It’s really dark down there: Uncertainty in groundwater hydrology

Larry Winter
University of Arizona

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Spatial scales and typical dynamics

Individual pore: 10 μm – 10 mm radii, 0.1 – 10 cm length

Dynamics: Poiseuille Eqn, Navier-Stokes Eqns

Explicit porous microstructures: 1 cm – 1 m sample lengths

Dynamics: Navier-Stokes Eqns

Laboratory: 1 – 10 m^3 blocks

Dynamics: Stokes Flows / Darcy's Law

Field: 10m – 1 km

Dynamics: Darcy's Law

Typical Scales of Measurement/ Observation

Local aquifer: 1 – 10 km Dynamics: Diffusion (Darcy's Law)

Basin-scale: 1 – 10^4 km Dynamics: Diffusion (Darcy's Law)

Flow through porous media: alternate representations

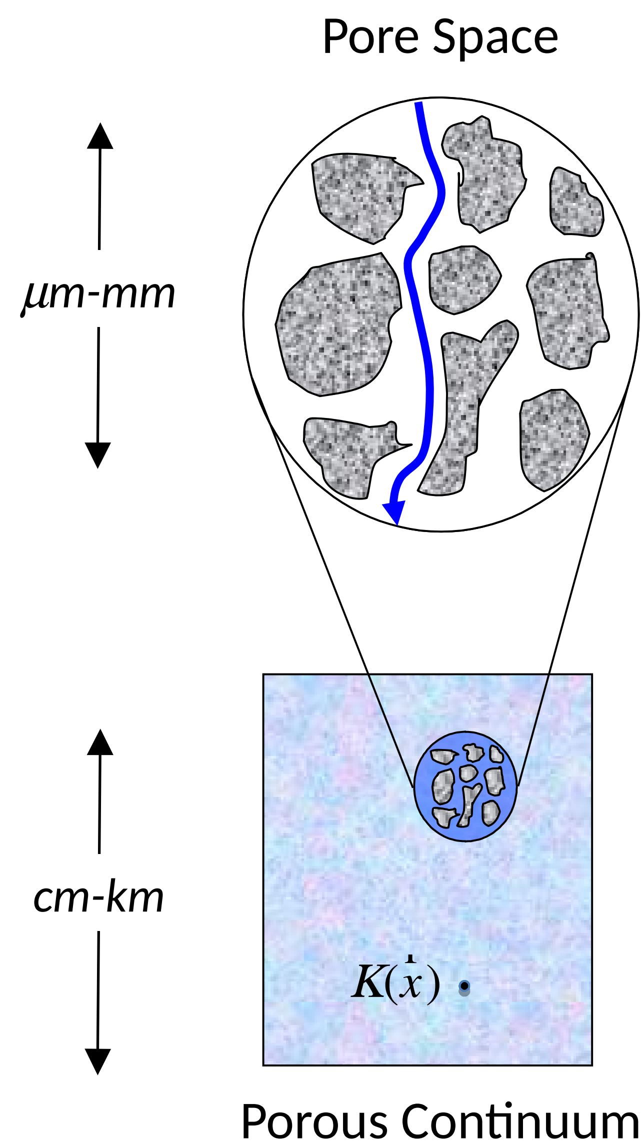
Porous microstructure

- Void and solid phases
- Navier-Stokes equations
- Detailed pore geometry

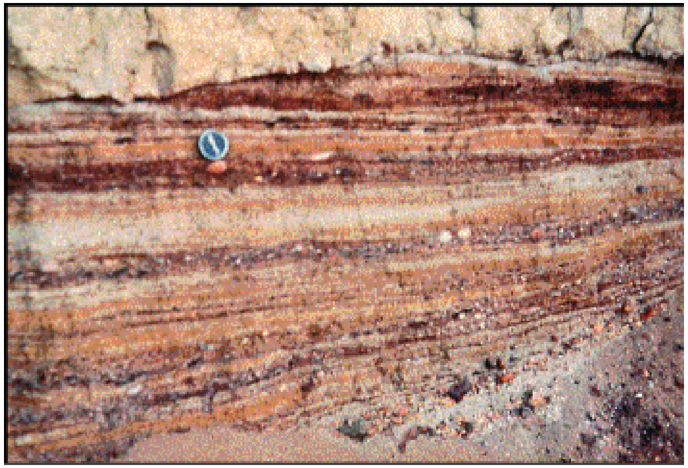
$$\chi(x) = \begin{cases} 1 \text{ if } x \in \text{ pore space} \\ 0 \text{ otherwise} \end{cases}$$

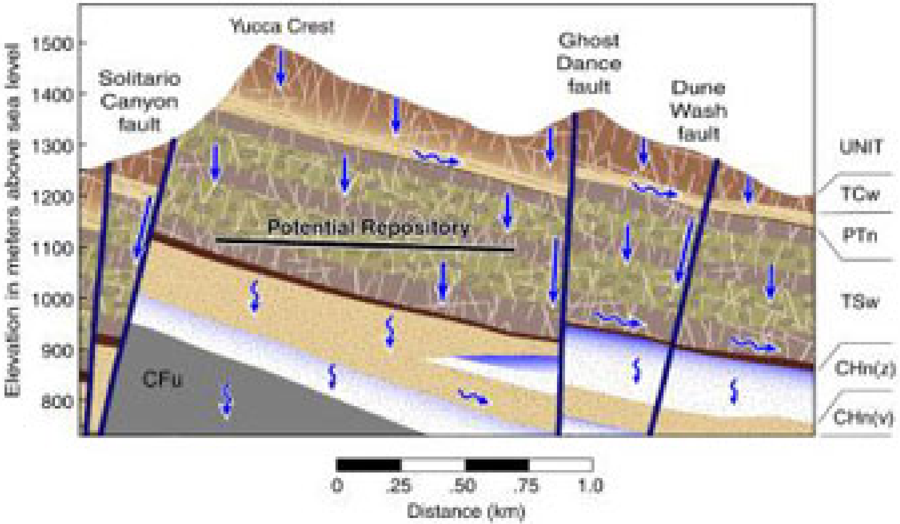
Continuum

- Darcy's Law, advection-diffusion
- Effective parameters
- Hydraulic conductivity [L/t]
- Head [L], velocity, concentration



Highly heterogeneous media





Geologic cross-section with flow patterns

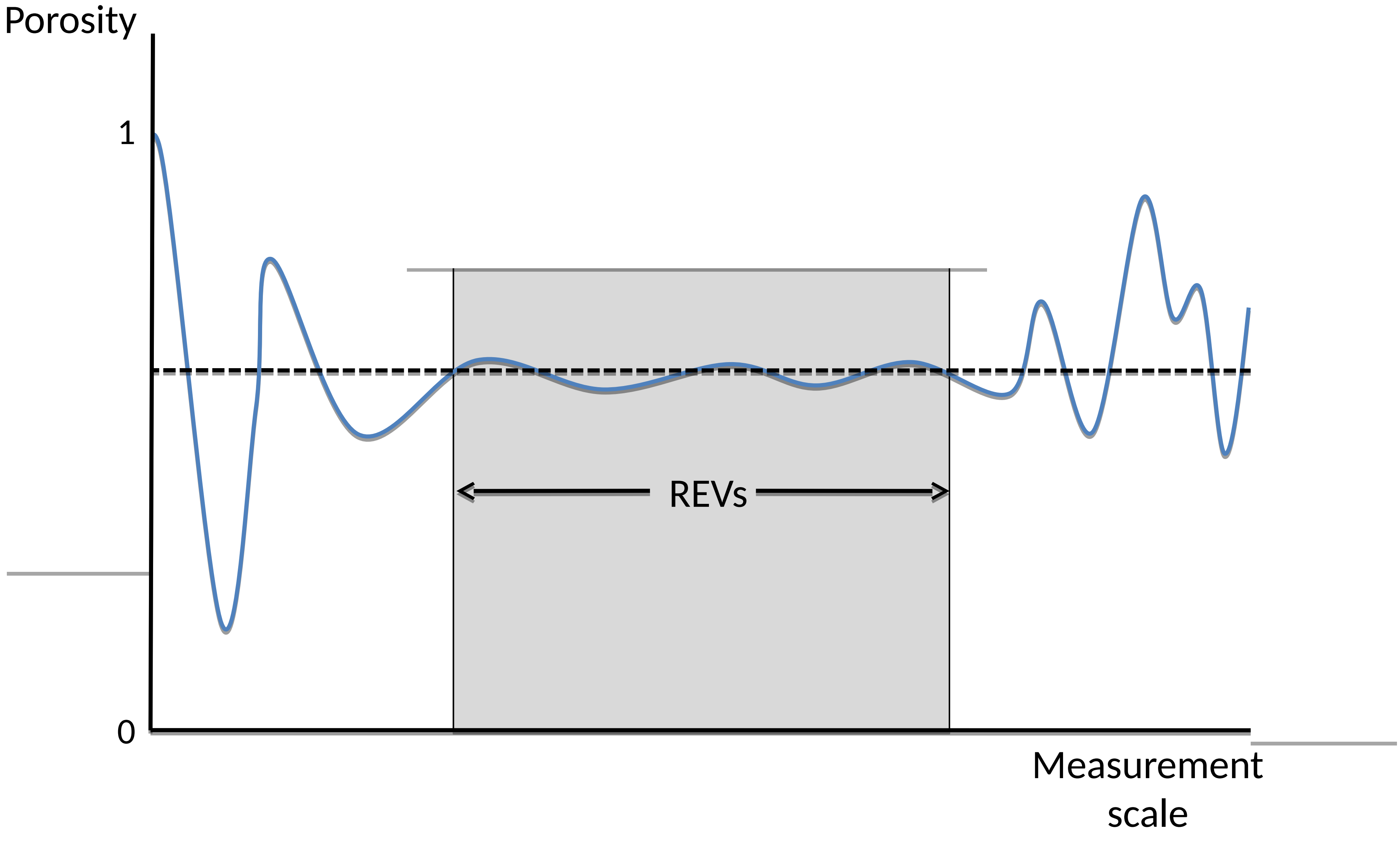
Models, their applications, scales, and assumptions

Model (theory)	Domain of Application	Scales	Assumptions in addition to IBCs & forcing functions
NSE	Pore-Pore network	10μ - cms	(1) Newton's 2nd Law (2) Conservation of mass
Darcy's law Continuity eqn Eqn of state Flow eqn	Elementary volume of a porous medium	cm-m	Continuum representation of porous medium. Uniform material
2D Transmissivity with S_y	Unconfined aquifer	km	**T** doesn't vary with head
2D Transmissivity with S	Confined aquifer	km	(1) Confining beds are plane and parallel, (2) One principal direction of **K** perpendicular to confining beds, (3) head gradient independent of z, (4) $\Delta h/\Delta t$ doesn't depend on z
Diffusion eqn		cm-km	Known **K**(**x**)

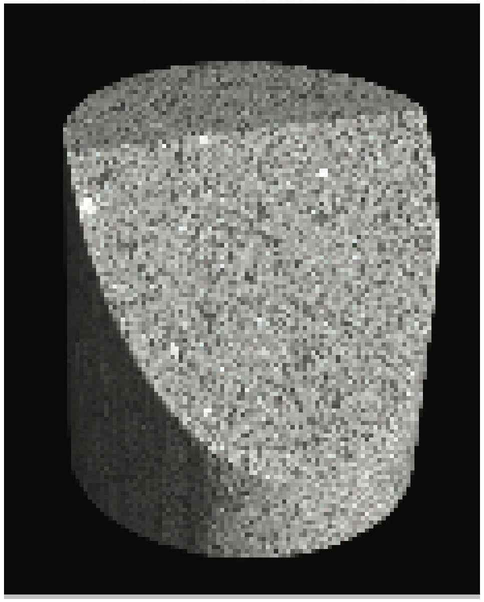
The … equations for the circulation of a fluid in a porous medium [relating to Darcy's law] *are significant only for* [small] *volumes of a porous medium*

