SUBSURFACE HYDROLOGY: PHYSICAL PROCESSES AND DATA AVAILABILITY

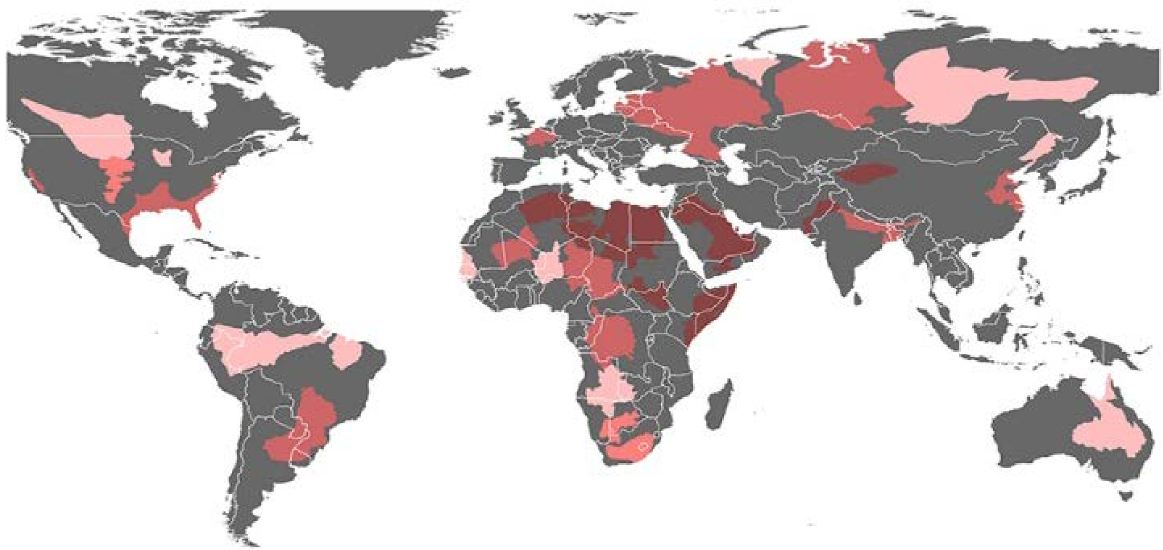
A. Fiori

Roma Tre University, Italy

DOCTORAL WINTER SCHOOL on DATA RICH HYDROLOGY
Villa Colombella, January 28th, February 1st, 2019

Relevance and applications of subsurface hydrology: Quantitative aspects

Changes in Storage vs. Aquifer Stress

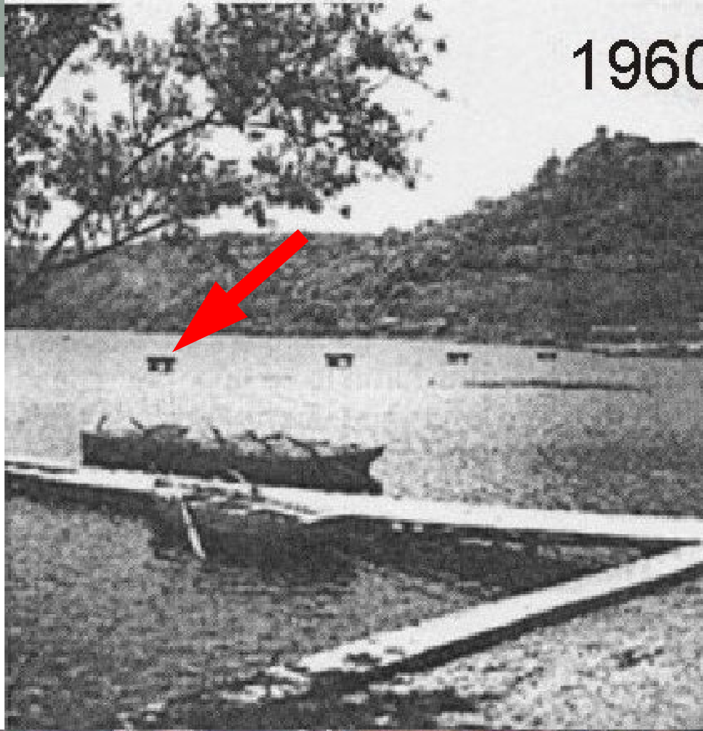


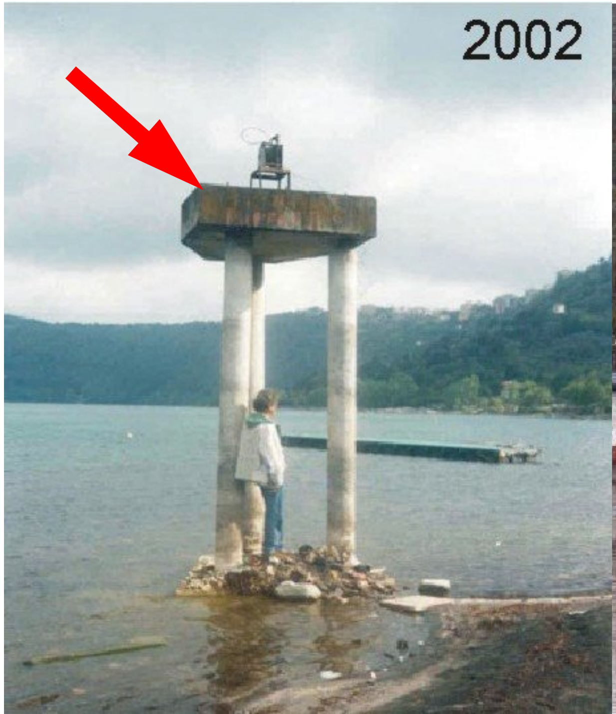
Type of Stress

- Unstressed
- Human-Dominated Stress
- Variable Stress
- Overstressed

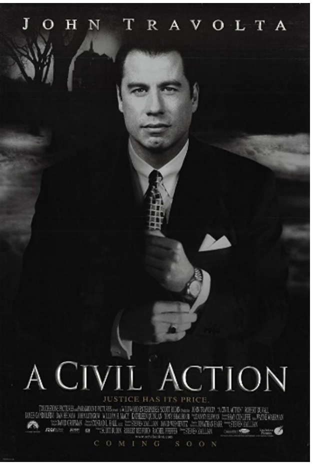
Not all groundwater stress is the same, and changes in storage have a complex relationship with 'stress'. The water supplies of overstressed aquifers are not experiencing any replenishment. Variable stress refers to an aquifer that is in decline but is still experiencing some replenishment. Some aquifers, while actually seeing an increase in storage, are classified as experiencing human-dominated stress. This means that without artificial recharge from human activities, such as water applied to land for irrigation, the aquifer would not record storage increases.

Consequences of overexploitation: the Lake Albano

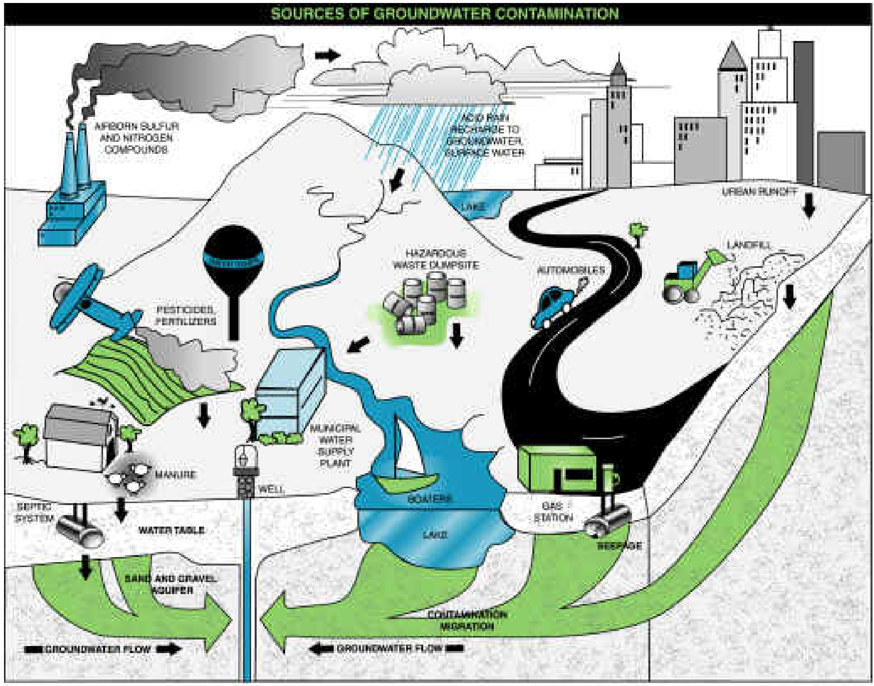




Relevance and applications of subsurface hydrology: Qualitative aspects



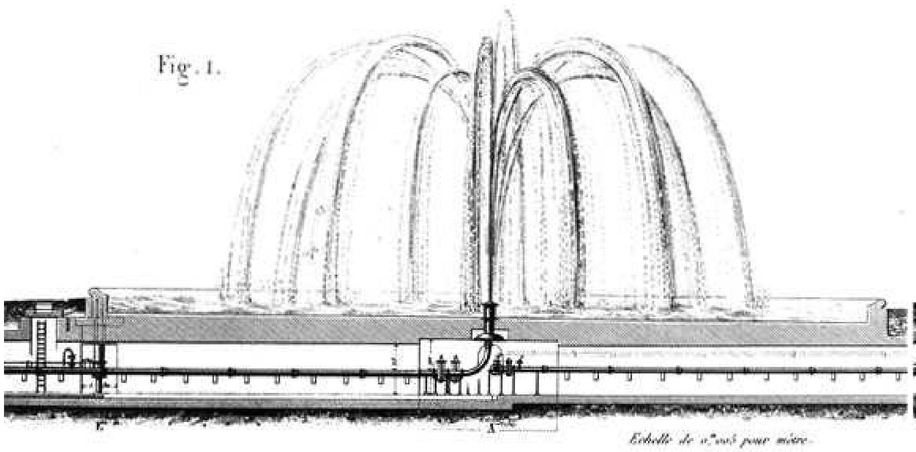
- Groundwater pollution is a widespread phenomenon
- It can occur from on-site sanitation systems, landfills, effluent from wastewater treatment plants, leaking sewers, petrol stations, fertilizers in agriculture.
- Contamination can also occur from naturally occurring contaminants, such as arsenic or fluoride.
- <u>New issues: emerging contaminants and fracking</u>
- Using polluted groundwater causes hazards to public health through poisoning or the spread of disease.



©2000 The Groundwater Foundation. Illustration by: C. Mansfield, The Groundwater Foundation

Birth and development of subsurface hydrology

- Symbolically it starts from 1856, when Hency Darcy Publishes “*Les fontaines publiques de la ville de Dijon*”
- The first 100 years are characterized by the assumption of <u>determinism and homogeneity</u>
- The last 50 years have seen a tremendous development of the discipline



Impact on society and legislation:
The English Rule (Rule of Capture)

1843: Acton v. Blundell

"English Rule"

The landowner can pump groundwater at any rate even if an adjoining property owner were harmed.

1861: Frazier v. Brown

English Rule in Ohio

Groundwater is "…occult and concealed…" and legislation of its use is "…practically impossible."

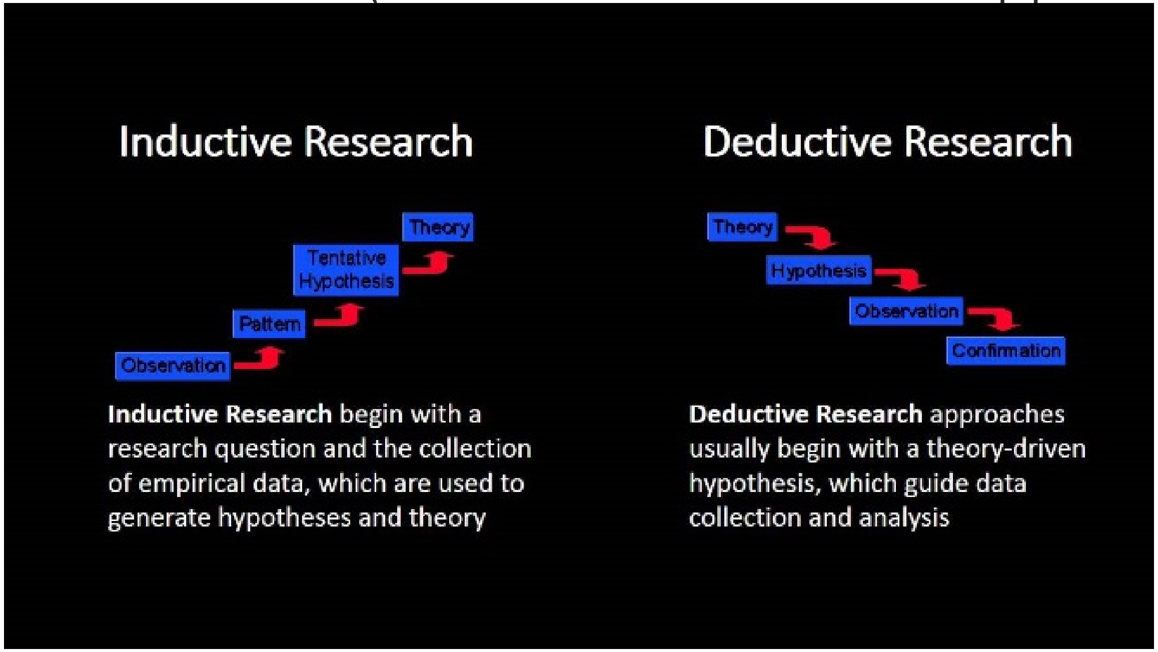
1984: Cline v. American Aggregates

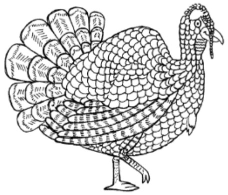
English Rule overturned in Ohio

Justice Holmes: "Scientific knowledge in the field of hydrology has advanced in the past decade…" so it "…can establish the cause and effect relationship of the tapping of underground water to the existing water level."

