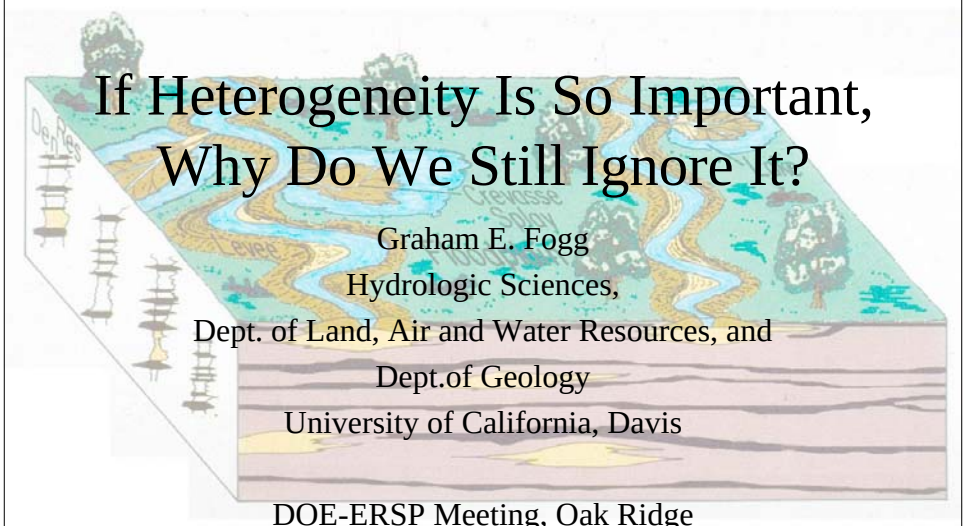

If Heterogeneity Is So Important, Why Do We Still Ignore It?

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Hydrologic Sciences,
Dept. of Land, Air and Water Resources, and
Dept.of Geology
University of California, Davis

DOE-ERSP Meeting, Oak Ridge
10/24/06

Qualifier and "but"….

- Much excellent work on heterogeneity being done.
- Nevertheless, significant misunderstanding persists.
  - Misinterpretation of subsurface hydrologic measurements.
  - Lack of geologic context.
  - Overemphasis of parsimony.
  - Lack of appreciation of significance of heterogeneity (especially among those who need to use simplified hydrologic models, e.g., managers, ecologists, groundwater tracer scientists, natural attenuation scientists & engineers).

Other Reasons

- Difficult (esp. multi-scale)
- Need for more, better tools
  - Fast simulation (esp. flow and reactive transport; less so for nonreactive transport)
  - Front ends for simulating flow and transport in large, heterogeneous systems
  - Upscaling methods to reduce need for explicit modeling of heterogeneity
- Sometimes, homogeneous models are OK.

Popular Approaches for Modeling Heterogeneity

- Gaussian: log-Gaussian assumption, typically ln K $\sigma^2 < 1\text{-}2$, exp covariance.
- Multi-modal: e.g., multiple categories, facies or flow units within which heterogeneity is moderate compared to inter-facies heterogeneity.

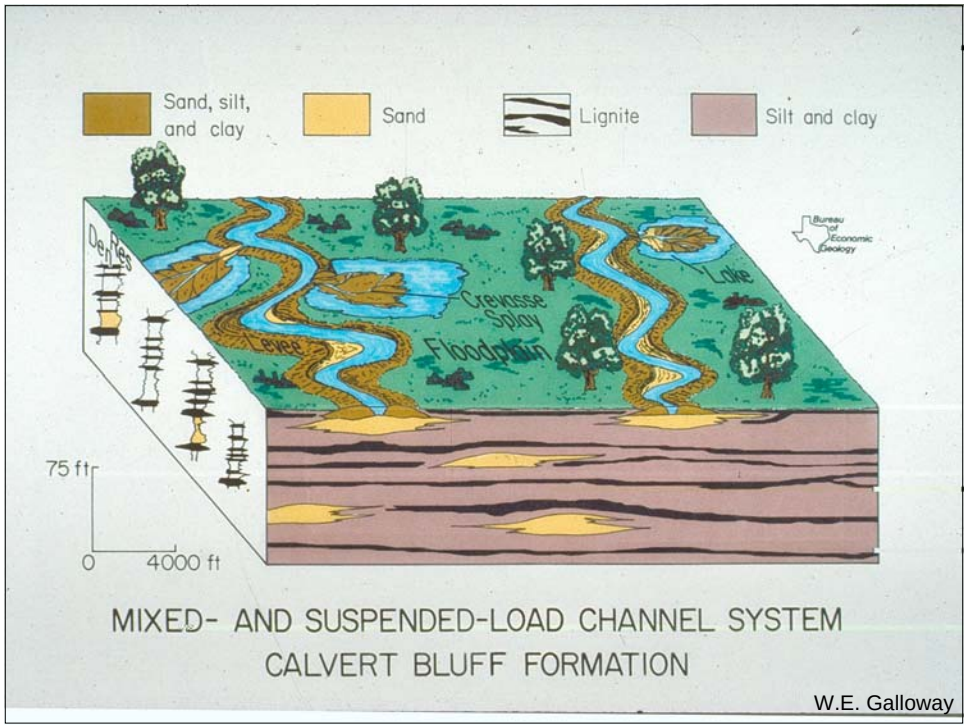
Gaussian Approach: Summary

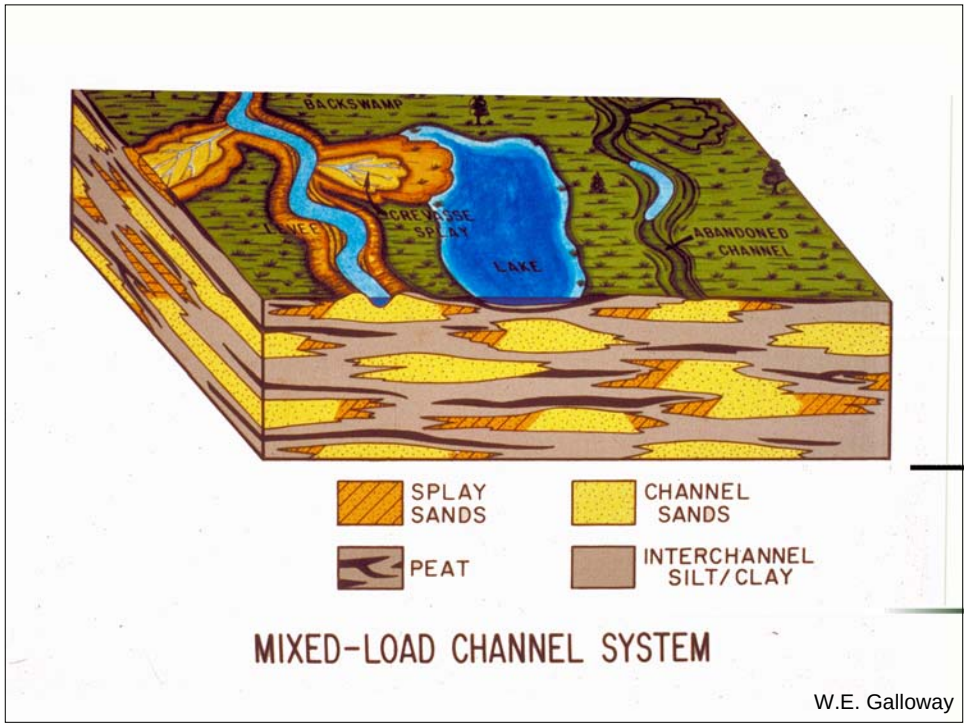
- Assumption that ln K σ^2 < 1-2 is common in stochastic groundwater literature.
- Small ln-K variance can only occur if the sediments are essentially without fines ("mud" or silt & clay).
- Sediments devoid of fines are rare, hence small ln-K variance is rare.
- The contrary is implied by the literature because of unintentional, biased measurement and sampling.

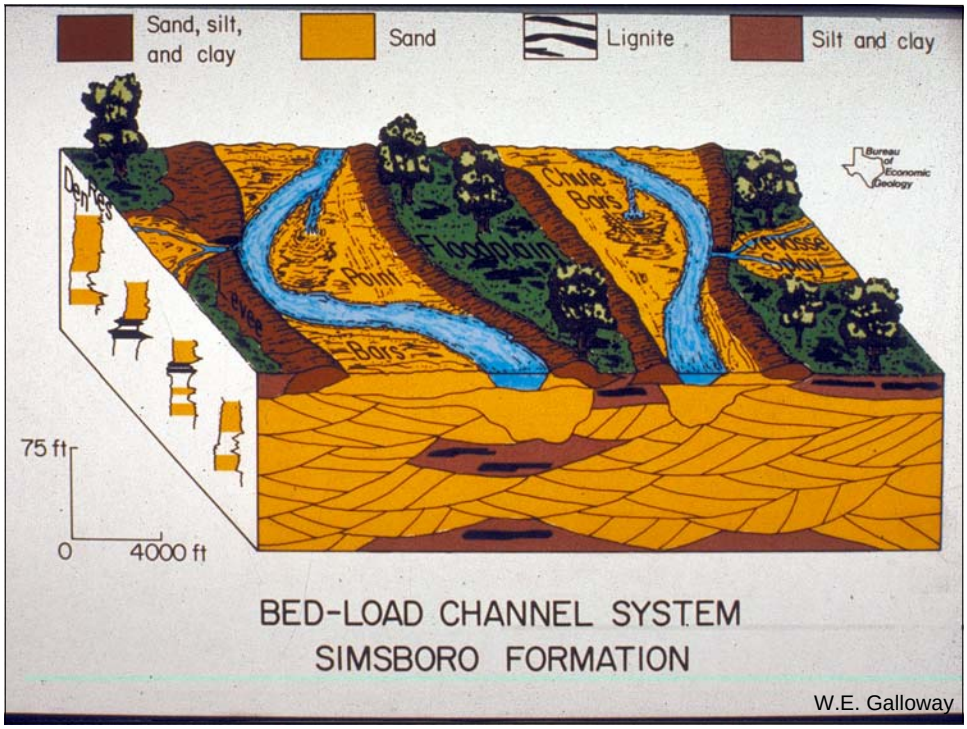
Multi-Modal (Facies) Conceptual Model for ln K σ^2:

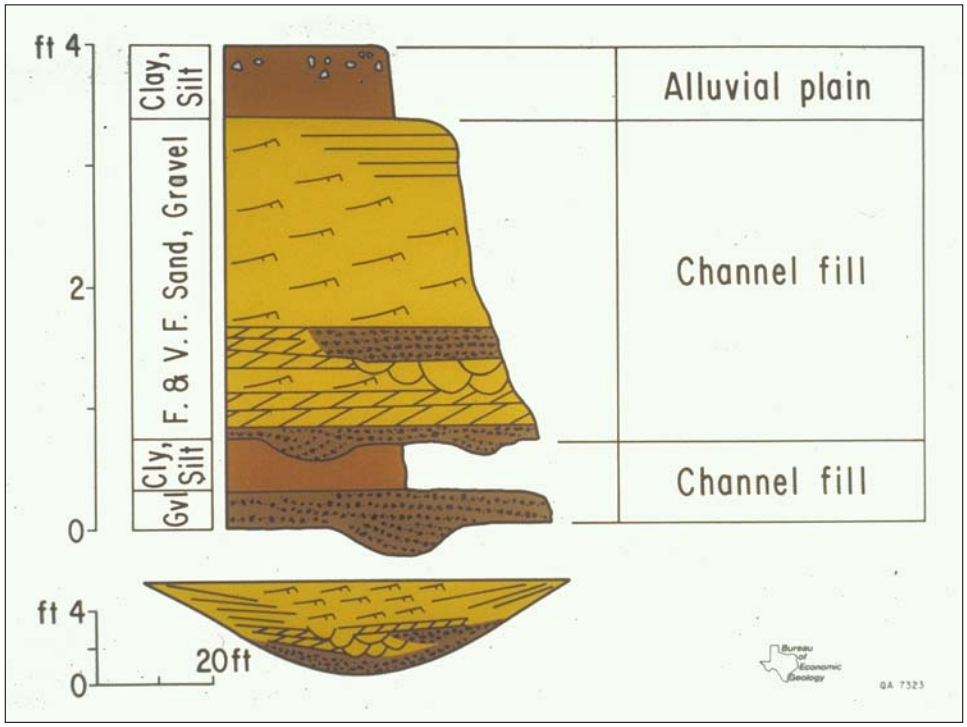
- Although available K data typically form apparent, unimodal distributions (e.g., Gaussian).

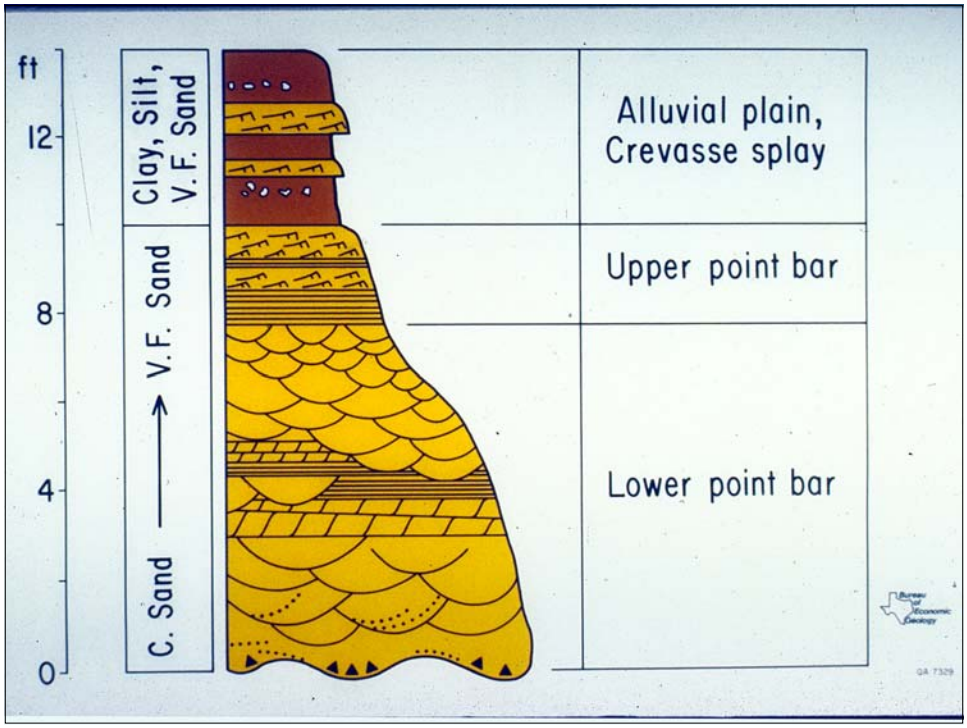
>> When one attempts to characterize K of all geologic facies present, a different paradigm of subsurface heterogeneity emerges, as compared to the Gaussian paradigm.


Sand, silt, and clay
Sand
Lignite
Silt and clay
Bureau of Economic Geology
Levee
Crevasse Splay
Floodplain
Lake
75 ft
0
4000 ft
MIXED- AND SUSPENDED-LOAD CHANNEL SYSTEM
CALVERT BLUFF FORMATION
W.E. Galloway

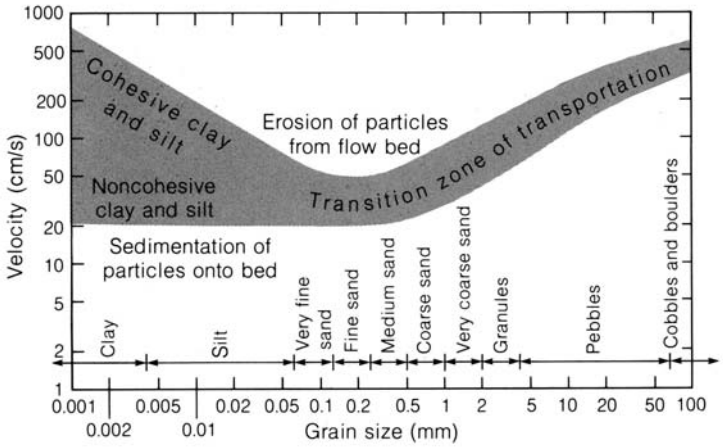

BACKSWAMP
LEVEE
CREVASSE SPLAY
LAKE
ABANDONED CHANNEL
SPLAY SANDS
CHANNEL SANDS
PEAT
INTERCHANNEL SILT/CLAY
MIXED-LOAD CHANNEL SYSTEM
W.E. Galloway


Sand, silt, and clay
Sand
Lignite
Silt and clay
Dennes
Levee
Point
Bars
Floodplain
Chute Bars
Crevasse Splay
75 ft
0
4000 ft
BED-LOAD CHANNEL SYSTEM
SIMSBORO FORMATION
W.E. Galloway


ft 4
2
0
Clay, Silt
F. & V.F. Sand, Gravel
Cly, Silt
Gvl
Alluvial plain
Channel fill
Channel fill
ft 4
0
20ft
QA 7323

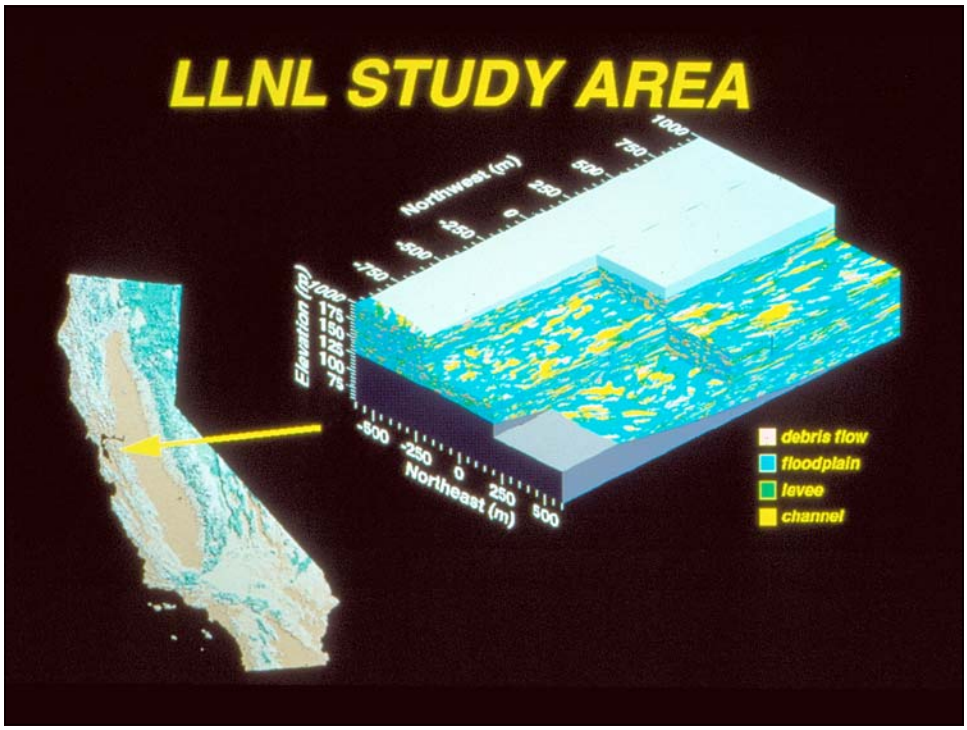


Nature Includes a Spectrum of Water Velocities, and Hence a Spectrum of Grain Sizes in Sediment



After Hjulstrom as modified by Sundberg (1956)

Example 1: Lawrence Livermore National Lab site, alluvial fan, Coast Ranges of California, U.S.; Fogg et al., 1998