-- *Marsily*

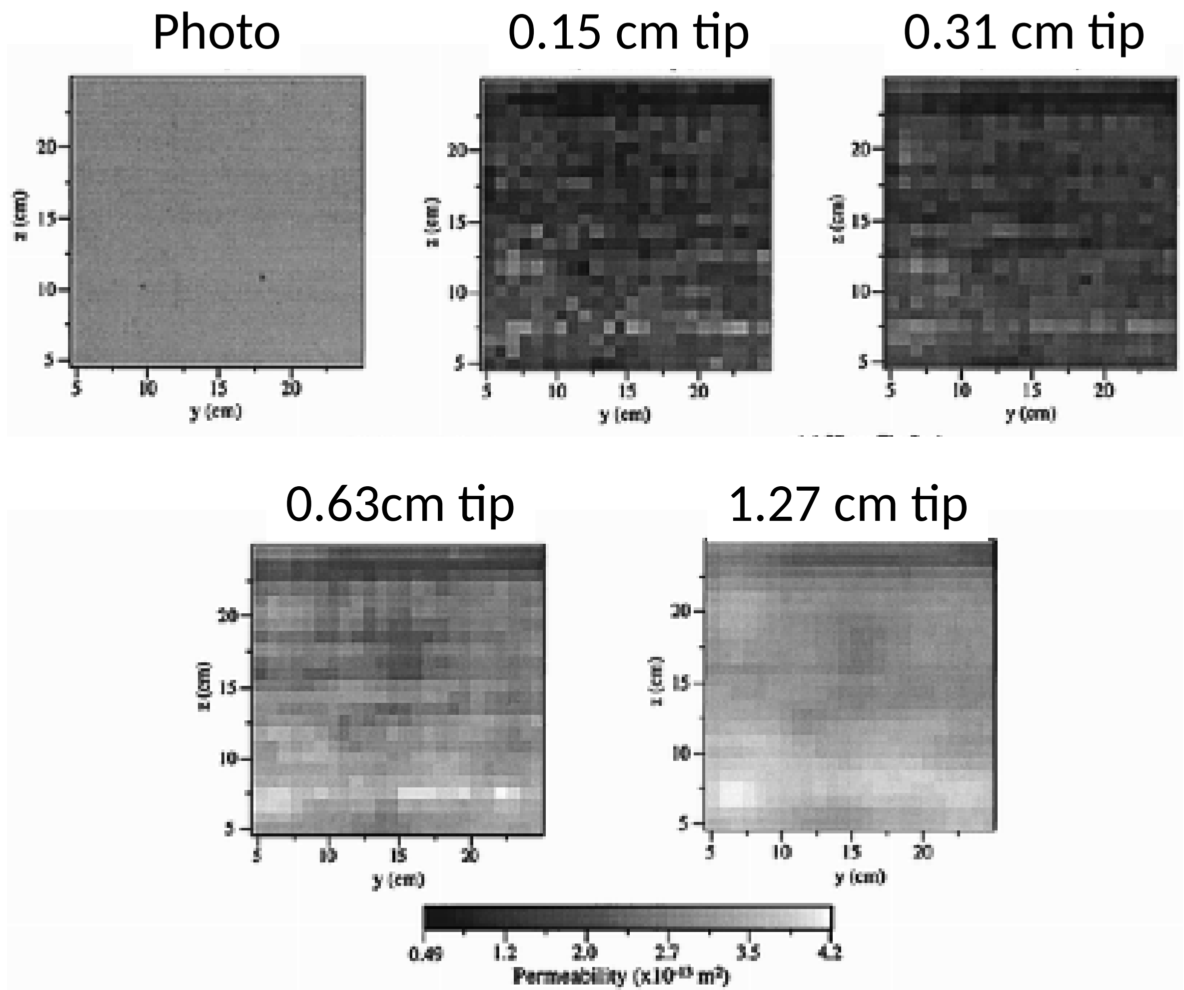
Measurement scales: REV



REV?



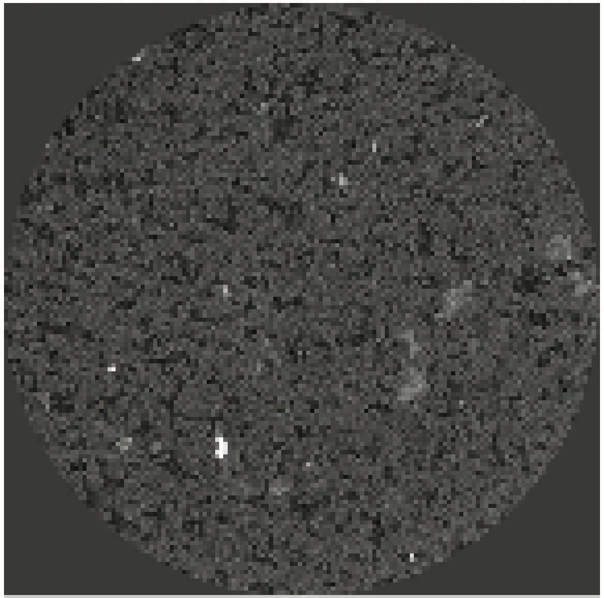
Berea sandstone

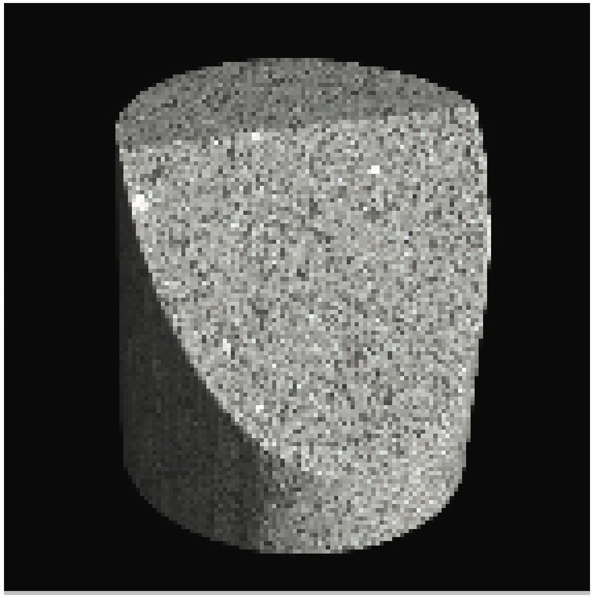


Puff permeameter images.

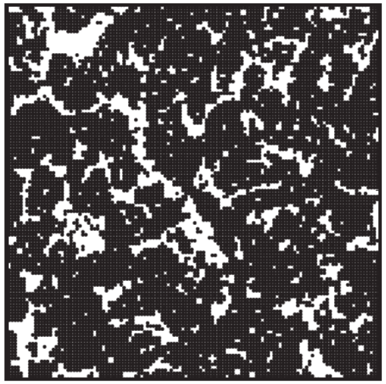
Tidwell et al., 1999

Pore microstructures



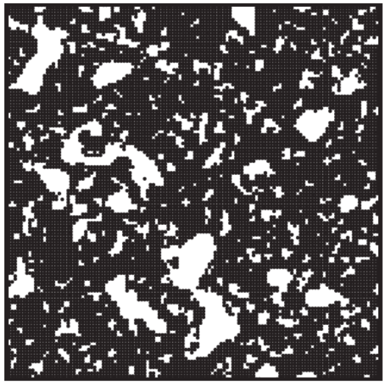


(a) Real Berea Sandstone



Berea Sandstone

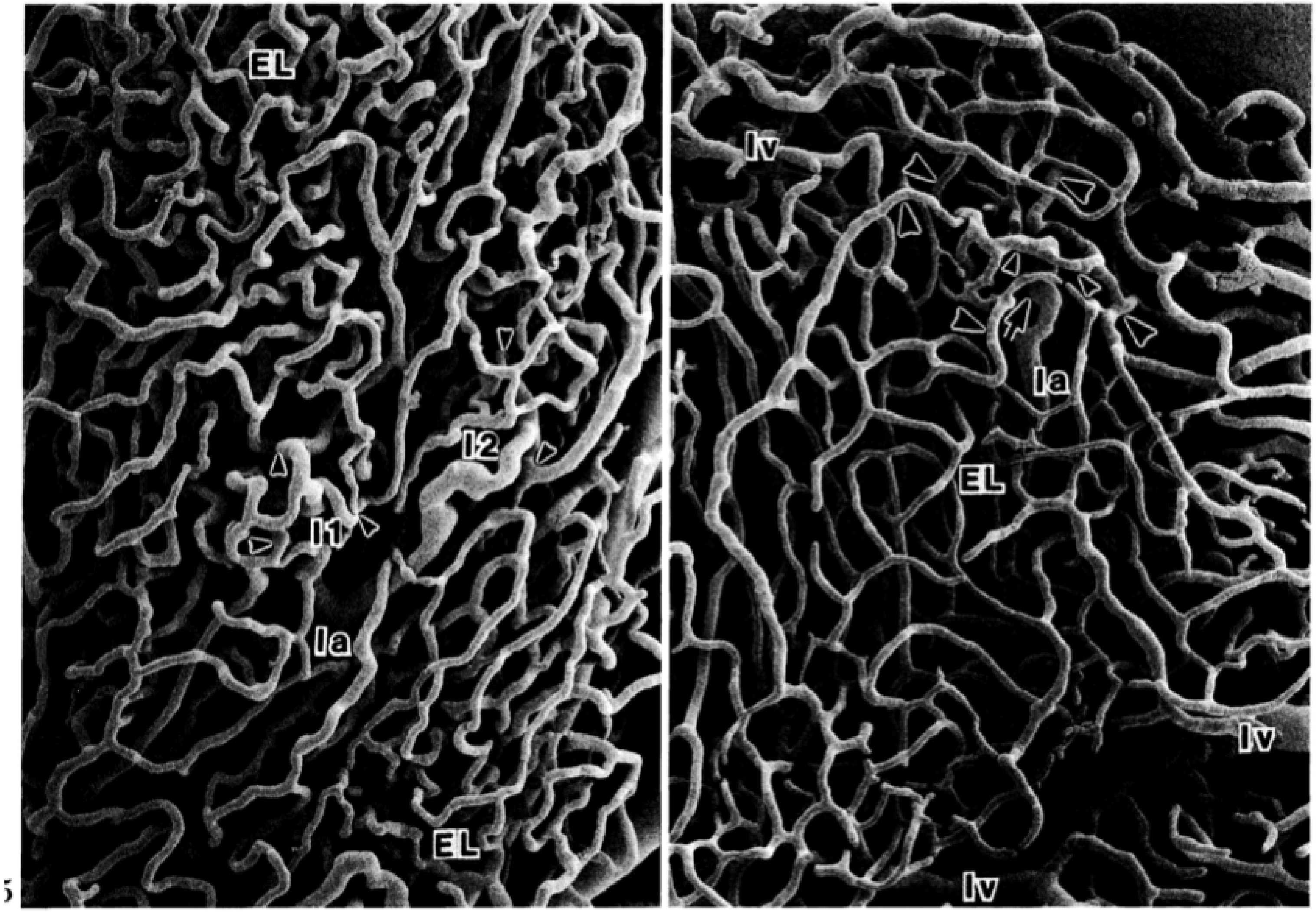
(b) Synthetic Berea Sandstone



Simulation

Berea Sandstone
(Courtesy Ming Zang)

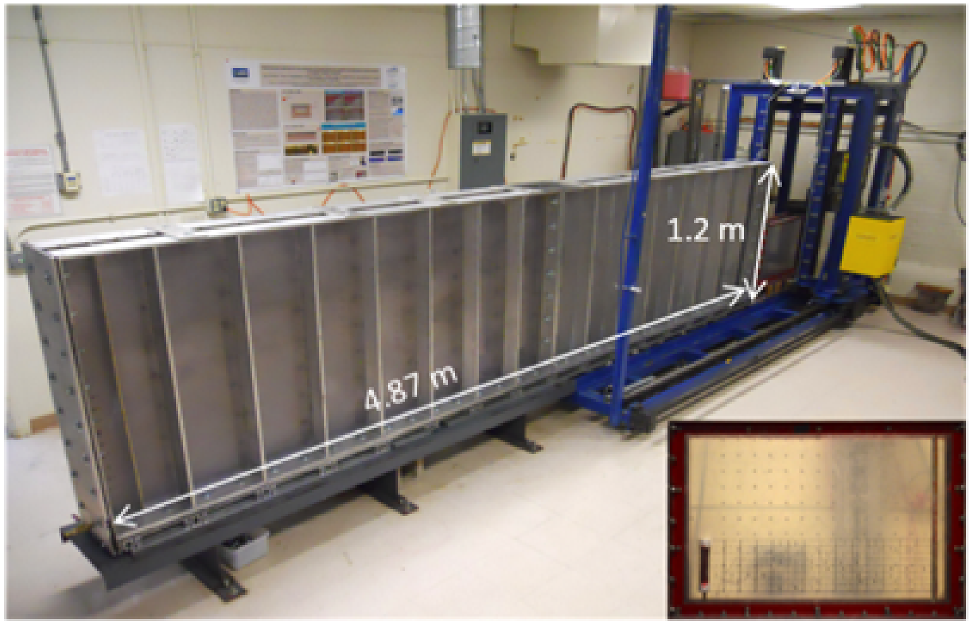
Biological Porous Media: Human Pancreas



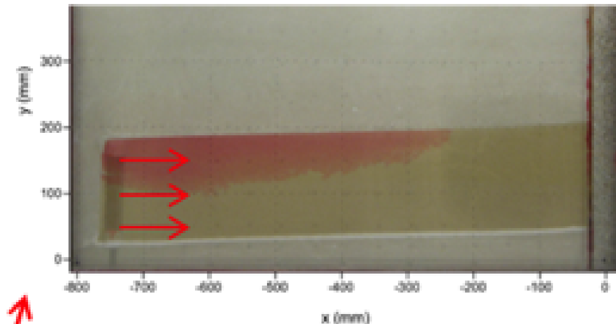
Murakami et al., “Microcirculatory Patterns in Human Pancreas,” (1994)