Subsurface hydrology and the curse of data availability: A push toward *deductive reasoning*

- Subsurface data has always been very scarce, the aquifer environment is known only approximately (ref English Rule).
- The chronic lack of data has led to a significant development of the theoretical aspects of the discpline, leading to a tremendous advancement (deductive vs inductive approach).





Russel's inductiviste turkey

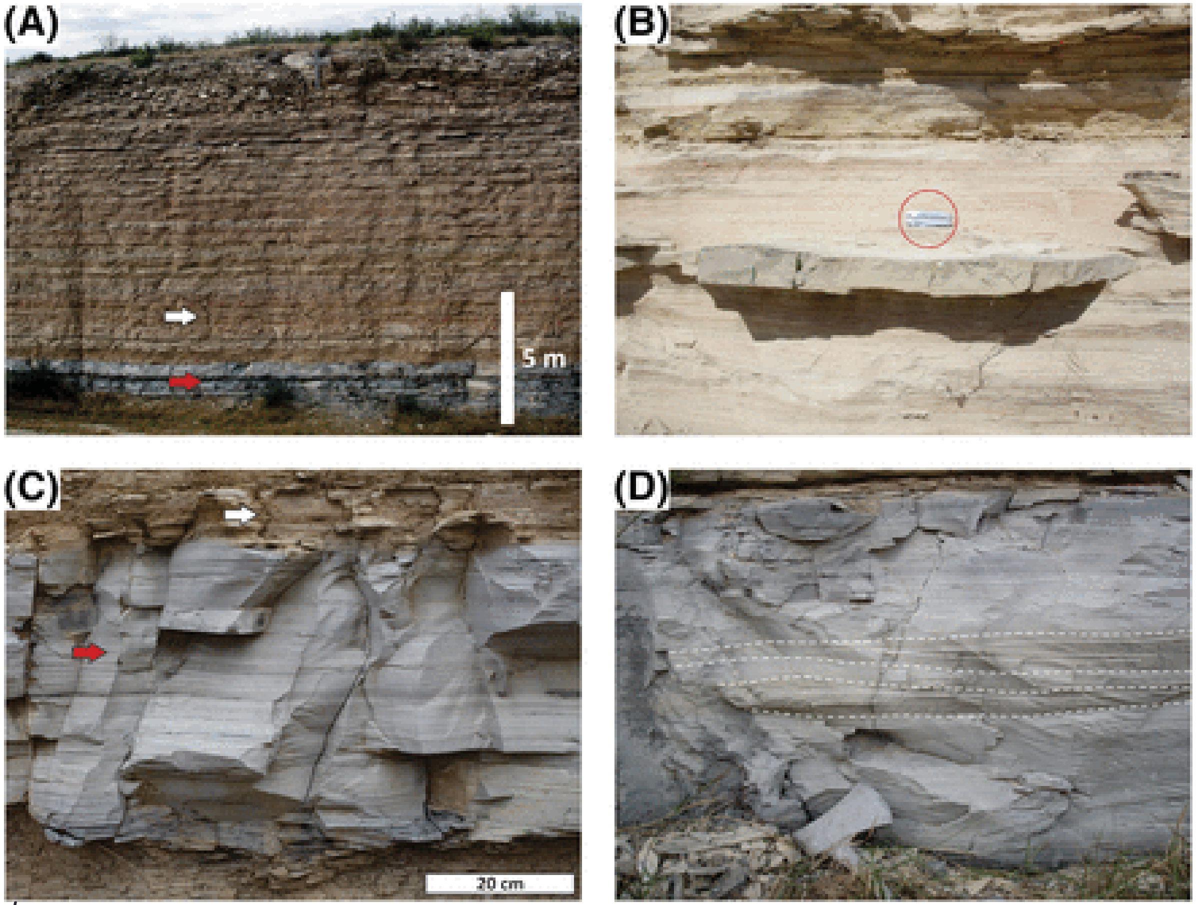
"Induction and Deduction in Physics“, Einstein, 25 December 1919

The truly great advances in our understanding of nature originated in a manner almost diametrically opposed to induction. The intuitive grasp of the essentials or a large complex of facts leads the scientist to the postulation of a hypothetical basic law, or several such basic laws. From the basic law (system of axioms) he derives his conclusion as completely as possible in a purely logically deductive manner. These conclusions, derived from the basic law (and often only after time-consuming developments and calculations), can then be compared to experience, and in this manner provide criteria for the justification of the assumed basic law.

Basic law (axioms) and conclusions together form what is called a "theory." Every expert knows that the greatest advances in natural science, e.g., Newton's theory of gravitation, thermodynamics, the kinetic theory of gases, modern electrodynamics, etc. all originated in this manner, and that their basis has this, in principal, hypothetical character. So, while the researcher always starts out from facts, whose mutual connections are his aim, he does not find his system of ideas in a methodical, inductive way; rather, he adapts to the facts by intuitive selection among the conceivable theories that are based upon axioms.

Uncertainty: a paradigm for subsurface hydrology

- Reliable models of flow and contaminant transport are important tools for risk assessment and management
- Problem:Flow and transport in natural aquifers are largely determined by the spatial distribution of the hydraulic properties



*"I consider it certain that we need **a new conceptual model**, containing the known heterogeneities of the natural aquifer to explain the phenomenon of transport in ground water"*
(Theis, 1967)

*"all significant applications of hydrogeology are **intrinsically uncertain** [...] the only settings in which deterministic models are actually appropriate are primarily academic"*
(Winter, 2004)

Where is uncertainty located?

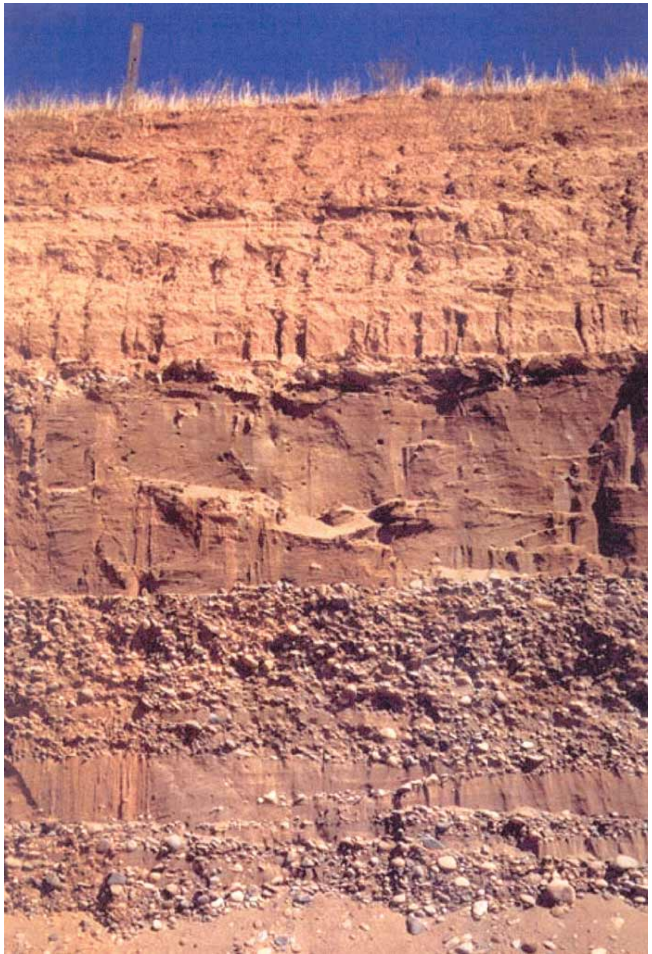
- Conceptual model
  - Geology
  - Boundary conditions
  - Input and output fluxes
  - …
- Spatial variability of hydraulic properties
- Measurement errors
- Errors in the solution of the PDEs
- Errors in the comparison with data (errors and different support scales)
- …

Why is important to quantify uncertainty

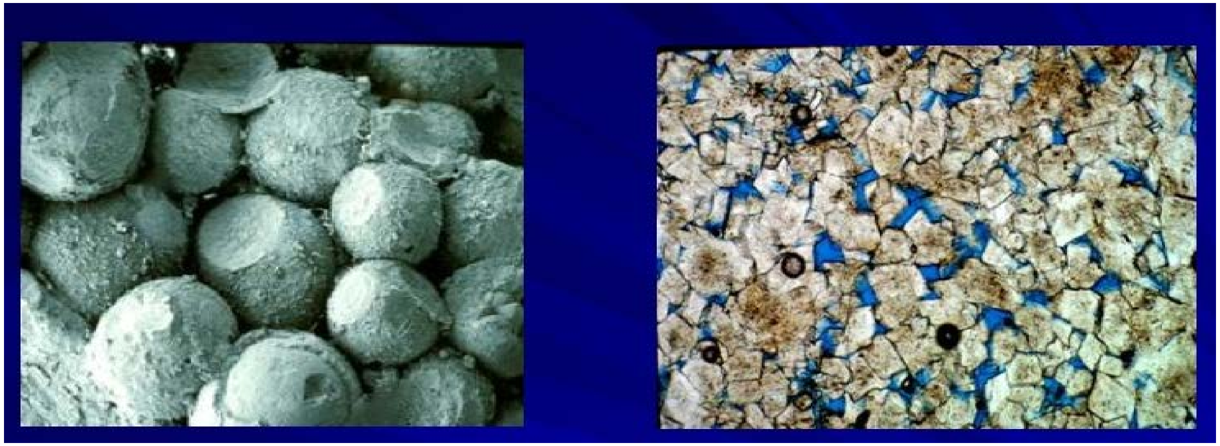
- Correct and effective evaluation of the hydrological processes occurring in complex, subsurface structures (scales etc.)
- Integrate the various hydrological quantities in a rational and coherent manner, considering the different support scales (measurements, heterogeneity, domain, etc.)
- Optimal analysis of the projects (e.g. in view of the WFD 2000/60)
- Design of optimal, “cost-effective” solutions such to incorporate uncertainty
- Risk analysis

Heterogeneity and its effects on subsurface hydrology

- Site characterization
- Water flow
- Contaminant transport
- Management of groundwater resources
- New awareness of the problem of scales



The pore-scale

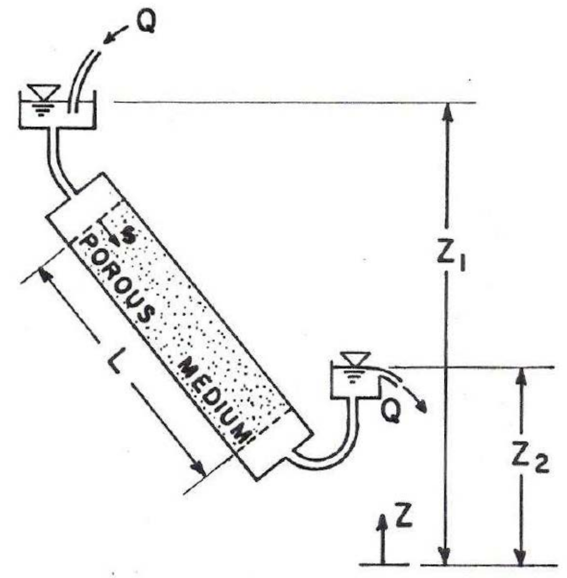


- A porous medium is an interconnected network of voids (pores) in a solid material
- The characteristic length scale *d* is the pore size: from µm to mm.
- The interest is generally in porous bodies of scale *L*>>*d*.
- <u>Macroscopic variables</u> constitute continuous space fields: the porous medium is replaced by a continuum.
- Value of variable at a point *x*: average over a volume (area) of scale ℓ whose centroid is at *x*.
- Homogeneous medium: no change with *x*.