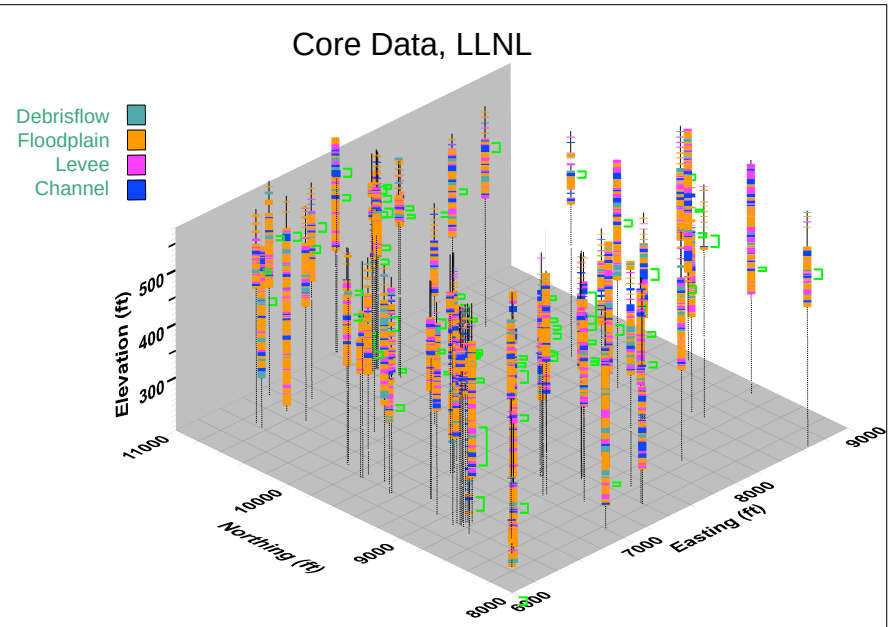
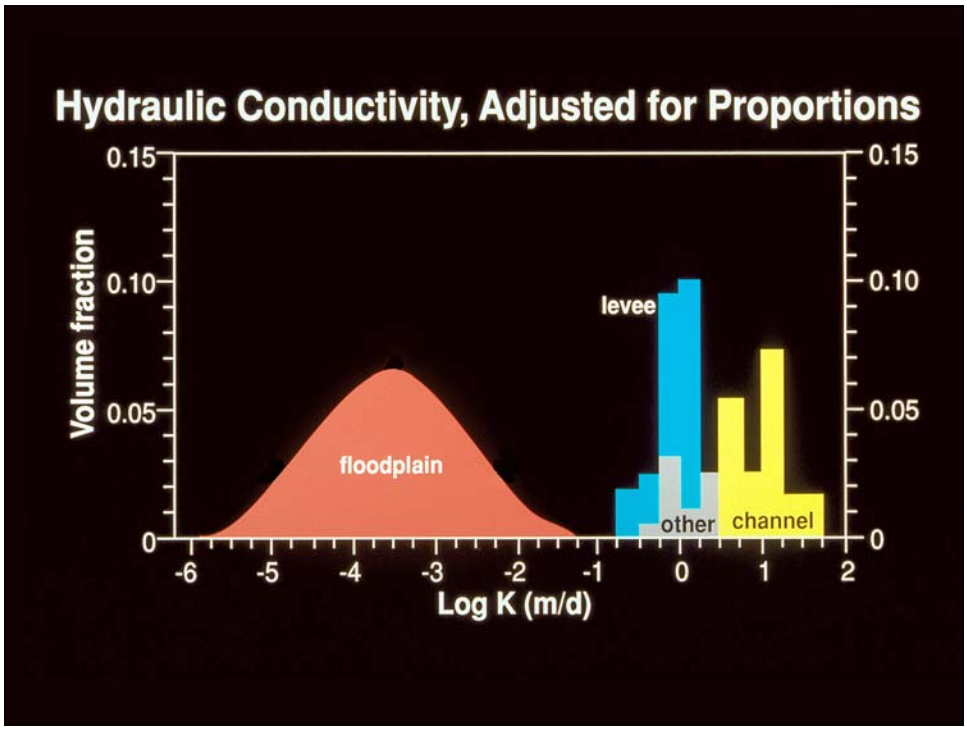
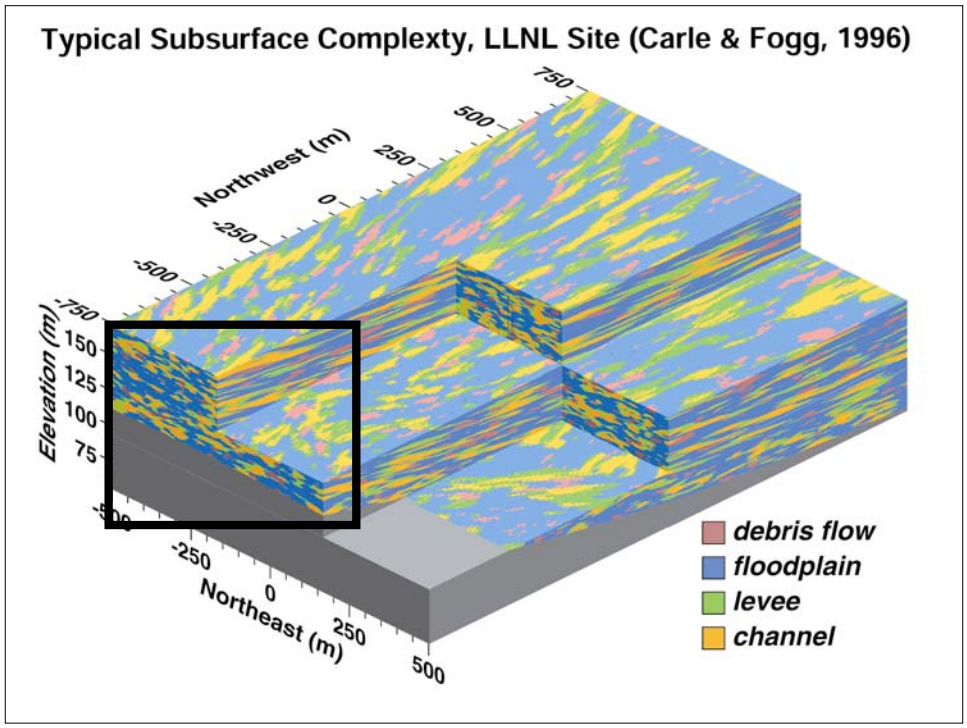
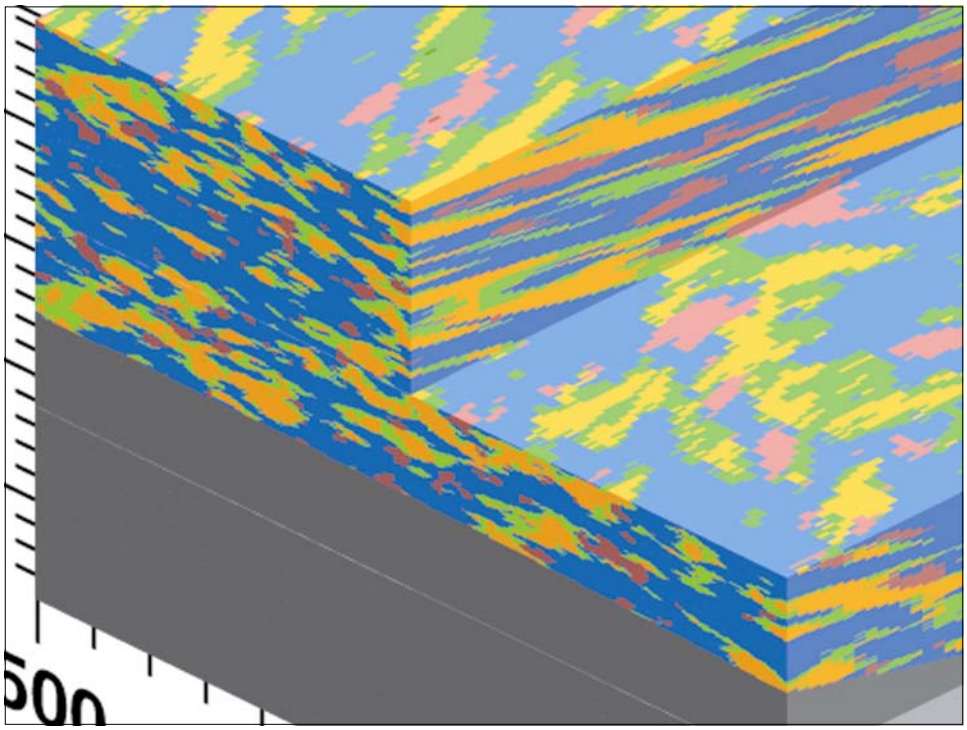


Fig. 1 *Core descriptions (from Carle, 1996)*




Typical Subsurface Complexty, LLNL Site (Carle & Fogg, 1996)
Northwest (m)
750
500
250
0
-250
-500
Elevation (m)
150
125
100
75
-250
0
250
500
Northeast (m)
debris flow
floodplain
levee
channel



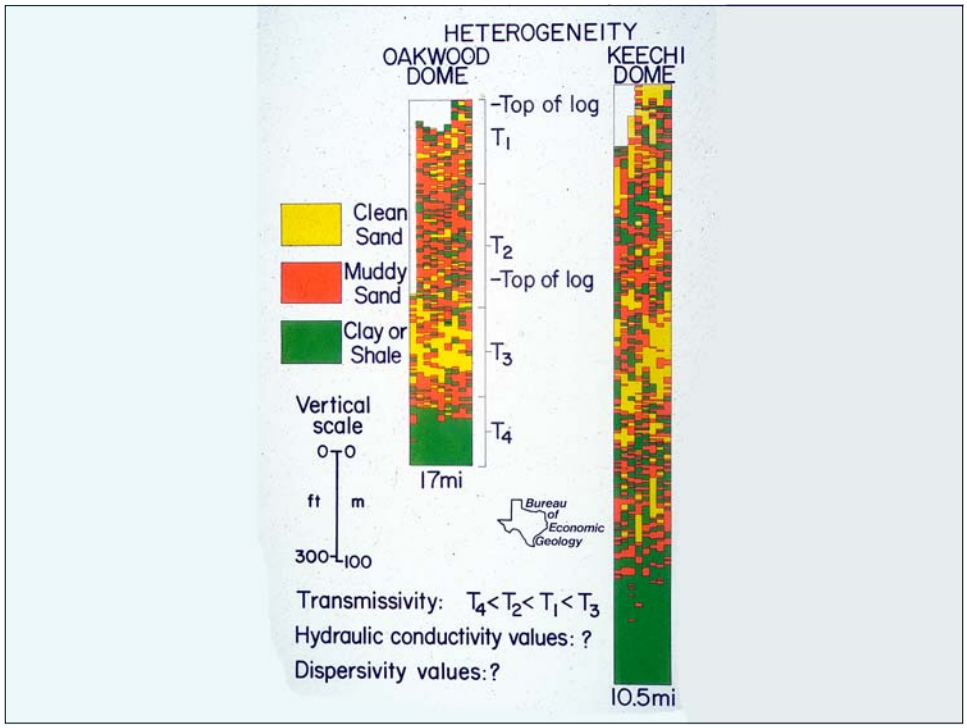
HYDRAULIC PROPERTIES
for
Ground-Water Flow Experiments

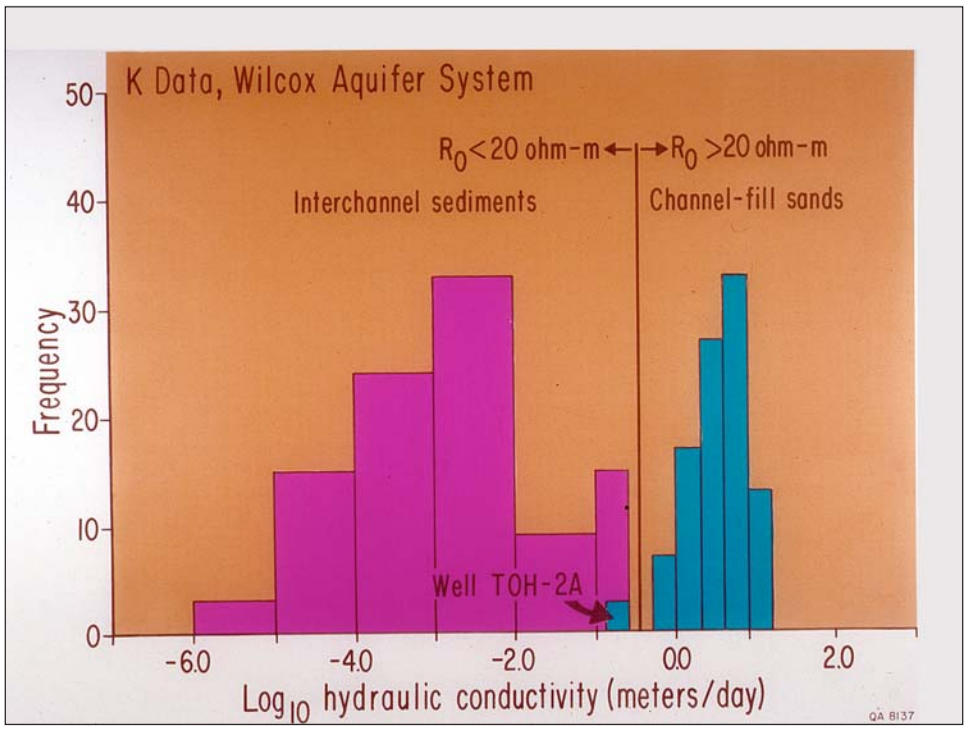
	ORIGINAL		REVISED	
	K (m/s)	S_s (m^{-1})	K (m/s)	S_s (m^{-1})
Debris Flows	5e-6	2e-5	5e-6	2e-5
Floodplain	2e-9	5e-4	5e-10	7e-4
Levee	3e-6	5e-5	2e-6	3e-5
Channel	6e-5	1e-5	6e-5	1e-5

