Computational Science and Engineering at DuPont

October 14, 2011

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Excerpt from the Proceedings of the 2011 COMSOL Conference in Boston

Topics

The DuPont Company and our diverse portfolio of science and engineering problems

Flagship problems

- underground injection
- stratospheric ozone depletion and greenhouse warming
- computational chemistry
- computational material science
- finite-element analysis and CFD
- bio-informatics
- data processing

Final comments about modeling

The Foundation of DuPont

CORE VALUES

Safety and Health

Environmental Stewardship

Highest Ethical Behavior

Respect for People

The Vision of DuPont

WE ARE A MARKET-DRIVEN SCIENCE COMPANY

Our vision is to be the world's most dynamic science company, creating sustainable solutions essential to a better, safer, healthier life for people everywhere.

The Mission of DuPont

SUSTAINABLE GROWTH

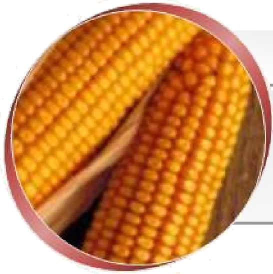
The creation of shareholder and societal value while we reduce the environmental footprint* along the value chains in which we operate.

* DuPont defines “footprint” as all injuries, illnesses, incidents, waste, emissions, use of water and depletable forms of raw materials and energy.

DuPont Continues to Evolve

*DuPont Pro Forma Sales – 2010**

$3.0 B
Nutrition & Health



$7.8 B
Agriculture

$3.8 B
Performance Coatings

$2.8 B
Electronics & Communications

$34.2B*

$6.3 B
Performance Materials

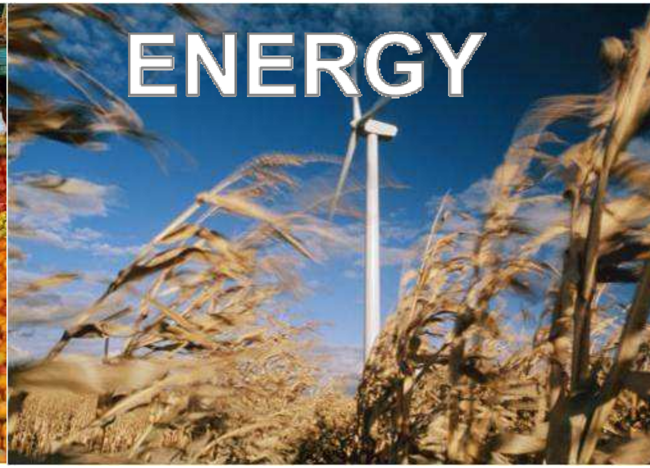
$6.3 B
Performance Chemicals

$3.4 B
Safety & Protection

$0.9 B
Industrial Biosciences

** Includes $0.2B in 'other' sales.*
Total company sales exclude transfers.

Sometime in 2011, the earth's population will reach 7 billion.
By 2050, it will be 9 billion.



Feeding The World

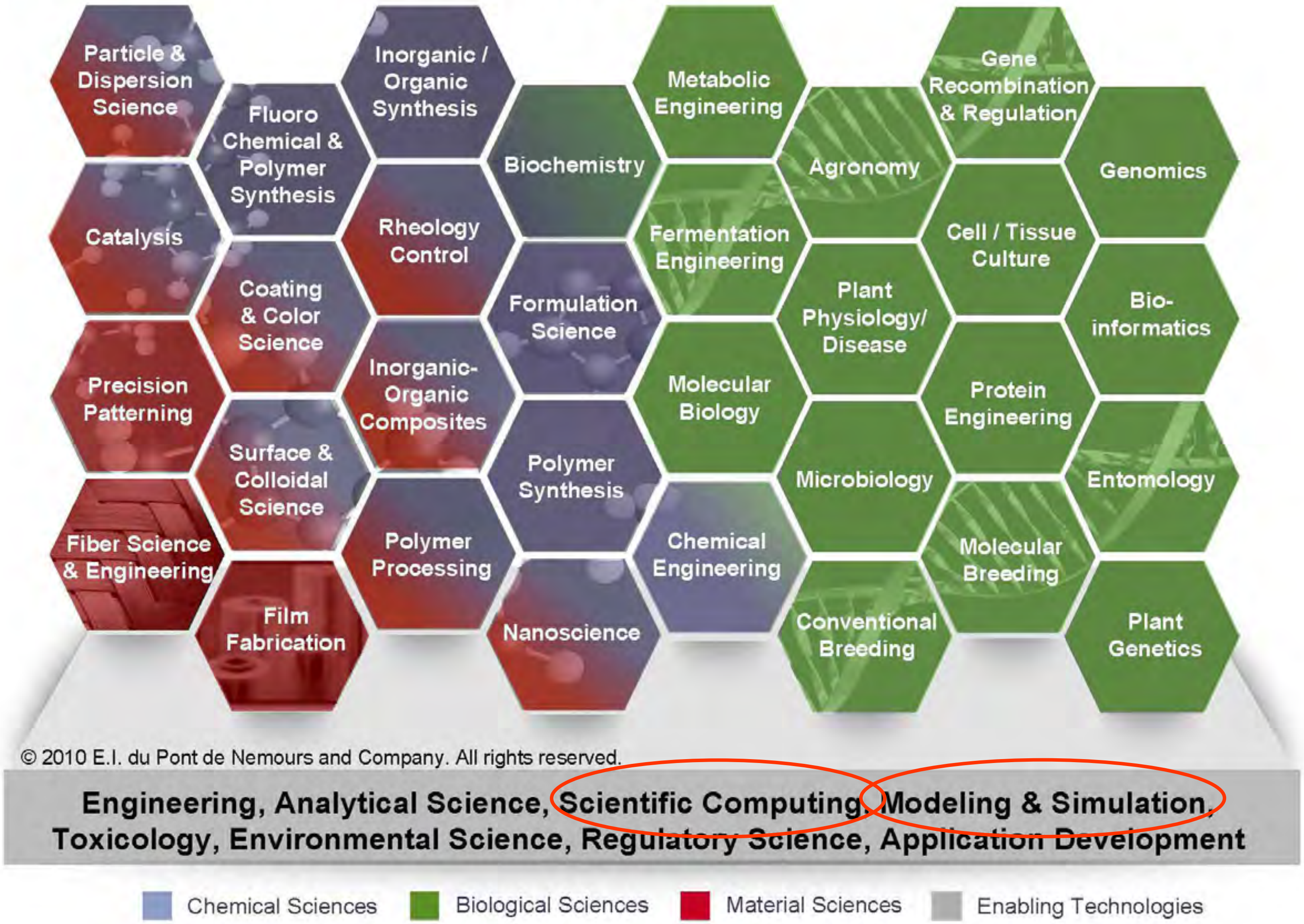
Reducing Our Dependence On Fossil Fuels

Keeping People And The Environment Safe

67,000 DuPont employees in more than 90 countries are working to find solutions through are applying our SCIENCE to find solutions to some really BIG challenges…

$1.7 billion DuPont Actual R&D Spend in 2010

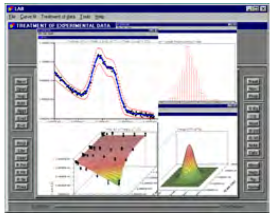
Integrating our science & technology to find solutions.

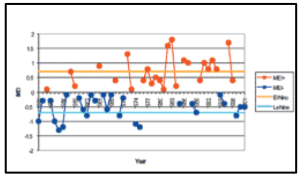


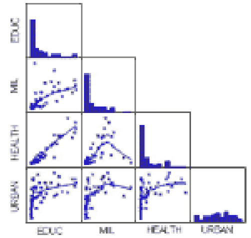
Modeling is a powerful technology used to:

(0) help define the problem

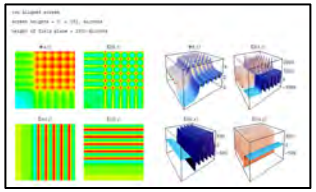
(1) organize & interpret data



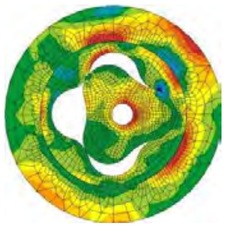


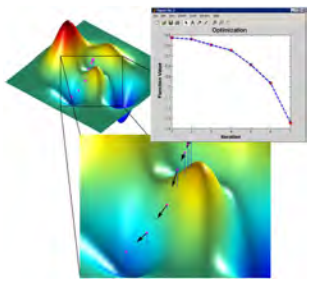


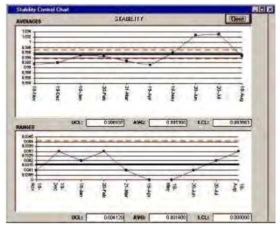
(2) capture fundamental understanding
-- qualitatively & quantitatively



(3) support the design, optimization, & control of products & processes







Good tools are critical: you *can* model electrostatic fields with Excel, but …

E.g.: metallic enclosure, grounded except for four short segments, where we apply positive and negative voltages as shown

be sure to turn on "Iteration" in the Tools/Options…/Calculation menu

Laplace's equation | **Successive overrelaxation**

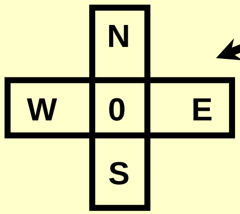
Dirichlet problem

SOR parar 1.8 1.8

ba/4 0.45 1-ba -0.8

x/y	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	1							
0	0	0	-500	-1000	-500	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0							
0.05	0	-104	-322	-481	-335	-134	-63	-33	-19	-12	-8	-5	-4	-3	-2	-1	-1	0	0	0			0	500	1000	500	0
0.1	0	-94	-203	-268	-223	-139	-83	-51	-32	-21	-14	-10	-7	-5	-3	-2	-2	-1	0	0			0	266	432	266	0
0.15	0	-67	-129	-163	-151	-115	-80	-55	-38	-26	-18	-13	-9	-6	-4	-3	-2	-1	-1	0			0	131	197	131	0
0.2	0	-45	-84	-105	-105	-89	-69	-51	-37	-27	-19	-14	-10	-7	-5	-4	-2	-1	-1	0			0	63	92	63	0
0.25	0	-30	-55	-70	-73	-66	-55	-44	-33	-25	-19	-14	-10	-7	-5	-4	-2	-2	-1	0			0	30	43	30	0
0.3	0	-20	-36	-47	-50	-48	-42	-35	-28	-21	-16	-12	-9	-7	-5	-3	-2	-1	-1	0	0	0	0	15	21	14	0
0.35	0	-13	-23	-30	-34	-33	-30	-26	-21	-17	-13	-10	-7	-6	-4	-3	-2	-1	-1	0	0	1	3	8	10	7	0
0.4	0	-8	-14	-18	-21	-21	-19	-17	-14	-11	-9	-7	-5	-4	-3	-2	-1	-1	0	0	0	1	2	4	5	3	0
0.45	0	-4	-7	-9	-10	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	-1	-1	0	0	0	0	1	1	2	2	1	0
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.55	0	4	7	9	10	10	9	8	7	6	5	4	3	2	1	1	1	0	0	0	0	-1	-1	-2	-2	-1	0
0.6	0	8	14	18	21	21	19	17	14	11	9	7	5	4	3	2	1	1	0	0	0	-1	-2	-4	-5	-3	0
0.65	0	13	23	30	34	33	30	26	21	17	13	10	7	6	4	3	2	1	1	0	0	-1	-3	-8	-10	-7	0
0.7	0	20	36	47	50	48	42	35	28	21	16	12	9	7	5	3	2	1	1	0	0	0	0	-15	-21	-14	0
0.75	0	30	55	70	73	66	55	44	33	25	19	14	10	7	5	4	2	2	1	0			0	-30	-43	-30	0
0.8	0	45	84	105	105	89	69	51	37	27	19	14	10	7	5	4	2	1	1	0			0	-63	-92	-63	0
0.85	0	67	129	163	151	115	80	55	38	26	18	13	9	6	4	3	2	1	1	0			0	-131	-197	-131	0
0.9	0	94	203	268	223	139	83	51	32	21	14	10	7	5	3	2	2	1	0	0			0	-266	-432	-266	0
0.95	0	104	322	481	335	134	63	33	19	12	8	5	4	3	2	1	1	0	0	0			0	-500	-1000	-500	0
1	0	0	500	1000	500	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0							

algorithm



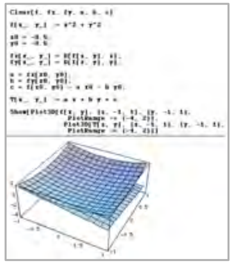
$$V_0 = \tfrac{1}{4}(V_N + V_S + V_E + V_W)$$

must be satisfied everywhere

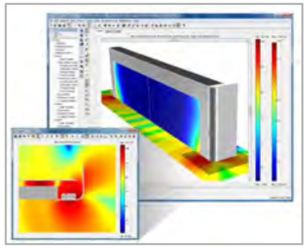
We need a diverse set of tools to attack a rich set of problems efficiently:

Utilities, programming, “low level”

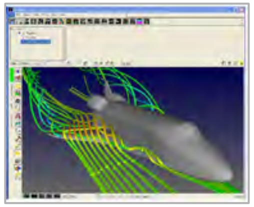
Numerical libraries



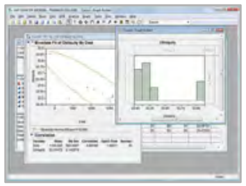
General mathematical analysis



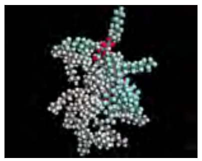
Engineering analysis



Visualization



Statistical applications



Special purpose

Over the years, the DuPont HPC Environment has followed developments in hardware -- and hardware costs.

