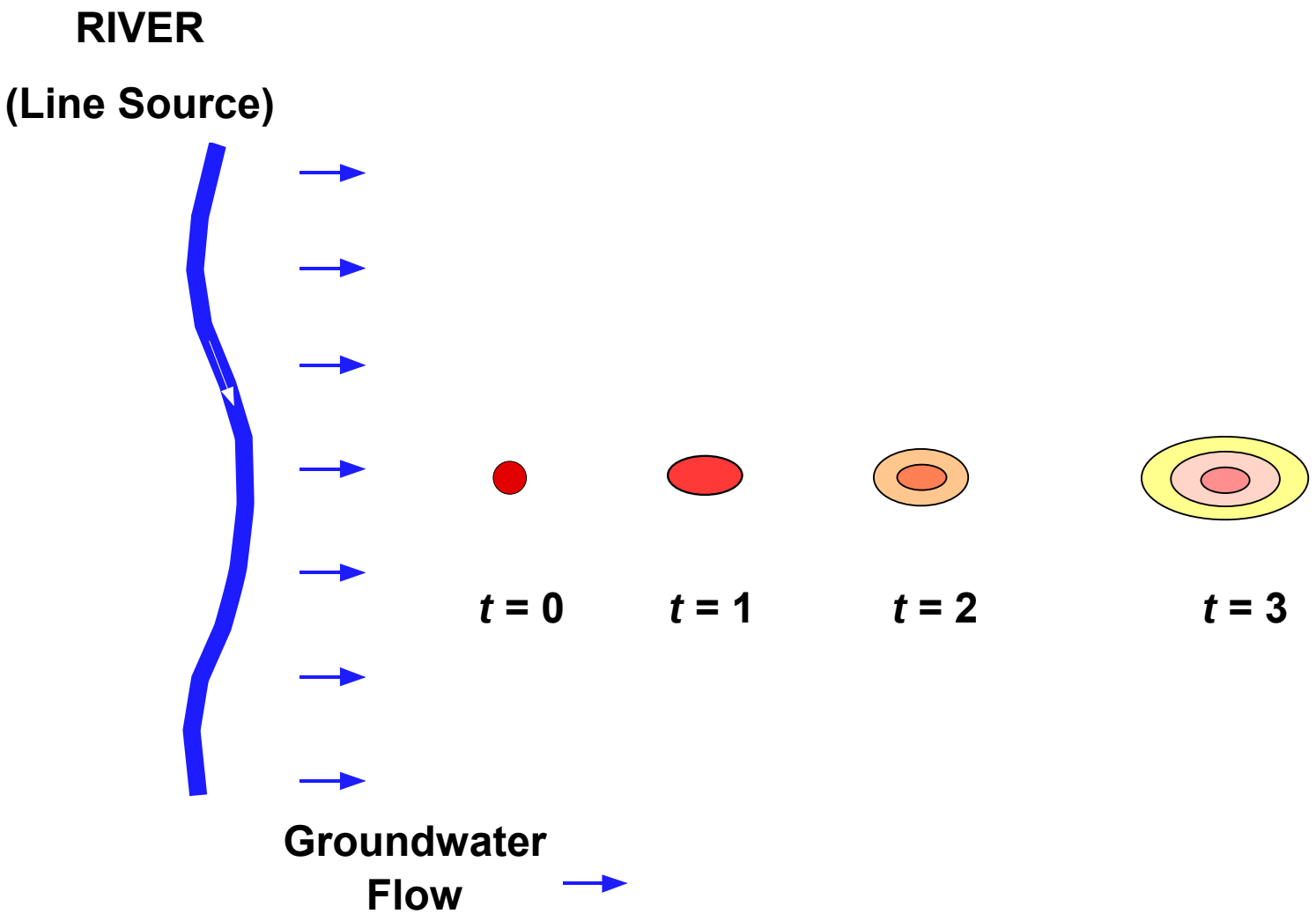
DISPERSION **ADVECTION**


SPILL
RIVER
(Line
Source)
Groundwater
Flow
Observation
Well
C
t1
time
C
t1
t2
time

POINT INITIAL CONDITION



Characteristics of Fickian Model:

- dispersive flux proportional to concentration gradient
- concentration>0 at all locations
- upstream dispersion
- Gaussian normal distribution
- no scale effects (macrodispersion)
- irreversible spreading

COEFFICIENT OF HYDRODYNAMIC DISPERSION (L^2/T)

$$D_{ij} = \alpha_{ijmn} \frac{V_m V_n}{|V|} + D_m$$

where: D_m is the effective coefficient of molecular diffusion (L^2/T), and
α is the dispersivity tensor (L)

The dispersivity (α) of an isotropic porous medium can be defined by two constants:

α_L and α_T

VARIATION OF DISPERSIVITY WITH DISTANCE (OR SCALE OF MEASUREMENT).

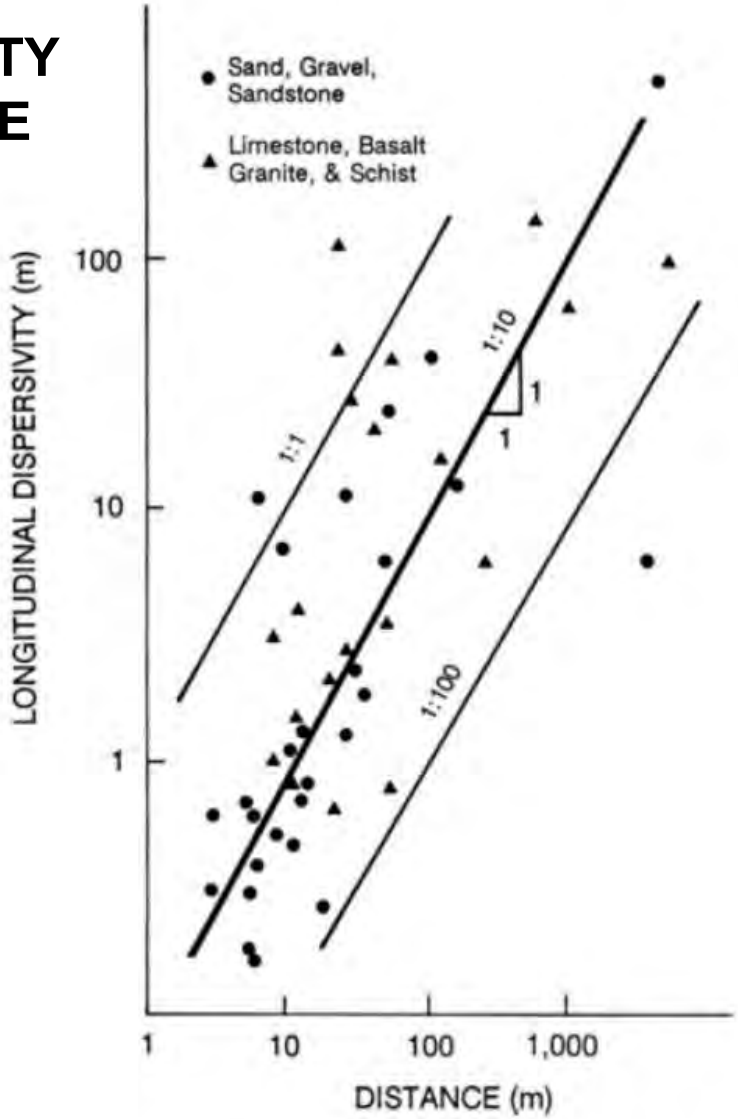
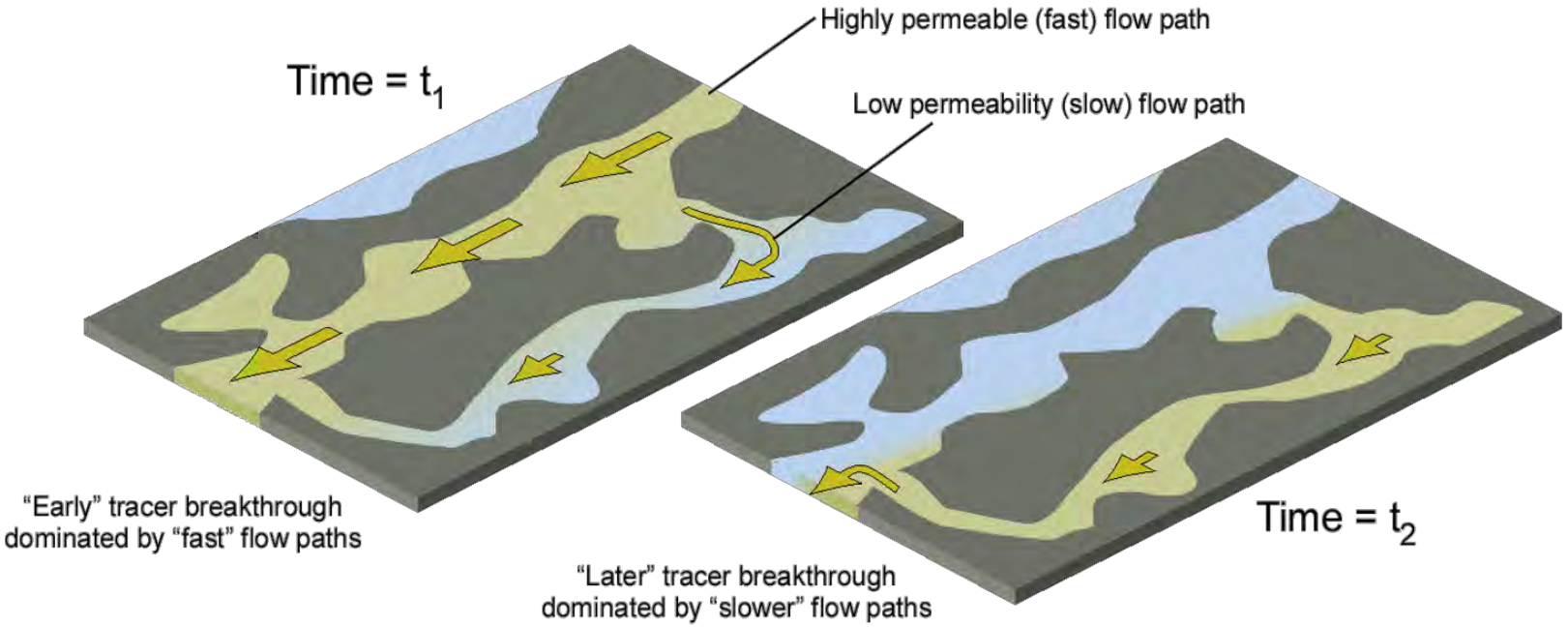