$\mathrm{Ln}\ K\ \sigma^2 = 25$

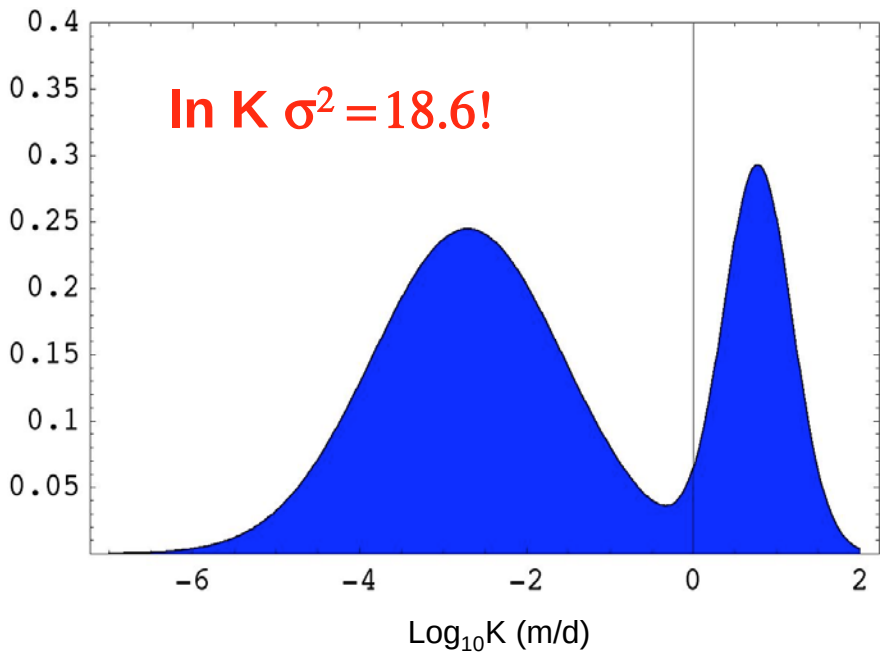
* *from pumping tests*
* *from barometric efficiency*

Example 2: Wilcox Group, East Texas Basin (fluvial); Fogg (1986)


HETEROGENEITY
OAKWOOD DOME
KEECHI DOME
-Top of log
T1
T2
-Top of log
T3
T4
Clean Sand
Muddy Sand
Clay or Shale
Vertical scale
0
0
ft
m
300
100
17mi
10.5mi
Bureau of Economic Geology
Transmissivity: T4< T2< T1< T3
Hydraulic conductivity values: ?
Dispersivity values: ?


K Data, Wilcox Aquifer System
R0<20 ohm-m
R0 >20 ohm-m
Interchannel sediments
Channel-fill sands
Frequency
50
40
30
20
10
0
Well TOH-2A
-6.0
-4.0
-2.0
0.0
2.0
Log10 hydraulic conductivity (meters/day)
QA 8137

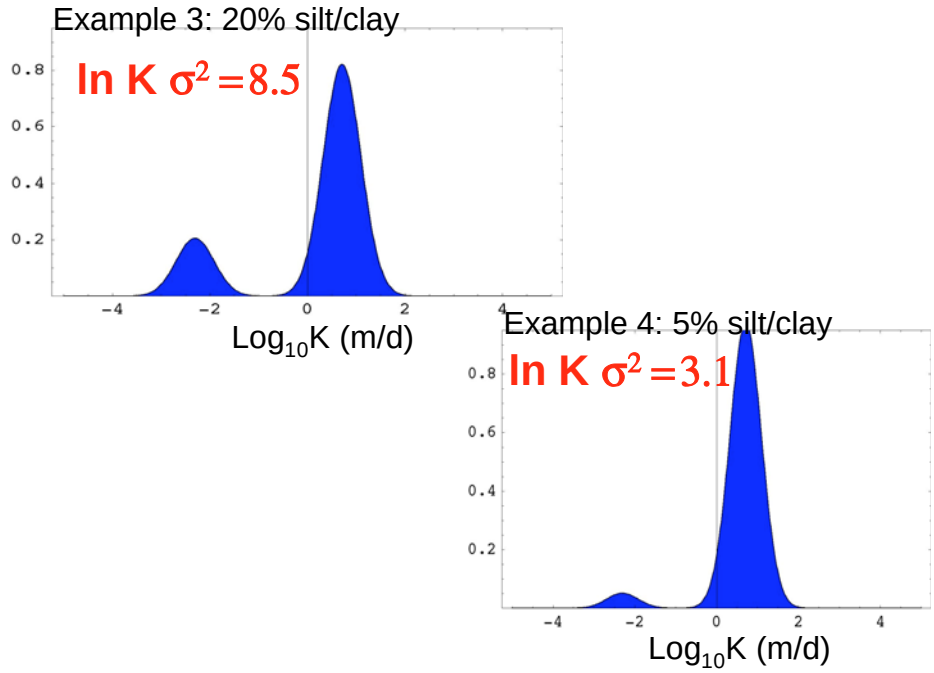
Composite PDF from 2 Gaussians



But what if an aquifer is very coarse-grained?

- **Then should the variance be as low as 1-2?**
- **Not likely, because coarse-grained formations usually contain some silt/clay materials.**

Consider 2 clean sands containing a modest amount of silt/clay facies: **Ex. 3**, 20% silt/clay; **Ex. 4**, 5% silt/clay. For simplicity, we assume that the composite system consists of 2 Gaussian distributions, each having ln K σ^2 = 0.8 and each with modest (10^3) separation in their modes.



Thus, as a general rule, one should not expect ln K σ^2 to be less than 2, even in very clean, sandy systems

- Where then, are the data suggesting ln K $\sigma^2 < 2$? Much of these data are summarized in Gelhar (1993; Table 6.1, p. 291) and Rubin (2003; Table 2.2, p. 35).
- Close examination reveals that all but a few of these data sets are biased and fundamentally cannot represent most of the low-K facies….

Reasons for Bias

- **"Well tests"** (pumping and slug) which tend to arithmetically average K's of all strata intersecting the well screen, neglecting low-K materials.
- "**Borehole flowmeter"** tests which are incapable of quantifying the low-end K values (muddy sediments).
- **"Soil"** which is inherently less heterogeneous than geologic depositional facies due to pedogeneisis, including biological (plants and animals) and mechanical (tillage) amplification of K of fines and geochemical (clay authigenesis) as well as mechanical (infiltrated fines) conversion of sand and gravel facies into finer-grained soils.
- **"Silt/clay"** was present at the site but K values apparently were not measured.

Ln K (and T) variance data from Gelhar (1993)

Table 6.1, p. 291

	Source	Medium	Type†	σ_Y	σ_Y^2	Biased?	Why?
1.	Aboufirassi and Marino (1984)	alluvial-basin aquifer	T	1.22	1.5	yes	well tests
2.	Bakr (1976)	sandstone aquifer	A	1.5–2.2	2.3-4.8	?	
3.	Binsariti (1980)	alluvial-basin aquifer	T	1.0	1.0	yes	well tests
4.	Byers and Stephens (1983)	fluvial sand	A	0.9	0.8	yes?	silt/clay
5.	Delhomme (1979) Delhomme (pers. communication)	limestone aquifer	T	2.3	5.3	yes	well tests
6.	Aquitane	sandstone aquifer	T	1.4	2.0	yes	well tests
7.	Durance	alluvial aquifer	T	0.6	0.4	yes	well tests
8.	Kairouan	alluvial aquifer	T	0.4	0.2	yes	well tests
9.	Normandy	limestone aquifer	T	2.3	5.3	yes	well tests
10.	Nord	chalk	T	1.7	2.9	yes	well tests
11.	Devary and Doctor (1982)	alluvial aquifer	T	0.8	0.6	yes	well tests
12.	Gelhar et al. (1983, Fig. 6.15)	fluvial soil	S	1.0	1.0	yes	soil
13.	Goggin et al. (1988)	eolian sandstone outcrop	A	0.4	0.2	no	
14.	Hess (1989)	glacial outwash sand	A	0.5	0.3	yes	borehole flowmete
15.	Hoeksema and Kitanidas (1985)	sandstone aquifer	T	0.6	0.4	yes	well tests
16.	Hufschmied (1986)	sand and gravel aquifer	A	1.9	3.6	yes	well tests
17.	Loague and Gander (1990)	prairie soil	S	0.6	0.4	yes	soil
18.	Luxmoore (1981)	weathered shale subsoil	S	0.8	0.6	yes	soil
19.	Rehfeldt et al. (1989a)	fluvial sand and gravel aquifer	A	2.1	4.4	yes	borehole flowmete
20.	Russo and Bressler (1981)	Homra red mediterranean soil	S	0.4–1.1	0.2-1.2	yes	soil
21.	Russo (1984)	gravelly loamy sand soil	S	0.7	0.5	yes	soil
22.	Sisson and Wierenga (1981)	alluvial silty-clay loam soil	S	0.6	0.4	yes	soil
23.	Smith (1978)	glacial outwash sand and gravel outcrop	A	0.8	0.6	no?	
24.	Sudicky (1986)	glacial-lacustrine sand aquifer	A	0.6	0.4	no?	
25.	Viera et al. (1981)	alluvial soil (Yolo)	S	0.9	0.8	yes	soil

†Types of data: T, transmissivity; S, soils; A, three-dimensional aquifer.