Run a host of applications
- CFD, FEA, Comp Chem, Bioinformatics, DB, etc.

Include storage & backup services

Use multiple platforms (SMP, Clusters, etc)

Run batch jobs through LSF

Provide a cloud computing environment for large jobs

CPU Hr. = $1000 $500 $300 $150 $20 $5 $3 <$2

Overview: underground injection

Modeling is one of the means required by USEPA to demonstrate that operations are protective of human health and the environment.

The demonstration of safe operations may be based on:

flow and containment: advective transport, diffusion
injectate is confined both vertically and horizontally

chemical fate: chemical kinetics and transport
injectate is rendered non-hazardous

There are also structural integrity issues to demonstrate:

induced seismicity evaluation
changes in stresses due to fluid injection do not de-stabilize the rock mass

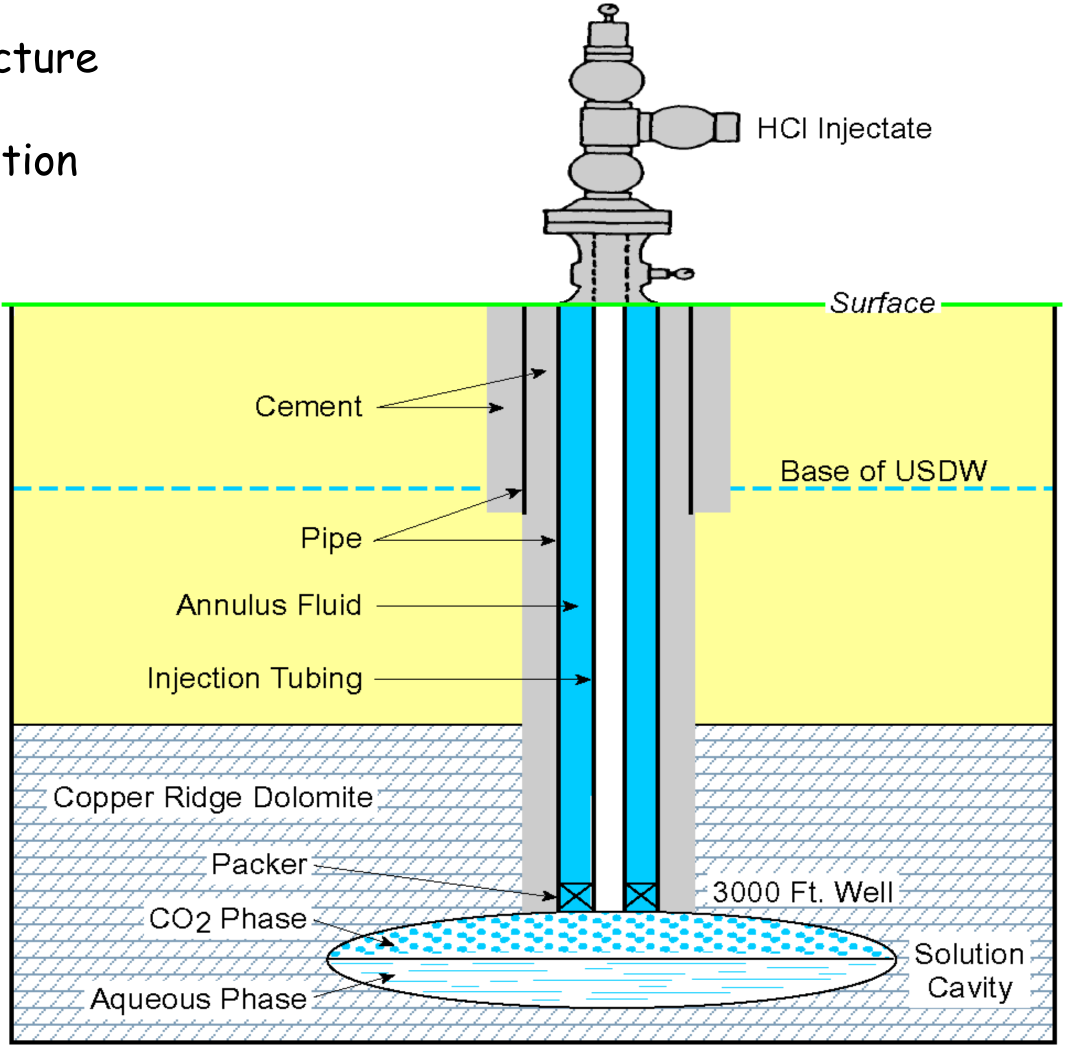
stability of nearby rock mass
presence of well and cavity (if present) do not de-stabilize the rock mass

Class I injection wells are regulated by USEPA and state and local authorities.

"... not just a hole in the ground"

a highly engineered structure

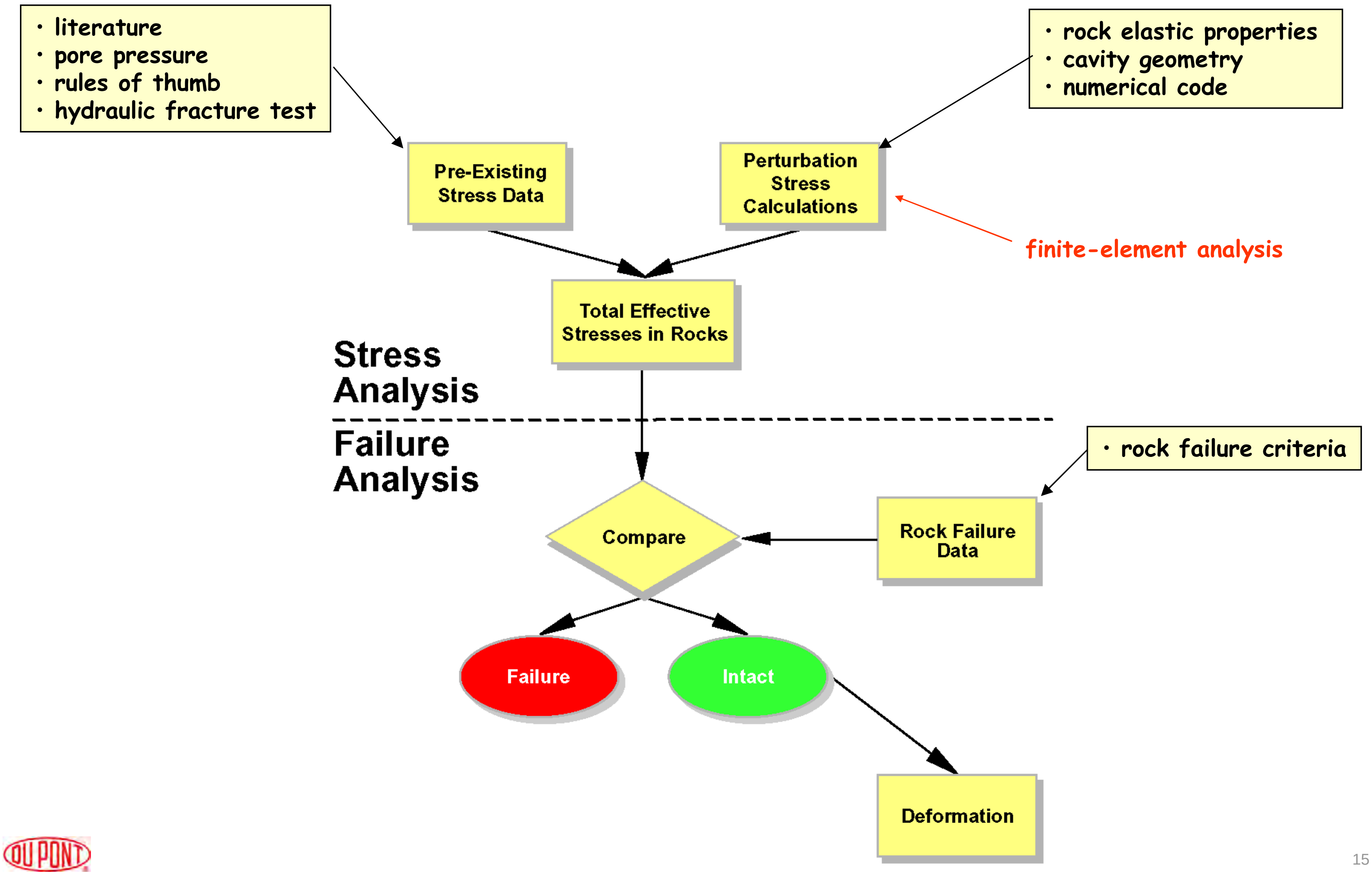
multiple layers of protection



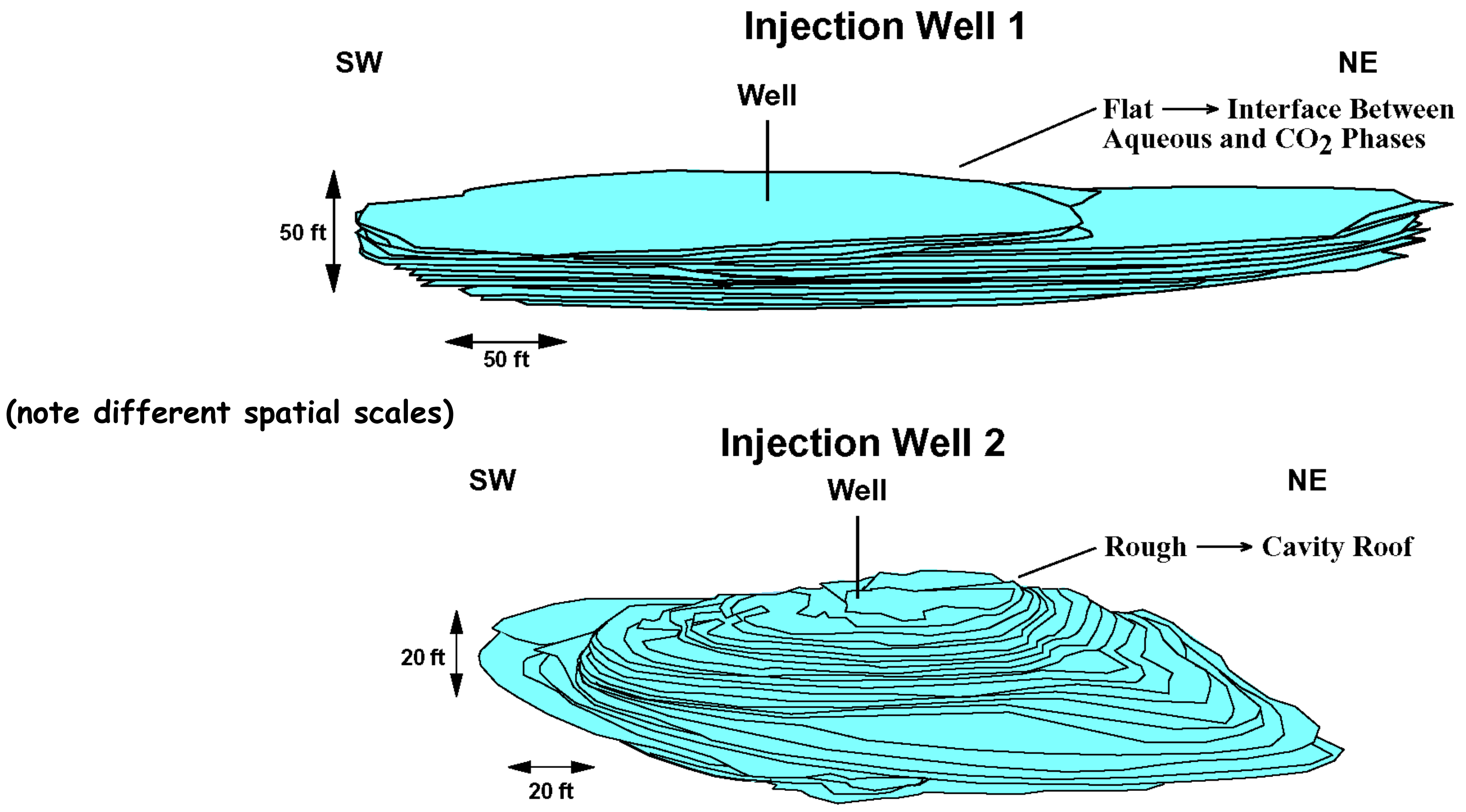
Case study. Acidic fluid injected into a carbonate rock creates a solution cavity.