FIGURE 4.1 Variation of dispersivity with distance (or scale of measurement).
SOURCE: Modified from Anderson, 1984.

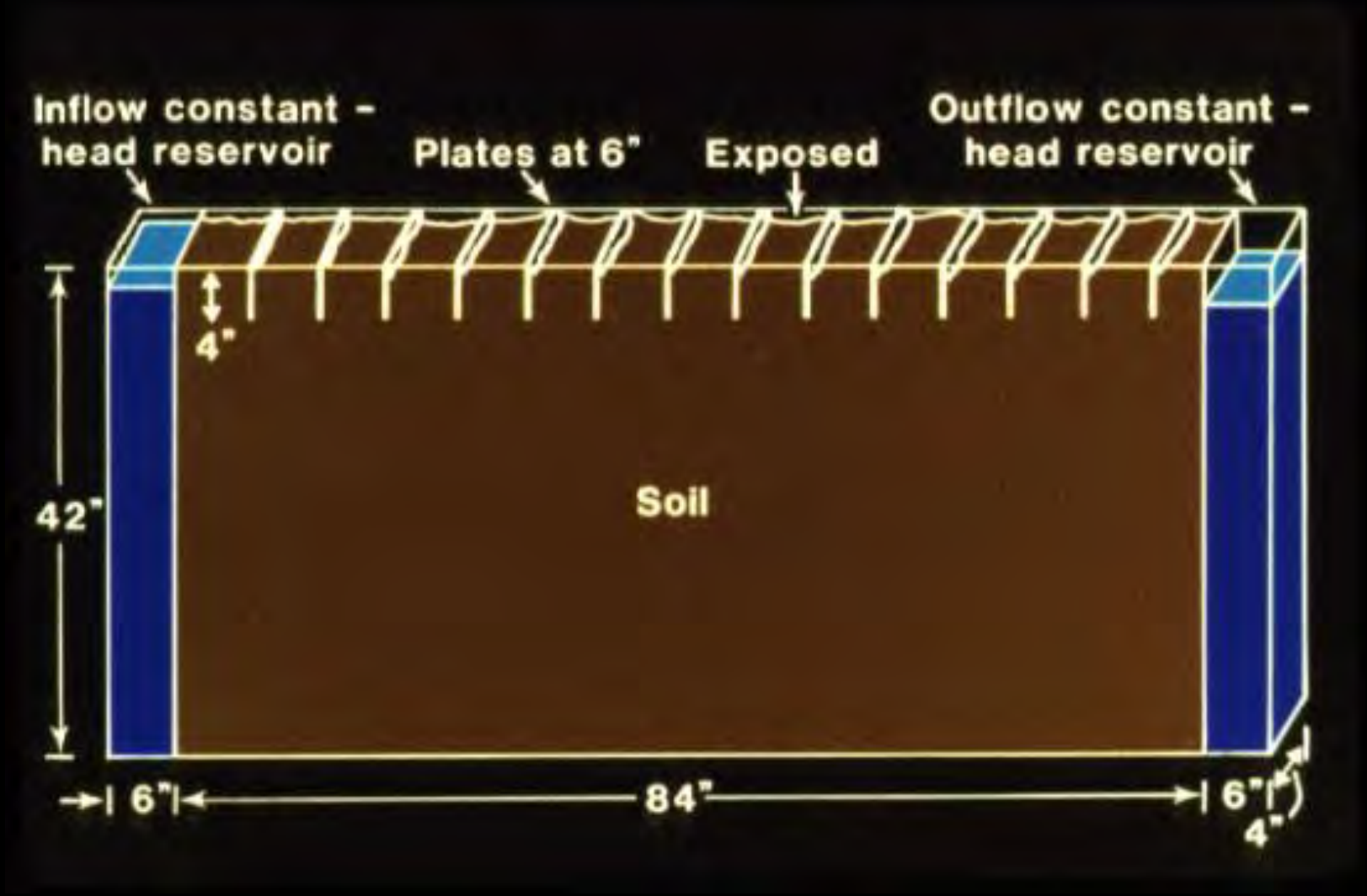
From: National Research Council (1990) *Ground Water Models: Scientific and Regulatory Applications*, National Academy Press

Matrix Diffusion vs Variable Advection

"Effective" matrix diffusion is an artifact of large variability in fluid advection. . .



Source: Al Shapiro, USGS



Courtesy of Steve Silliman, University of Notre Dame
(experiments performed at University of Arizona)