Flow through porous media: Lab scale

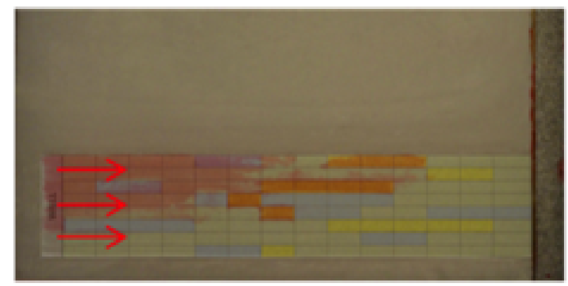
X-ray frame hosting 2 experimental flow cells



Homogeneous reservoir

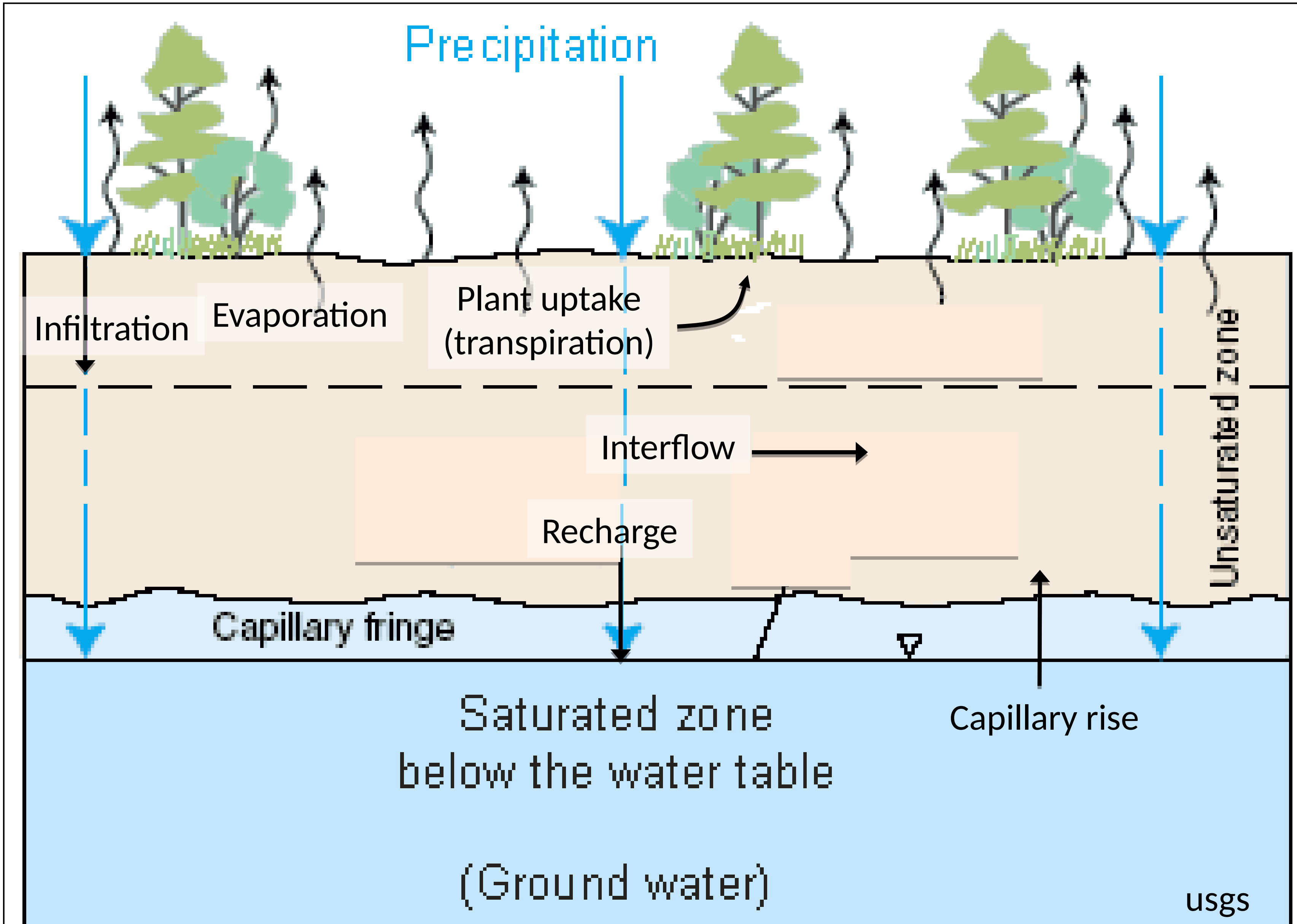


Heterogeneous reservoir

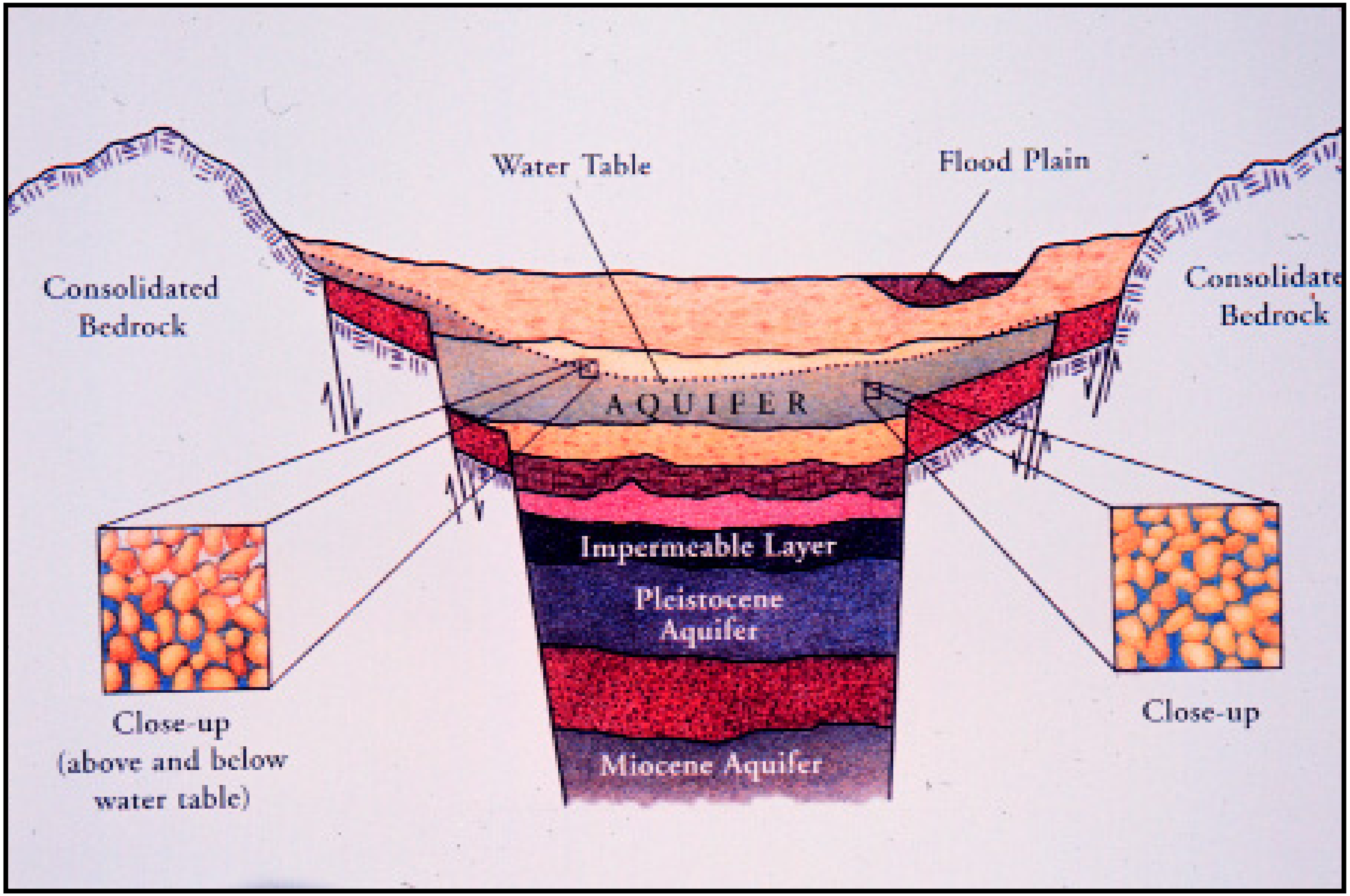


Center for experimental study of subsurface environmental processes
Colorado School of Mines