Is the cavity stable?

The structural integrity analysis is composed of a stress analysis, followed by a failure analysis.



Geometry of cavities as measured by Sonar Caliper Survey and confirmed by borehole televiewer.



Question: Could these cavities fail?

The stress calculation is straightforward once the basic data are in hand.

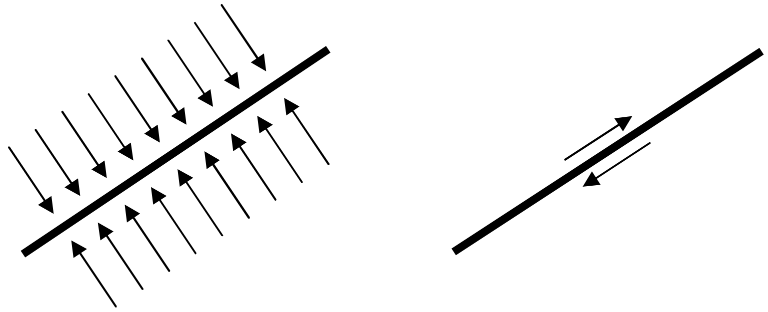
The test for failure is straightforward, although tedious.

Specify a set of potential failure planes

- at various locations near the cavity
- at various orientations

Calculate normal and shear stresses for each

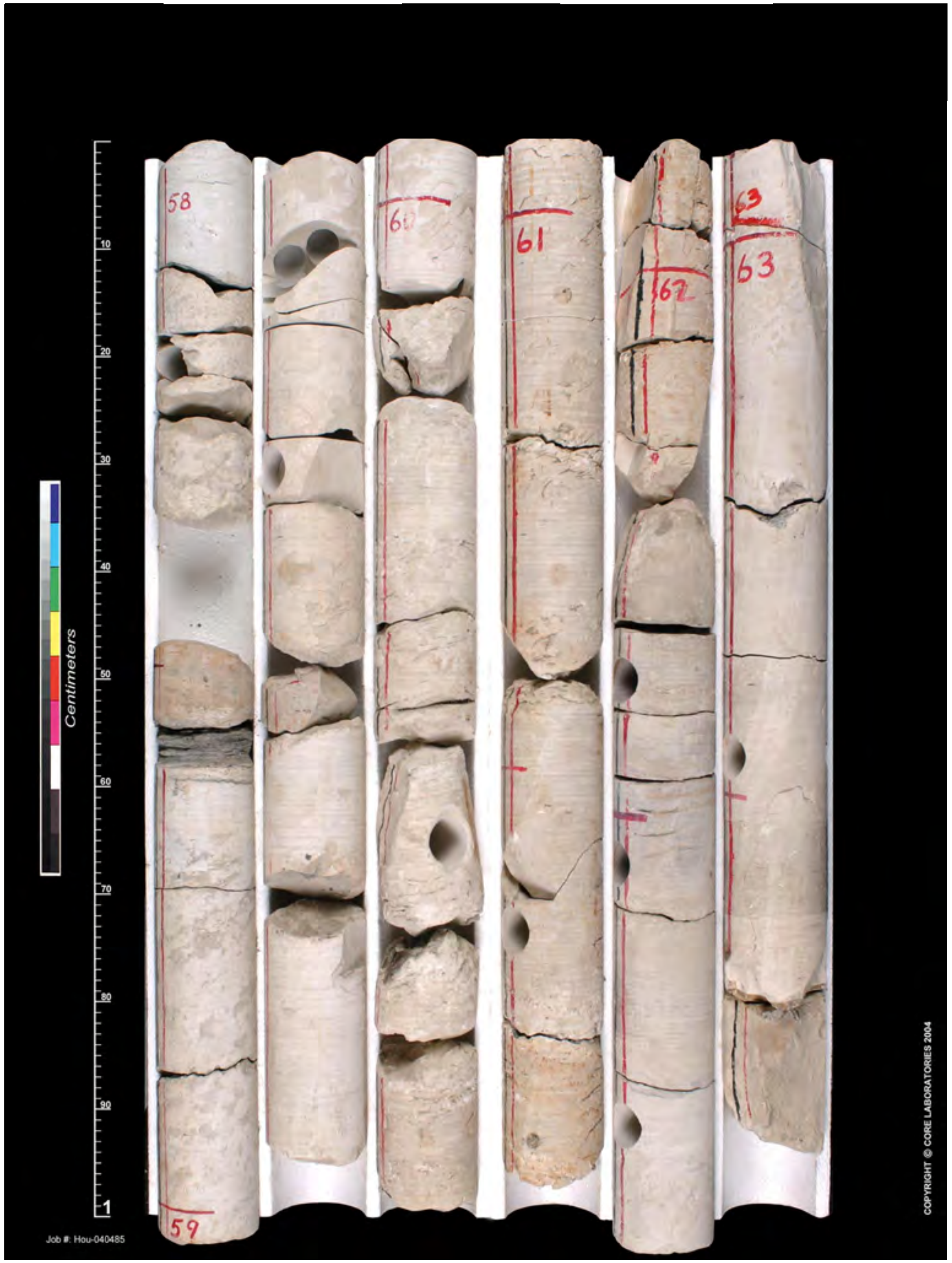
Observe whether failure envelope is exceeded



normal stress **shear stress**

Rock mechanical data come from selected core samples.

Core showing plugs cut out for rock mechanics and permeability testing.



Rock elastic properties were measured both statically and ultrasonically.

static values from "rock squeezing" for the structural integrity analysis

ultrasonic values from wave propagation studies for correlation with well logs

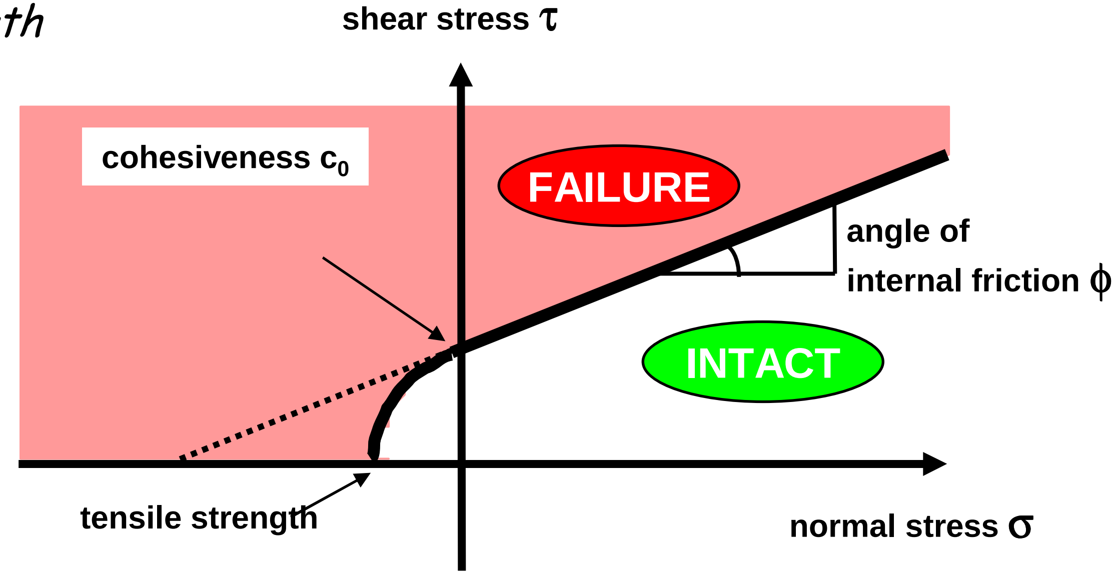
Isotropic elastic materials are characterized by density ρ, Young's modulus E, & Poisson's ratio ν

E = stress / strain

$$\nu = \frac{\text{lateral strain}}{\text{axial strain}}$$

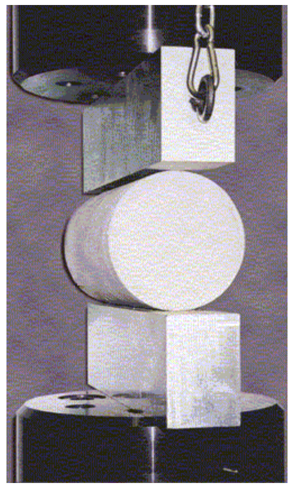
Static "rock squeezing" determined the failure envelope for each cored interval.

cohesiveness (related to unconfined compressive strength)
angle of internal friction
tensile strength



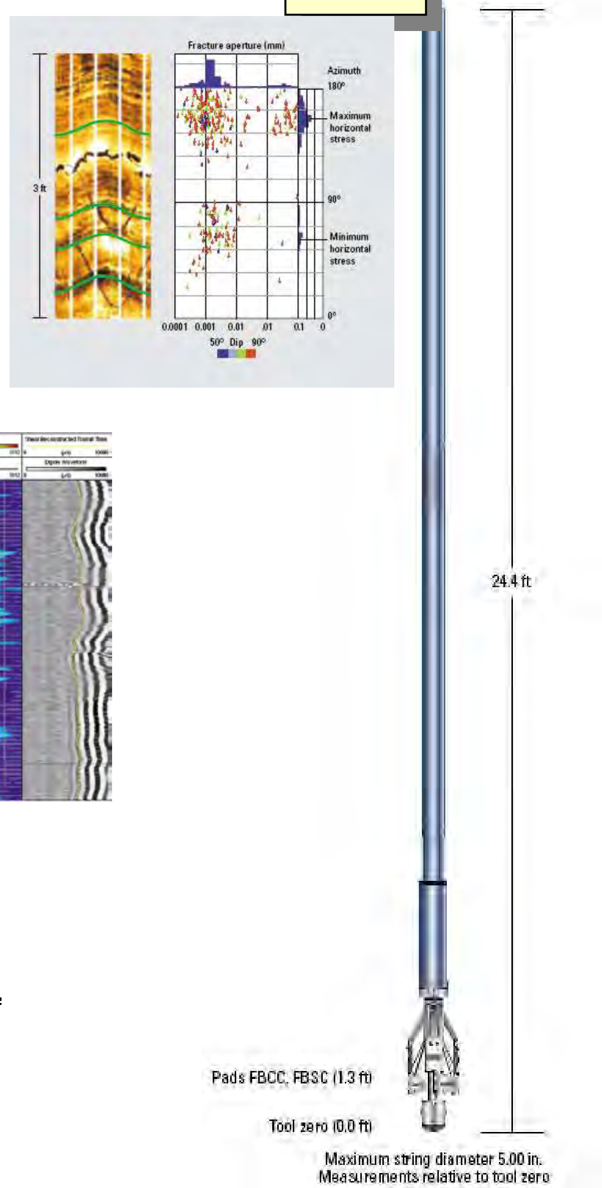
triaxial test stand

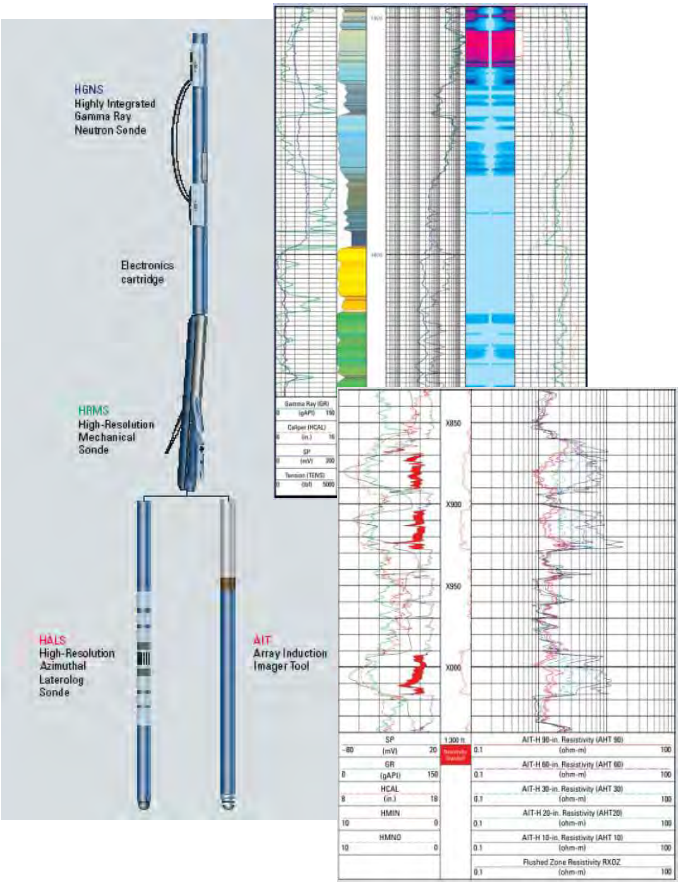
"Brazilian test" measures the tensile strength



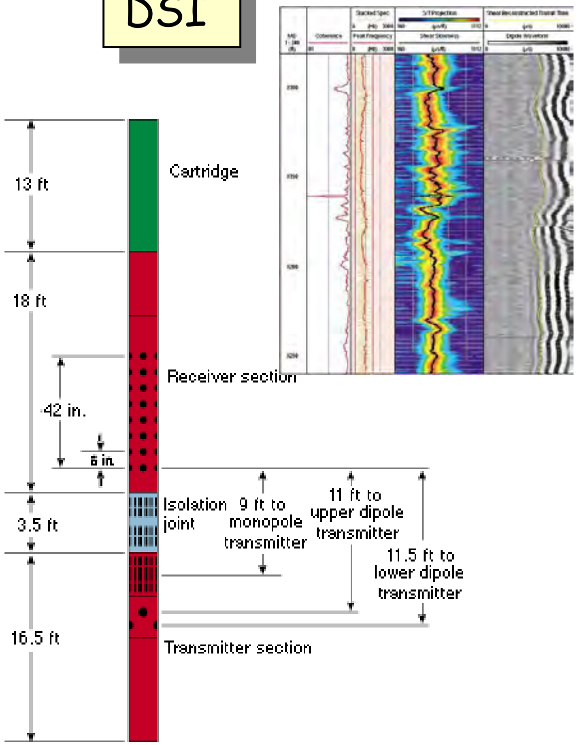
Wireline well logs provided continuous coverage down the well.