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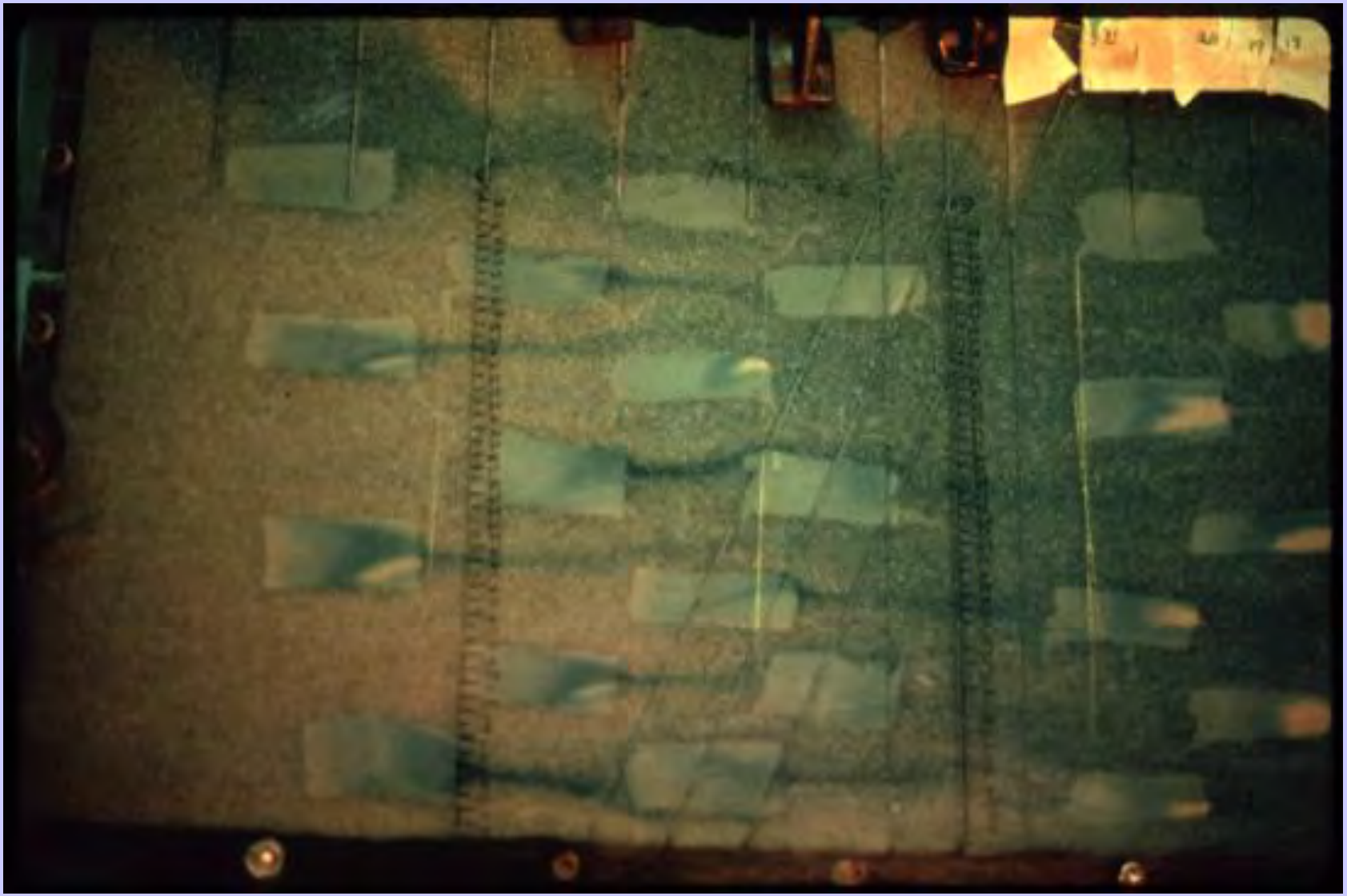

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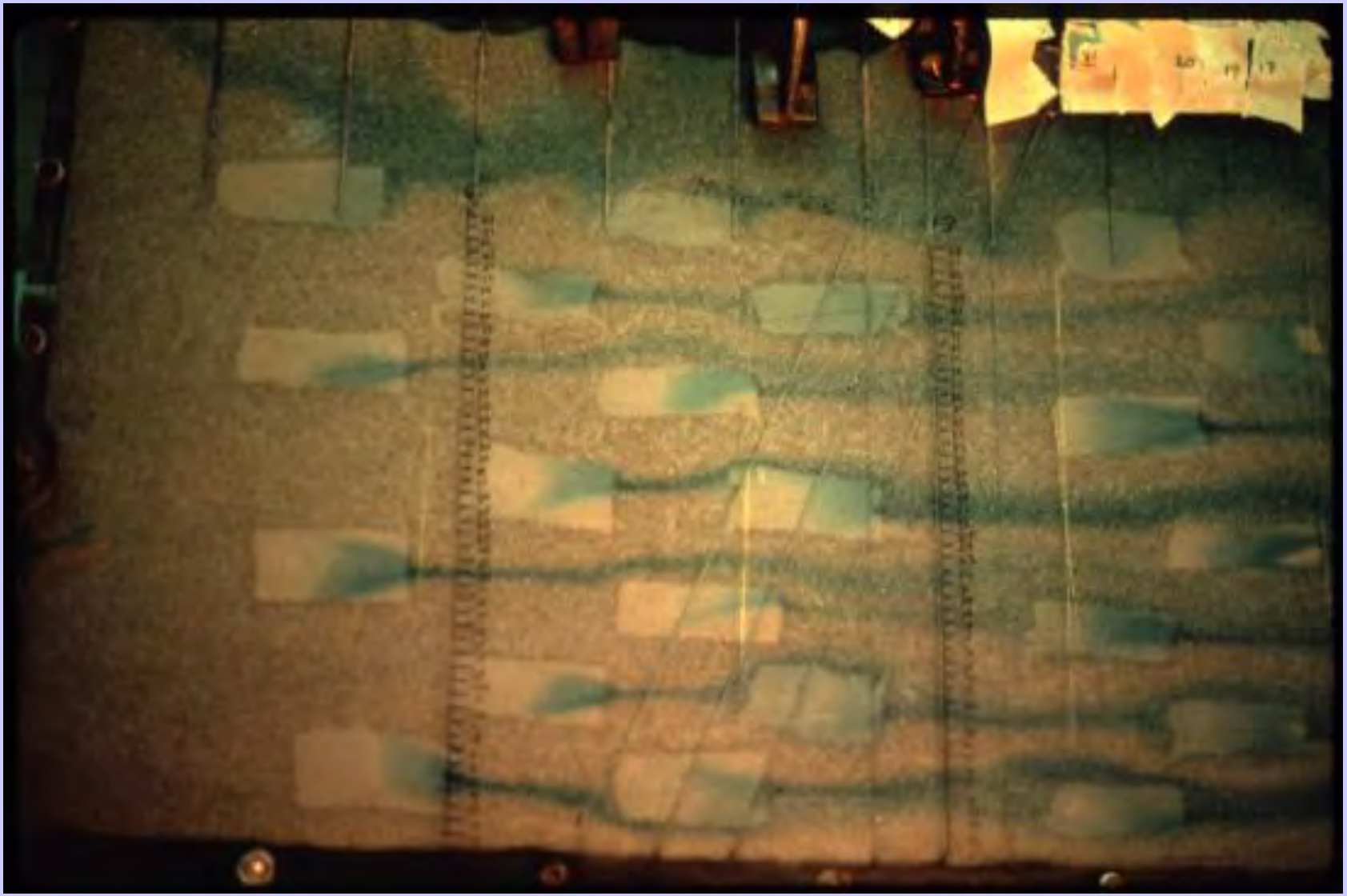