From the pore-scale to Darcy scale

- Darcy's law: $$q = Q/A = K\,(H_{inlet} - H_{outlet})/L.$$
- K : hydraulic conductivity.
- In nature: $10^{-1} \lesssim K(\mathrm{cm/sec}) \lesssim 10^{-6}$
- Generalization for 3D flow in space

$$\mathbf{q} = -K\,\nabla H$$



- For incompressible matrix and fluid, conservation of mass

$$\nabla.\mathbf{q} = 0$$

Solute transport

- At t=0 a conservative solute (tracer) at constant concentration C_0 is inserted at the column entrance x=0; water flows at constant velocity $U=q/n$.
- The BTC (breakthrough curve) at the outlet C(L,t) has an inverse Gaussian shape. C(x,t) obeys the ADE (advective dispersion equation) of solute mass conservation + Fick's law

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D_{d,L}\frac{\partial^2 C}{\partial x^2}$$

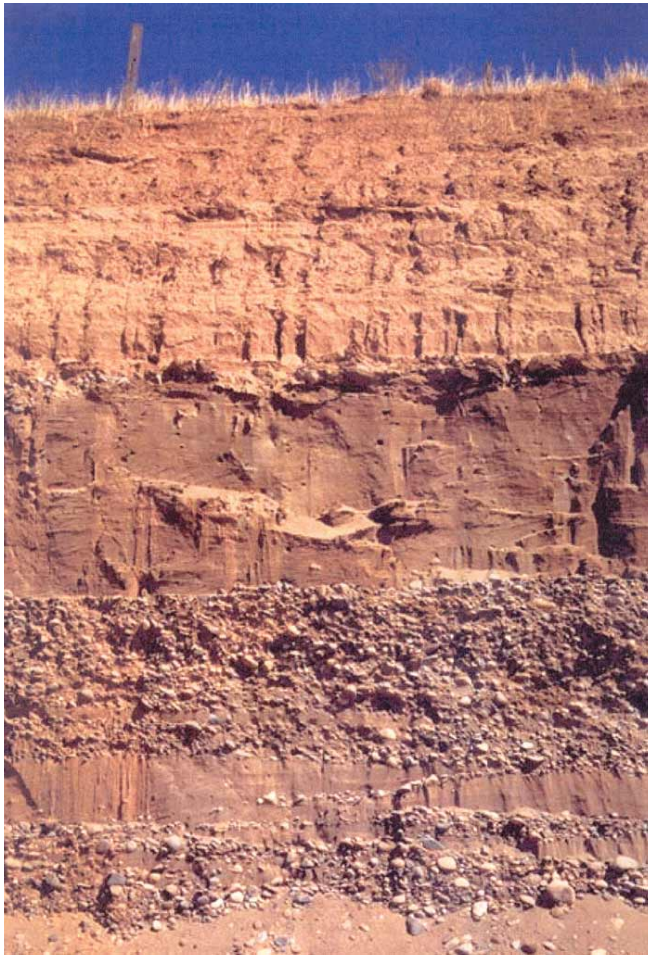
- 3D generalization: $$\frac{\partial C}{\partial t} + \mathbf{V}.\nabla C = \nabla.(\mathbf{D}_d \nabla C)$$

General problem of transport

- Given a space domain Ω, given the velocity field V(**x**) solution of the flow problem, given $\alpha_{d,L}$ and $\alpha_{d,T}$, given initial and boundary conditions for C (e.g. instantaneous or continuous injection in a subdomain of Ω), determine C(**x**,t) satisfying the transport equation.
- Simple case: instantaneous injection of a fluid body of constant concentration C_0 at t=0, for constant U. The centroid of the solute body moves with U, and surfaces of constant C are elongated ellipsoids.

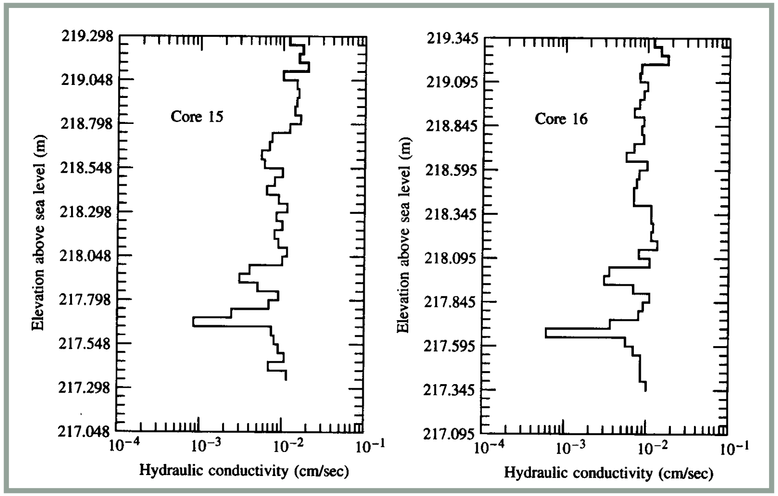
From the Darcy scale to the local scale

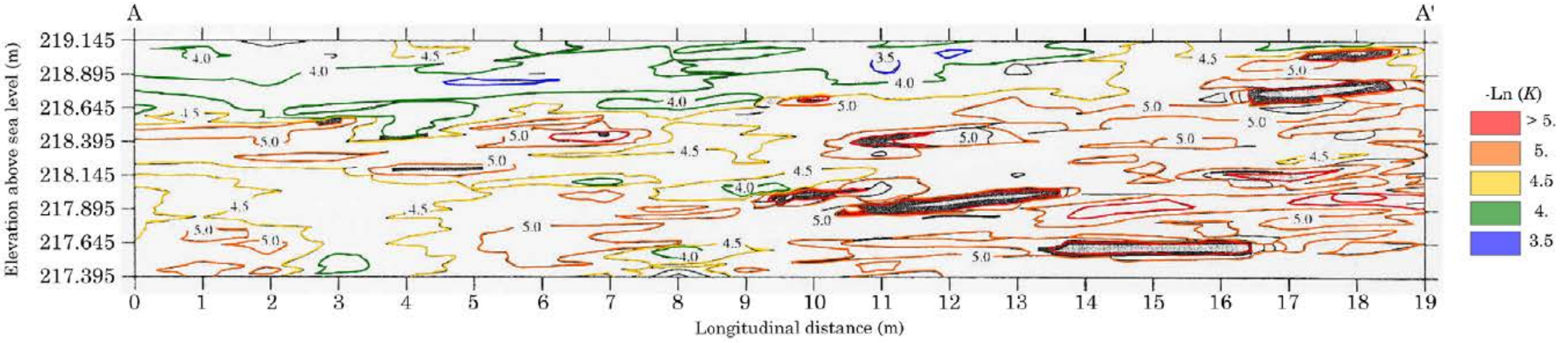
- Natural formations (aquifers, petroleum reservoirs) are characterized by scales *L* =O(10^1-10^3meters). Their properties vary in space over scales *l* much larger than the laboratory scale ℓ.
- The hierarchy L>>l>>ℓ>>d is assumed to prevail.



Heterogeneity: the hydraulic conductivity

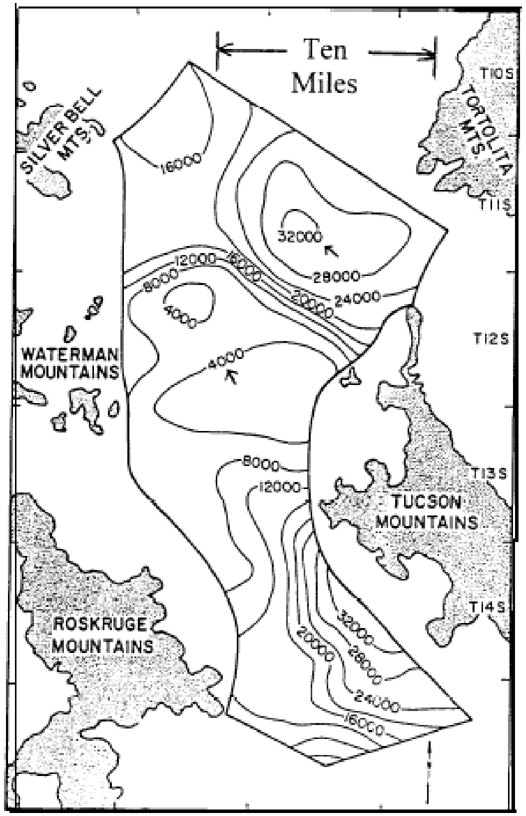
The property of highest spatial variability is *K*, which may vary by orders of magnitude in the same formation. It is irregular (seemingly erratic) and generally subjected to uncertainty due to scarcity of data.





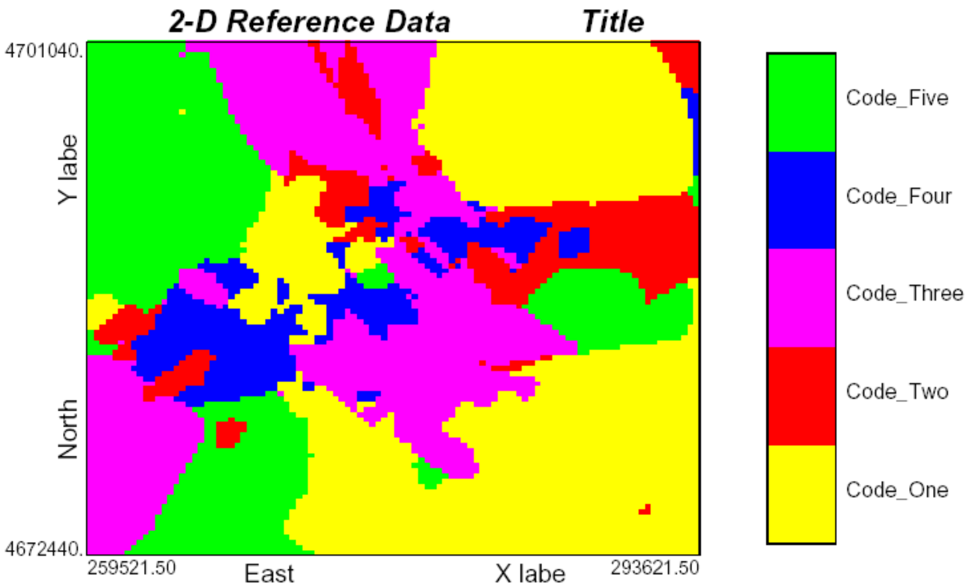
Borden Site, Canada

From the local scale to the regional scale



Transmissivity Distribution (m²lday)
(Based on Kriged Data from 148 Pumping or Recovery Tes

Avra valley; USA (Clifton and Neuman, 1982)

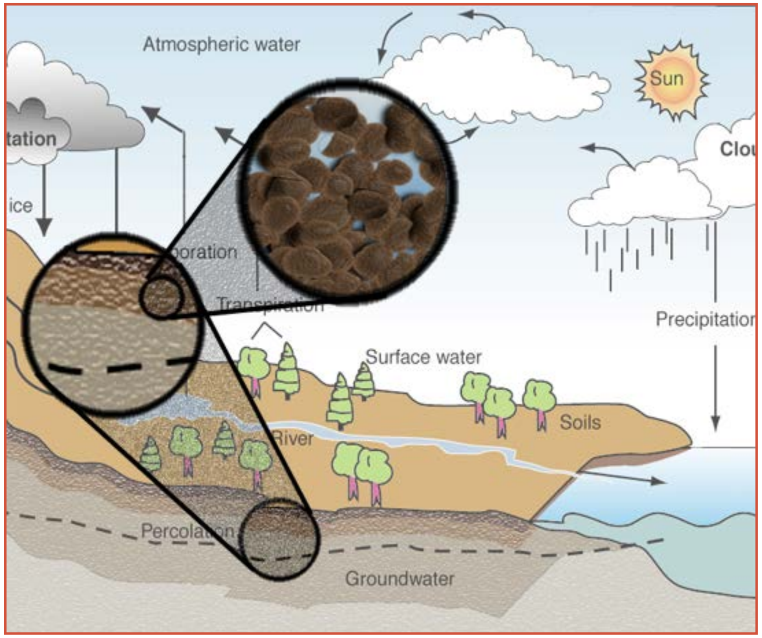


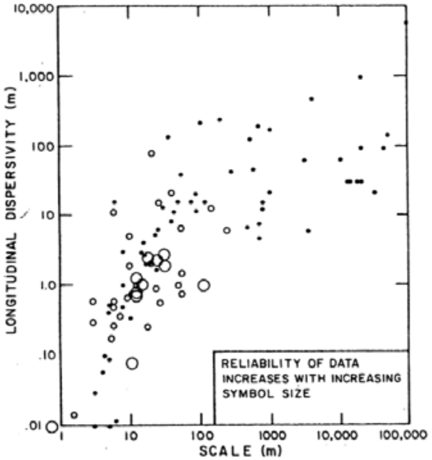
Treja valley; Italy (Conte, 2004)

The scale effect

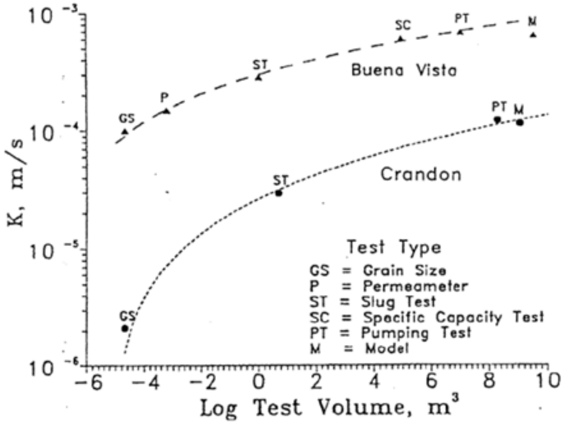
May depend on the observation scale:

- The nature and type of heterogeneity;
- Observed flow and transport phenomena;
- The observed physical quantities (concentration, velocity, etc.)