FMI





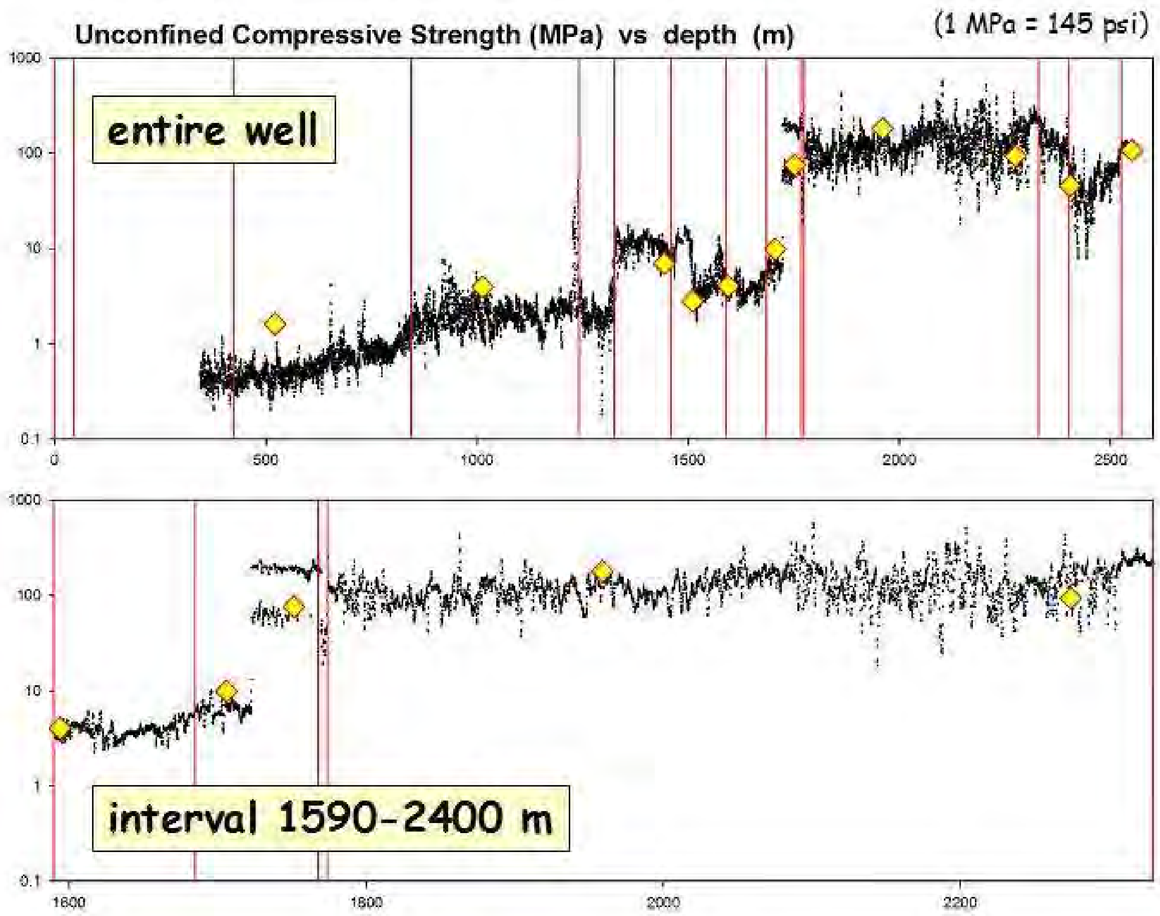
DSI



standard tools

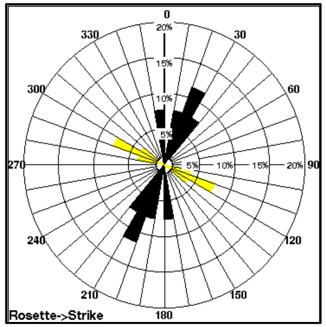
The MEM provides a **"log" of the rock mechanical properties** down the well. For example, the unconfined compressive strength (UCS), here shown with

- the geological interpretation (red vertical lines) and
- the Core Lab measurements (yellow diamonds)



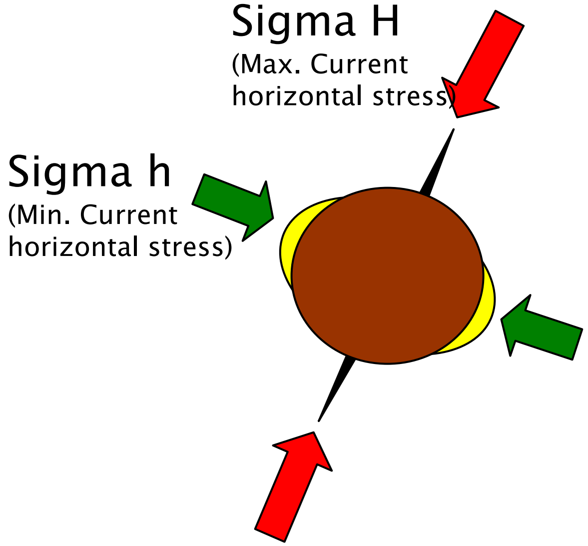
Well measurements allow us to estimate the orientation and magnitude of the background stress field.

Schlumberger FMI log



Breakouts and drilling-induced fractures observed in well logs indicate local **stress field orientation**

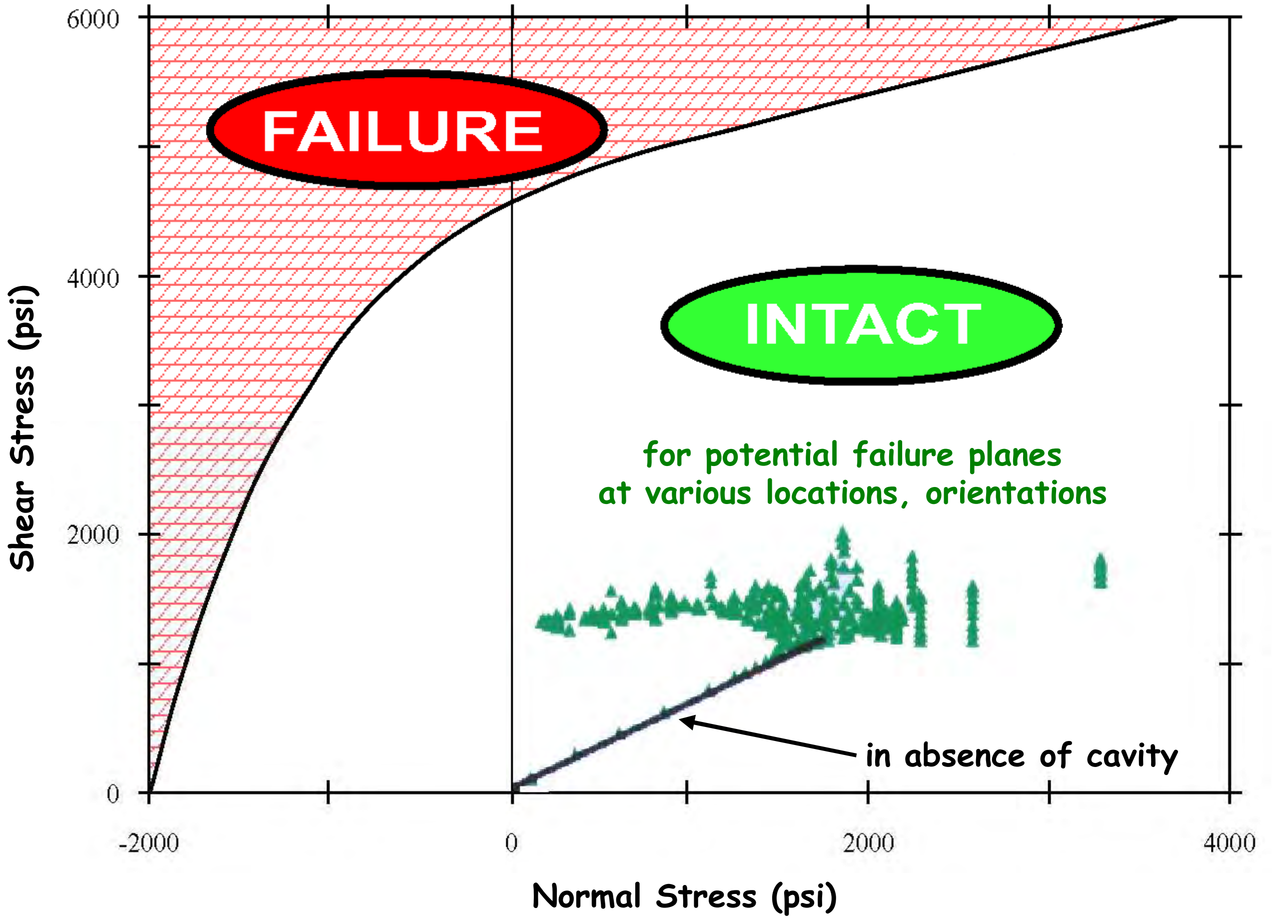
A hydrofrac test is the best available estimate of the **least horizontal stress.**



From Schlumberger's DSI log, we infer **greatest horizontal stress.**

From the density log, we estimate the **vertical stress**, which comes from the "overburden" (gravity acting on mass density).

We pass the test for failure on both cavities. Both are expected to remain stable for the duration of injection operations.



Overview: stratospheric ozone depletion and global warming

Modeling is used by the world scientific community to unravel the mechanisms of ozone depletion and to predict the greenhouse warming caused by chemicals emitted on a large scale.

global chemistry-transport model

- chemical kinetics, gas phase and heterogeneous
- atmospheric dynamics: advective and diffusive transport
- radiative forcings
- Ozone Depletion Potential

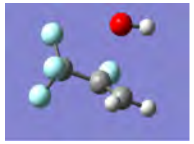
warming model & emissions inventories

- estimate/predict atmospheric loadings
- Global Warming Potential

$$GWP_i \equiv \frac{\int_0^{TH} RF_i(t)dt}{\int_0^{TH} RF_r(t)dt} = \frac{\int_0^{TH} a_i \cdot [C_i(t)]dt}{\int_0^{TH} a_i \cdot [C_i(t)]dt} = \frac{\int_0^{TH} a_i \cdot \left[C_i^0 \exp(-t/\tau)\right]dt}{\int_0^{TH} a_i \cdot [C_i(t)]dt}$$

quantum chemistry models

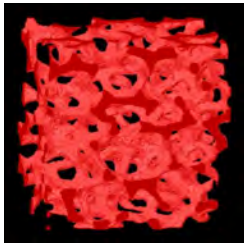
- estimate energy balances due to molecular degradation of greenhouse gases
- provide inputs to the models above

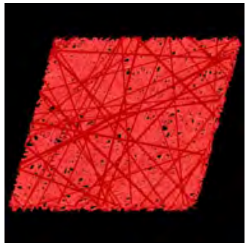


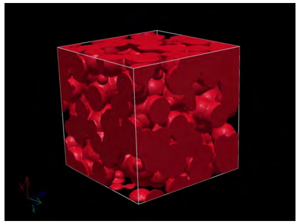
Transport properties of disordered media
(computational material science).