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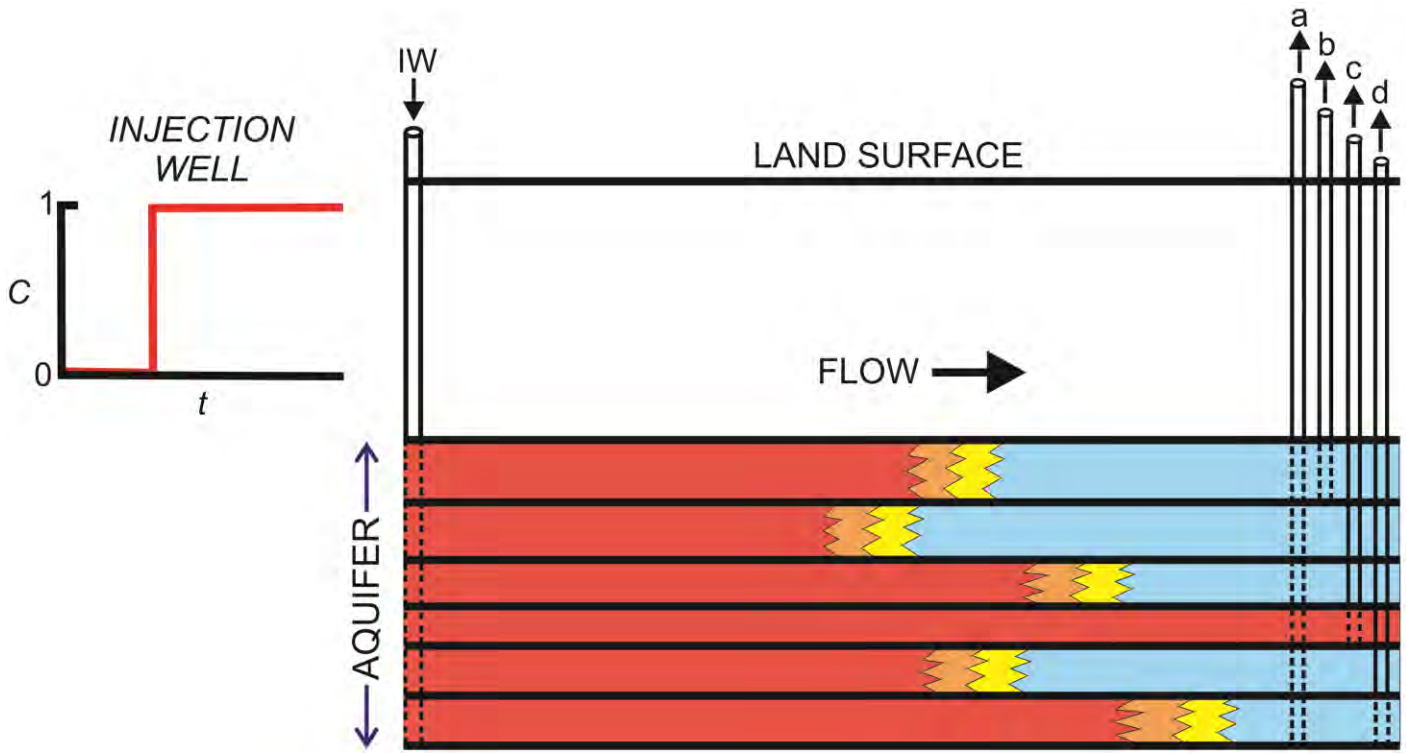
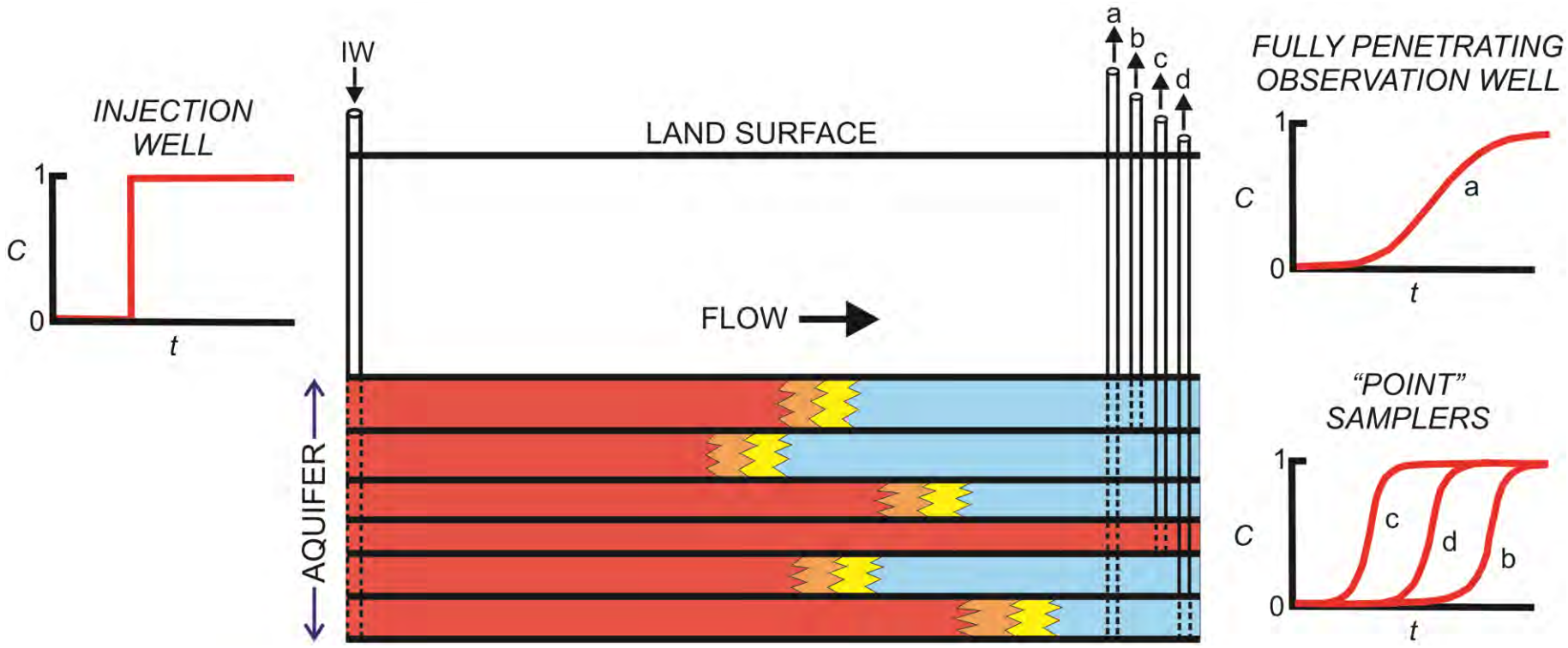
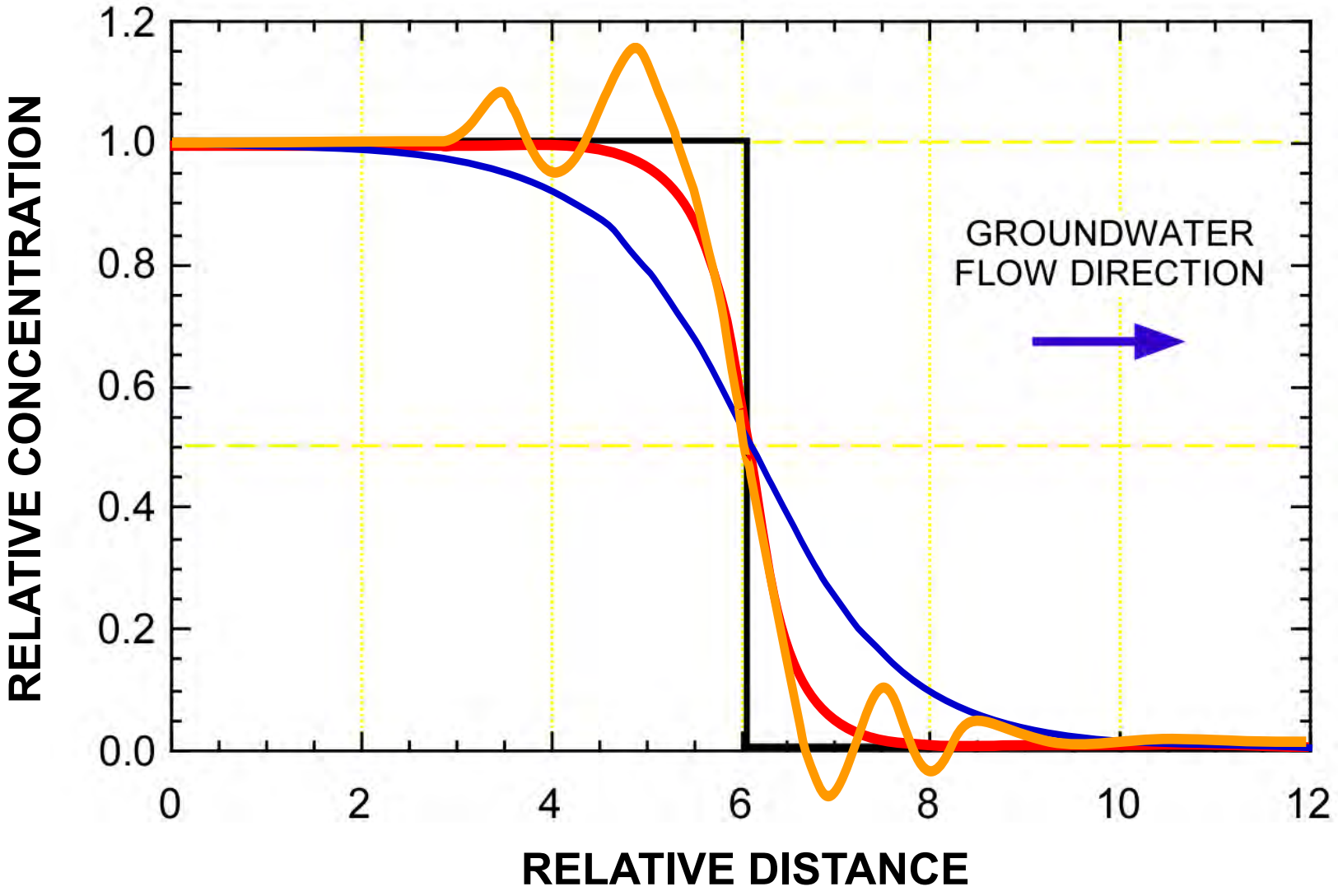