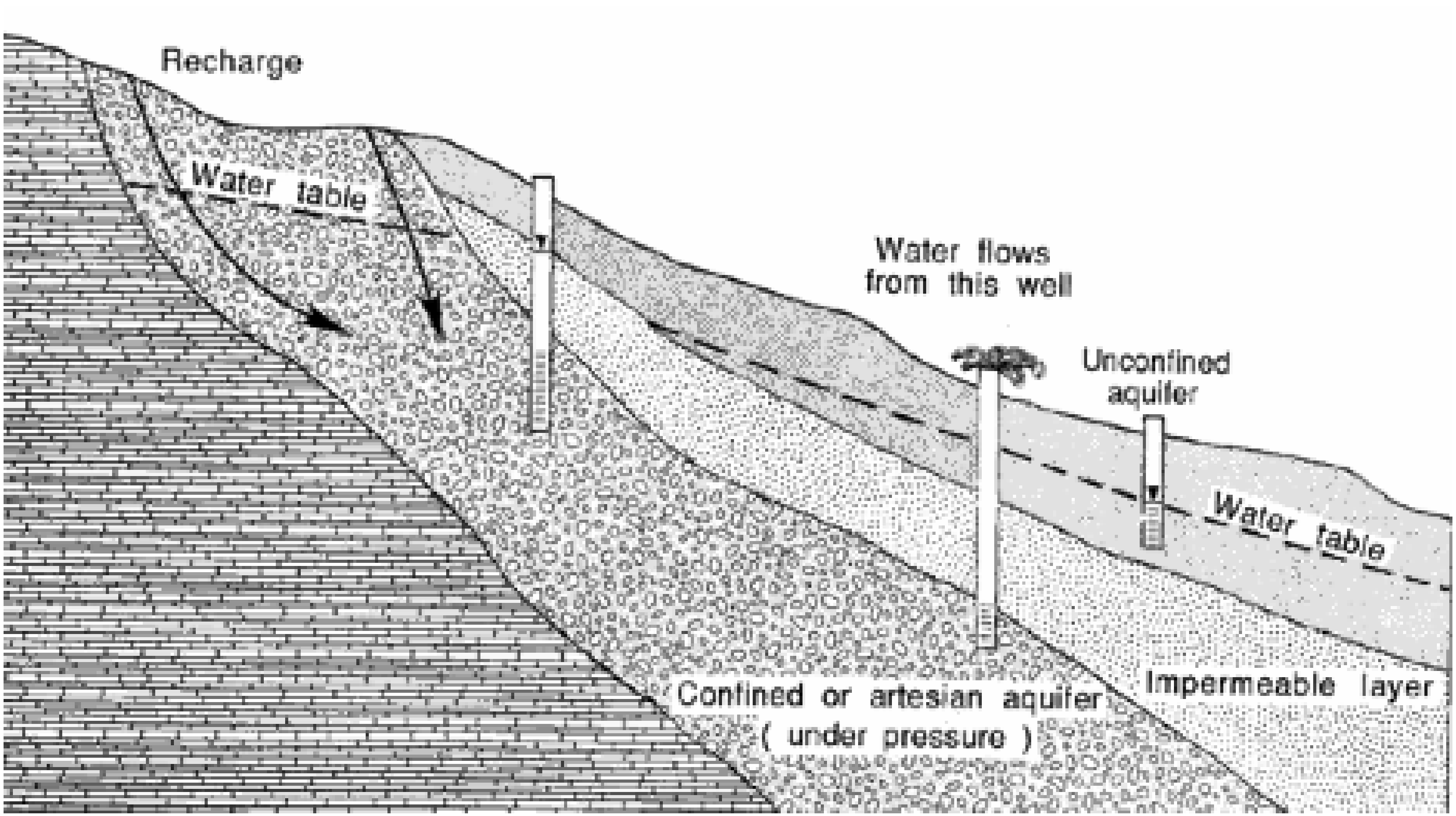
Flow through porous media: Field scale



System of aquifers



Aquifer systems



High Plains Aquifer

450,000 km^2

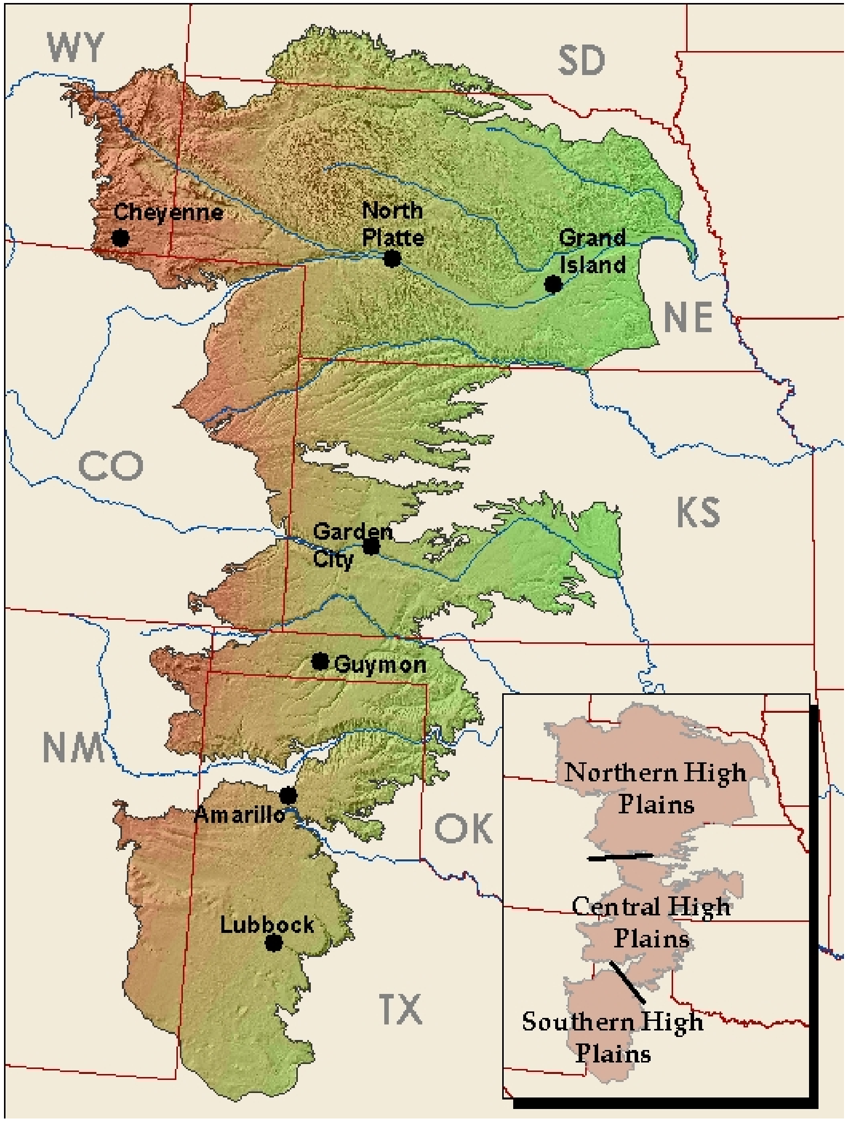
Elevation: 2400m – 355m

Few streams

The Great Plains produce about 25% of US crops and livestock.

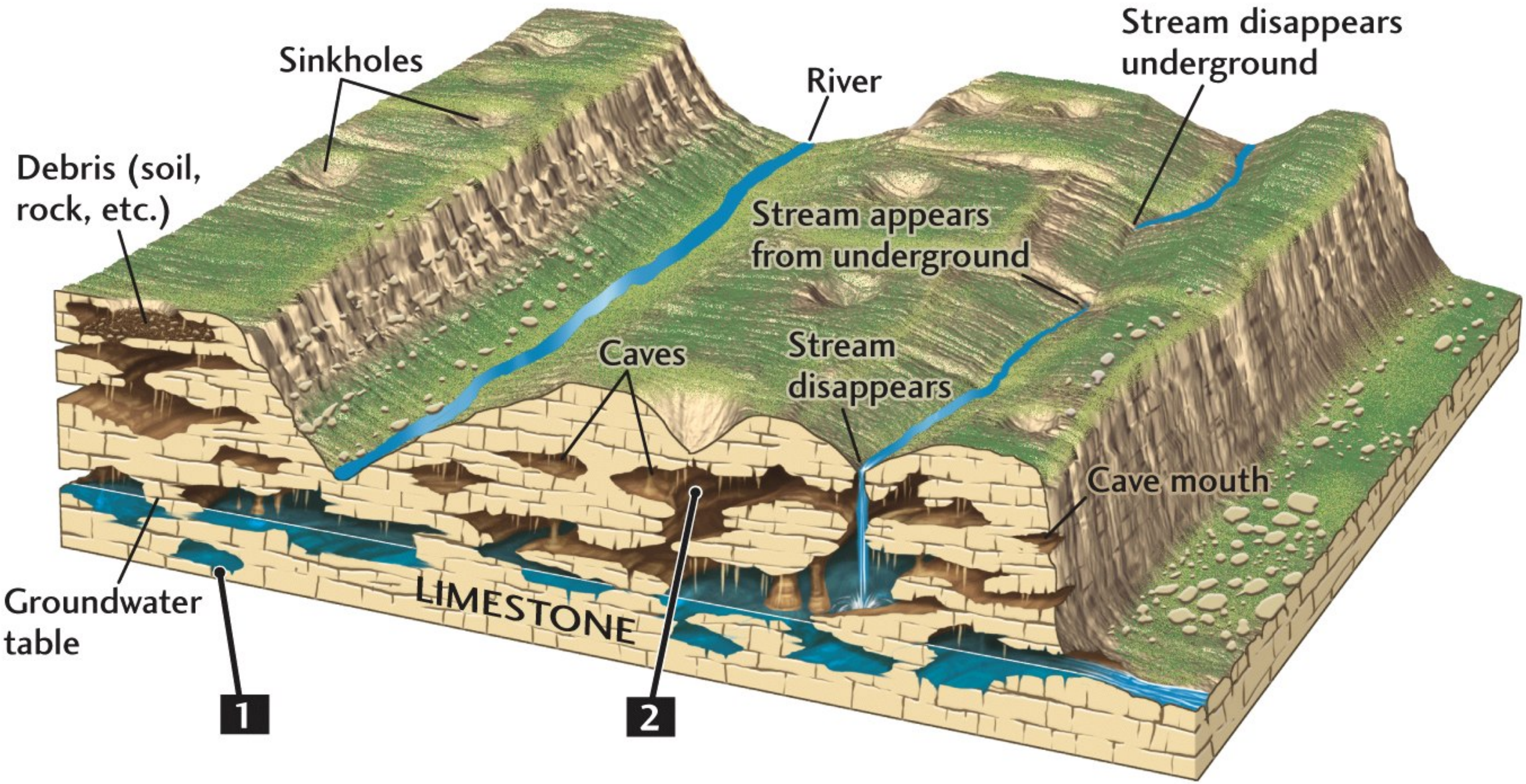
Great reliance on ground water for agriculture

30% of all ground water pumped for irrigation in the United States.



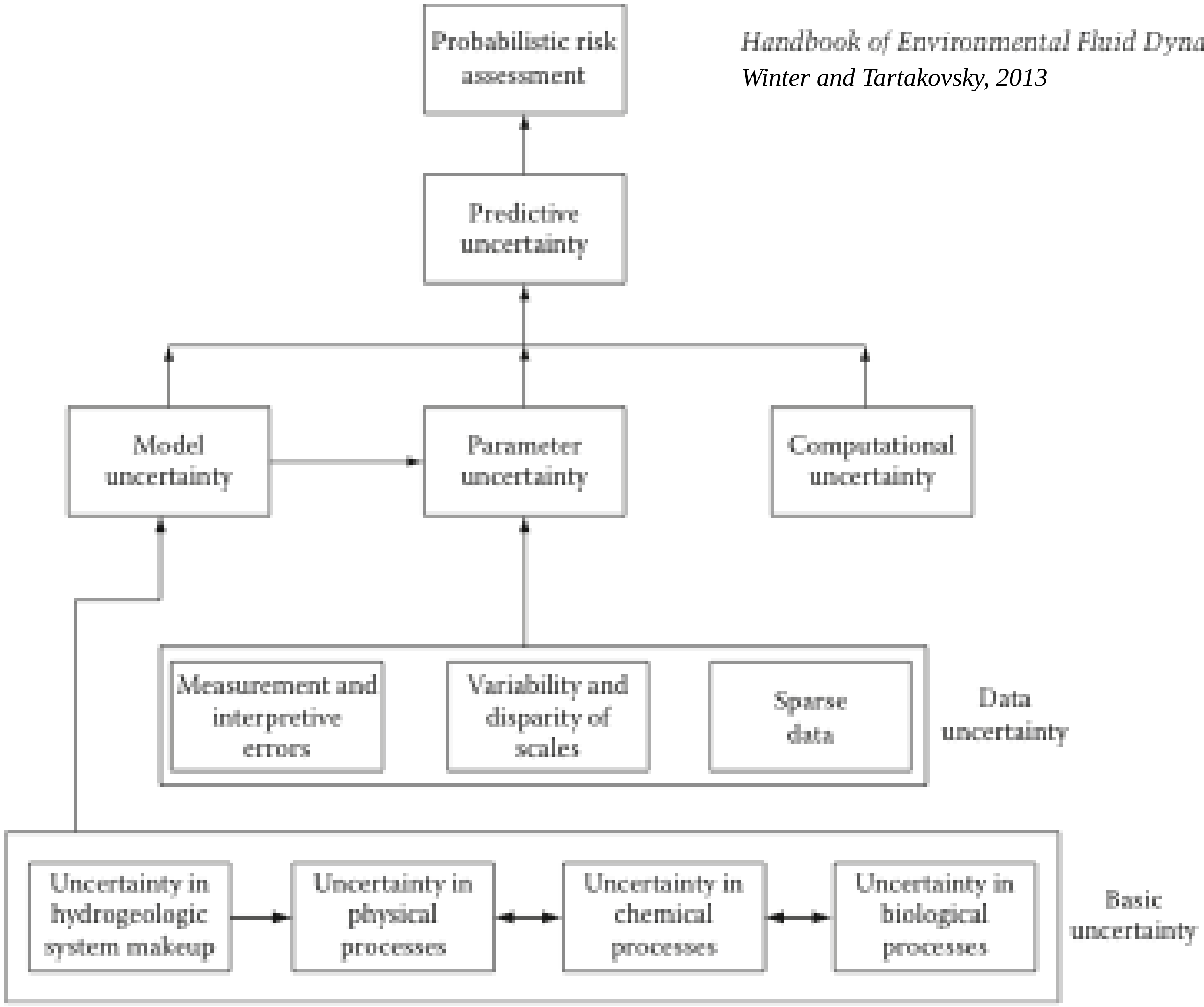
Courtesy USGS

Karst systems



Sources of uncertainty

Handbook of Environmental Fluid Dynamics, Volume One
Winter and Tartakovsky, 2013