Many DuPont processes and products involve disordered media.

fuel cell components
filter and barrier media
thermal insulation, sound/noise control
clothing and hygiene products
composite materials
packed beds
aquifers







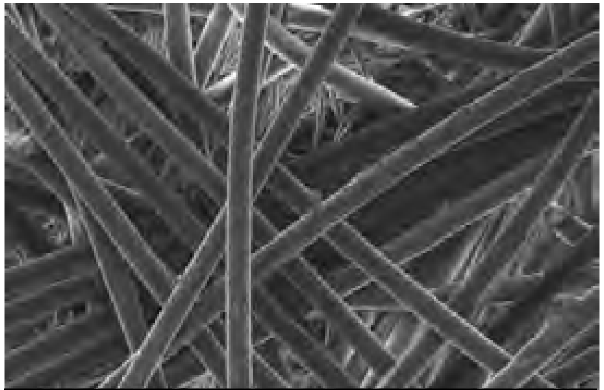
Difficult for a finite-element approach!

GeoDict can simulate a wide variety of structures.

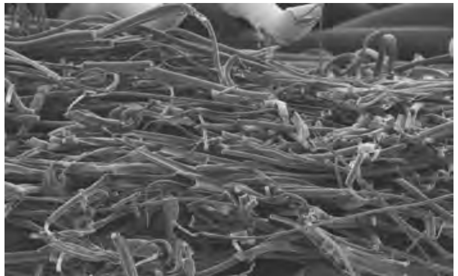
synthesize geometry
analyze porosity
calculate flow field
simulate filtration/barrier performance

Case study. Predict the barrier performance of a 3-layer fibrous medium.

SEMs



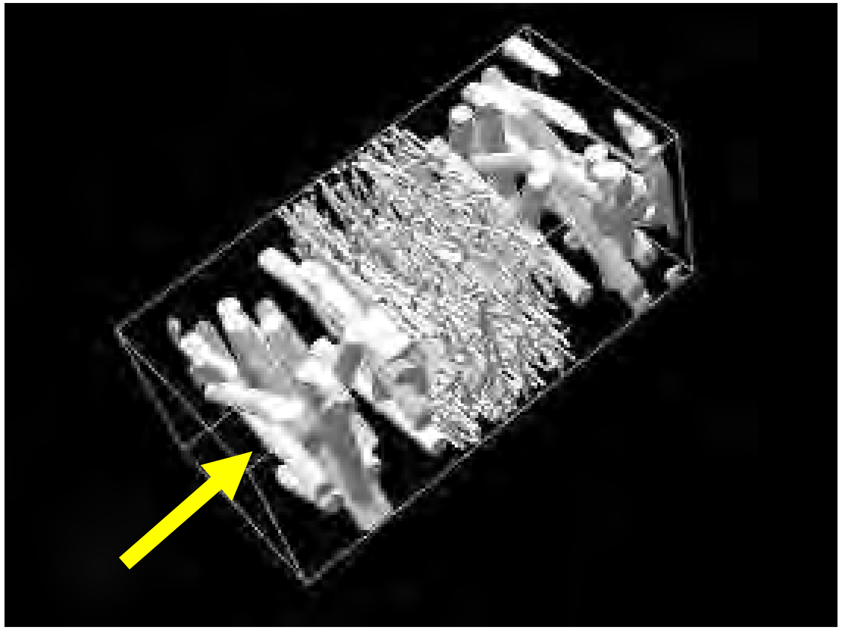
plan view



cross section view

Step one: generate a virtual sample.

model of medium

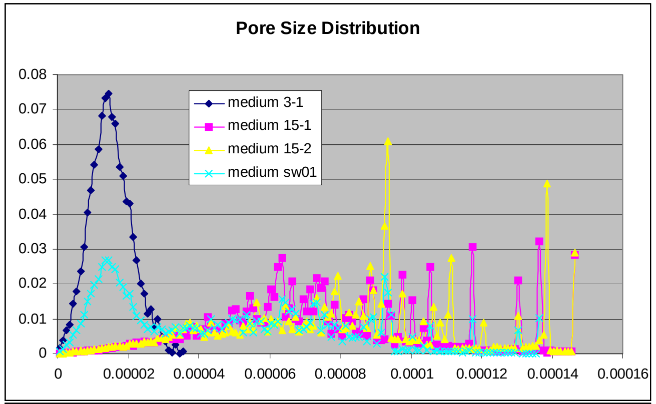


simulated SEMs

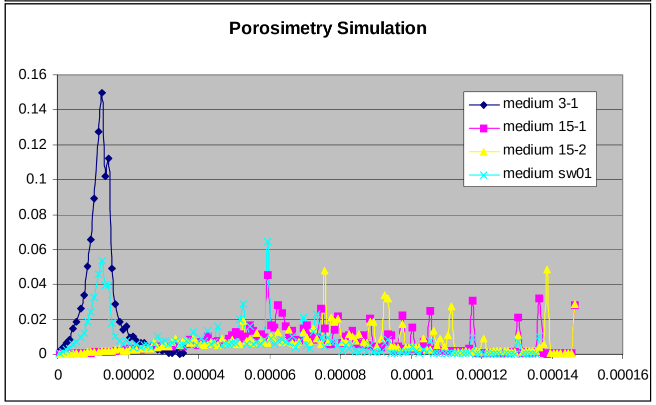
Given a synthetic structure, the code can predict its pore properties.

pore size distribution for

all pores

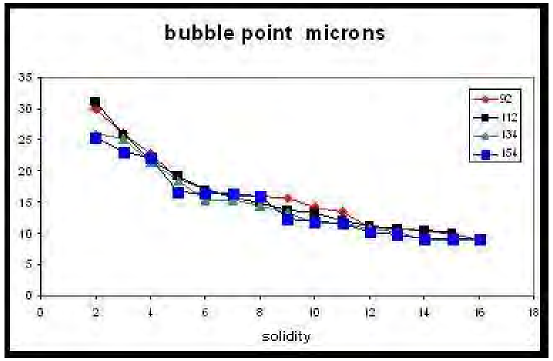


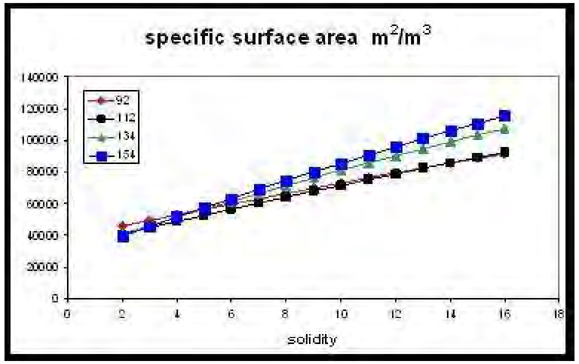
through-pores only

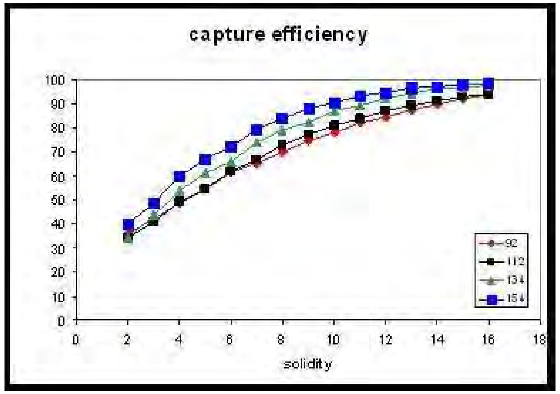


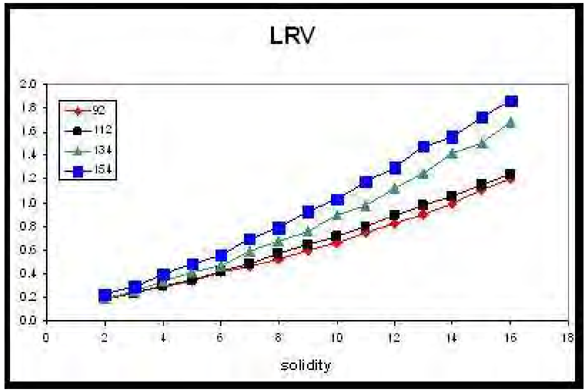
percolating sphere emulates bubble point

Scripting the runs allows a large number of number of models to be run efficiently with minimal intervention.









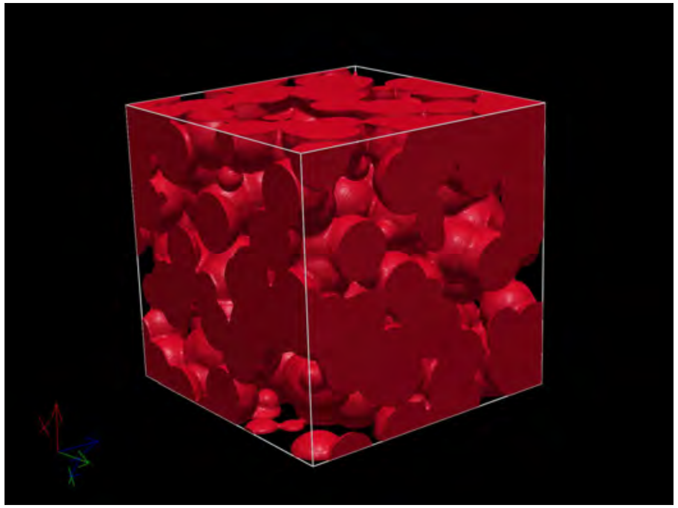
This procedure generates quantitative relationships, showing sensitivities to key parameters.

These can be used as properties in a finite-element model of the overall device.

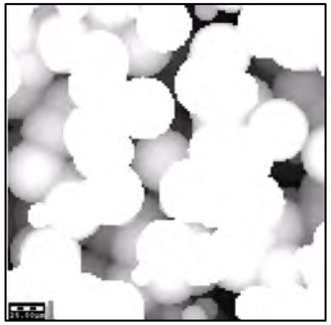
Case study. The loss of permeability in a sandstone aquifer due to the presence of fine particles.

Consider, e.g., 80% / 20% mixture of 50 mm / 20mm sand grains:

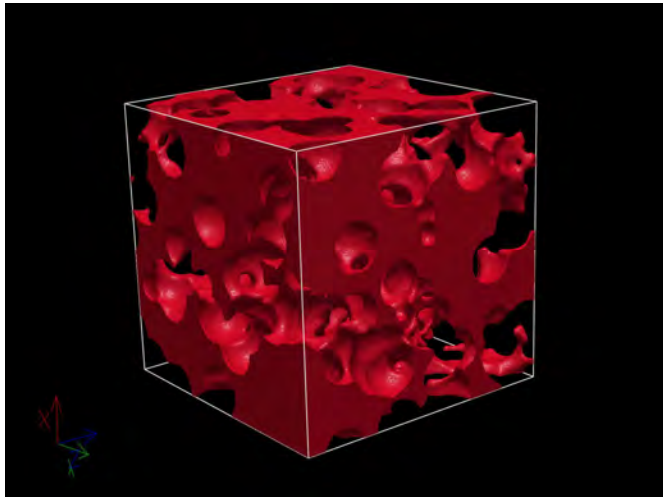
structure with 30% porosity



simulated SEM

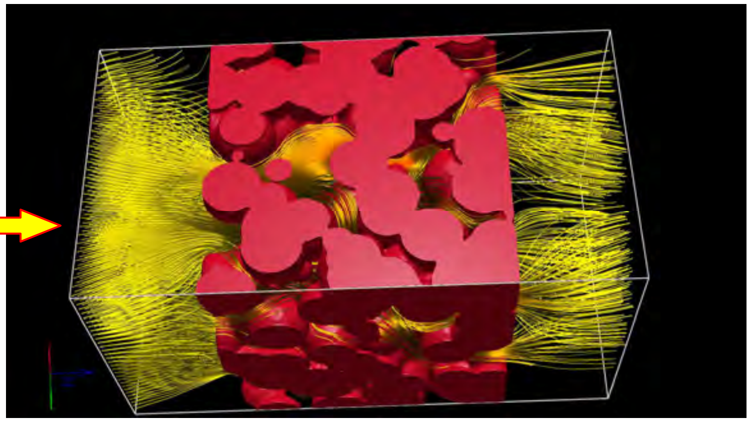


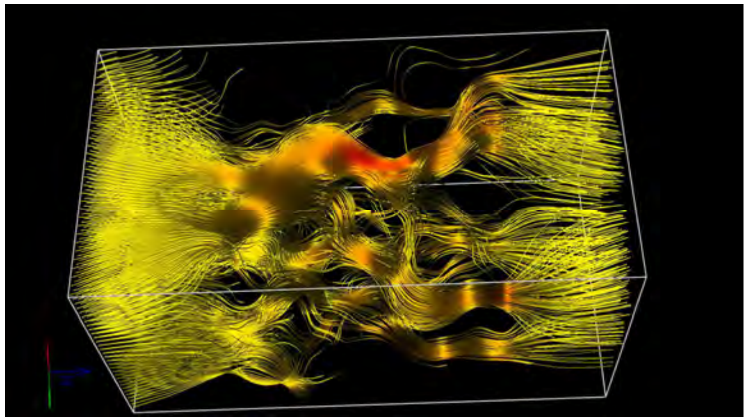
pore structure



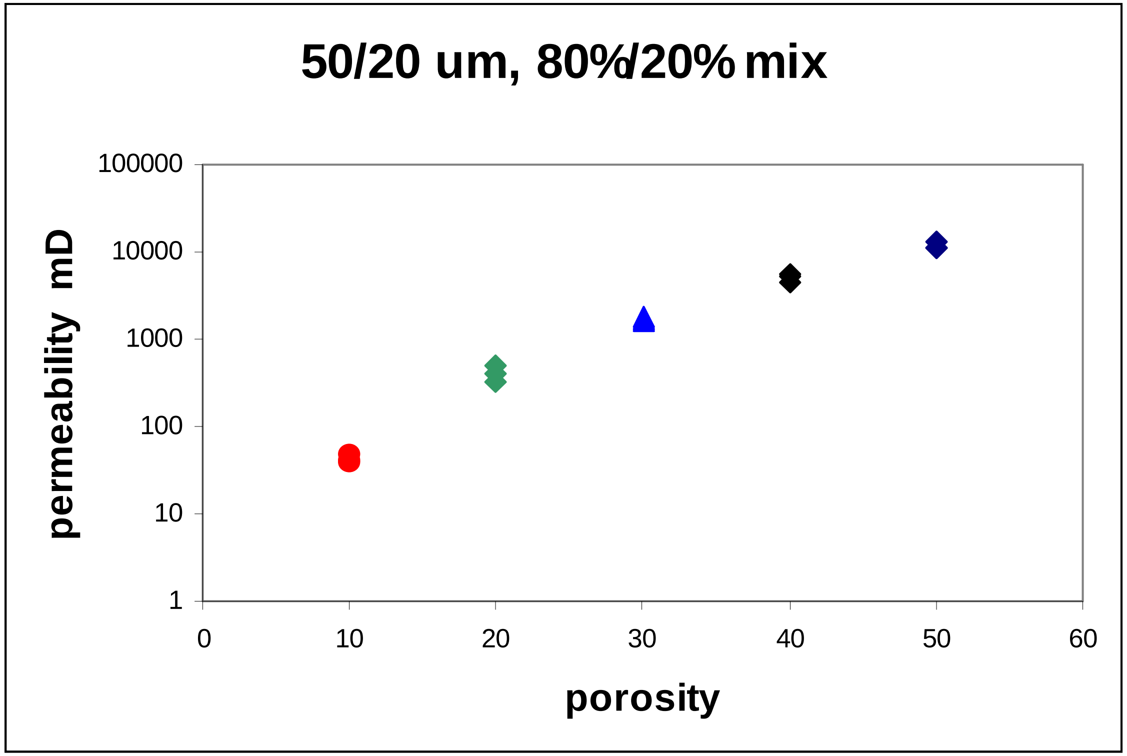
streamlines through the structure

flow





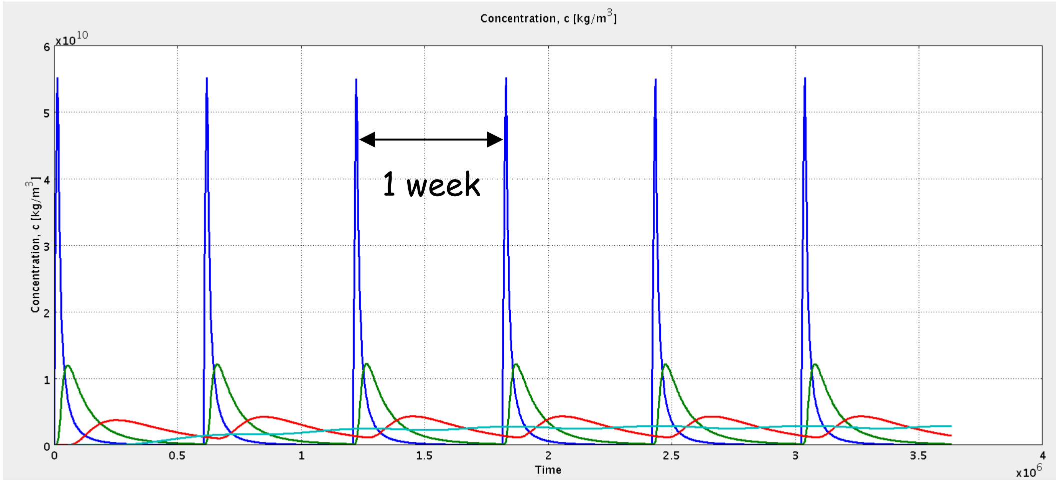
A scripted suite of flow models gives us a quantitative relationship for permeability as a function of porosity -- with no adjustable parameters -- that agreed well with lab measurements.



Case study: Transport and dispersion of a train of treatment pulses injected into an aquifer.

goal: design dosing of the aquifer (concentration, pulse length, frequency)

typical result: a 4-hr pulse every week, seen at 1, 3, 6, 10 m from well



Two step procedure, using COMSOL:

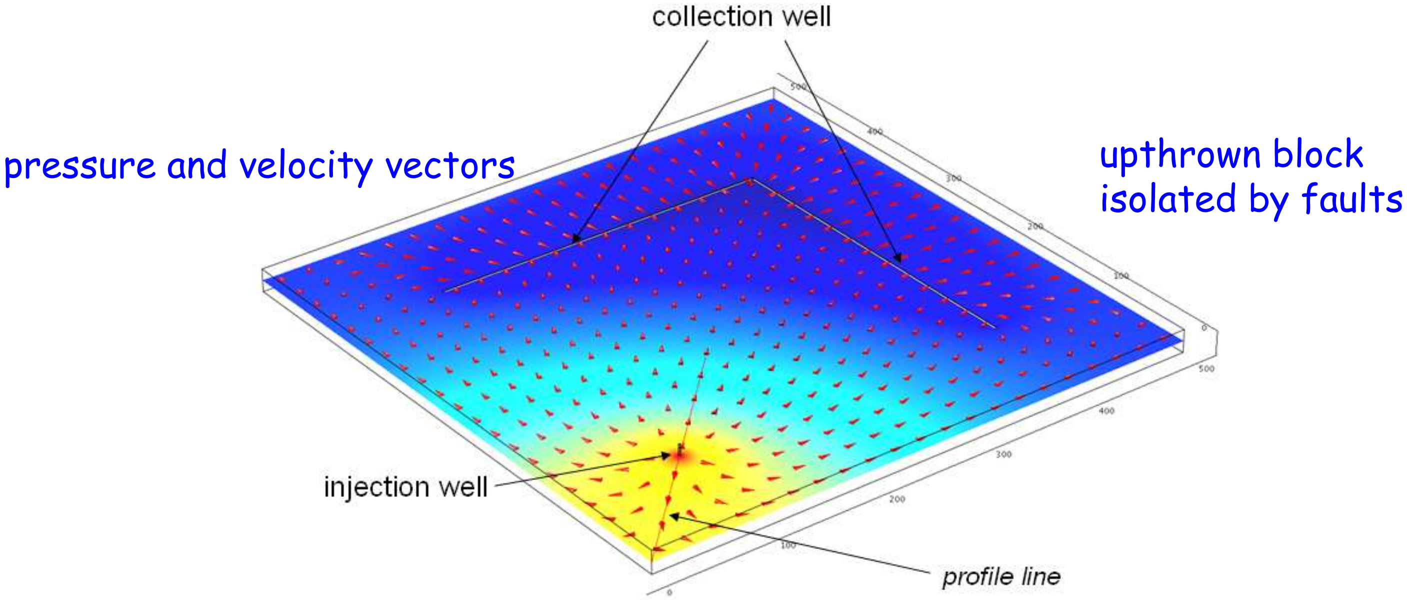
1. Darcy's Law.
   Pump pressure establishes a background steady-state pressure and flow fields (the well is pumping water for some time before our solute pulses are introduced).

$$S\frac{\partial p}{\partial t} + \nabla\cdot\left[-\frac{\kappa}{\eta}(\nabla p + \rho_f g \nabla D)\right] = Q_s$$

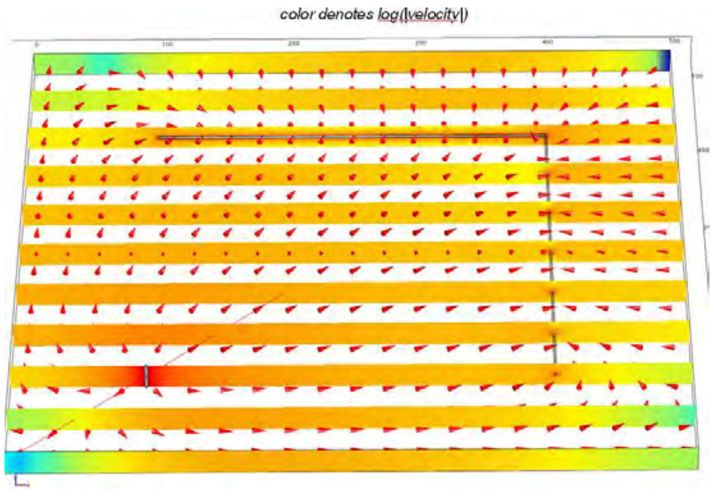
2. Advection-dispersion equation.
   Pulses of solute are transported by the background flow field, dispersing as they travel.

$$\theta_s \frac{\partial c_i}{\partial t} + \rho_b \frac{\partial c_{Pi}}{\partial c}\frac{\partial c_i}{\partial t} + \nabla\cdot[-\theta_s D_{Li}\nabla c_i + \mathbf{u}c_i] = R_{Li} + R_{Pi} + S_{ci}$$

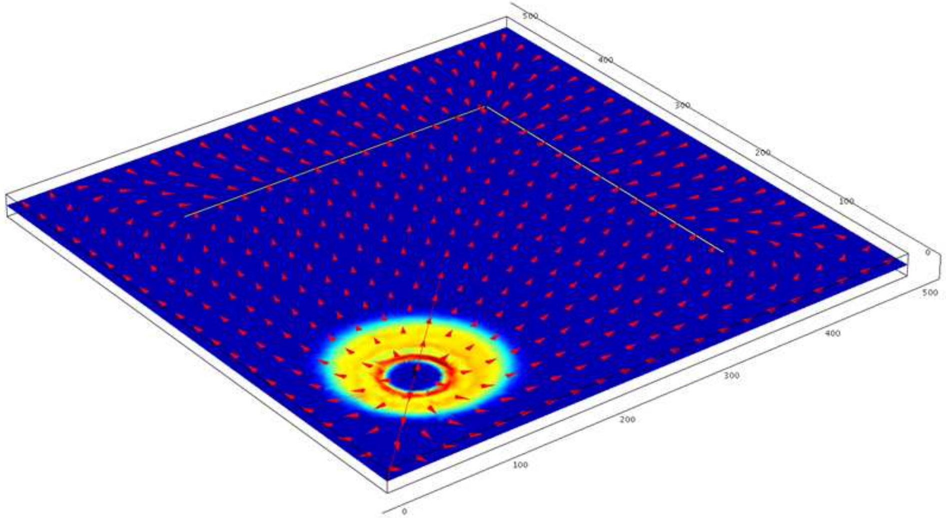
A 3-D model shows the injector/producer geometry.