INJECTION
WELL
1
C
0
t
IW
LAND SURFACE
a
b
c
d
FLOW
AQUIFER


INJECTION WELL
1
C
0
t
IW
LAND SURFACE
FLOW
AQUIFER
a
b
c
d
FULLY PENETRATING OBSERVATION WELL
1
C
0
a
t
"POINT" SAMPLERS
1
C
0
c
d
b
t

NUMERICAL PROBLEMS IN SOLVING ADVECTIVE-DISPERSIVE EQUATION



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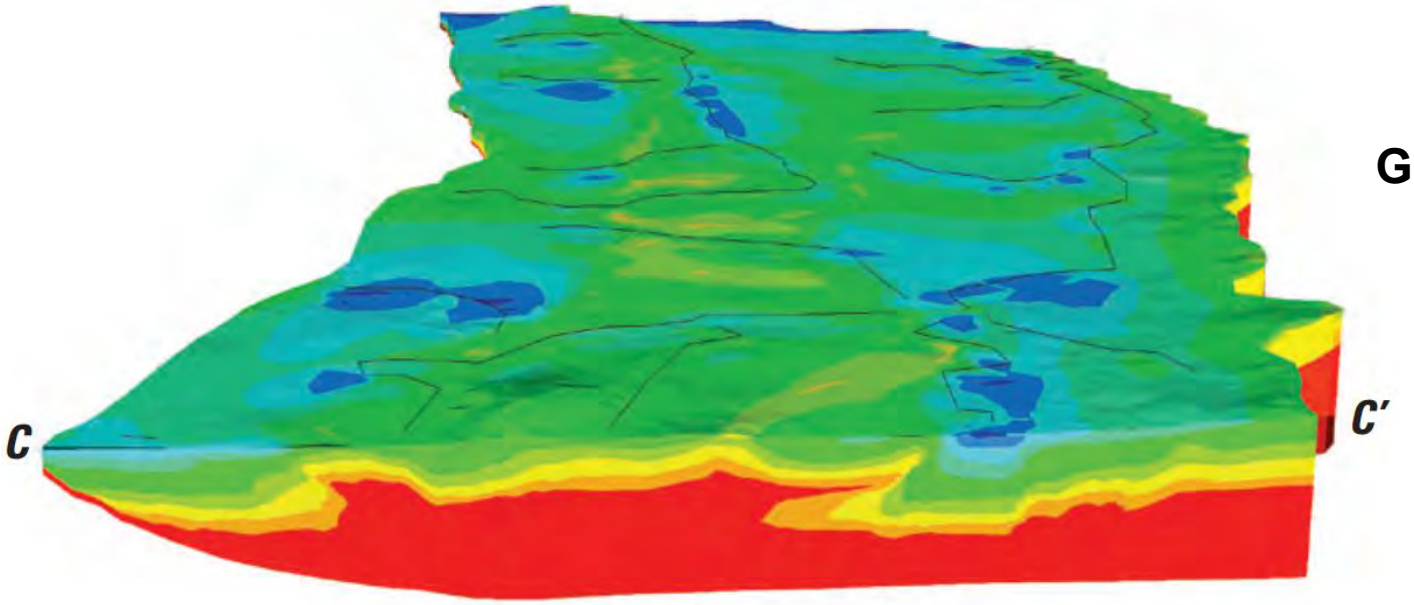
DISPERSION **ADVECTION**

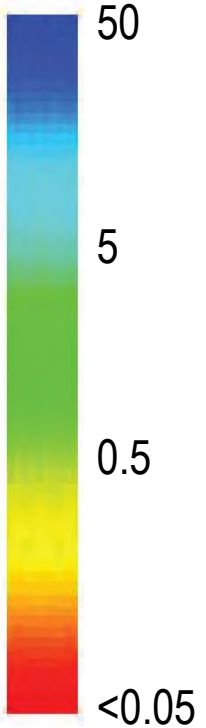
SIMULATED MAGNITUDE OF GROUNDWATER VELOCITY FROM MODEL OF GROUNDWATER FLOW IN SHENANDOAH VALLEY, VIRGINIA & WEST VIRGINIA