Dispersivity (Gelhar, 1986)

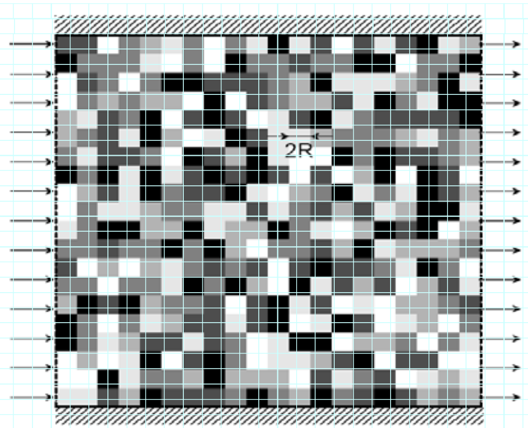


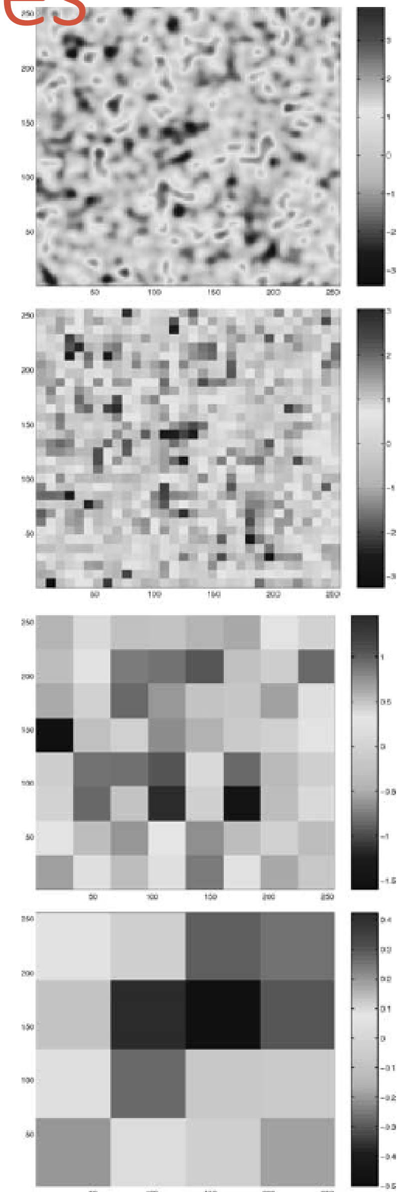
Hydraulic conductivity
(Bradbury & Muldoon, 1990)

Upscaling: the passage accross scales

- How do we model the structure so that flow and transport solutions lead to same quantities of interest (e.g. Mean velocity and macrodispersion)?

- Applications:
  - Effective/equivalent conductivity
  - Block-scale conductivity
  - Effective dispersion coefficient
  - ....

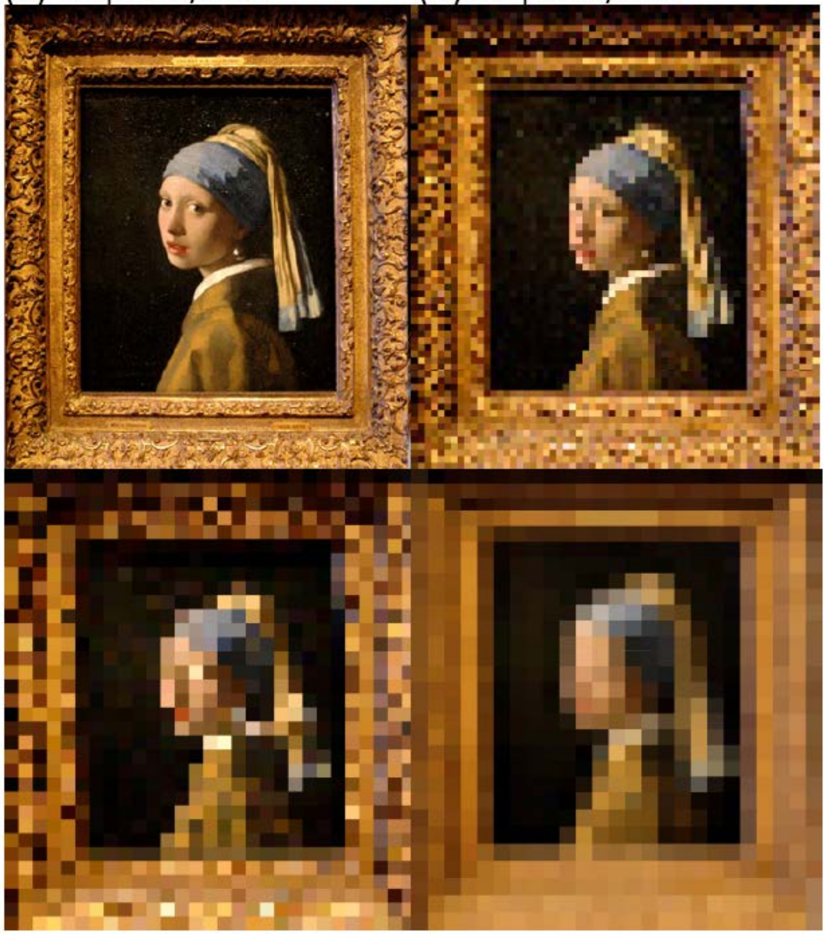




Effective properties and *goal-oriented* characterization

- There is the need to limit the level of information («weight» of the image)
- The final result depends on the available information and the interpolation scheme
- The choice of the resolution/interpolation depends on the particular goal at hand (*goal-oriented*), for instance the recognition of the shape represented in the image or only a particular detail.

(a) 72 pixels/inch (b) 10 pixels/inch



(c) 4 pixels/inch - nearest neighbor interpolation (d) 4 pixels/inch – cubic spline interpolation

The stochastic approach

- Detailed characterization of hydraulic properties is unfeasible;
- It is convenient to describe *K* as a space random function, with assigned statistical properties;
- As a consequence, the flow and transport variables (e.g. piezometric head, discharge, concentration) are also random functions
- The solution of the goverving equations is not simple, even in terms of statistical moments.

Heterogeneity as a random property

- $K(\mathbf{x})$, or equivalently $Y=lnK$, is modeled in statistical terms as RSF (random space function).
- The actual formation is regarded as a realization of an ensemble of replicates of same statistical properties.
- The ensemble is a convenient mathematical construction to tackle variability and uncertainty.
- Replicates can be generated numerically by Monte Carlo simulations.

Statistical characterization of hydraulic conductivity

- The statistical structure of the RSF Y(**x**) can be quantified by the joint PDF (probability density function) of its values at an arbitrary set of points $Y_i=Y(x_i)$: $f(Y_1,Y_2,\ldots,Y_N)$.

- In many formations the univariate f(Y) was found to fit a normal distribution

$$f(Y) = (2\pi\sigma_Y^2)^{-1/2} \exp[-(Y')^2/(2\sigma_Y^2)]$$

where $Y'=Y-\langle Y \rangle$, $\langle Y(\mathbf{x}) \rangle$ is the ensemble mean, σ_Y^2 is the variance.

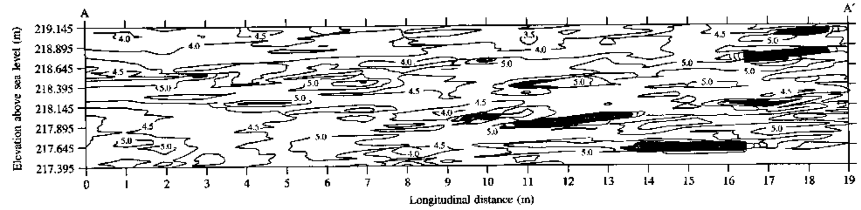
Statistical characterization (cont.)

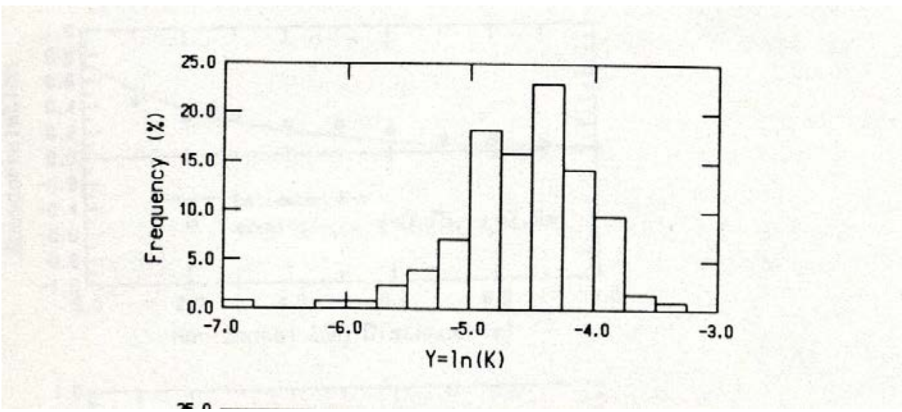
- The bivariate $f(Y_1,Y_2)$ is characterized at second order by the means, the variances and the two-point covariance $C_Y(\mathbf{x}_1,\mathbf{x}_2)=\langle Y'(\mathbf{x}_1)Y'(\mathbf{x}_2)\rangle$.

- If Y is multivariate normal, it is completely defined by these moments.

- Stationary RSF:
  - $\langle Y(\mathbf{x})\rangle$=const, σ_Y^2=const
  - $C_Y(\mathbf{x}_1,\mathbf{x}_2)=\sigma_Y^2\rho_Y(\mathbf{r})$ ($\mathbf{r}=\mathbf{x}_1-\mathbf{x}_2$). Isotropic: $\rho_Y(r)$, $r=|\mathbf{r}|$
  - Integral scale: $I = \int_0^\infty \rho_Y(r)\, dr$ Anisotropic: I_x, I_y, I_z

Example: Borden Site





$$Y = \ln K$$

$$Y \in N(\langle Y \rangle, \sigma_Y^2)$$

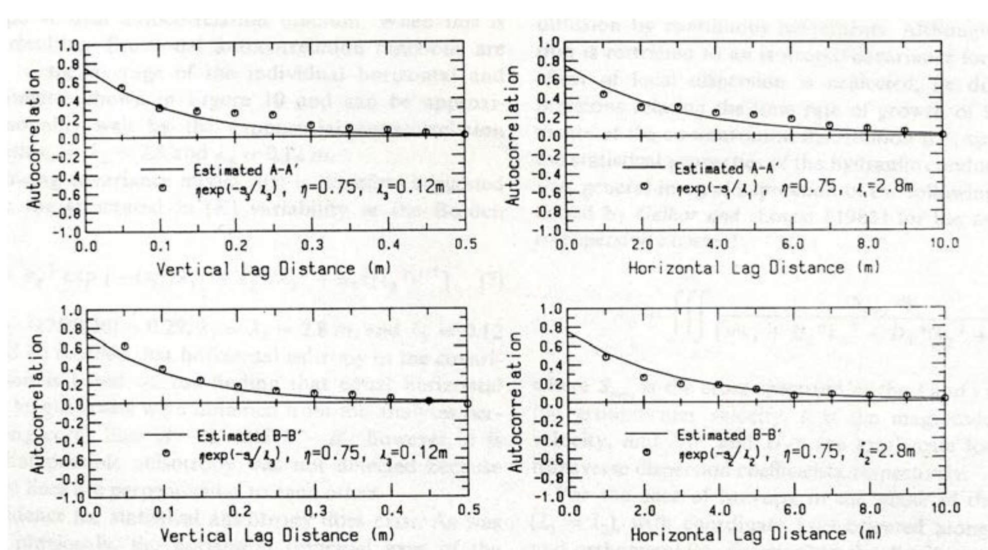


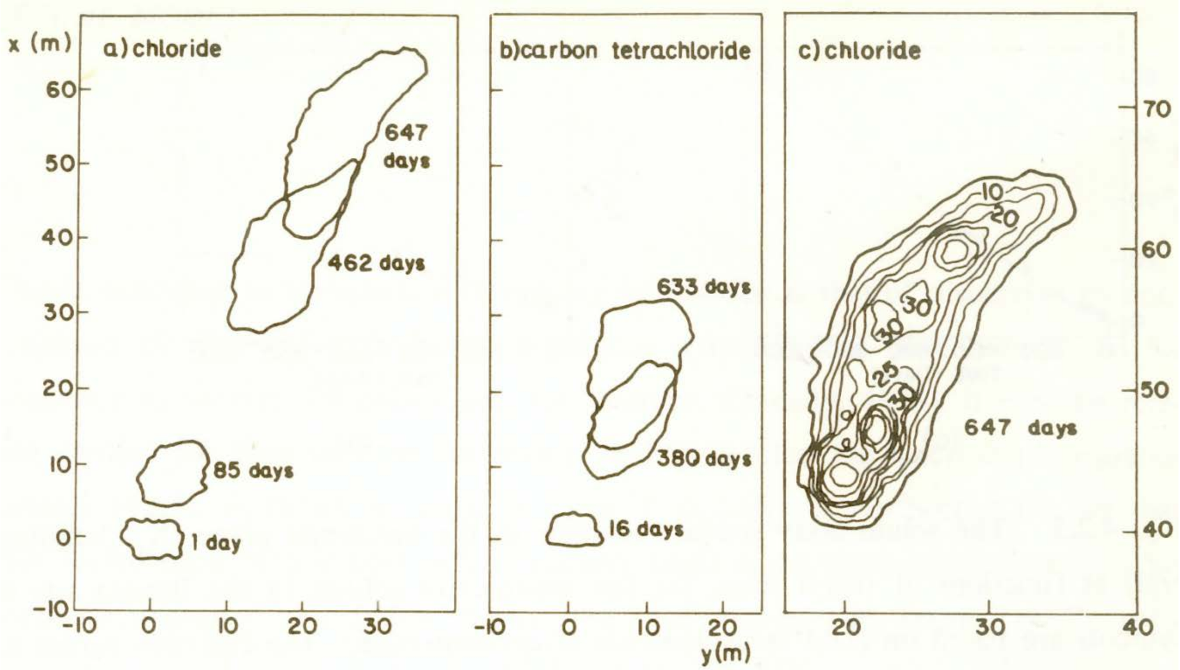
Fig. 10. Vertical and horizontal autocorrelation functions for ln (K) along cross-sections $A - A'$ and $B - B'$.

Stochastic modeling of flow and transport in natural formations

- Since the flow equation $\nabla^2 H + \nabla H . \nabla Y = 0$ contains the RSF *Y*, it is a stochastic equation.
- The variables $H(\mathbf{x},t)$, $\mathbf{q}(\mathbf{x},t)$, $\mathbf{V}(\mathbf{x},t)$, $C(\mathbf{x},t)$ are RSF and are defined by the joint PDF of their values at different **x** and t
- The general problem of stochastic modeling: given a space domain Ω, given the RSF Y(**x**) i.e. K(**x**), given *n*, $\alpha_{d,L}$, $\alpha_{d,T}$ (generally assumed constant), given initial and boundary conditions for H and for C, determine the RSF H,**V** by solving first the flow equation and subsequently the RSF C(**x**,t) satisfying the transport equation.