	Source	Medium	Type†	σ_f	σ_f^2	Biased?	Why?
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†Types of data: T, transmissivity; S, soils;
A, three-dimensional aquifer

Scale Issue

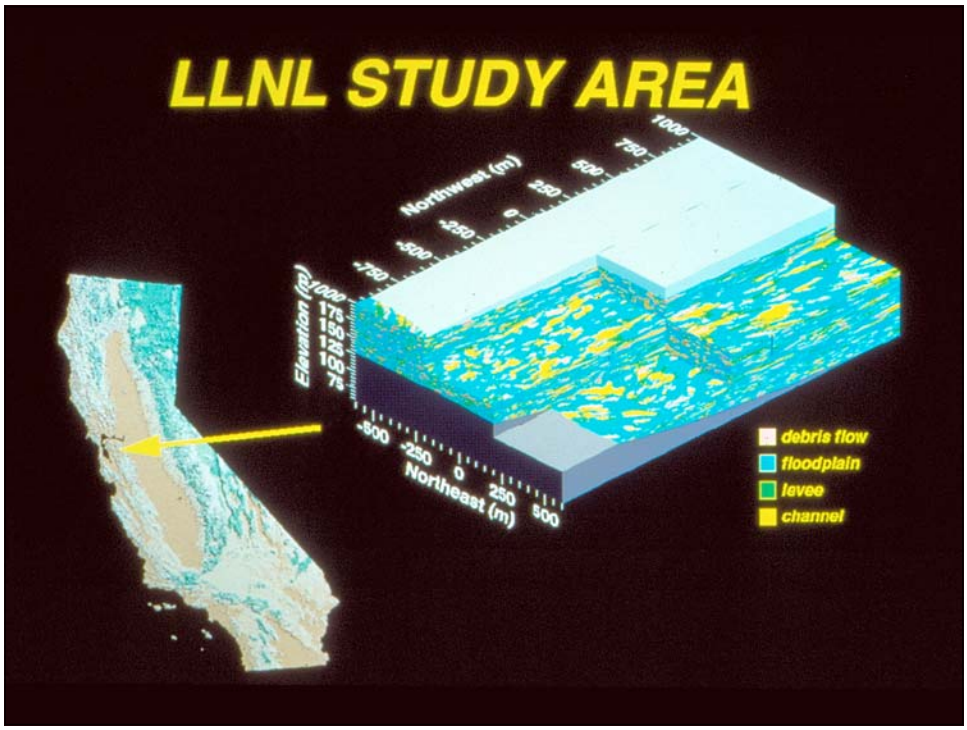
- The assumption is often made that the low-K media can be neglected because the plume is primarily ‘seeing’ the high-K materials.
- This is only likely to be true in unusually clean deposits or at very local scales.
- As a plume spreads, the likelihood of it encountering low-K material increases.
- Sequestration of mass in the low-K materials can explain apparent, scale-dependent dispersion (LaBolle and Fogg, 2001).

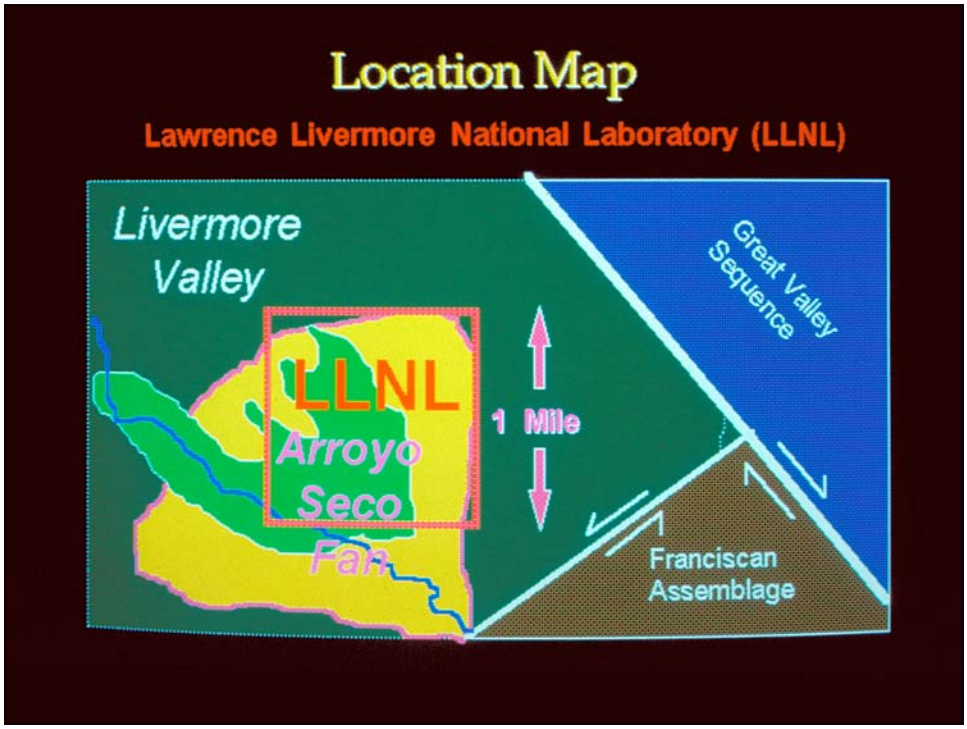
The Low-K Media Are Important and Often Critical

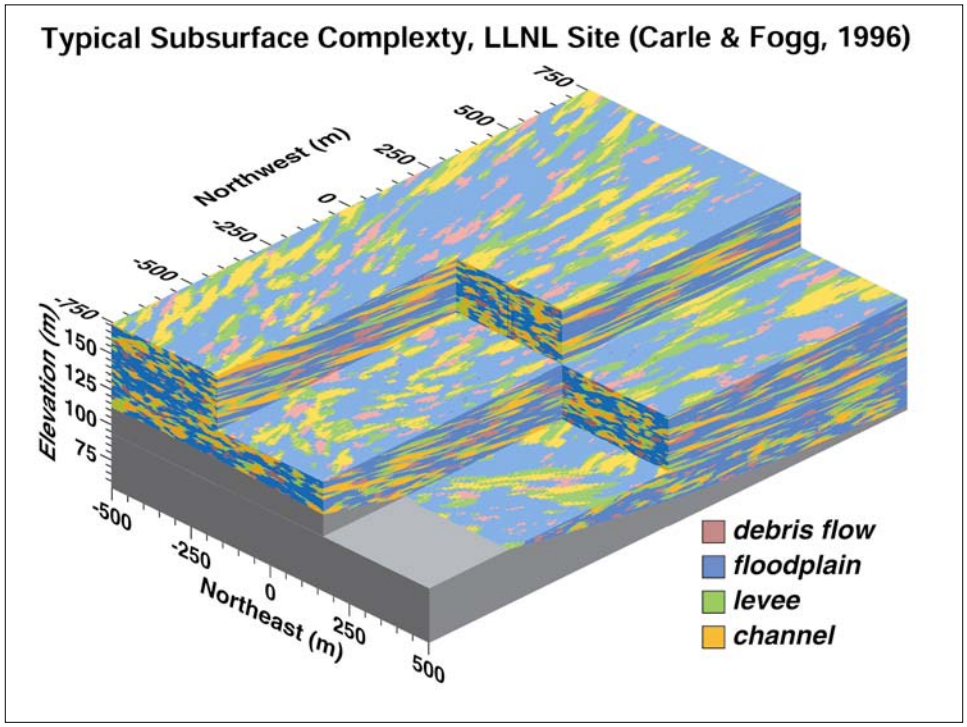
- Preferential flow and extreme tailing (Zheng & Gorelick, 2003; Zinn & Harvey, 2003; LaBolle & Fogg, 2001.
- Difficult remediation, including pump-and-treat rebound (LaBolle & Fogg, 2001).
- Significant, unanticipated mixing of groundwater ages (Weissmann et al., 2002).
- Fractionation of isotopes (LaBolle et al., in press).

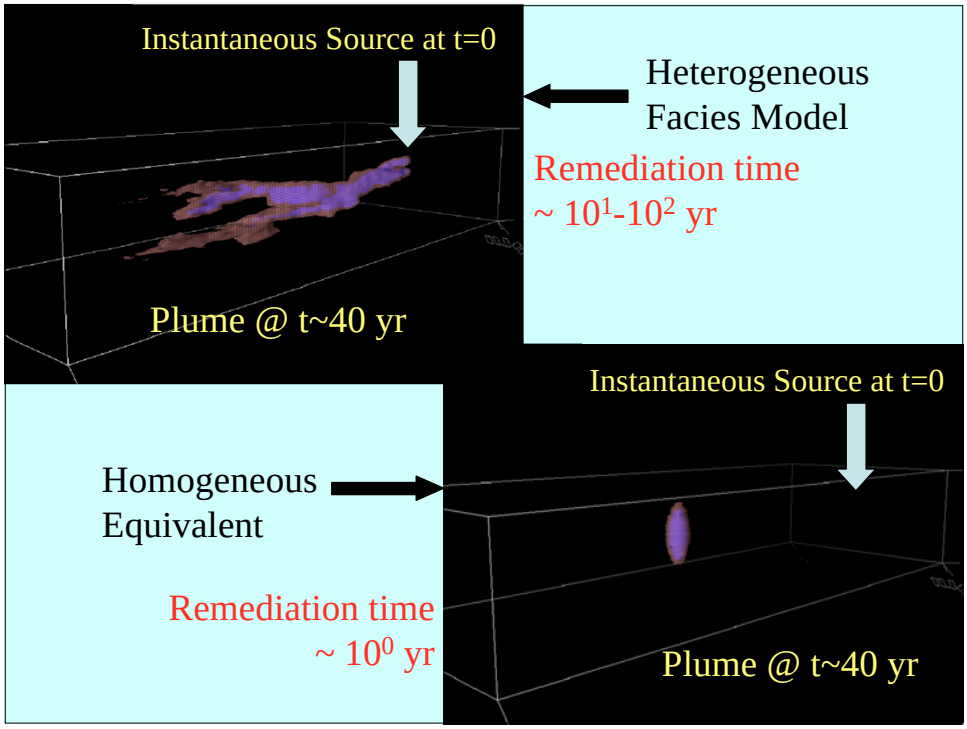
Remediation Example

- Remediation is, at best, very difficult and, at worst, impossible.
- Even remediation of non-reactive compounds like Cl^- or MTBE is difficult because of diffusion (e.g., pump-and-treat [PAT] rebound).
- Conventional models of remediation tend to predict short PAT clean-up times, whereas experience shows PAT clean-up on decadal time scales.
- Can a low ln K σ^2 model simulate PAT realistically?