Block cropped along section **C-C′**

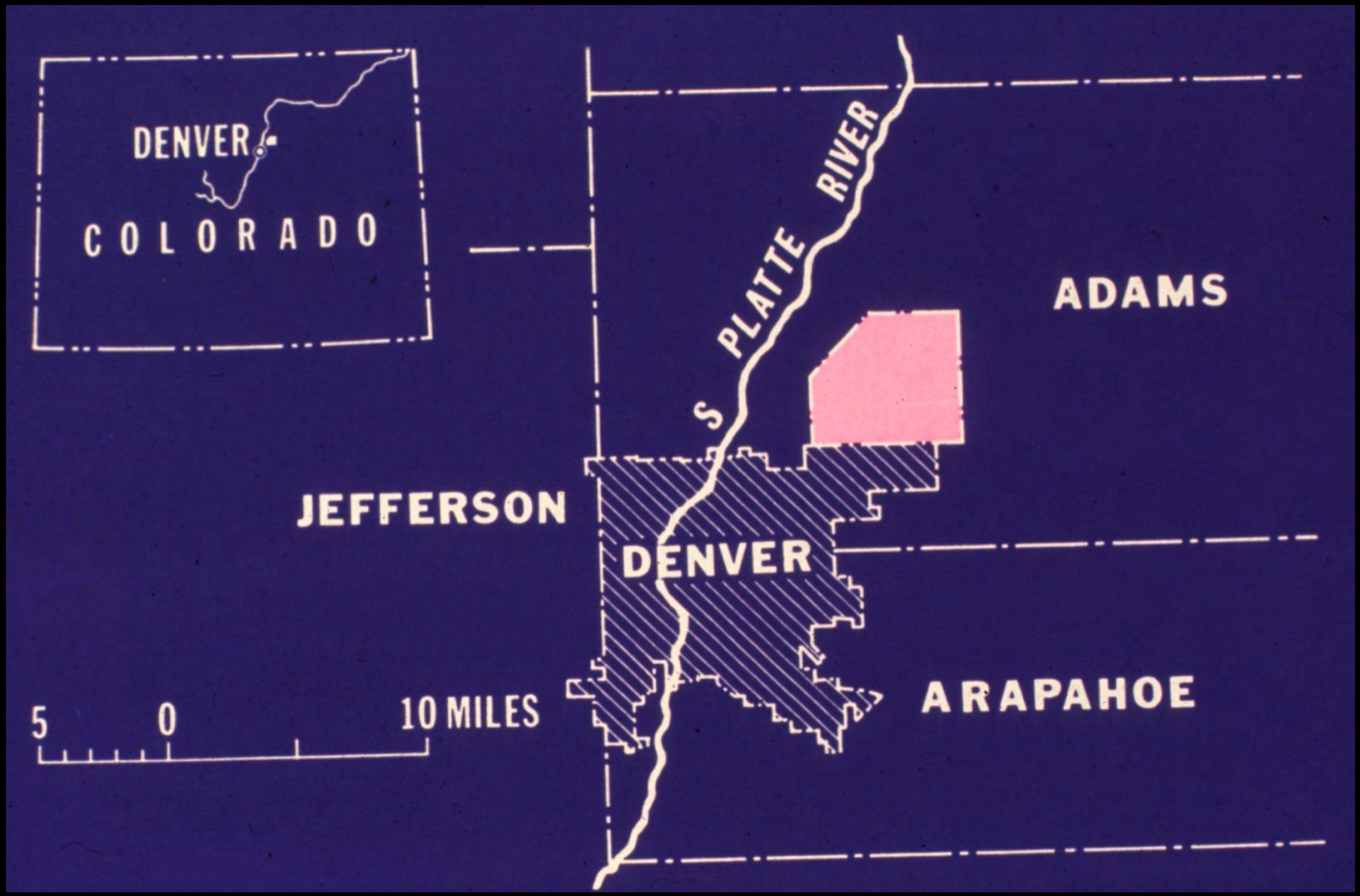
EXPLANATION

Groundwater velocity, in m/day



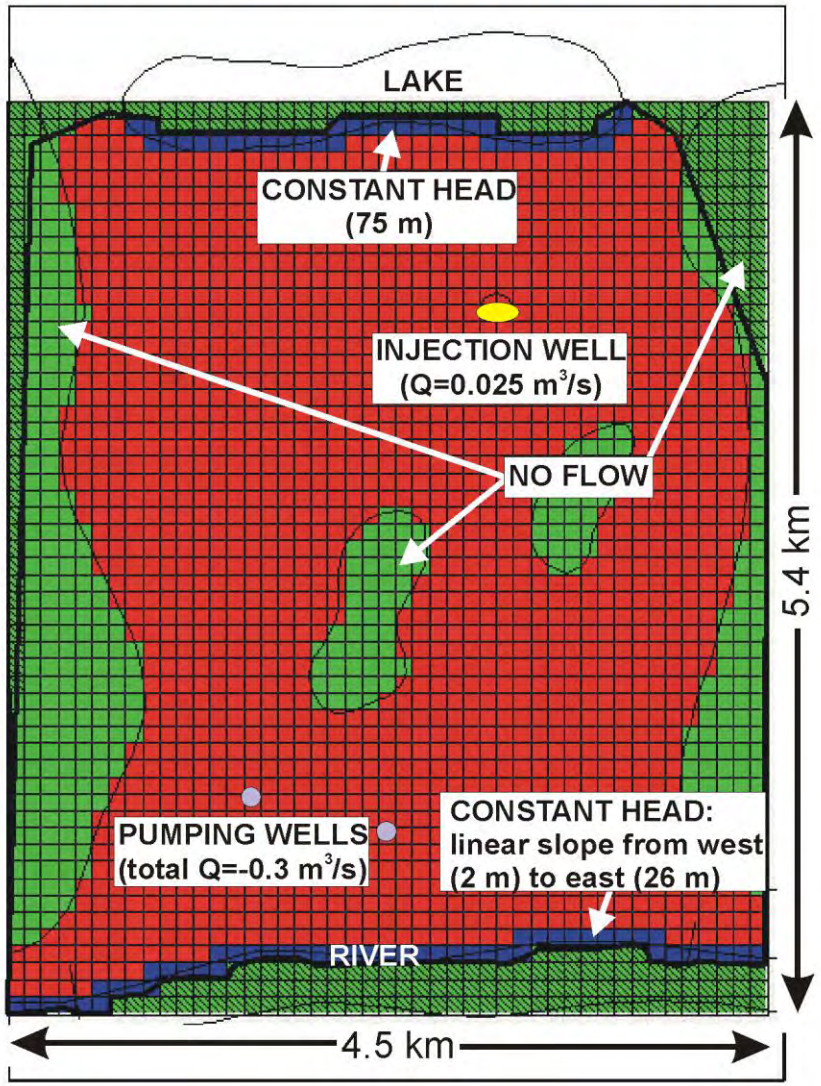
Modified From: Yager, Southworth, and Voss (2008), USGS Sci. Inv. Report 2008-5002