Impact of heterogeneity on transport: the Borden experiment

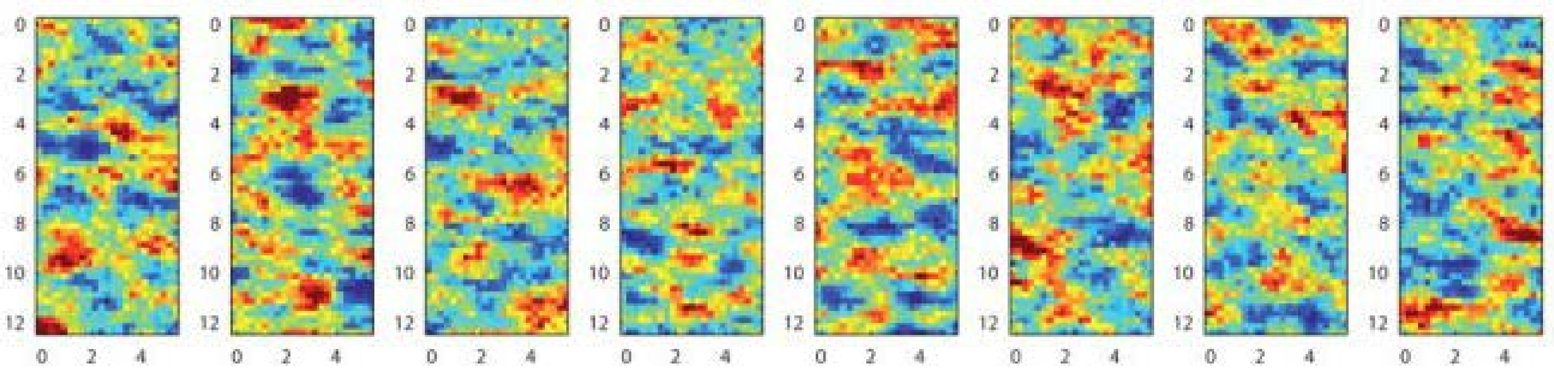
- Heterogeneity of K(**x**) has a major effect on transport, which is enhanced by orders of magnitude as compared to local pore scale dispersion.



Isoconcentration lines for the Borden experiment

Solutions: numerical Monte Carlo

- The conceptually simple and most general approach is by Monte Carlo simulations: realizations of Y are generated, the deterministic equations for each realizations are solved M times, and the complete statistics is determined at N points.
- It is computationally demanding and does not lead to significant insight. At present and for highly heterogeneous formations, they are numerical experiments at most.



Solutions: approximate analytical

- Approximate solutions are sought for simplified conditions, such as:

  - Stationary logconductivity $Y \ (\langle Y \rangle, \sigma_Y^2, I_h, f)$
  - unbounded domain Ω (i.e. **x** is far from the boundary)
  - steady flow, uniform in the mean **⟨V⟩**=**U**=const (caused by a uniform mean head gradient ∇⟨H⟩=-J applied on the boundary approximately valid for natural gradient flow)

Lagrangian approach and quantification of transport

- The initial solute body is regarded as made up from indivisible particles of mass ΔM. In the case of injection in a volume in the resident mode: $\Delta M = C_0 \Delta V_0$. For instantaneous injection in a plane $\Delta M/M_0 = m_0 \, \Delta A_0$ where M_0 is total mass and m_0 is (relative mass of solute)/area, i.e. $\int_{A_0} m_0 dA_0 = 1$
- In the resident mode m_0=const, in the flux proportional mode $m_0(\mathbf{a}) = [V_x(\mathbf{a})/U](\Delta M/M_0 \, \Delta A_0)$ where $\mathbf{x}=\mathbf{a}$ is a coordinate in A_0 or V_0.

Transport equation

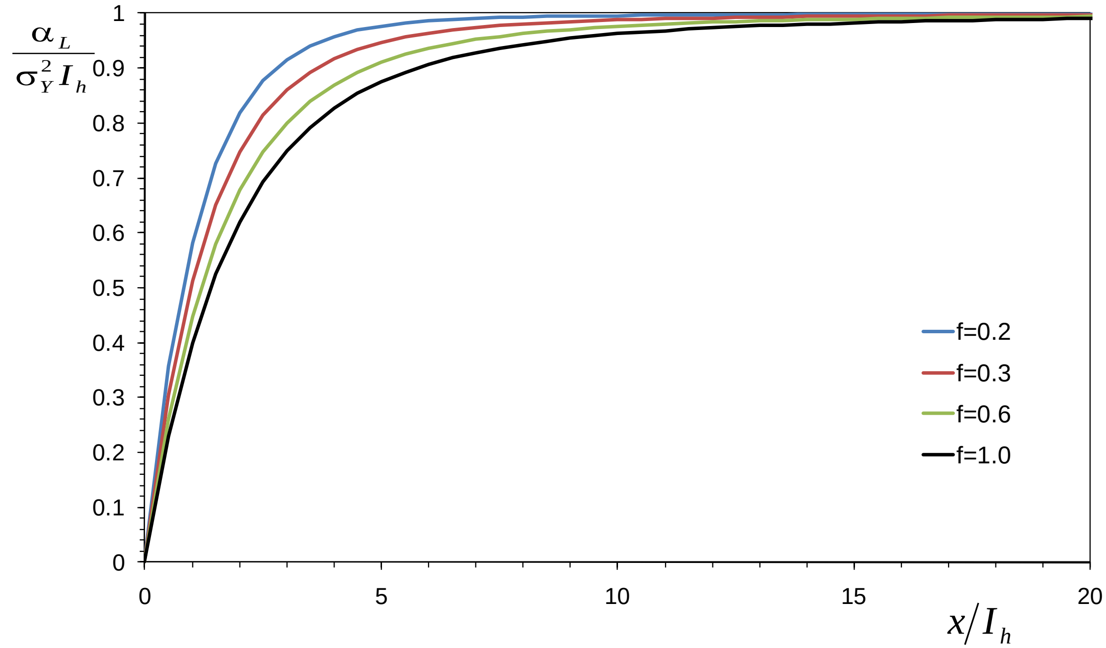
- The mean concentration in transport of Gaussian travel time or trajectories distributions satisfies the ADE

$$\frac{\partial \langle C \rangle}{\partial t} + U \frac{\partial \langle C \rangle}{\partial x} = \alpha_L U \frac{\partial^2 \langle C \rangle}{\partial x^2}$$

where α_L is the macrodispersivity, characterizing spreading of solute due to heterogeneity $\alpha_L(x) \rightarrow \sigma_\tau^2/(2U^2x) = \sigma_u^2 I_u/U^2$ for $x/I_h > 1$.

Longitudinal macrodispersivity

- It is seen that α_L is <u>non-Fickian</u> and reaches the asymptotic constant value after a "setting" distance x/I_h~10.
- The asymptotic value is does not depend on anisotropy and from the solution of the flow problem it is given by **$\alpha_L = \sigma_Y^2 I$**

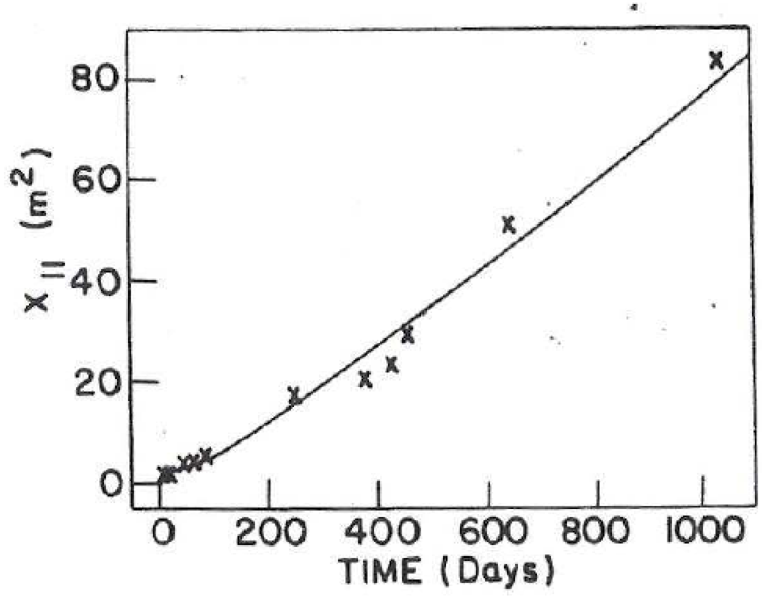


- For common values of σ_Y^2 and I_h, $\alpha_L >> \alpha_{d,L}$. For example for the Borden Site aquifer, $\sigma_Y^2=0.38$, $I_h=2.8$m, $\alpha_L=0.36$ m whereas $\alpha_{d,L} \cong 0.001$ m

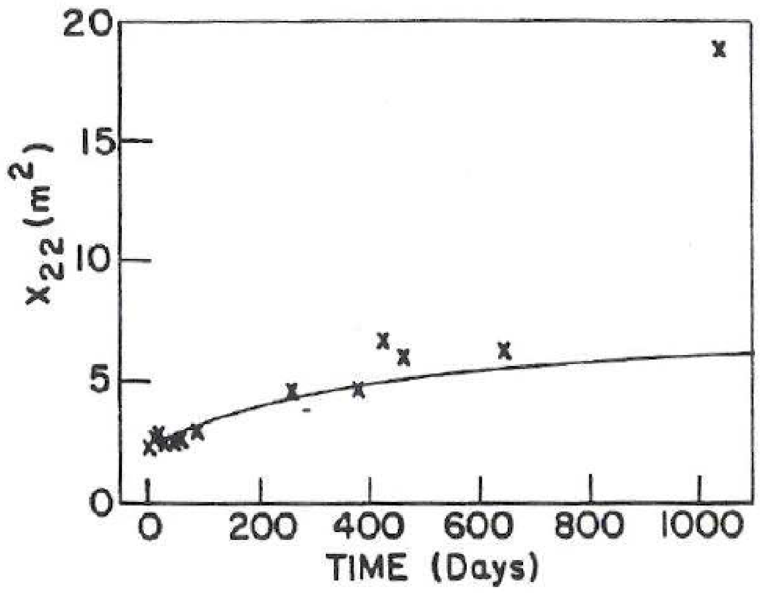
Longitudinal macrodispersivity (cont.)

- Numerical simulations and field tests have showed that the first order approximation is quite accurate for $\sigma_Y^2 \leq 1$, making it useful for many aquifers of weak heterogeneity.
- The first-order solutions have successfully explained several flow and transport features, like e.g. macrodispersion and non-Fickianity

Application to the Borden Site



(a)



(b)

from Dagan, 1984

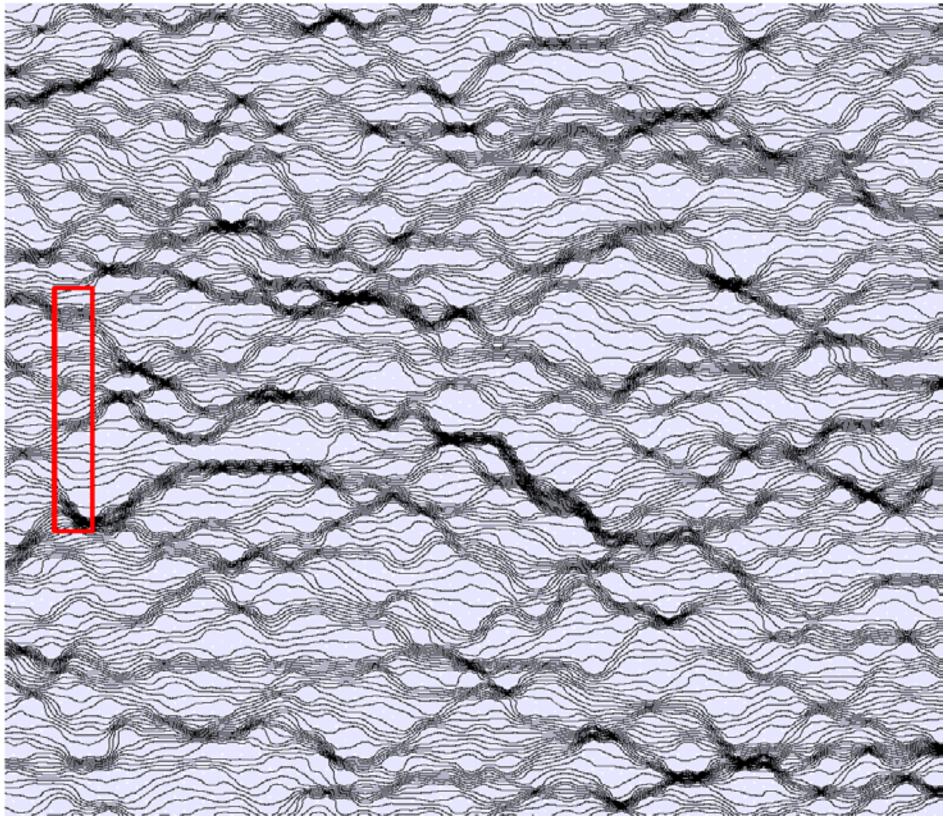
A few unresolved issues (strongly heterogeneous formations)

- Large dispersivities (scale effect?)
- Large “setting times”, non-Fickian stage (non-Fickian transport?)
- Non-Gaussian breakthrough curve (ADE solution / Gaussian model not appropriate?)
- Anomalous transport?
- Connectivity?