Flow through porous structures: experiments

Physical

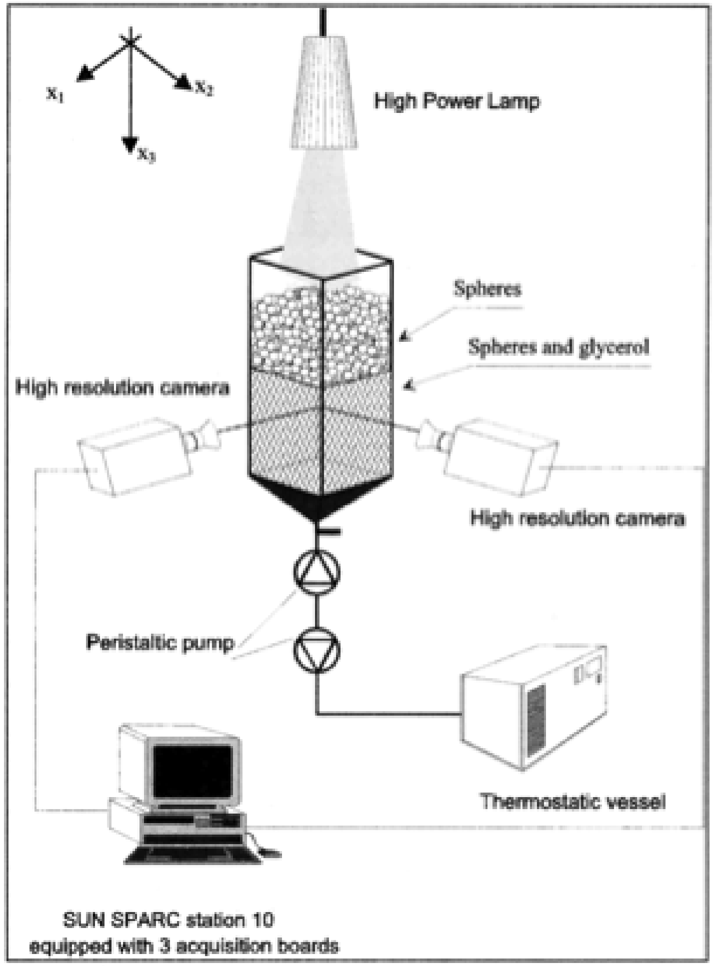


Figure 1. Sketch of the experimental setup.

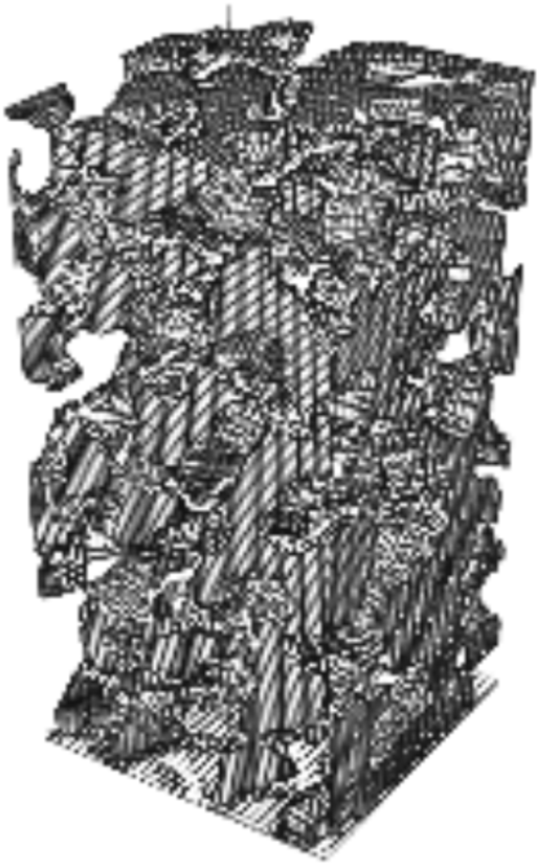
Moroni et al., 2001

Computational

- Cartesian Domain
  $L_x \times L_y \times L_z = 1.27 \times 10^{-2} \times 1.27 \times 10^{-2} \times 2.55 \times 10^{-2}$ m^3
- Resolved with $N_x \times N_y \times N_z = 128 \times 128 \times 256$
- $\Delta x = \Delta y = \Delta z = 10^{-4}$ m
- $\Delta t = 5 \cdot 10^{-5}$ s
- $\nu = 10^{-6} m^2 s^{-1}$, ρ constant.
- Periodic in the vertical with Neumann Boundary Conditions along horizontal boundaries.
- Run the simulation past steady state then evaluate the velocity and pressure fields.
- Eulag CFD Simulator (Prussa et al., 2006).
- Immersed boundary method for pore spaces (Smolarkiewicz and Winter, 2010)

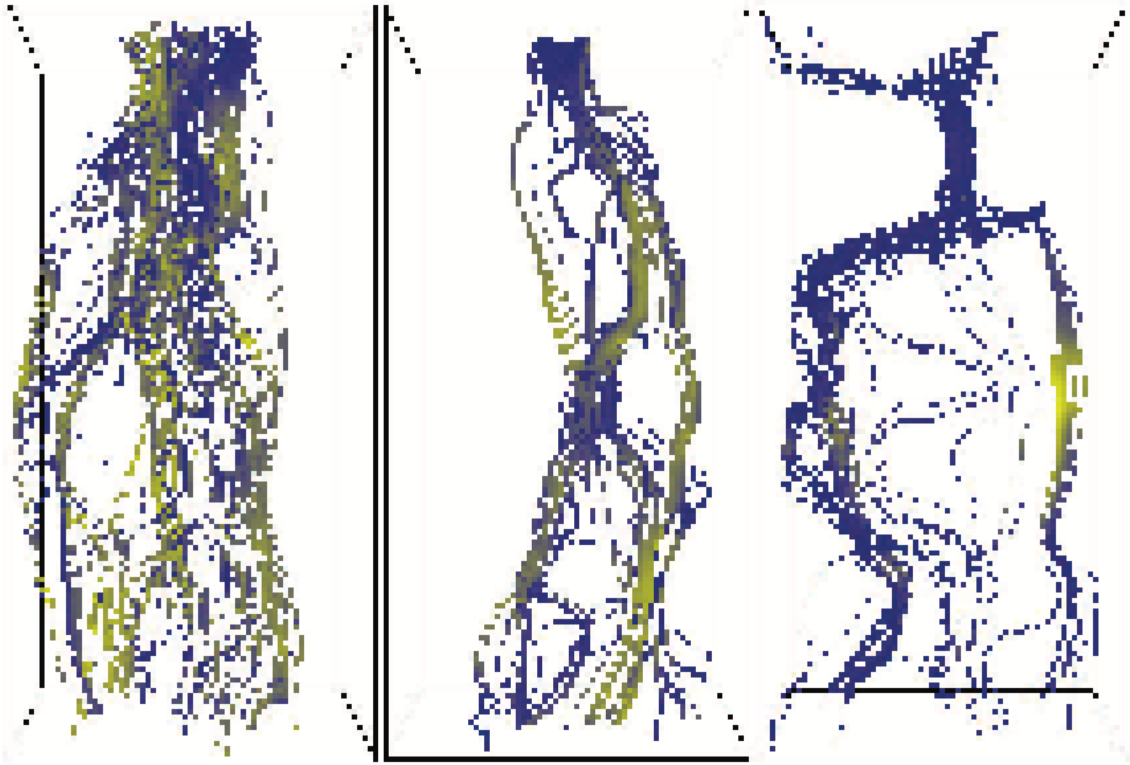
Computational experiments

Synthetic medium



Smolarkiewicz and Winter (2010)

Particle trajectories – Yellow is fast



Hyman et al. (2012)

Heterogeneous velocities

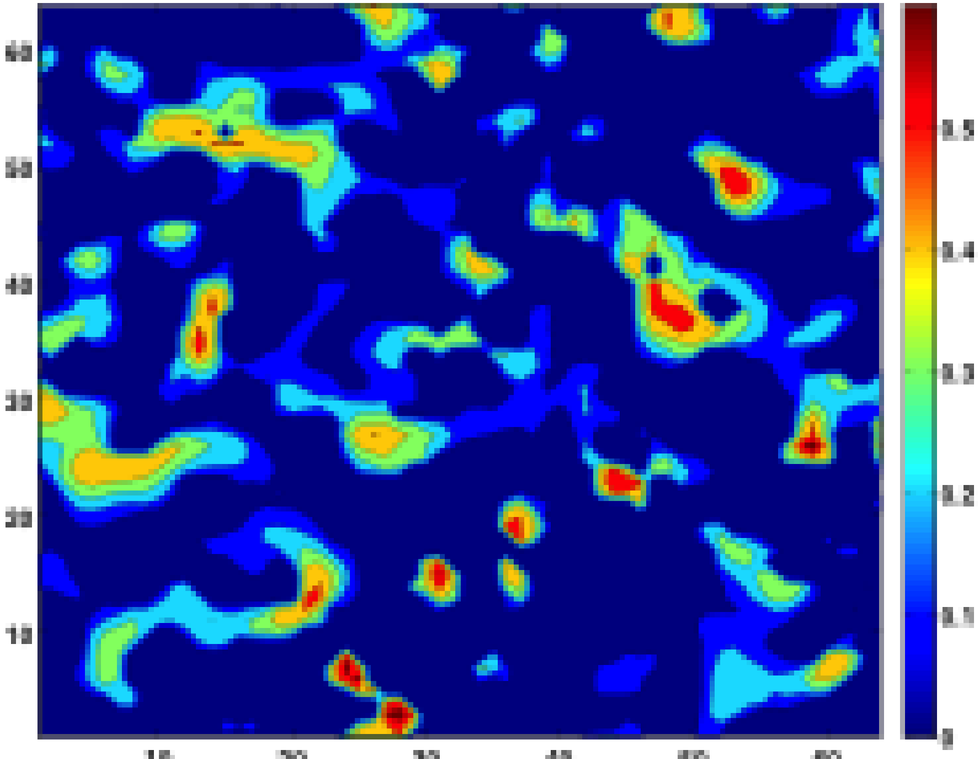


Figure: Normalized velocity magnitudes for a cross sections of a porous medium with of expected porosity of 0.50

Expanding (left) and Contracting Regions (right)