Rocky Mt. Arsenal, Colorado

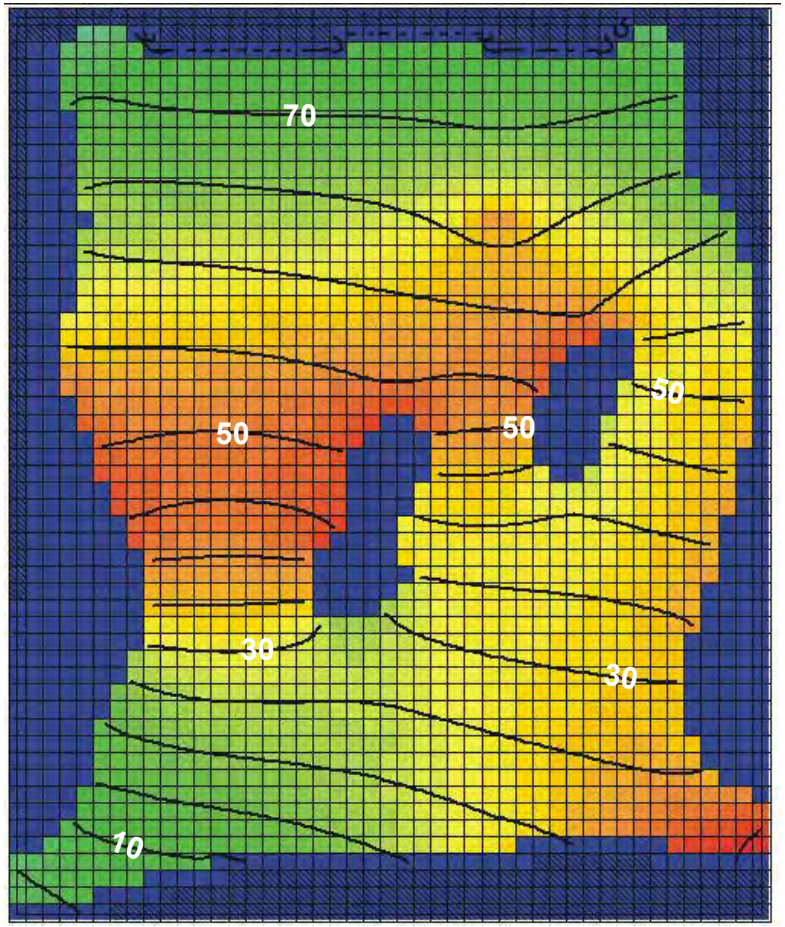


SIMPLIFICATION OF ROCKY MOUNTAIN ARSENAL CONTAMINATION PROBLEM TO COMPARE NUMERICAL ALGORITHMS

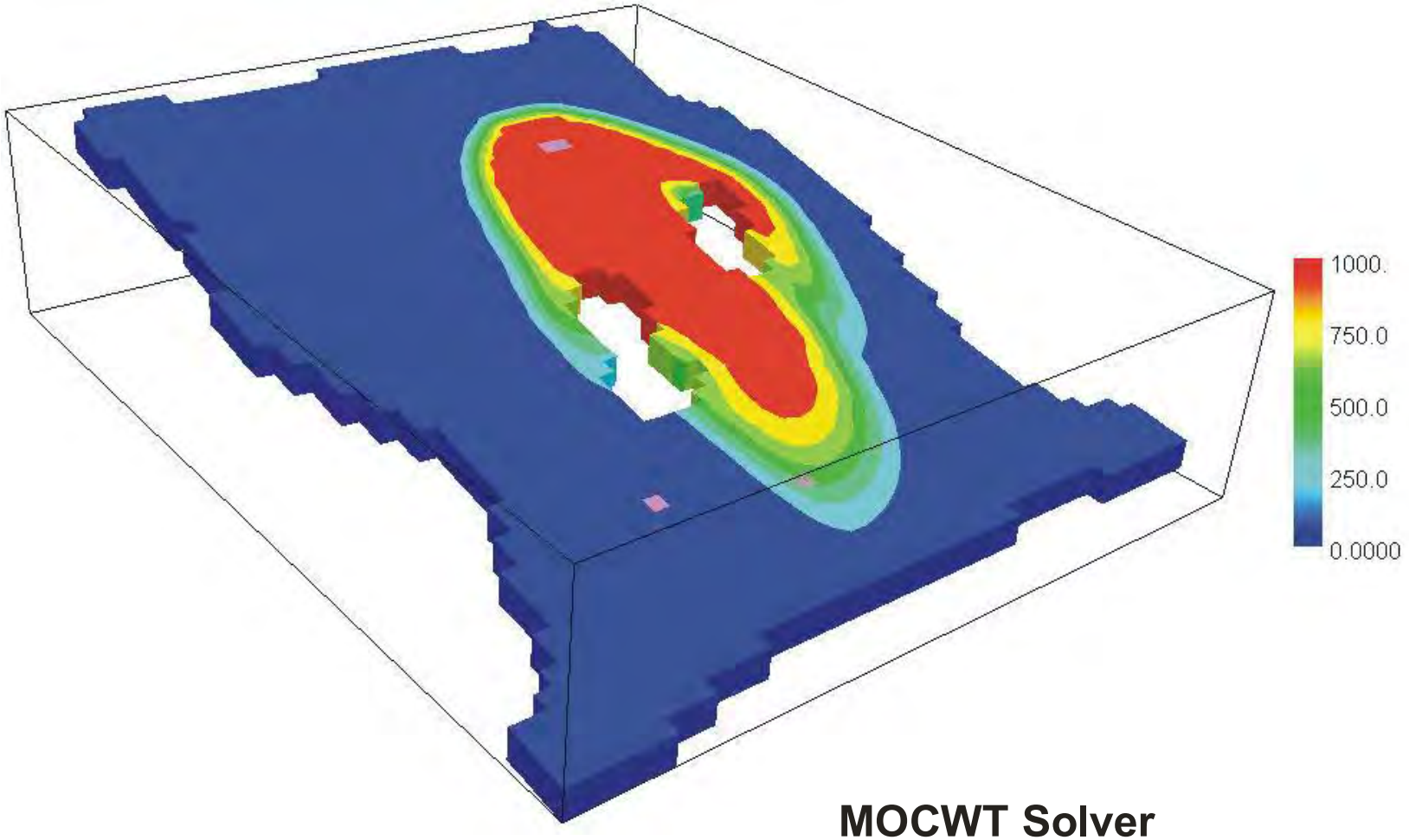
FINITE-DIFFERENCE GRID & BOUNDARY CONDITIONS FOR TEST PROBLEM



WATER-TABLE ELEVATION & SATURATED THICKNESS (b)



CALCULATED SOLUTE CONCENTRATIONS



MOCWT Solver
Unconfined; constant porosity
Time = 30 yrs.

RESULTS OF NUMERICAL EXPERIMENTS

SIMPLIFIED ANALOG TO ROCKY MT. ARSENAL, CO, PROBLEM

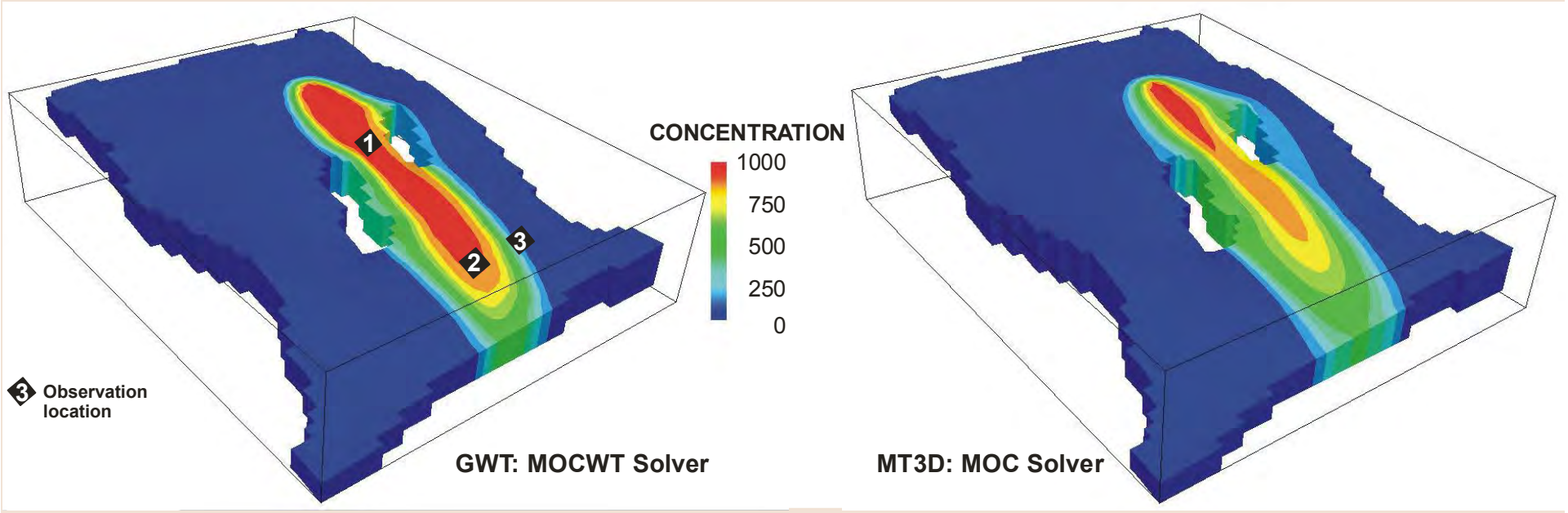
Unconfined aquifer; variable thickness; randomly distributed heterogeneous porosity

	MODFLOW-GWT					MT3D				
	MOC	MOCWT	MOCWT[1]	MOCIMP	ELLAM	MOC	MMOC	HMOC	FD	TVD
Transport time steps	190	99	99	99	99	194	194	194	433	433
Run time (seconds)	15.5	10.0	5.7	8.7	8.5	3.0	2.5	3.0	2.9	5.1
Maximum concentration	1009	1005	1001	1026	1342	999	999	999	986	1053
Minimum concentration	-3.0	-0.8	-4.0	-38	-88	0	0	0	0	-9
Mass-balance error (%)	2.3	$5x10^{-5}$	$7x10^{-6}$	0.6	$4x10^{-5}$	2.8	5.7	3.3	$2x10^{-5}$	$1x10^{-4}$