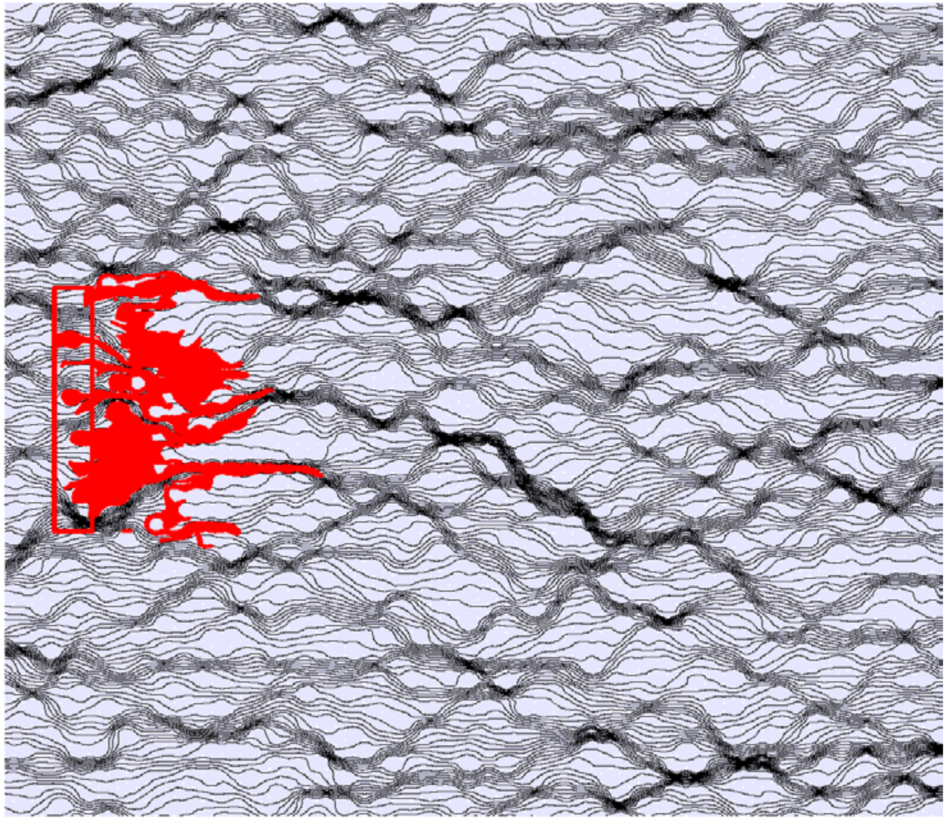
Numerical Laboratory (2D example)

$\sigma_Y^2=4$, n=0.9

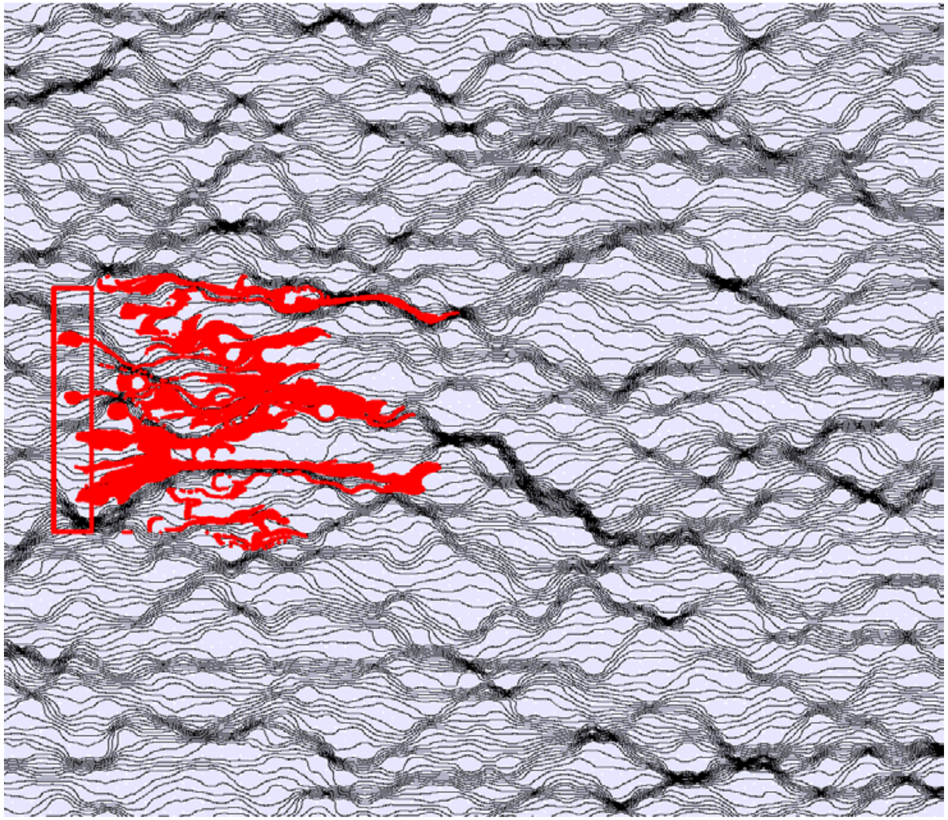
$tU/I_h=0$



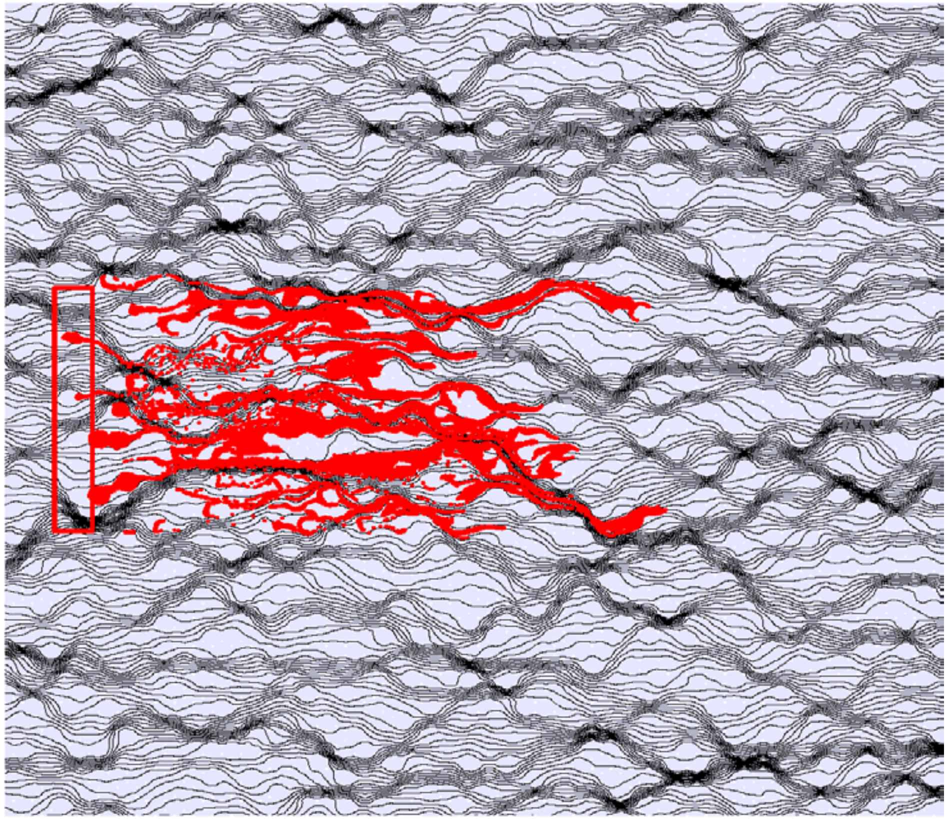
tU/l_h=7.5



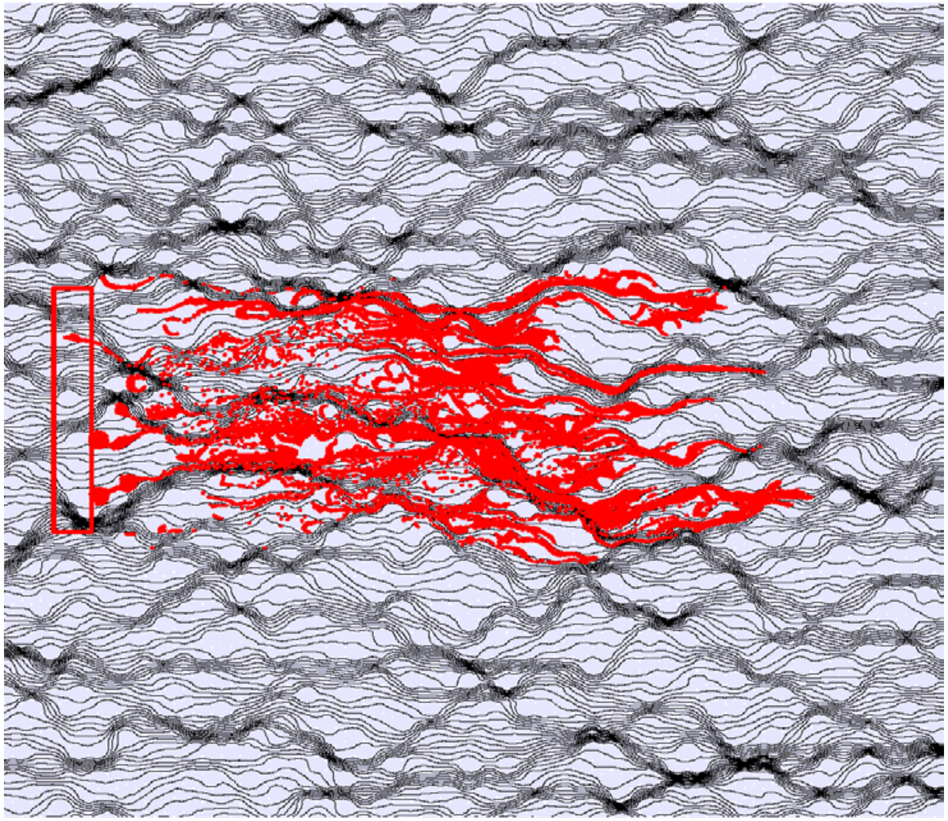
$tU/l_h=15$



tU/l_h=22.5

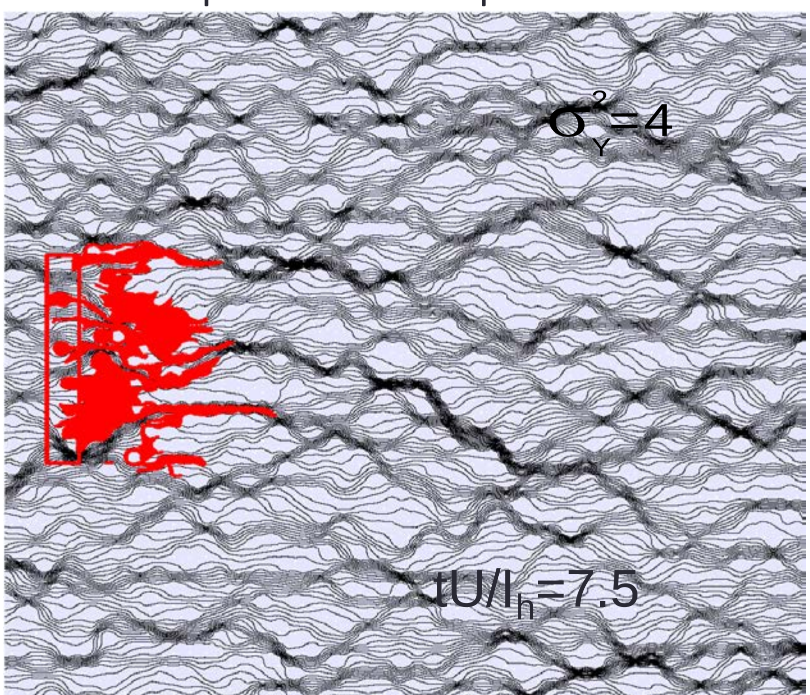


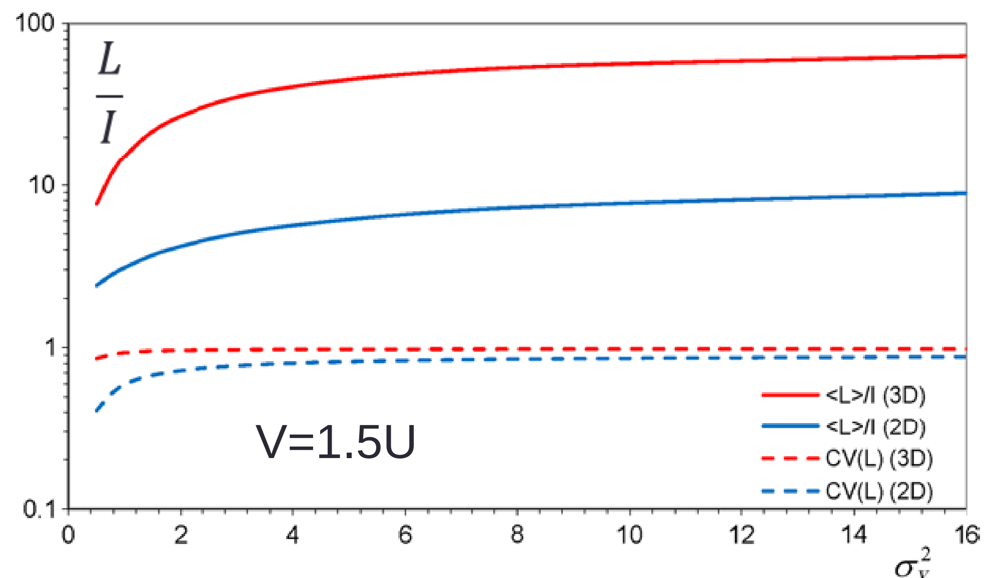
tU/l_h=30



Connectivity / Channeling

- Channeling emerges naturally in highly heterogeneous formations, even in stationary *K* structures with finite correlation length of *K* (it is a *flow-related* feature)
- The distribution of the length of connected pathways strongly depends on space dimensionality