Location Map
Lawrence Livermore National Laboratory (LLNL)
Livermore Valley
LLNL
Arroyo Seco Fan
1 Mile
Great Valley Sequence
Franciscan Assemblage


Typical Subsurface Complexty, LLNL Site (Carle & Fogg, 1996)
Northwest (m)
750
500
250
0
-250
-500
Elevation (m)
-750
150
125
100
75
-500
-250
0
250
500
Northeast (m)
debris flow
floodplain
levee
channel



Transport In Composite Media Containing Discontinuities

RWHET

Random Walk particle method for HETerogeneous media

LaBolle, Fogg and Tompson (1996)

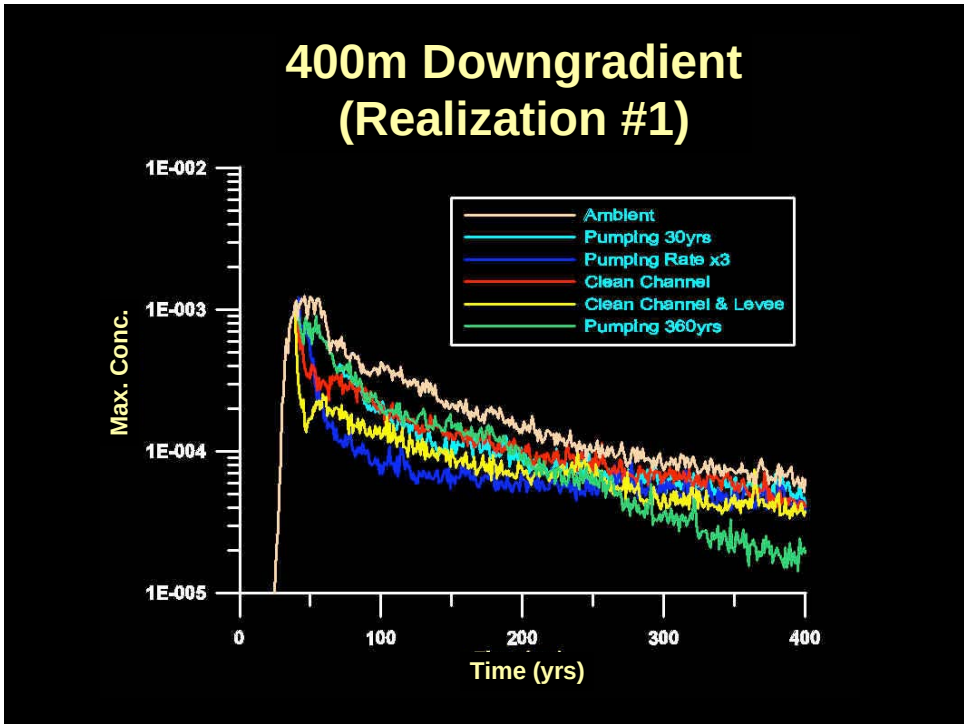
LaBolle, Quastel and Fogg (1998)

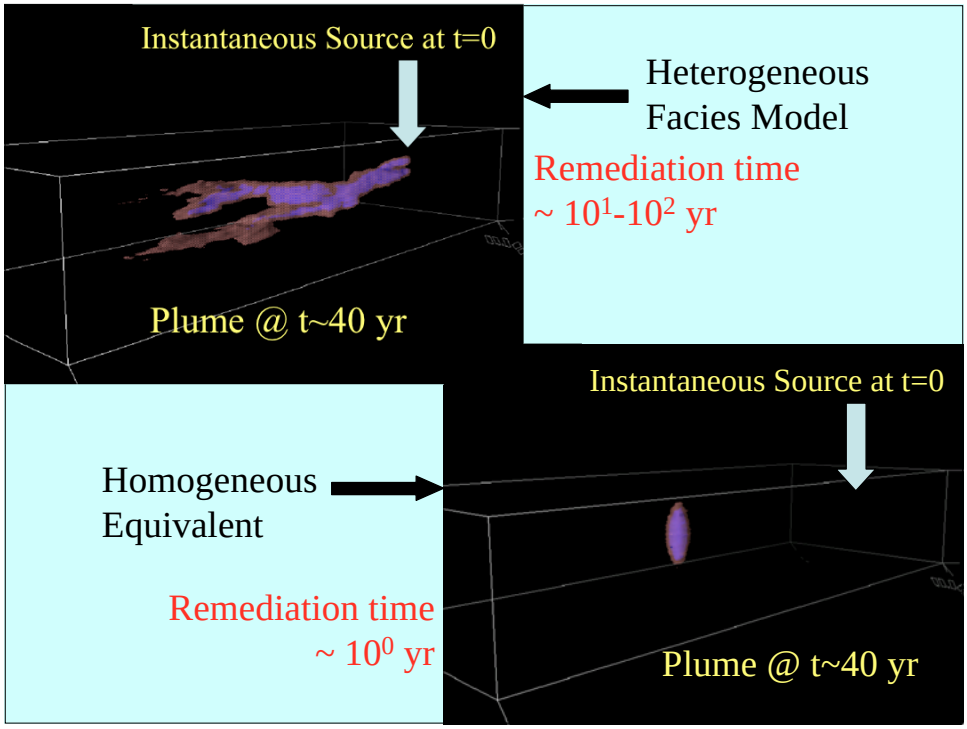
LaBolle, Quastel, Gravner and Fogg (2000)

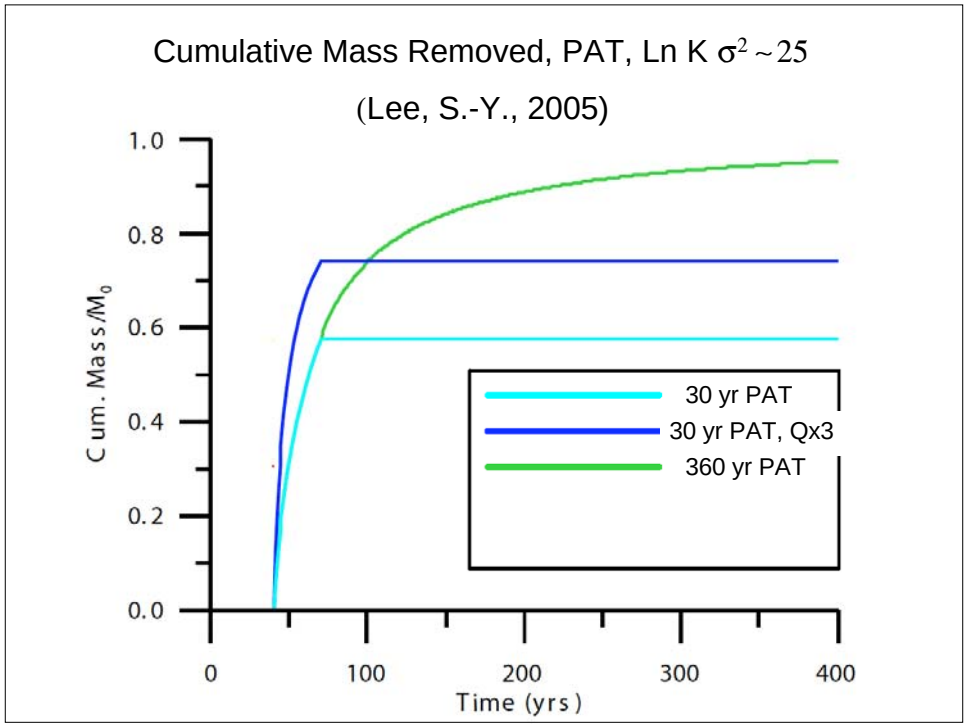
LaBolle and Fogg (2000)

Simulation Experiment: Pump-and-Treat (PAT)

- Simulate plume (TCE) development; 40 yr; 10 realizations.
- Simulate plume recovery via pumping well; yrs 41-70.
- α_T = 0.01 m (10 x 20 x 0.5 m grid blocks)
- α_L irrelevant.

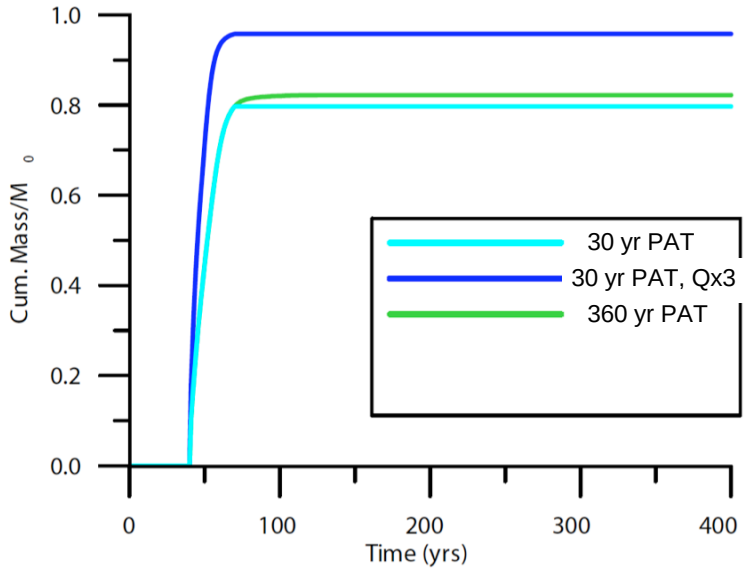



Instantaneous Source at t=0
Heterogeneous Facies Model
Remediation time ~ 10^1-10^2 yr
Plume @ t~40 yr
Instantaneous Source at t=0
Homogeneous Equivalent
Remediation time ~ 10^0 yr
Plume @ t~40 yr


Cumulative Mass Removed, PAT, Ln K $\sigma^2 \sim 25$
(Lee, S.-Y., 2005)
Cum. Mass/M_0
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400
Time (yrs)
30 yr PAT
30 yr PAT, Qx3
360 yr PAT

Cumulative Mass Removed, PAT, Ln K $\sigma^2 \sim 2.0$

(Lee, S.-Y., 2005)



Parsimony

•Fine, but the governing equation may no longer apply.

Albert Einstein:

Everything should be made as simple as possible,

but not one bit simpler.