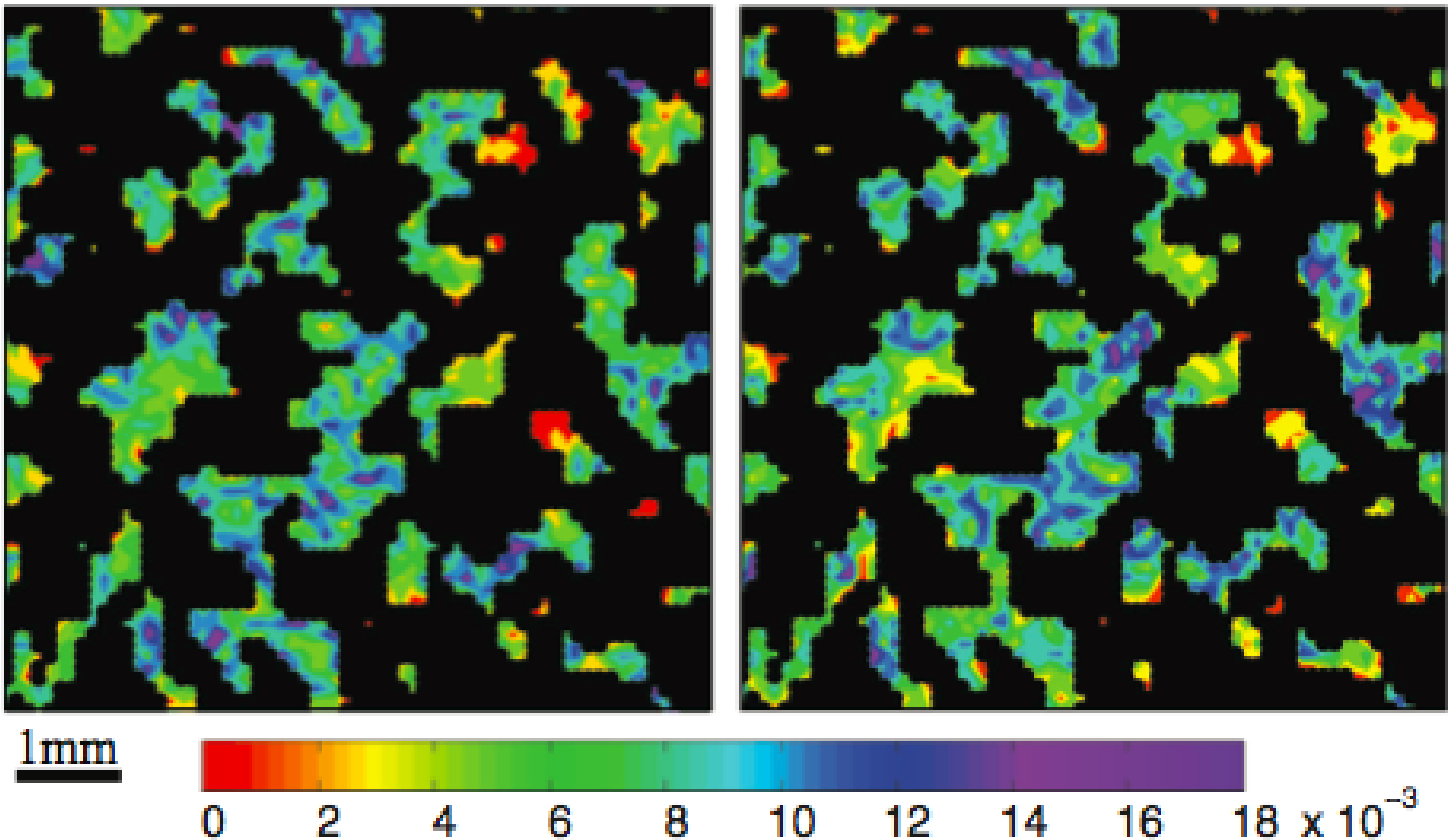
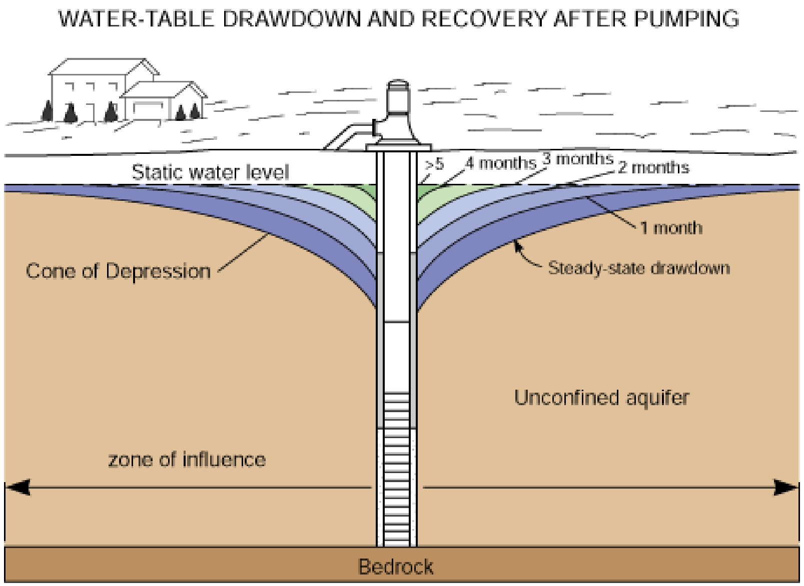


FIG. 1. (Color online) Contour plots of the forward (left) and backward (right) FTLE fields in one-fourth of a horizontal cross section from a porous medium with porosity 0.38 show that regions of high FTLE values are fragmented. Solid matrix shown in black.

(Hyman and Winter, *Phys Rev* E, 2013)

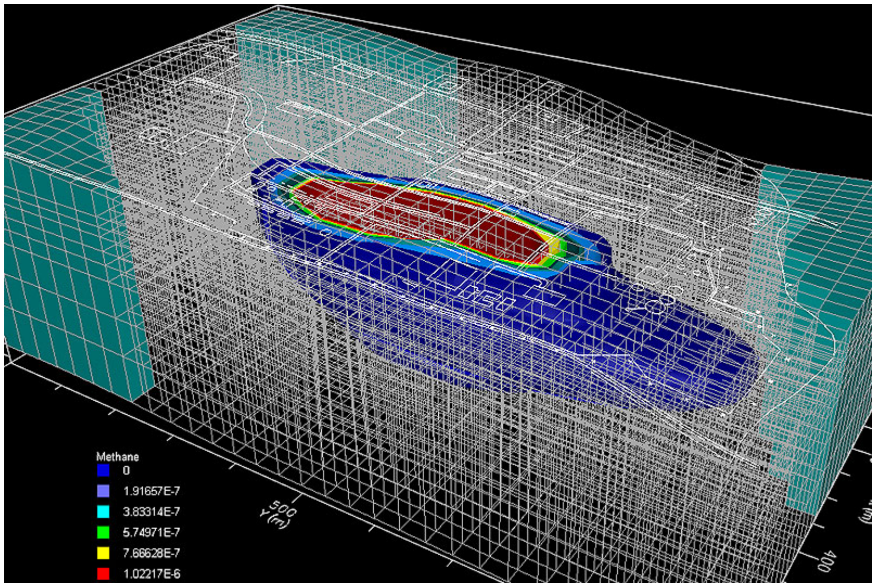
Field scale and larger

Physical



Kansas Geological Survey

Computational



https://www.swstechnology.com/

USGS Modflow
https://water.usgs.gov/ogw/modflow/

System dynamics: Continuum representation

Darcy's Law

$$q = -K(x)\nabla h$$

Continuity

$$\nabla \bullet q + (S\frac{\partial h}{\partial t} + F) = 0$$

Flow

$$\nabla \bullet K \nabla h = S\frac{\partial h}{\partial t} + F$$

Mass Transport

$$\frac{\partial C}{\partial t} = \nabla \bullet (D\nabla C - \mathbf{u}C)$$

Parameters

Conductivity: $K(x)$, $[K] = m/s$

Permeability: $k(x) = (\mu / g\ \rho)\ K = m^2$

Transmissivity: $T(x)$, $[T] = m^2/s$

Storativity: S, $[S] = 1$

Dispersion coefficient: D, $[D] = m^2/s$

State variables

Hydraulic head: $h(x, t)$, $[h] = m$

Darcy flux: $q(x, t)$, $[q] = m/s$

Flow rate: $Q(x, t)$, $[Q] = m^3/s$

Concentration: $c(x, t)$, $[c] = M/m^3$

Groundwater Flow: Some Foundational Problems

Inverse problem. Estimate basic parameters (hydraulic conductivity) at a given scale of analysis (porous microstructures -- aquifers) from data.

Most are highly heterogeneous, e.g., $K(x) = K_i(x)$ if $x \in$ material i

1st Forward Problem (Heterogeneities). Determine effects of material heterogeneities on flow/transport at a given scale.

Scale-up. Scale observations of heterogeneous parameters up to effective parameters at a larger scale.

Scale-Down. Scale parameters averaged at a larger scale down to realistic distribution of heterogeneities at a smaller scale.

2nd Forward Problem (Prediction). Quantify uncertainties about system states arising from incomplete knowledge of parameters and model structure for a specific aquifer.

Scale-up

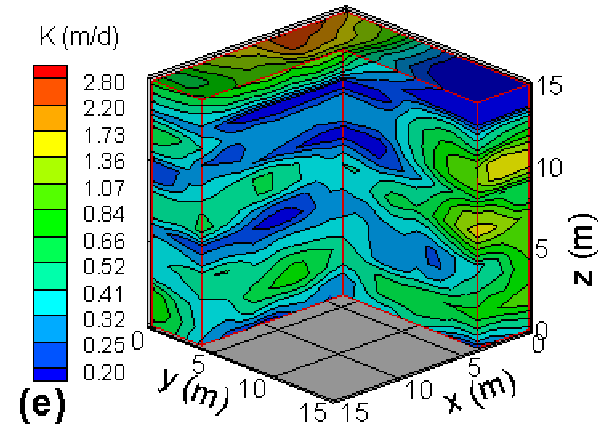
Effective parameters

Statistically uniform

- Stationary and ergodic. Glimm and Kim, 1998
- Single hydro-geological material produced at more or less the same time by more or less the same process.
- Asymptotic expansions. Gelhar and Axness, 1983, Winter et al., 1984; Fannjiang and Papanicolaou, 1997

Statistically heterogeneous media

- Separable scales. Winter and Tartakovsky, 2001. Clark et al., in prep.
- Self-similarity. Neuman, 1994. Molz, 2004



Yeh et al, 2009

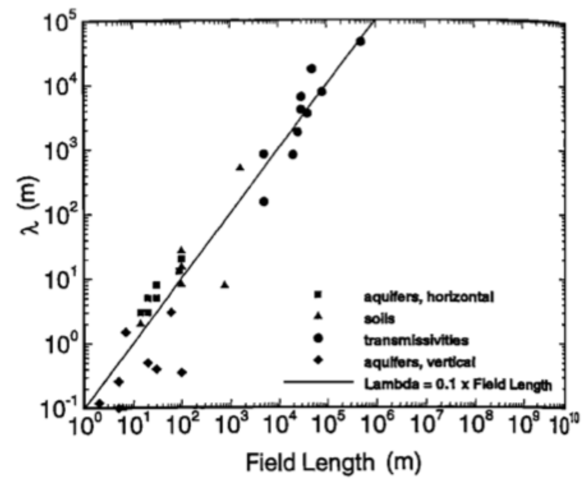


Fig. 1: Correlation scale λ of natural log hydraulic conductivities and transmissivities at various sites versus field length (data from *Gelhar* [1993, Table 6.1]).

Neuman, 1994

Scale-down and Inverse Problem

Statistical interpolation

- Spatial covariance, structure function, Kriging:

$$\gamma(\Delta x) = \mathrm{E}[\ ||K(x + \ ) - K(x)||^2]$$

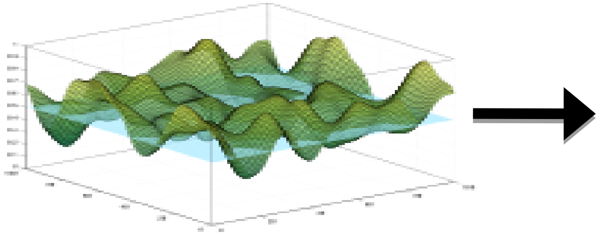
- Monte Carlo simulation

Sequential estimation

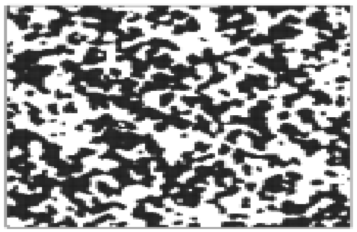
Thresholded fields

Realizations of pore spaces with specified correlations (Adler, 1992) or physical properties, e.g., Minkowski functionals of integral geometry (Hyman and Winter, 2014) can be produced by thresholding Gaussian random fields.

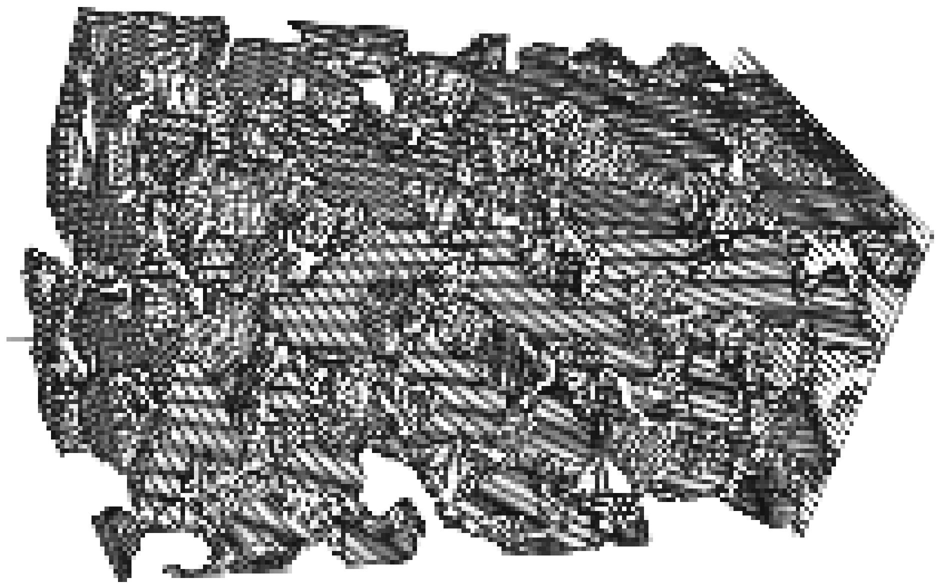
Thresholded Gaussian Fields



Thresholded surface



Simulated pore space



1st Forward problem: Effect of heterogeneities

Zhu et al, 2015
12 realizations

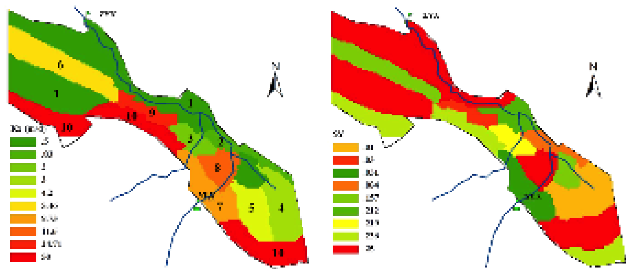


Figure 1. PEST estimated aquifer conductivity K_z and specific yield S_z.