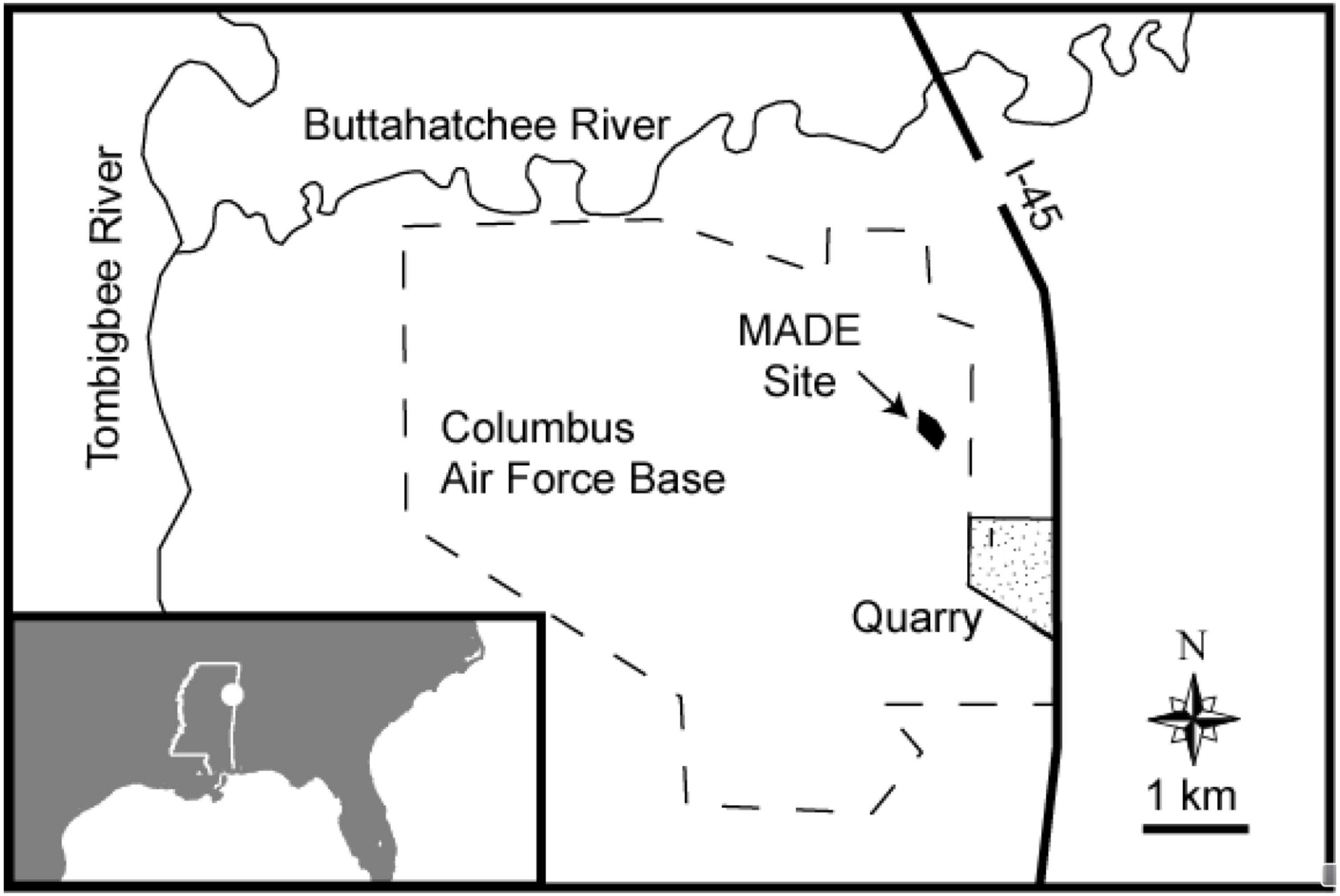


Fiori and Jankovic, MG 2012

The MAcroDispersion Experiment (MADE): Background

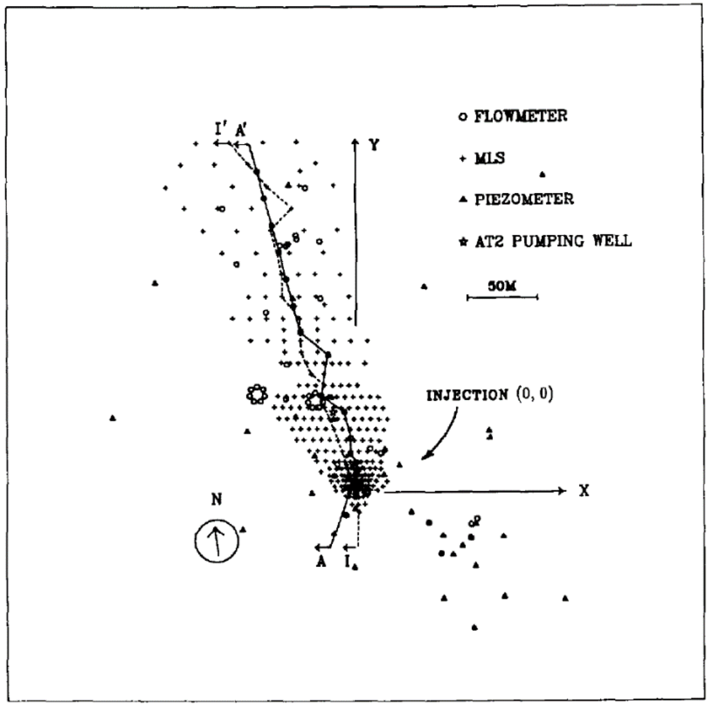
- In early 80’s, the success of the macro-dispersion theory in its application to the first large-scale tracer test at the Borden site spurred excitement that it was suitable for modeling field-scale transport processes;
- The MADE site was identified in mid 80’s as a more heterogeneous setting than Borden to test the macrodispersion theory in strongly heterogeneous aquifers;
- Along with several well-known tracer test sites, the MADE site has had a tremendous impact on how we view contaminant transport in the subsurface today.

The MADE site



Aerial view of the MADE site

- Columbus, MS (USA)

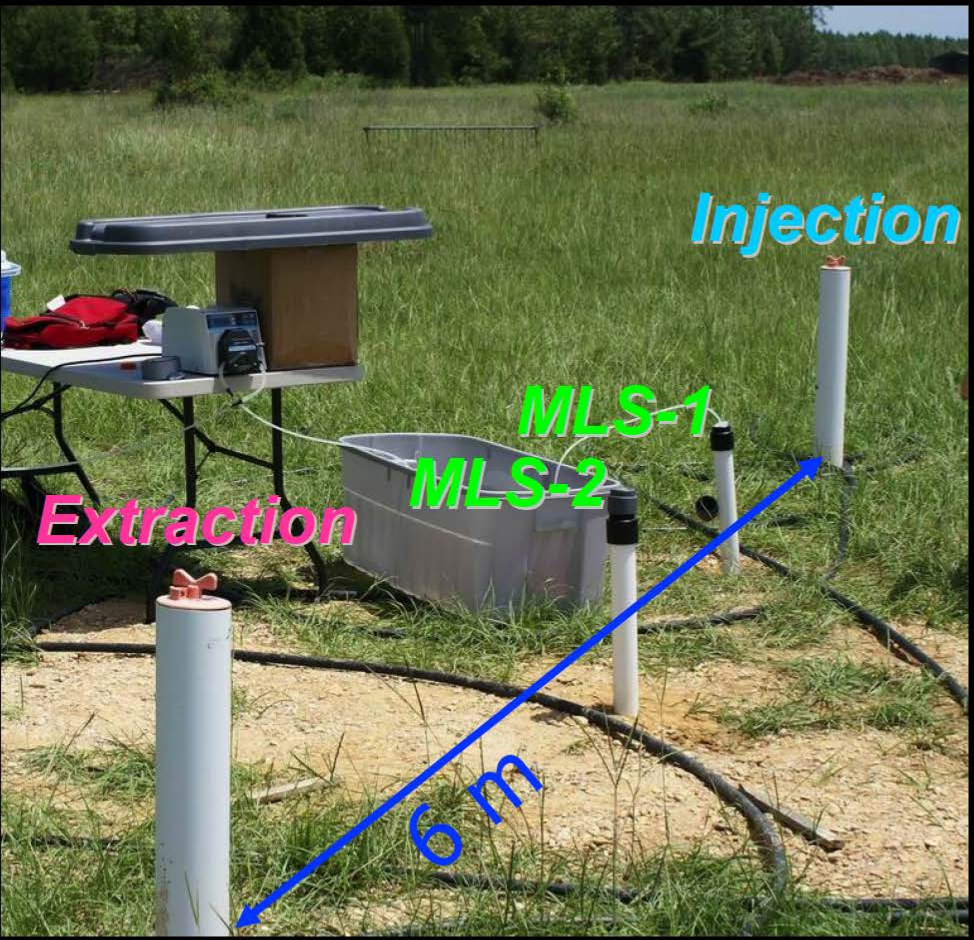


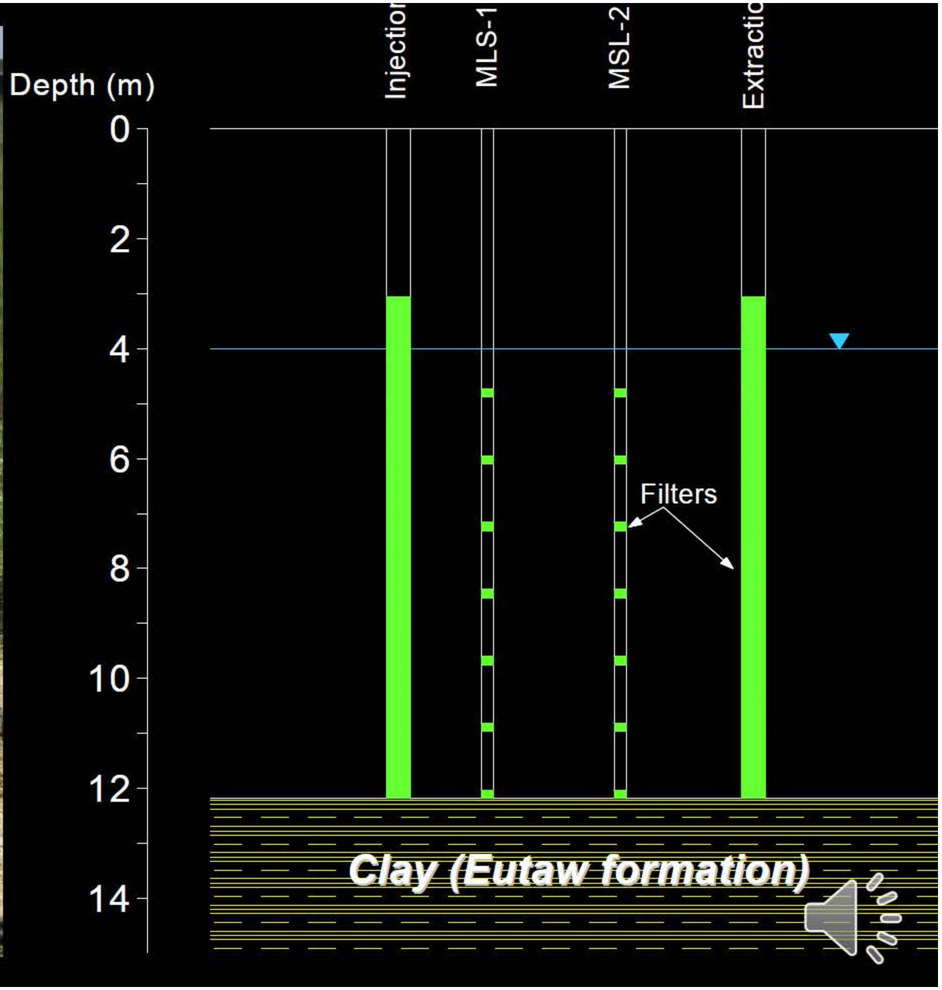
Porous material at MADE

View from a Quarry ~750 m from the MADE Site

- Shallow unconfined aquifer consisting of a highly heterogeneous mixture of sands, silts, and gravels;
- About 10m in saturated thickness, underlain by continuous clay layer.