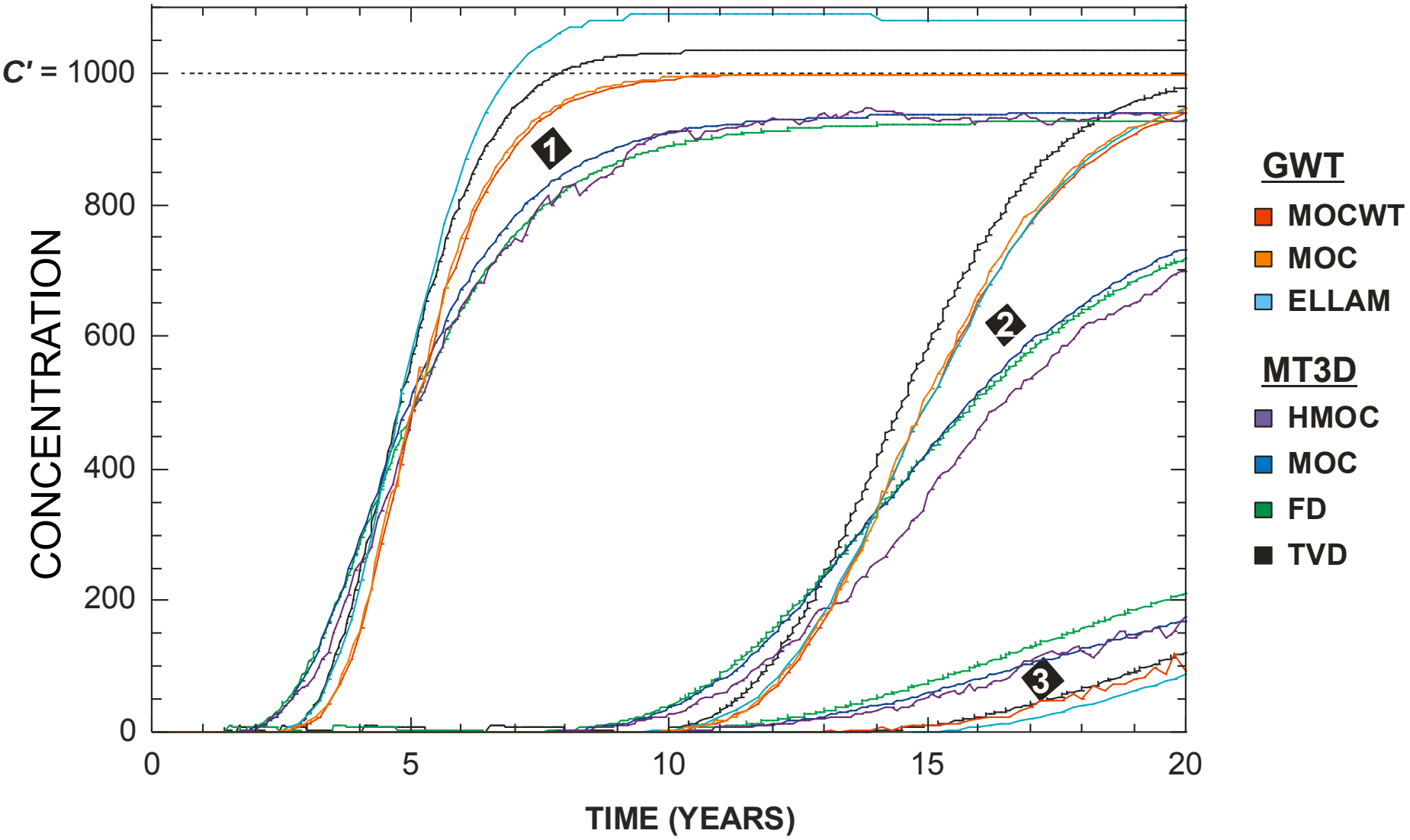
[1] Spatially varying distribution of particles, ranging from 25 to 4 per cell, decreasing in number with distance from plume

CALCULATED SOLUTE CONCENTRATIONS

Unconfined; randomly distributed porosity
Time = 20 yrs.



COMPARISON OF BREAKTHROUGH CURVES FOR 3 OBSERVATION POINTS

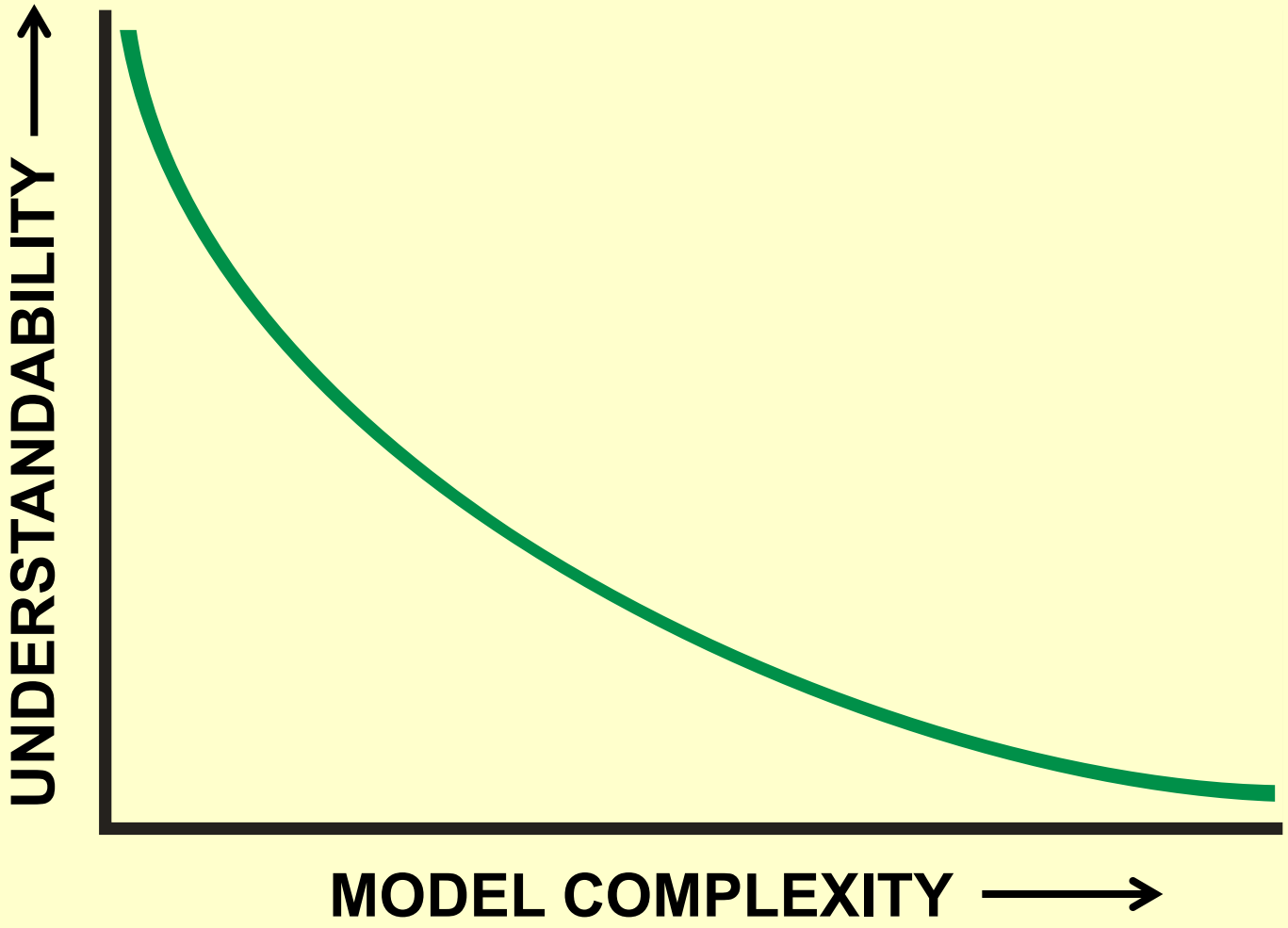


EMERGING TREND

- LARGER & MORE COMPLEX MODELS

- EXAMPLES:
  - Multi-scale (telescopic or adaptive meshes)
  - Detailed heterogeneity
  - Ecological problems
  - Reactive transport
  - Variable density
  - Stochatic processes

MODEL COMPLEXITY & EASE OF UNDERSTANDING MODEL BEHAVIOR



MAJOR CONCERN

Does model complexity mask conceptual & parameterization errors and biases?

GROUNDWATER MODELING:

- GROUNDWATER FLOW MODELING IS RELATIVELY EASY/SIMPLE COMPARED TO SOLUTE TRANSPORT

SUCCESSFUL SOLUTE-TRANSPORT MODELING:

- Start simple and add complexities in “bite-sized” increments

SUCCESSFUL SOLUTE-TRANSPORT MODELING:

- Grid size can make a difference (especially in transport modeling)

SUCCESSFUL SOLUTE-TRANSPORT MODELING:

- Calculated plumes will be sensitive to how heterogeneity is represented

SUCCESSFUL SOLUTE-TRANSPORT MODELING:

- Scale of heterogeneity adequate to simulate groundwater flow may not be satisfactory for simulating solute transport

SUCCESSFUL SOLUTE-TRANSPORT MODELING:

- Watch out for numerical errors—you will have some

SUCCESSFUL SOLUTE-TRANSPORT MODELING:

- Numerical dispersion can lead to erroneous estimates of risk (over or under, depending on nature of safety criteria)

SUCCESSFUL SOLUTE-TRANSPORT MODELING:

- Uncertainty in your conceptual model may dominate the errors in your solution & predictions

SUCCESSFUL SOLUTE-TRANSPORT MODELING:

- In simulating historical concentrations or in predicting future concentrations …

  the secret to successful solute-transport modeling is to …

  LOWER YOUR EXPECTATIONS!