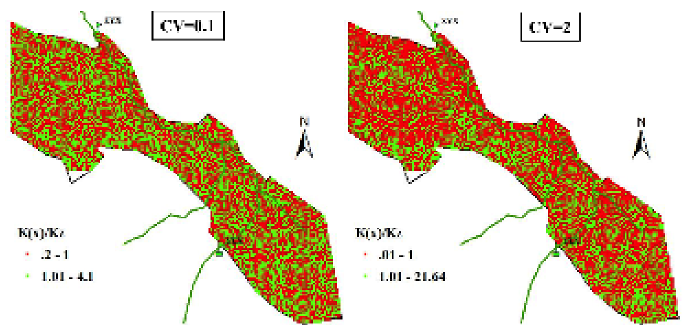
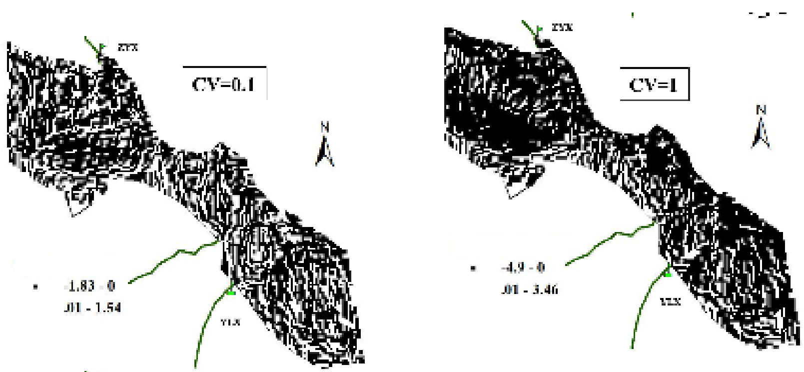


Figure 4. Grid-scale realization of K field perturbation when CV equals 0.1 and 2.



The field of normalized groundwater flow differences $\Delta q(x)$ with grid-scale $K(x)$.

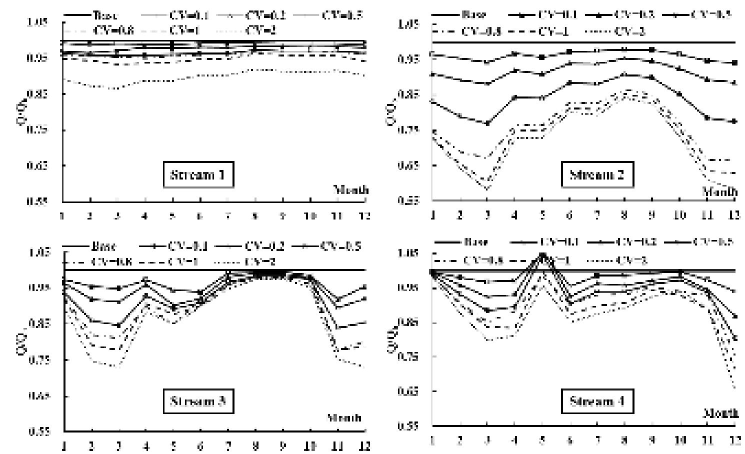


Figure 7. Aquifer–stream discharges of different streams from refined model.

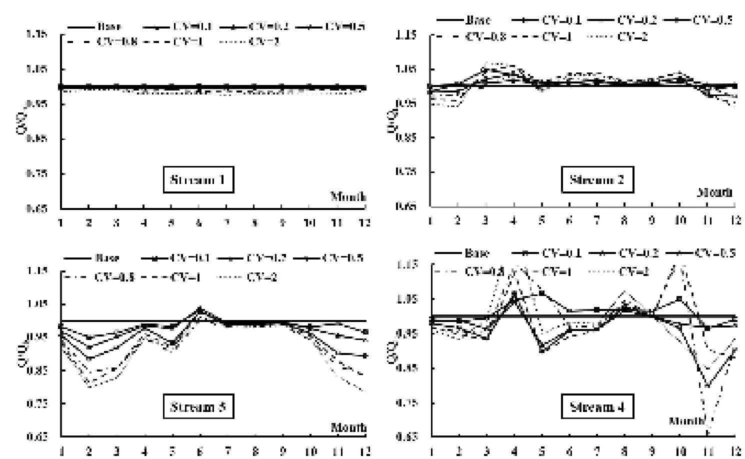


Figure 8. Stream–aquifer leakages of different streams from refined model.

1st Forward problem: Effect of heterogeneities

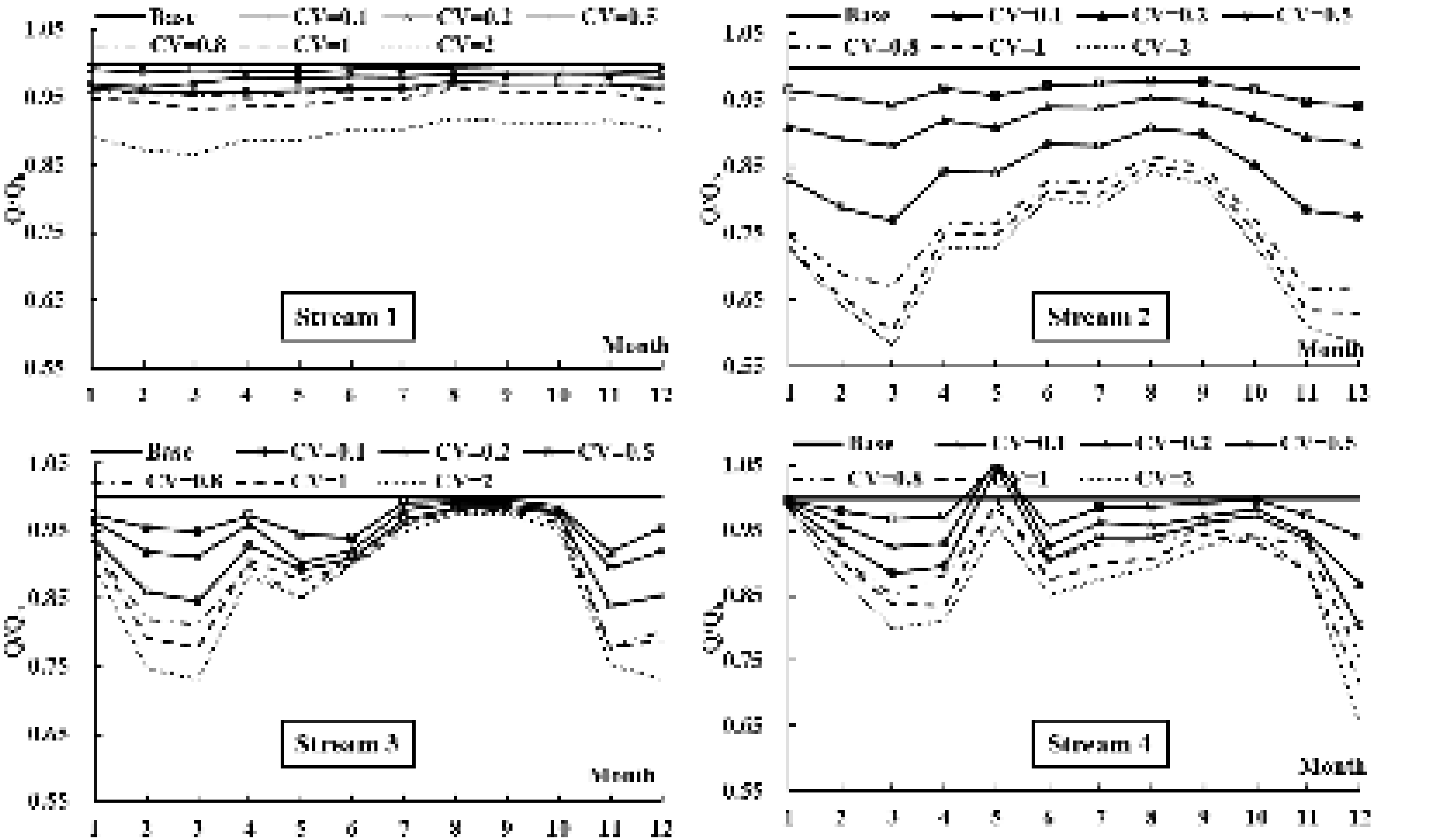


Figure 7. Aquifer–stream discharges of different streams from refined model.

Zhu et al, 2015

2nd Forward Problem: Prediction

Example. Predict hydraulic head, h, in an aquifer based on incomplete measurements, D, of parameters (Π), forcings, and initial and boundary conditions.

An Ill-Posed Problem

Solve the flow equation under these conditions.

It can't be done.

The usual response is to fill in the missing data via calibration, which makes a numerical solution possible, but doesn't solve the problem of uncertainty.

How good is that solution?

A Well-Posed Problem

First, it's not just the head, h, that we don't know.

We don't know the parameters, the forcings or the IBCs either. Call them Π.

The solution is the joint probability of the system state *and* parameters,

$$P[h, \Pi \mid D],$$

conditioned on the measurements.

Bayesian Hydrogeology

Start by making $P[h,\Pi|D]$ more precise,

$$P[h,\Pi|D]=P[M_h,M_\Pi|D]=\frac{P[D|M_h,M_\Pi]}{P[D]}P[M_h,M_\Pi]$$

M_h are the moments of the system state h, e.g., $\bar{h}$, σ_h^2.

M_Π are the moments of the system parameters like IBCs, forcings, K, S.

Determining $P[D|M_h,M_\Pi]/P[D]$ is a geo-statistical problem.

The 2nd term is hydrogeological. It can be further decomposed,

$$P[M_h,M_\Pi]=P[M_h|M_\Pi]P[M_\Pi]\ .$$

Berliner et al., 2000; Wikle, 2003

Predictions

Monte Carlo simulations. Freeze, 1975

Moment differential equations. Zhang and Neuman, 1995; Tartakovsky and Neuman, 1998

$$K(x) = \overline{K}(x) + K'(x)\ ,\ \overline{K'(x)} = 0 \text{ and } h(x) = \overline{h}(x) + h'(x)\ ,\ \overline{h'(x)} = 0$$

$$\overline{\nabla \bullet K \nabla h} = \nabla \bullet \overline{K} \nabla \overline{h} + \overline{\nabla \bullet K' \nabla h'}$$

Orthogonal polynomials. Xiu and Karniadakis, 2003; Zhang and Lu, 2004; Xiu and Tartakovsky, 2006

High heterogeneity. Winter and Tartakovsky, 2001; Guadagnini et al., 2003.

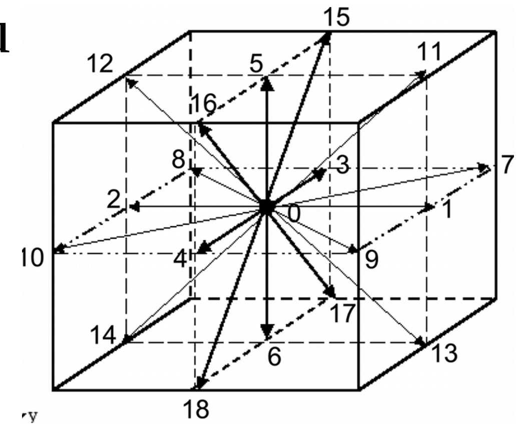
$$p(h, K) = p(h \mid K)\, p(K)$$

Models of reduced complexity

Reduced dimensionality

Orthogonal polynomials. Xiu and Karniadakis, 2003; Zhang and Lu, 2004; Xiu and Tartakovsky, 2006

Wavelet transforms. Foufoula-Georgieu



LBM

Reduced physics

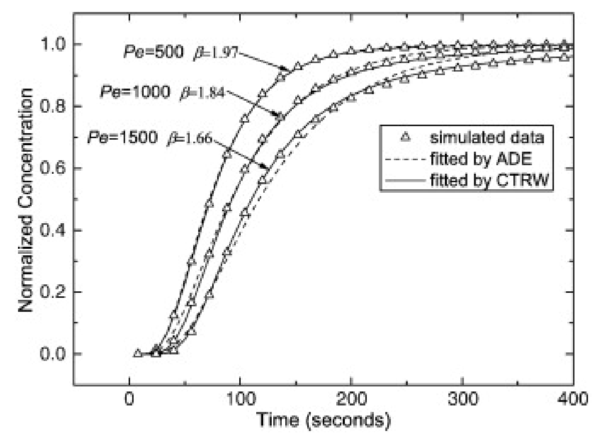
Lattice Boltzmann.