Groundwater Age

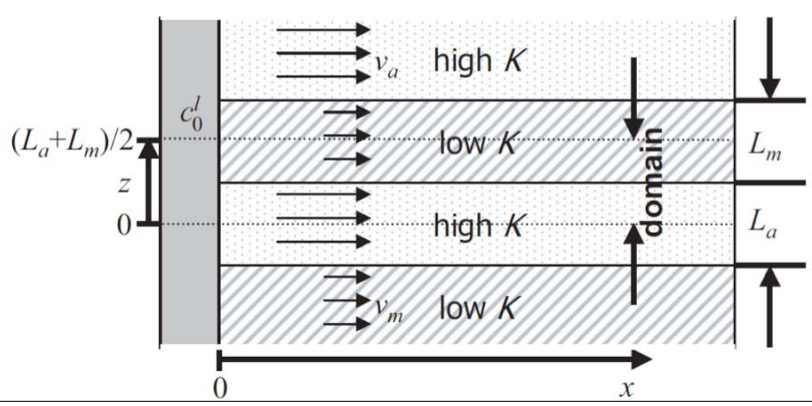
Gary Weissmann
Yong Zhang
Eric LaBolle
Si-Yong Lee
Juana Eweiss

The Diffusive Fractionation of ^{3}H and ^{3}He in Groundwater and its Impact on Groundwater Age Estimates

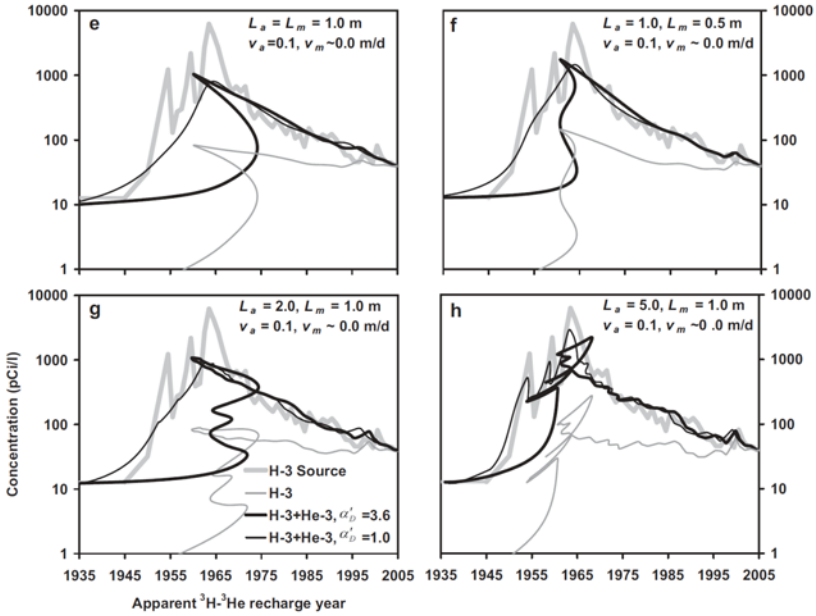
2006, WRR

Eric M. LaBolle and Graham E. Fogg
Hydrologic Sciences, University of California, Davis

Juana B. Eweis
E.L. Hydrologic Associates, Davis, CA



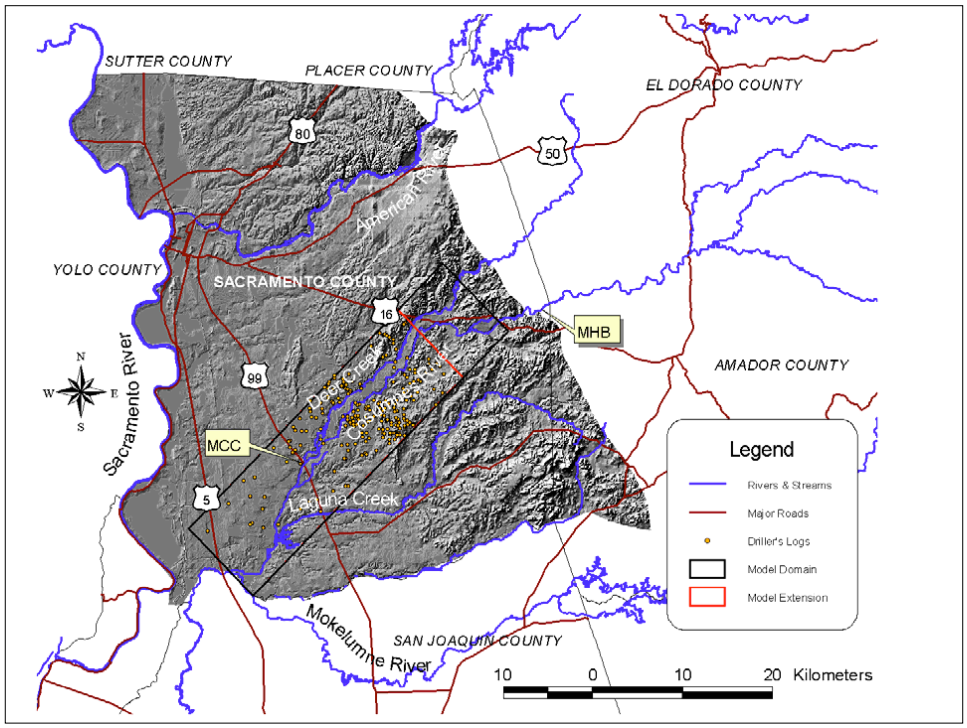
Effects of Diffusive Fractionation on ^3H-^3He Age



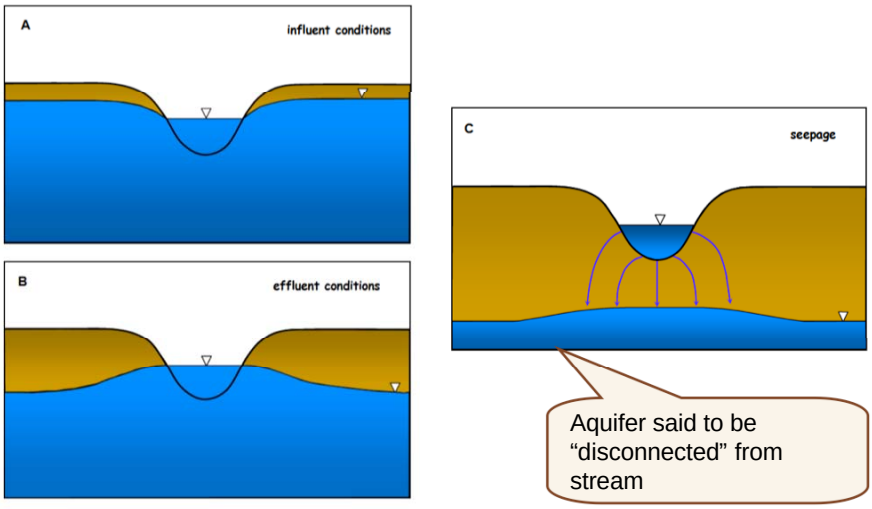
Groundwater and Surface Water Interaction