Dipole tracer test (MADE-5)





Interpretation of the dipole test (from Zech et al, GW, 2018)

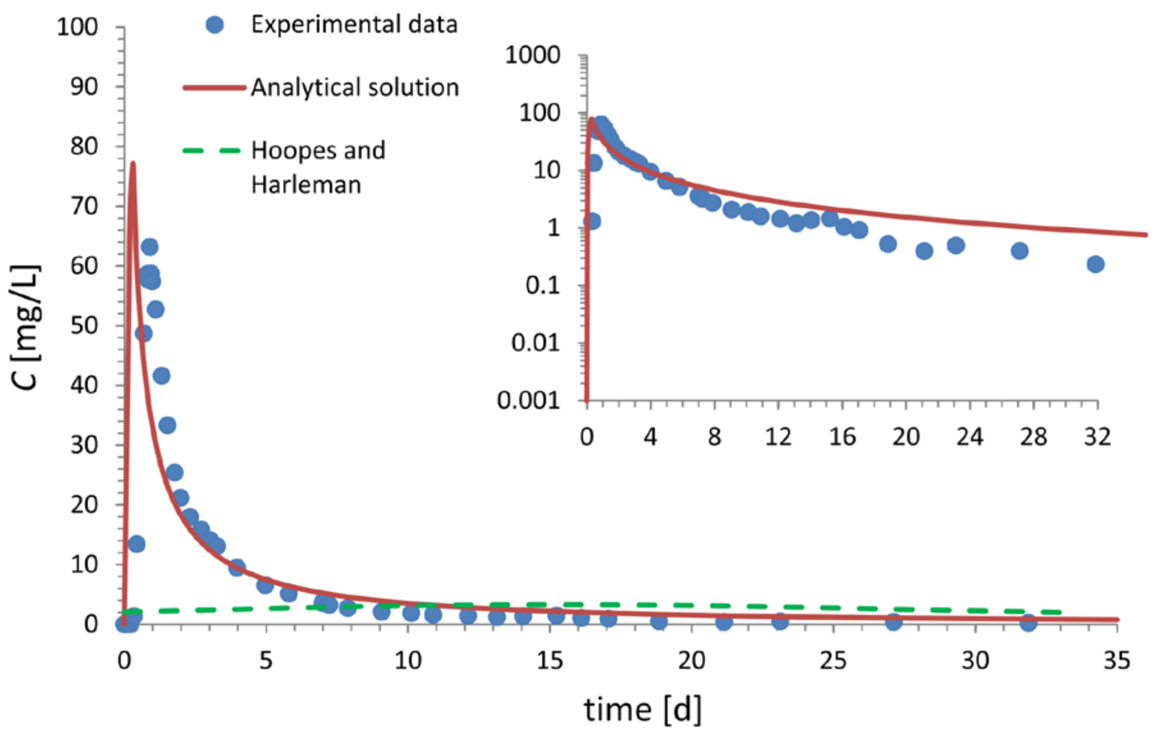
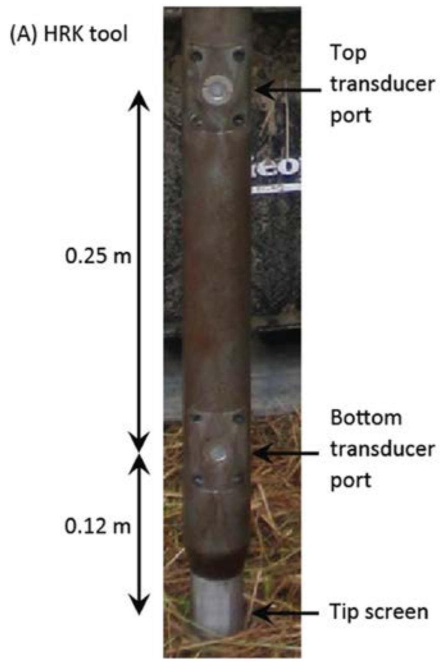
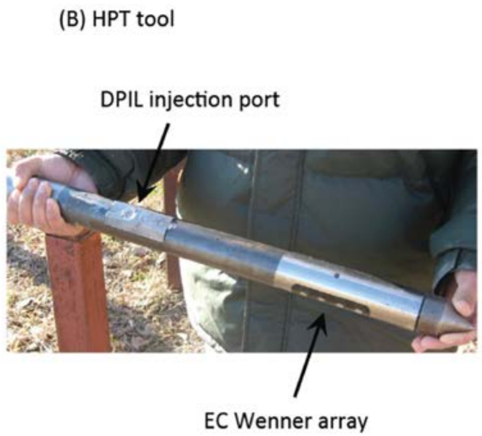
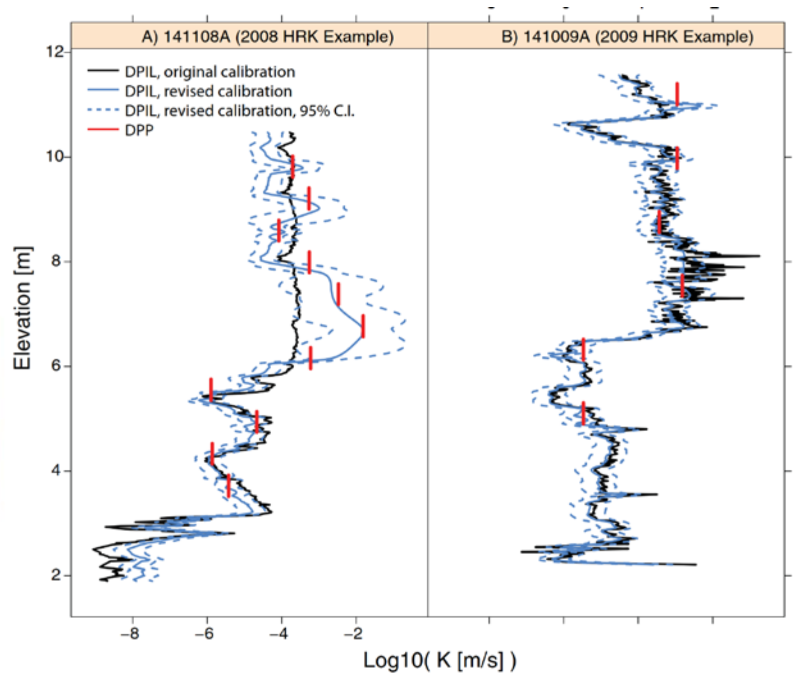


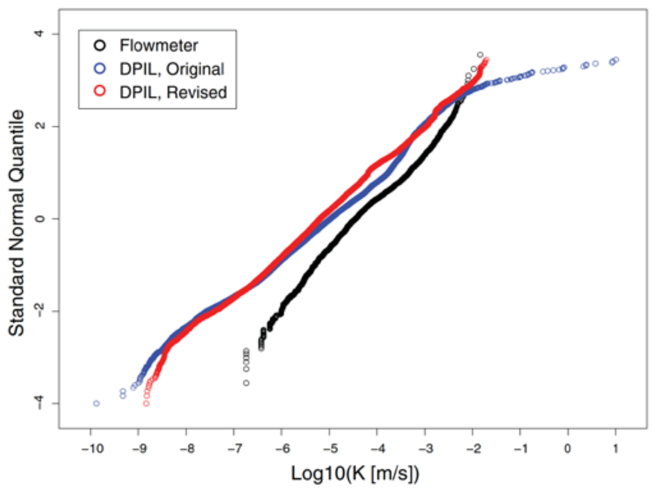
Fig. 6. Experimental results of the dipole tracer test at the MADE site and its interpretation by the proposed analytical model as well as the equivalent homogeneous solution of Hoopes and Harleman (1967); experimental data from Bianchi et al. (2011).

Breakthrough in measurements: the Direct Push method (DPIL)

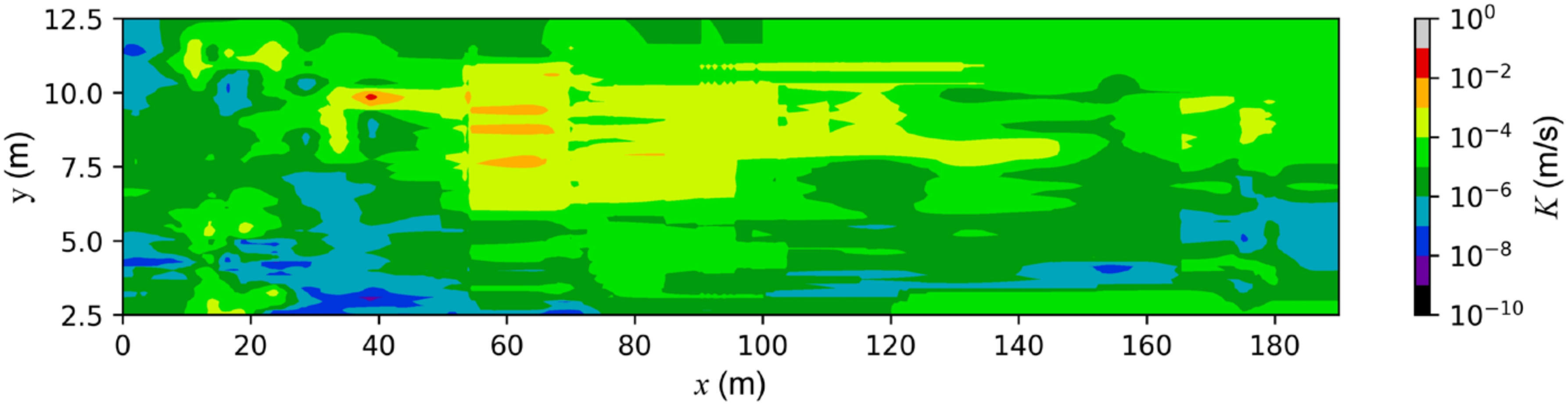






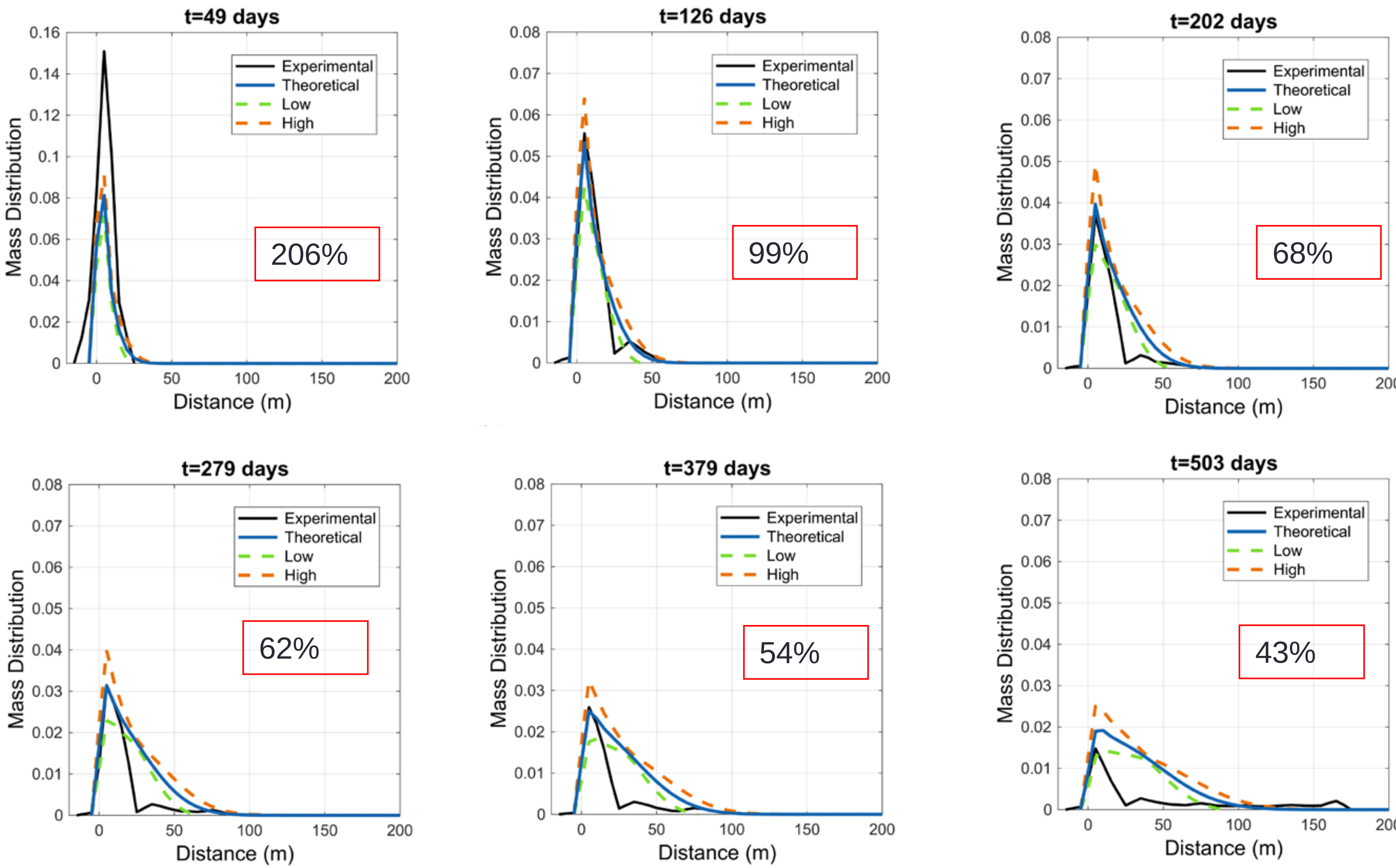


Vertical profile of hydraulic conductivity at MADE



from Fiori et al, submitted to Frontiers

Comparison of mass distribution (MADE-1)



Relative to injected mass

Fiori et al., WRR, 2013; Fiori et al, submitted to Frontiers

Conclusions

- Groundwater flow and transport is still a hot and debated topic after four decades of stochastic subsurface hydrology;
- The modeling of groundwater flow and transport in strongly heterogeneous formations is still a challenging problem, as well as uncertainty characterization;
- Despite of the recent and significant advances in characterization, subsurface hydrology is still a poor-data discipline, and the typical applications are very much exposed to uncertainty;
- More work is needed to develop and improve characterization techniques (hydrogeophysics etc), but more work is also needed to understand several fundamental processes that guide flow and transport in the complex subsurface environments.