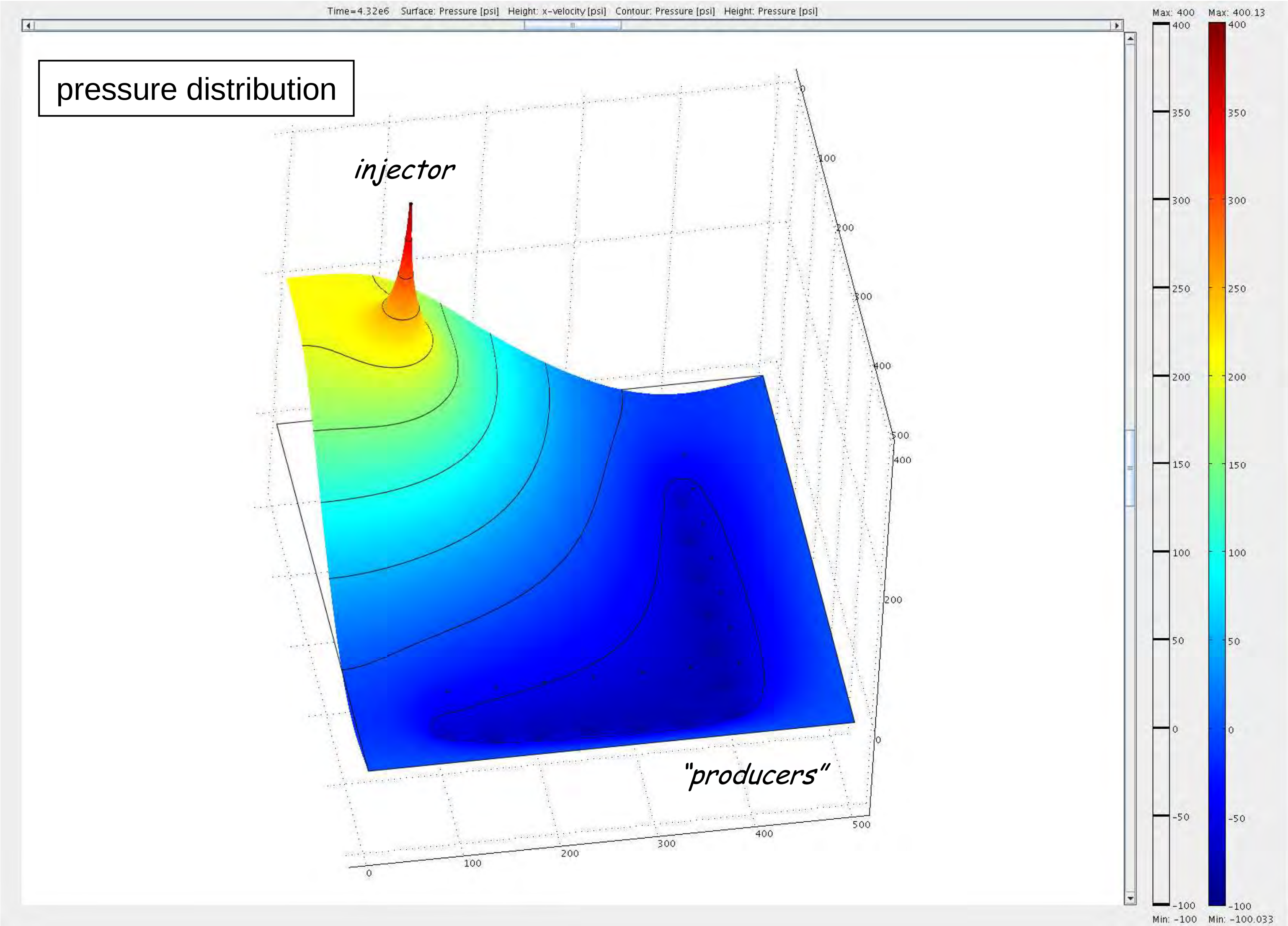
3-D velocity field



Outward solute transport after five weekly pulses

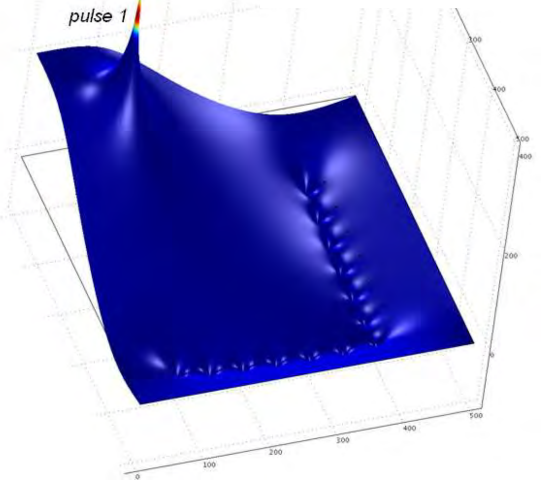


We can do it more conveniently in 2-D, however, since the aquifer is thin.

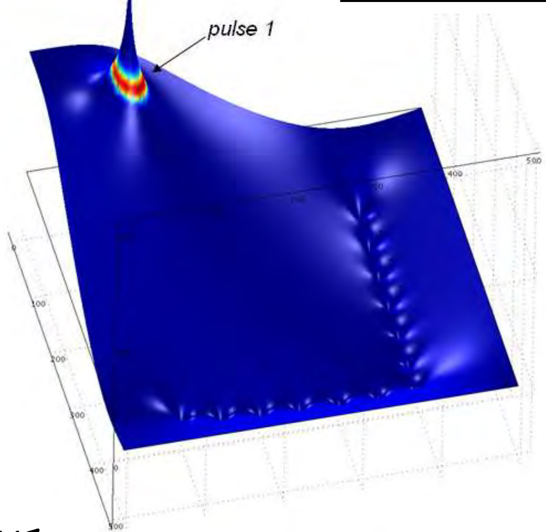


The pulses move down-gradient, spread geometrically, and disperse.

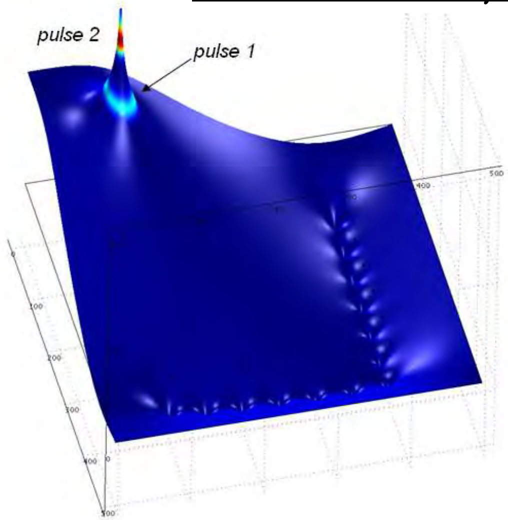
just after pulse 1



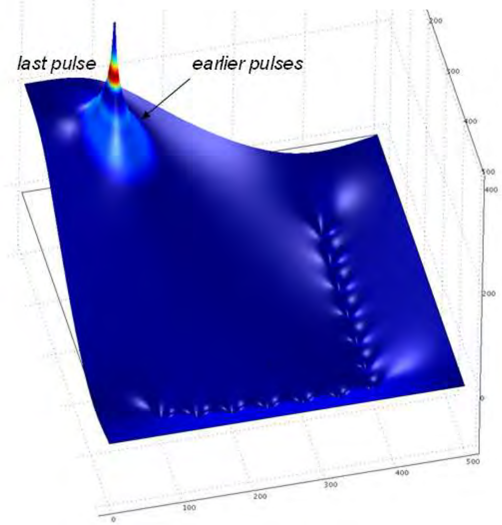
after six days



after 7-1/2 days



after 7+ weeks



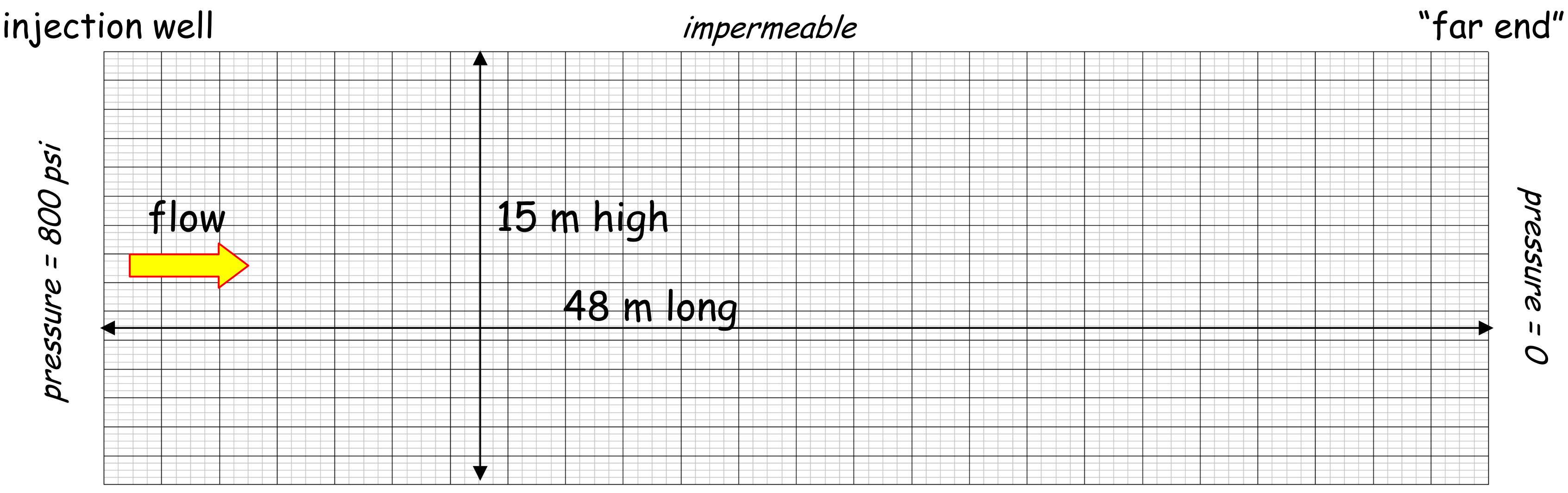
Case study. The numerical value of dispersivity is a key question in scaling up from lab to the field: empirically, its value depends on the scale size of the measurement.

$$\theta_s \frac{\partial c_i}{\partial t} + \rho_b \frac{\partial c_{Pi}}{\partial c}\frac{\partial c_i}{\partial t} + \nabla \cdot [-\theta_s D_{Li} \nabla c_i + \mathbf{u} c_i] = R_{Li} + R_{Pi} + S_{ci}$$

dispersivity -> hydrodynamic mixing

We show that heterogeneity of an aquifer can be important in dispersing a solute and can be the basis for a scale dependence of the dispersivity.

0. Model is planar 2-D
1. Darcy's law establishes the pressure and flow
2. Advection-dispersion equation transports solute (injected once a week for 4 hours)

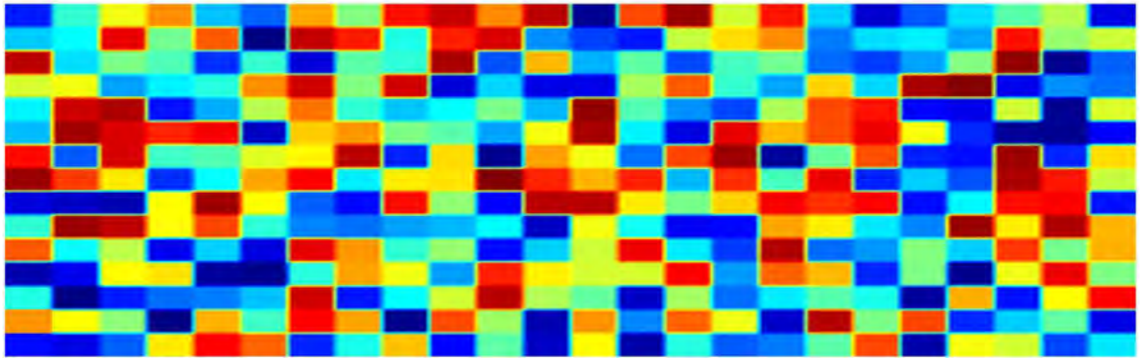


2m x 1m domains (large blocks)
16 elements (small blocks) per domain

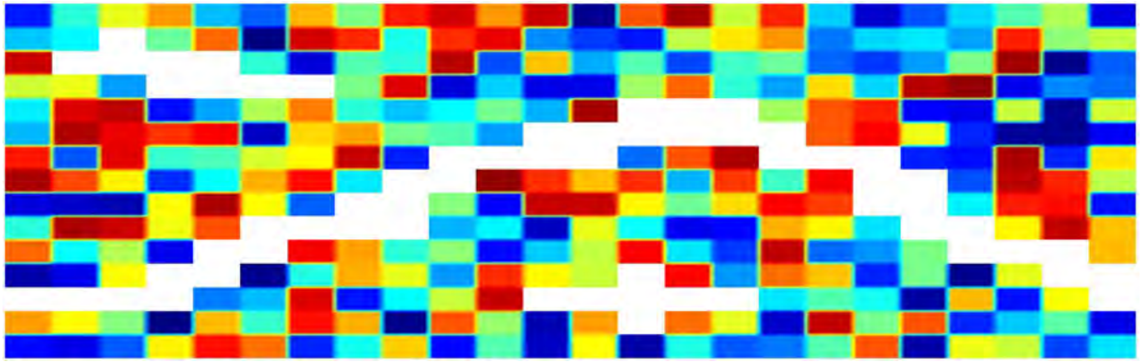
DUPONT

We look at two permeability distributions:

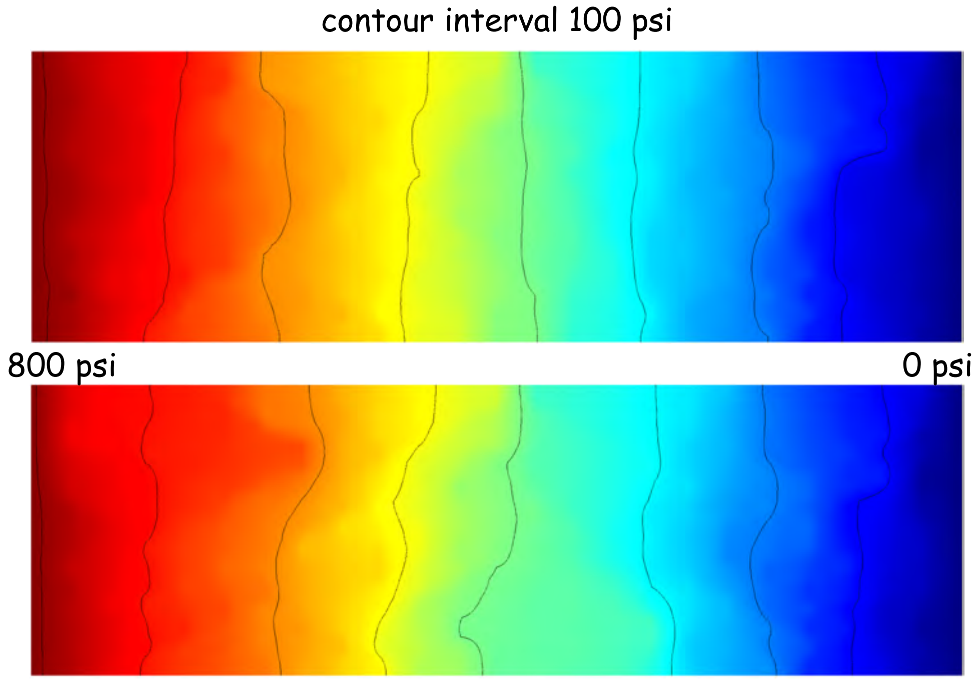
randomly assigned on [0, 100] milliDarcy



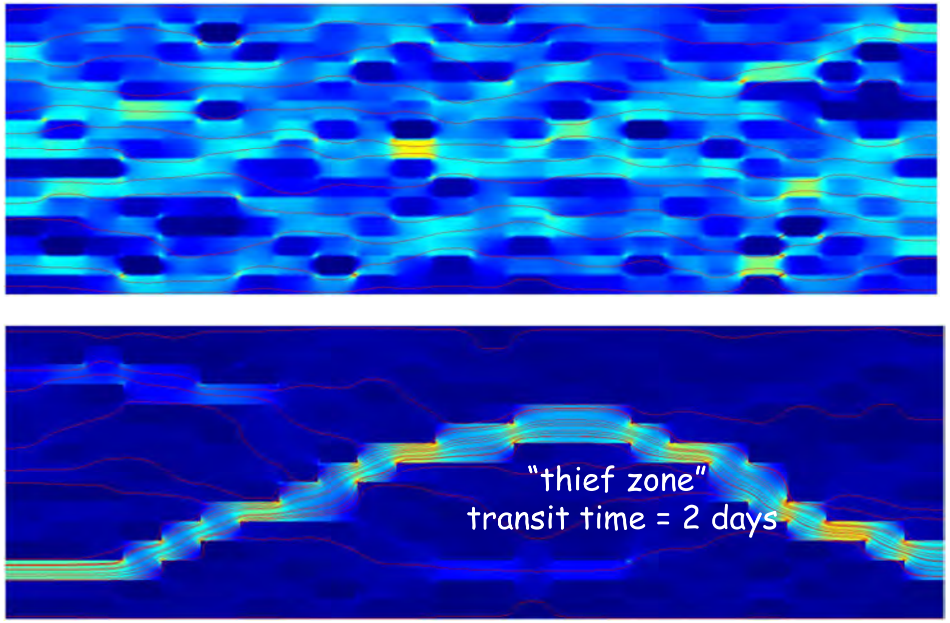
as above, with high perm zones (1 Darcy)



The pressure distributions are quite similar.



The high perm zones "attract" and channel the flow, as shown by |velocity| & streamline plots.

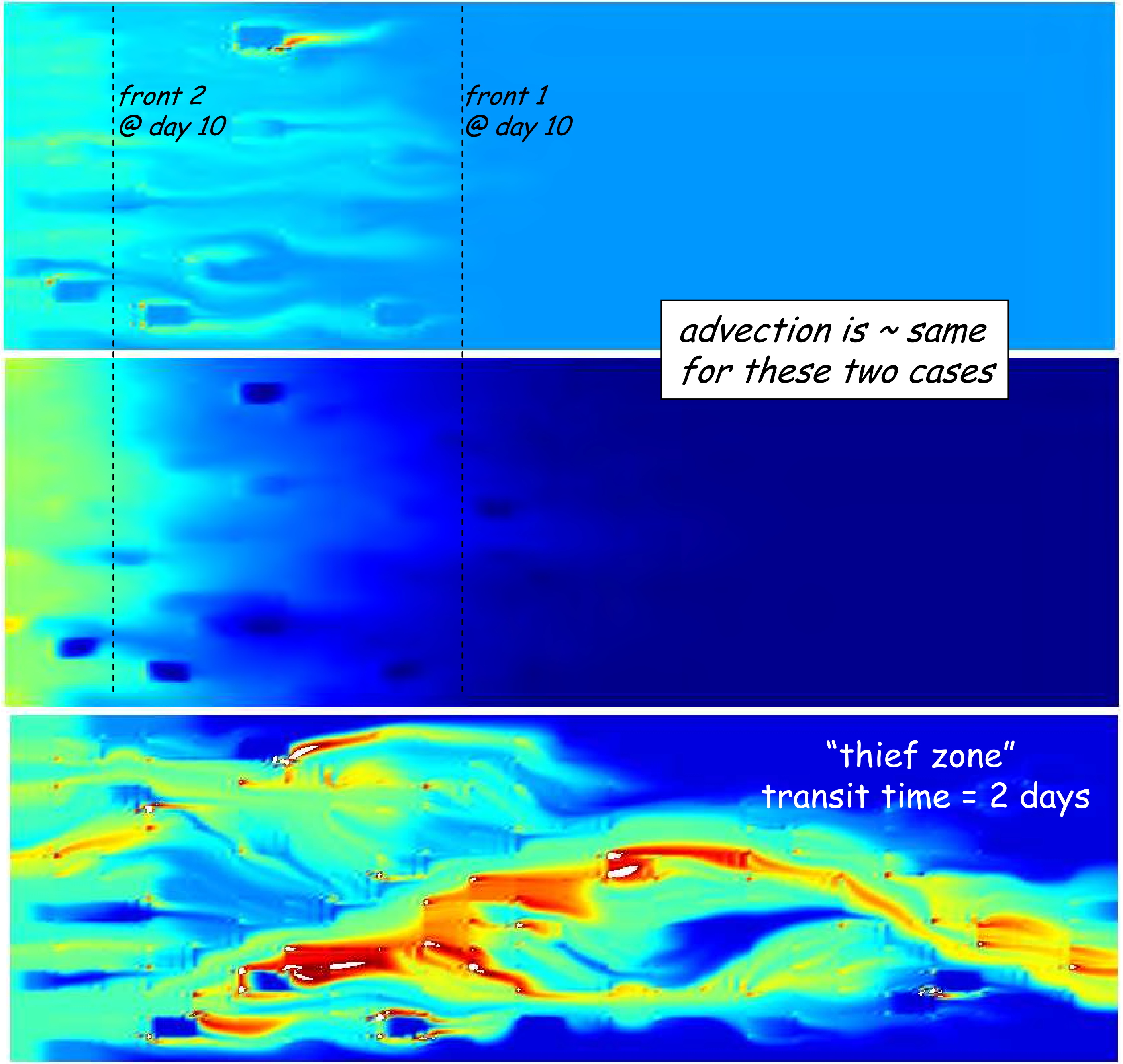


For comparison, here are the solute concentrations after ten days:

Solute dispersal for random perm, low dispersivity (0.05 m)

Solute dispersal for random perm, high dispersivity (1 m)

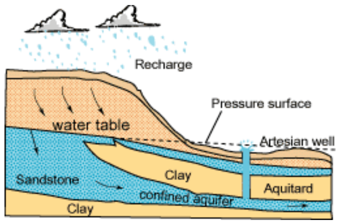
Solute dispersal for random perm with hi perm zones, low dispersivity (0.05 m)



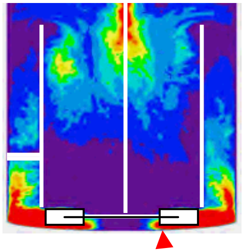
Challenges:

Many real life problems are **ill defined** at the outset.
Often, getting **good input data** is the most difficult task.
Many problems are “**multiphysics**.”
Many systems are **disordered in some sense**.
Many problems are structured across **multiple scale sizes**.
It is important to understand **sensitivities** to model parameters.

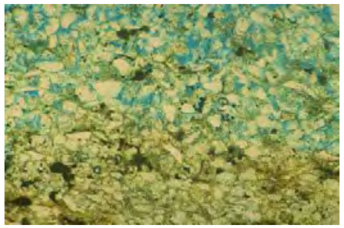
macro-scale

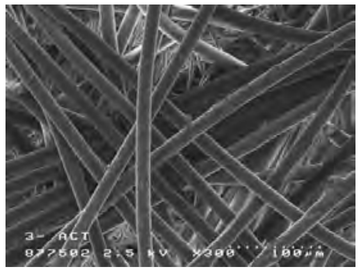


meso-scale



micro-scale

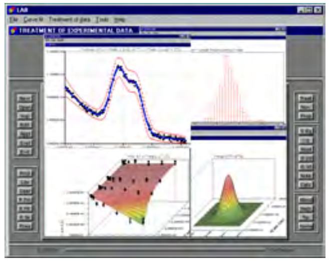


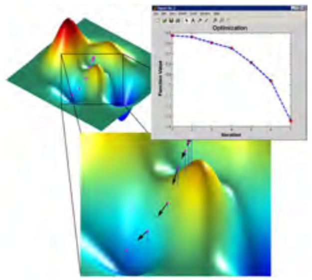


Advice to modelers (IMHO, of course):

Use “empirical” and “fundamental” modeling early on -- when it can really make a difference:

help define the problem
guide experiments and interpret and codify data
capture fundamental understanding
suggest product/process improvements





Use “empirical” and “fundamental” modeling early on -- when it can really make a difference:

- help define the problem
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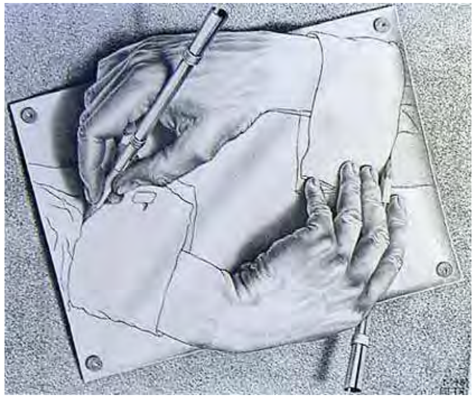
Do hand calculations. Perform a scale analysis of your problem to identify what is important and what is not. Draw things to scale.



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Develop tools and techniques to solve funky, non-standard equations.

$$z(1-z)\frac{d^2 y}{dx^2}+[c-(a+b+1)z]\frac{dy}{dx}-aby=0.$$

$$\frac{\partial\eta}{\partial t}=\frac{3}{2}\sqrt{\frac{g}{h}}\left(\eta\frac{\partial\eta}{\partial x}+\frac{2}{3}\frac{\partial\eta}{\partial x}+\frac{1}{3}\sigma\frac{\partial^3\eta}{\partial x^3}\right),$$

$$\frac{d^2 U}{du^2}-[a-2q\cosh(2u)]U=0$$

$$\frac{1}{3}u_{tt}-u_t u_{xx}-\frac{3}{2}u_x^2 u_{xx}+u_{xxxx}=0$$

Use "empirical" and "fundamental" modeling early on -- when it can really make a difference:

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guide experiments and interpret and codify data
capture fundamental understanding
suggest product/process improvements

Do hand calculations. Perform a scale analysis of your problem to identify what is important and what is not. Draw things to scale.

Have tools to solve funky, non-standard equations.

Use "multiphysics" tools which couple diverse and complex phenomena without requiring a major development effort.

(my personal favorite, but there are others, too)

Use “empirical” and “fundamental” modeling early on -- when it can really make a difference :

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- guide experiments and interpret and codify data
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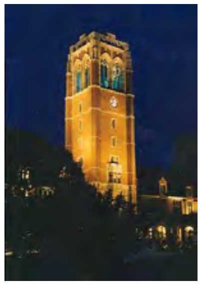
Do hand calculations. Perform a scale analysis of your problem to identify what is important and what is not. Draw things to scale.

Have tools to solve funky, non-standard equations.

Use “multiphysics” tools which couple diverse and complex phenomena without requiring a major development effort.

Maintain connections within the company and with vendors, academics, and government labs to gain access to the latest developments in modeling technology.



Many insightful statements have been made about modeling:

"There is nothing more practical than a good theory."
primarily attributed to Kurt Lewin, but also to Maxwell, Einstein, Hilbert, …

"A model should be as simple as possible, but not simpler."
Albert Einstein

"All models are wrong, but some are useful."
George Box

"The purpose of computing is insight, not numbers."
Richard Hamming

"But at some point you need numbers, too."
Rick Nopper