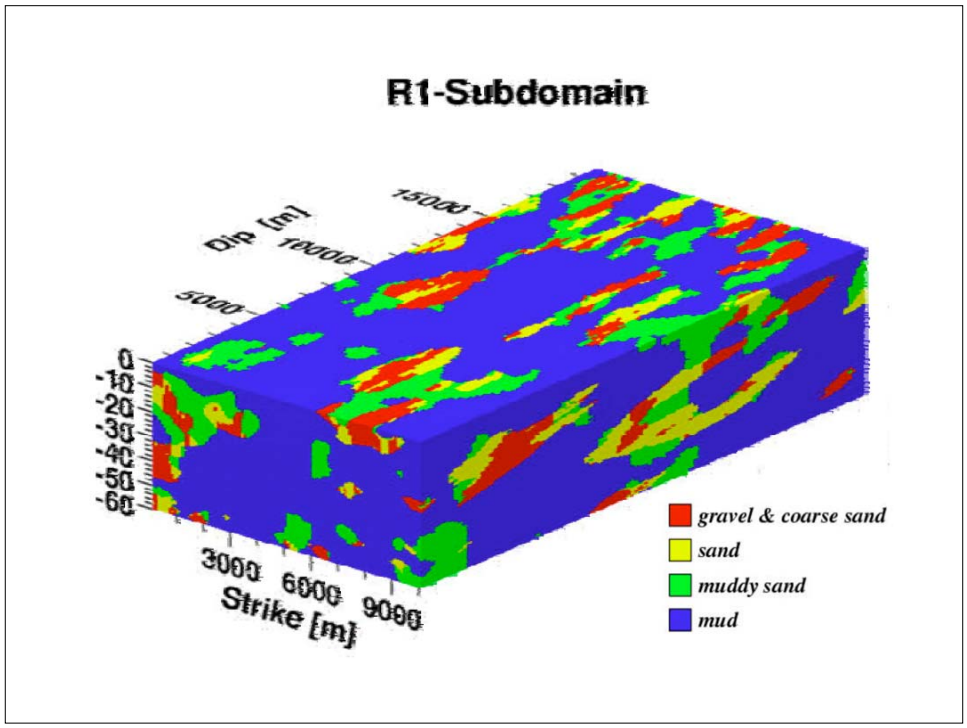
Jan Fleckenstein

Rich Niswonger



River-Aquifer Interaction Basics





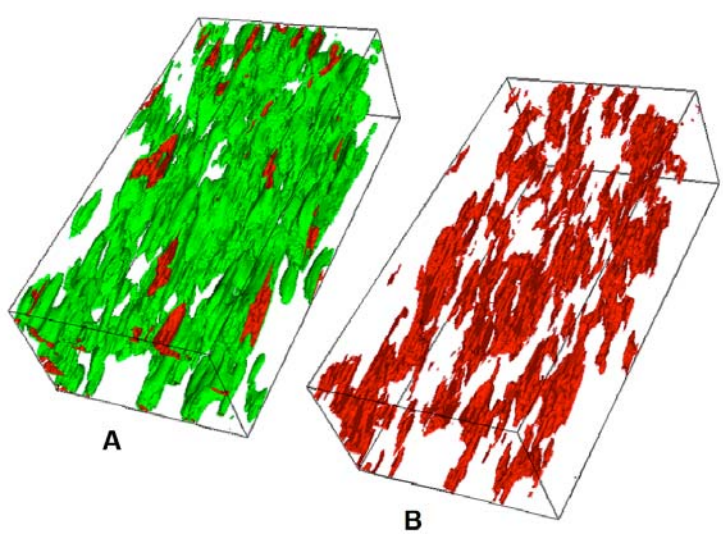
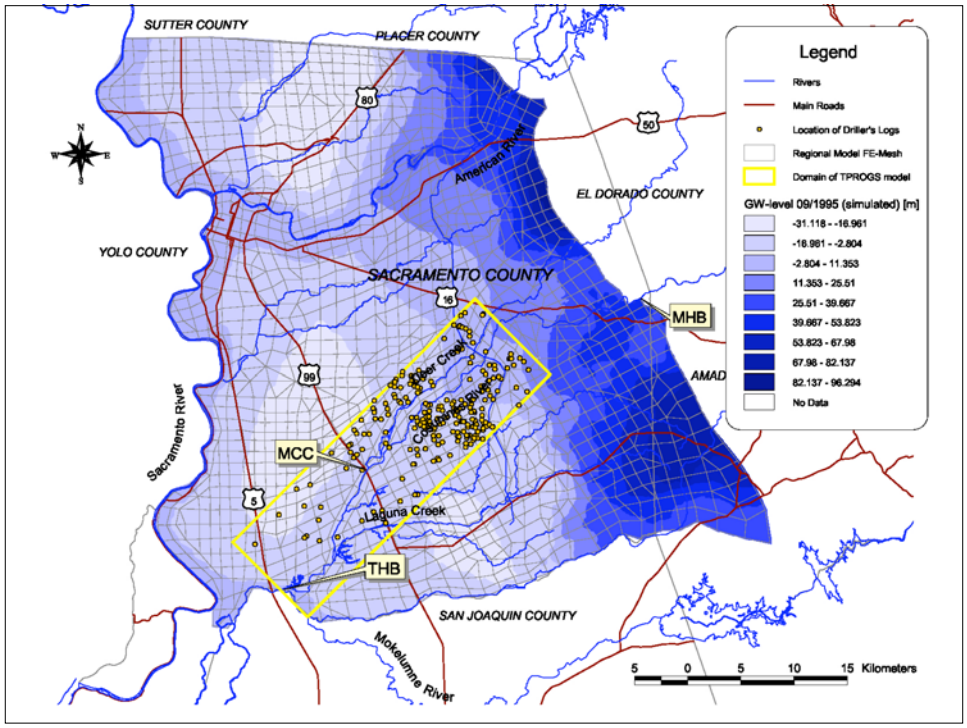
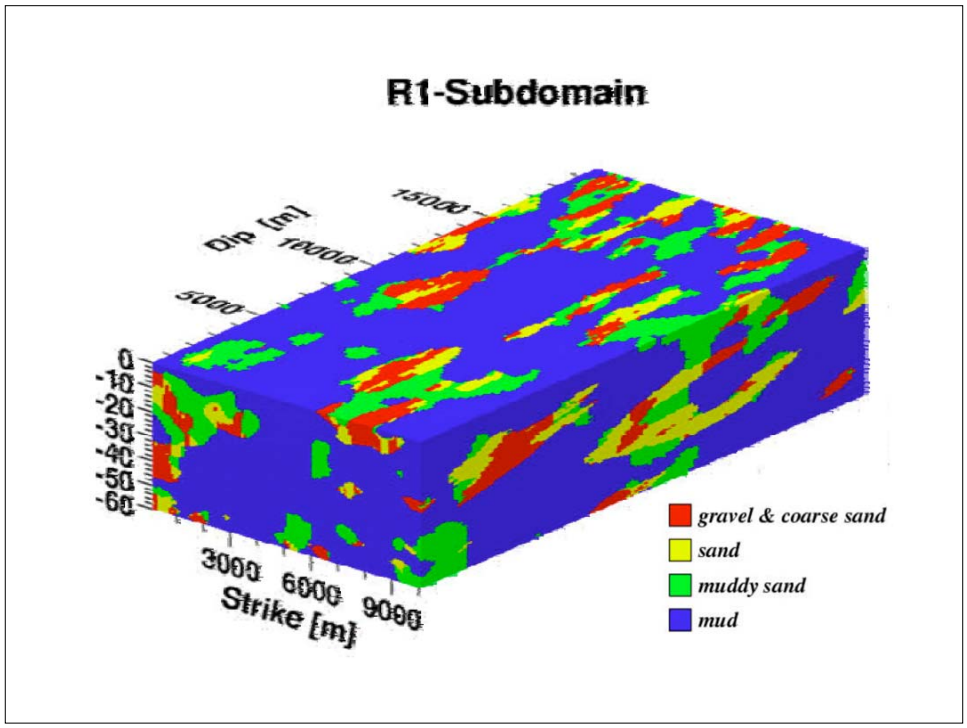
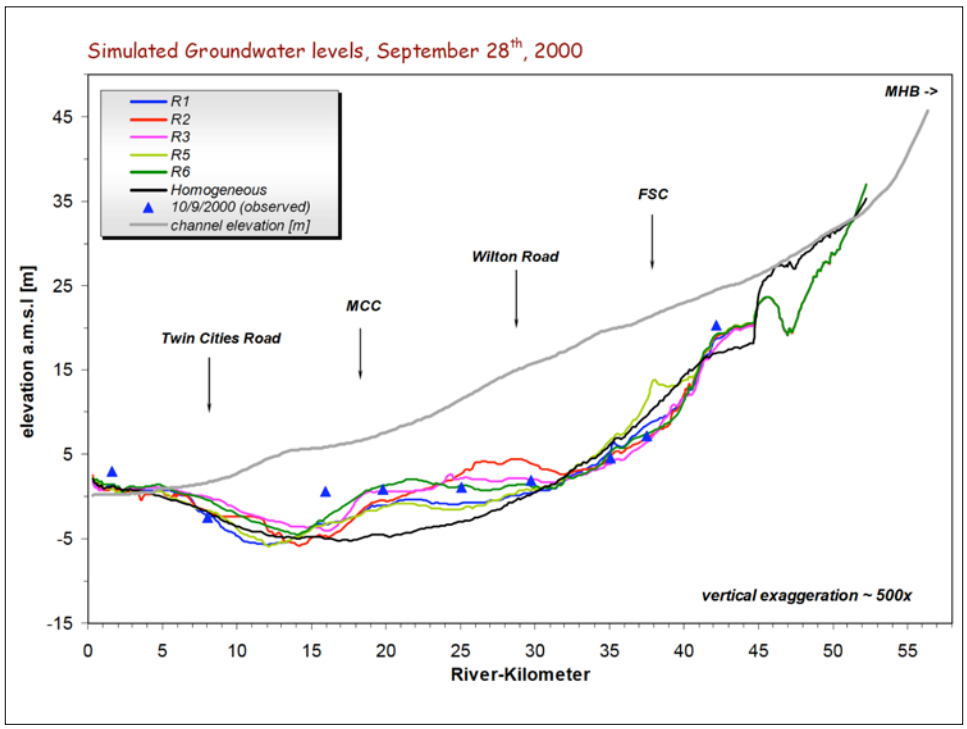


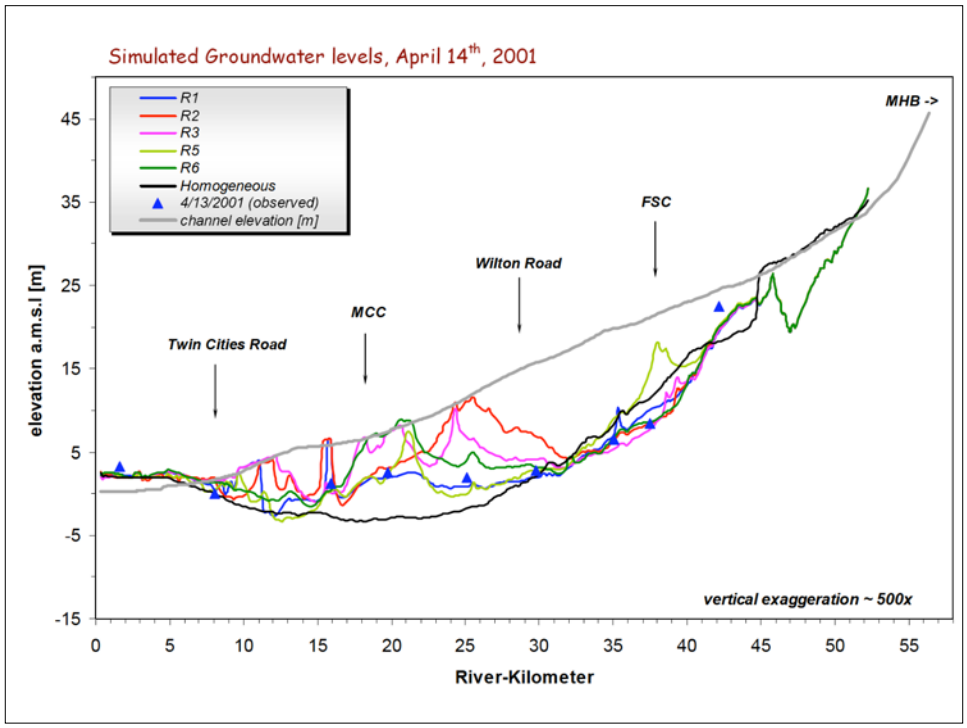
Figure 5.12 *Network of connected channel hydrofacies in the block of realization 1 used for the up-scaling simulations. A = hydrofacies 1 and 2, B = hydrofacies 1. Red colors indicate hydrofacies 1 (gravel and coarse sand) and green represents hydrofacies 2 (sands).*



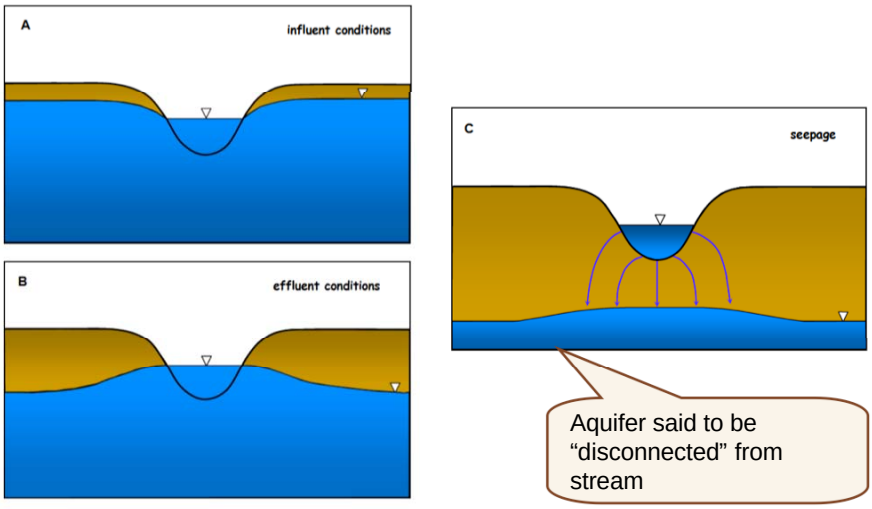
Simulation Results


R1-Subdomain
Dip [m]
5000
10000
15000
0
-10
-20
-30
-40
-50
-60
3000
6000
9000
Strike [m]
gravel & coarse sand
sand
muddy sand
mud


Simulated Groundwater levels, September 28th, 2000
R1
R2
R3
R5
R6
Homogeneous
10/9/2000 (observed)
channel elevation [m]
MHB ->
FSC
Wilton Road
MCC
Twin Cities Road
vertical exaggeration ~ 500x
elevation a.m.s.l [m]
River-Kilometer
45
35
25
15
5
-5
-15
0
5
10
15
20
25
30
35
40
45
50
55



River-Aquifer Interaction Basics



Summary

- Extraterrestrials reading the hydrology literature would likely conclude that ln-K $\sigma^2 < 2$.
- But sediments devoid of fines are rare, hence ln-K $\sigma^2 < 2$ is rare.
- Stems from interpretation of *hydrologic* data without adequate geologic context.
- This has led to confusion over the nature of geologic heterogeneity.

Summary continued

- Although much research being done on heterogeneity, in practice it is still seldom used in <u>conventional</u> models.
  - Lack of appreciation
  - Need for better computational tools (faster, wieldy)
  - Need for upscaling that accounts for transport processes
- Parsimony often invoked without realizing that it might invalidate the governing equation.

Summary continued

- Increasing attention to integrated analysis (gw-vadose-sw, environmental tracers, ecohydrology, etc.) is leading to neglect of heterogeneity - sometimes legitimately, sometimes not.
- Homogeneity still permeates our conceptual models (our subconscious?), leading to unanticipated consequences.