Chen and Doolen,

Continuous time random walk

https://www.weizmann.ac.il/EPS/People/Brian/CTRW/

Berkowitz, 2006.



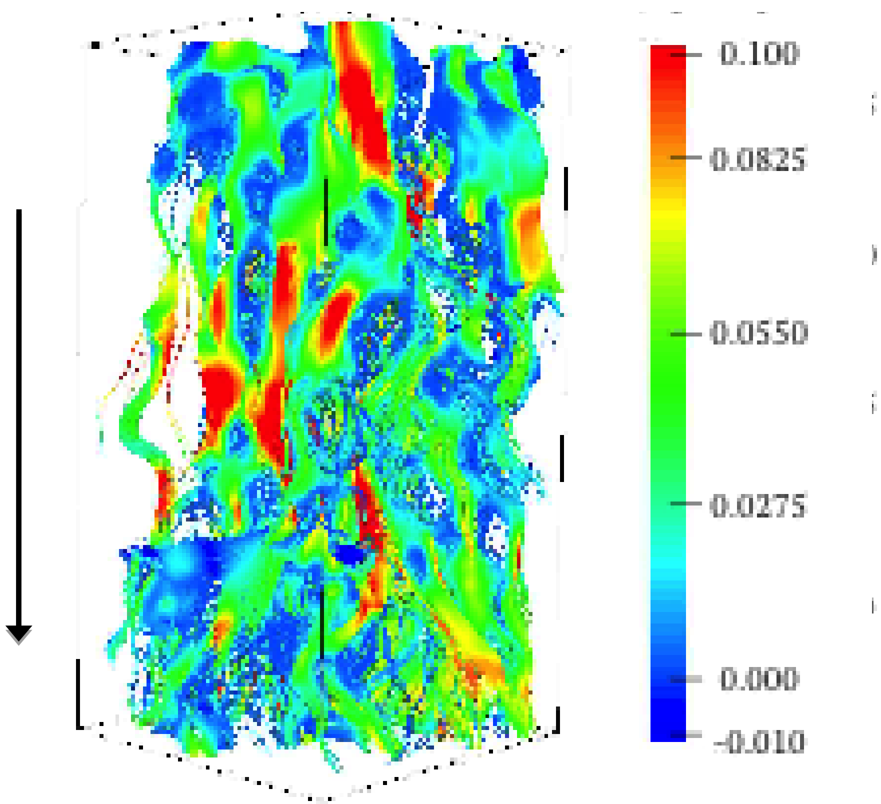
CTRW

State transition diagrams.

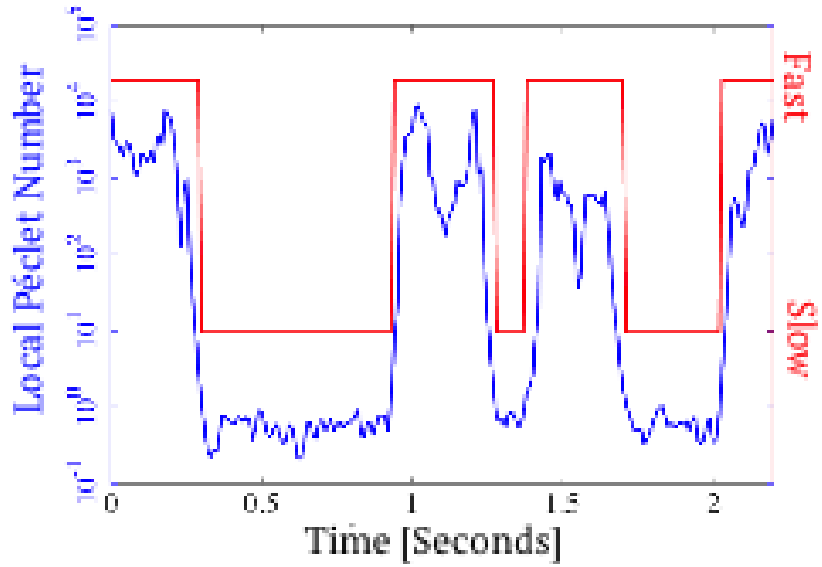
Winter and Tartakovsky (2009)

Jump processes

RCM for particcle breakthrough



Vertical velocities



10^5 particles

Σ, Φ ~ slow and fast states

$L_x = L_y = 1.28$ cm, $L_z = 2,56$ cm

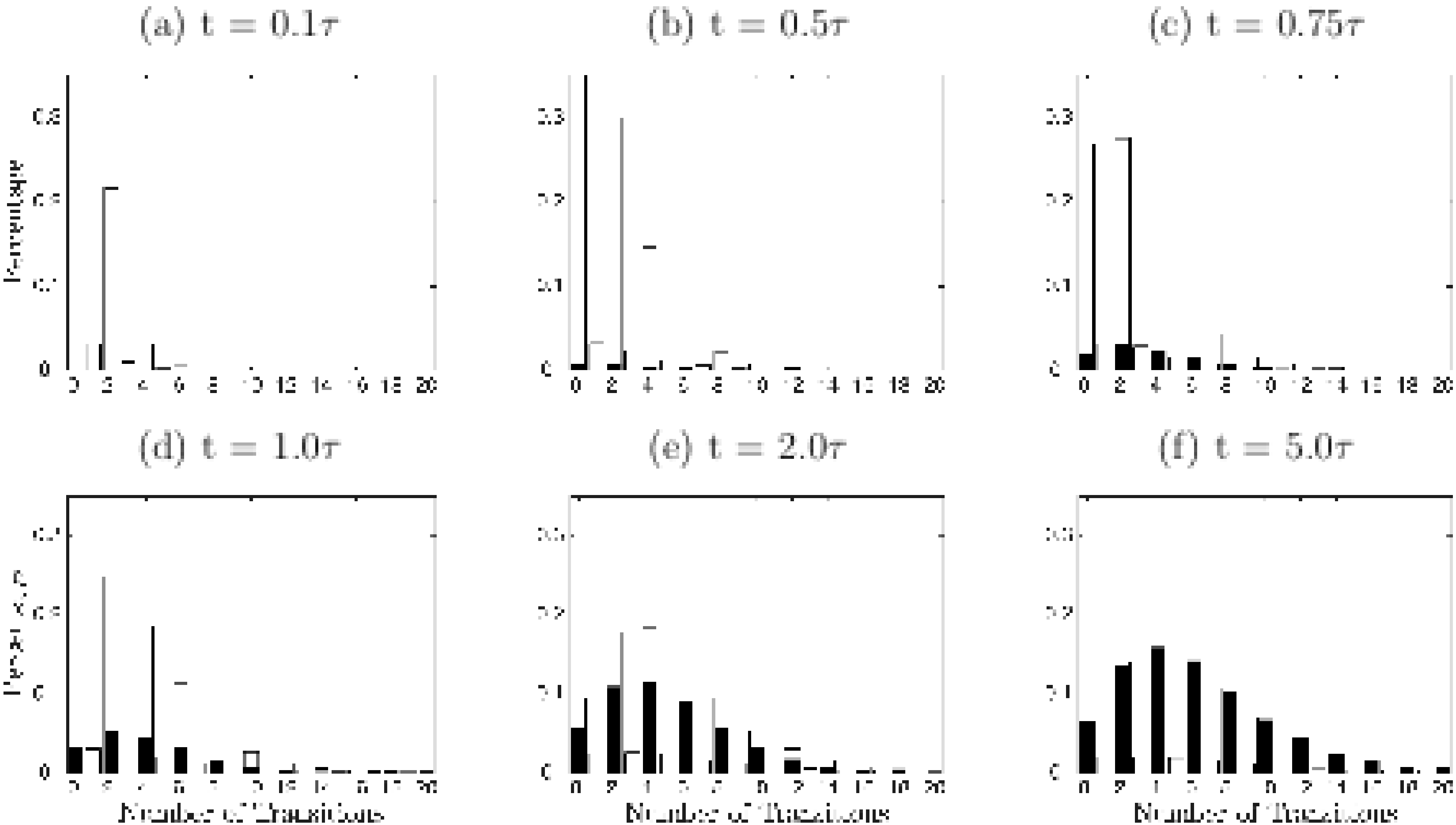
σ, ϕ ~ residence times per state

v_Σ, v_Φ ~ constant velocities

$v_\Phi >> v_\Sigma$

C. Clark – UA
J. Hyman – LANL
A. Guadagnini -- Politecnico

Transitions and break through



Results

n ~ number of transitions

$\nu_n(t)$ ~ # particles that have made n transitions by t

$B_n(t)$ ~ # particles that have broken thru by t after n transitions

$$\mathrm{P}[N(t) = n] = \frac{\nu_n(t)}{10^5}$$

$$\mathrm{P}_n[T < t] = \mathrm{P}[T < t \mid N(t) = n] = \frac{\beta_n(t)}{\nu_n(t)}$$

$$\mathrm{P}[T < t] = \sum_n P_n[T < t] P[N(t) = n]$$

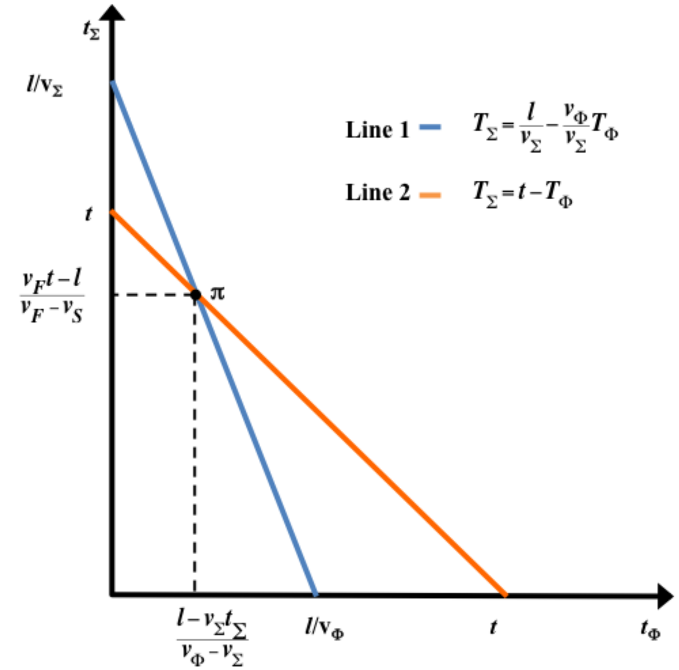
Continuous time Markov chain model

$\mathrm{P}_n[T < t] = \mathrm{P}_n[Z(t) > l]$ before t

$T_\Phi + T_\Sigma = t,\ \ Z(t) = \mathrm{v}_\Phi T_\Phi + \mathrm{v}_\Sigma T_\Sigma$

$\mathrm{P}[T < t] = \mathrm{P}[T_\Sigma = t - T_\Phi\ ,\ T_\Sigma = \frac{l - v_\Phi T_\Phi}{v_\Sigma} l]$

$\mathrm{P}[T < t] = \Sigma_n\ \mathrm{P}_n[T < t]\ \mathrm{P}[N(t) = n]$



Assume CTMC

Residence times exponential

$T^{(n)}{}_S \sim \Gamma(t_S; n_S, s)$

$$\mathrm{P}_n[T < t] \propto \int_{\frac{l - v_\Sigma t}{v_\Phi - v_\Sigma}}^{t} p_n(t - t_\Phi, t_\Phi) dt_\Phi$$

$$\mathrm{P}[N(t) = n] \propto \int_0^t p_n(t - t_\Phi, t_\Phi) dt_\Phi$$