Can we make accurate predictions of the long-term fate of CO2 stored in aquifers?

Gary A. Pope
The University of Texas at Austin

SIAM Conference on Mathematical &
Computational Issues in the Geosciences

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Short answer: NO
at least not if we are talking about 1000 years of CO2 in the subsurface

Does this mean it is a waste of time to use models to make predictions: NO

Is this a contradiction: NO

So why do modeling?

- **Models are useful for understanding fluid flow in the subsurface and what is most important to measure**
- **Models are useful for exploring different CO2 injection strategies and alternatives**
- **Models are useful for quantifying the sensitivity of complex subsurface processes to important physical, chemical and biological phenomena**
- **Models are a useful aid to engineering design of experiments and subsequently subsurface processes and CO2 storage in particular**
- **Models are useful for communication of important ideas and uncertainties to both scientists and others**
- **Models are useful for explaining past events**

Some Examples of Why Predictions Are Difficult (predictions of the future that is)

- The model is incomplete in some way
- Some unexpected event or phenomena occurs, often completely outside our range of knowledge or experience
- The implementation of the process is flawed or changes for some reason that was not anticipated e.g. the CO2 is injected above fracture pressure so it does not stay in the target zone
- Someone a thousand years from now drills a well into a CO2 plume or some other similar event occurs--use your imagination

These factors are real but very hard to deal with except by simply acknowledging they exist and have the potential to matter.

When do we as a scientific community do that?

Examples of difficulties that we do know about

- The geological data input to the simulator is not sufficiently accurate, and of course it might be completely wrong. I'm not concerned here with a small scale pilot where huge amounts of time, effort and money have gone into a careful geological study to describe as accurately as possible the geology over the small volume related to the pilot. I'm more concerned with the very large scale where we have much less dense data. It seems almost hopeless that we will have sufficient characterization of large aquifers when it has been so difficult to do so in oil reservoirs where the incentive is much greater and the time scale much shorter.

Examples of difficulties that we do know about

- **Another intangible but very important factor is unintended bias. It is just human nature to delude ourselves into believing that our models are better than they are. We also want to believe that our results are right. We are mesmerized by the color images that modern visualization software produces with ease and in great abundance. The images are not reality. For a variety of reasons, they are not always even a good representation of the results of the model. We also want our predictions to be correct because we are predicting something we think is desirable e.g. that it is possible to store large quantities of CO2 in geological formations for thousands of years and keep it out of the atmosphere with little risk to human health and safety and little or no environmental consequences to the groundwater.**

Some Examples of Why Predictions Are Difficult

- The resolution of the model is simply not high enough. Under some circumstances, the transport of the CO2 is unstable. Such instabilities are extremely difficult to accurately model since they require a very fine grid and are so sensitive to small details in capillary barriers and so forth. Taking into account local heterogeneities and capillary pressure barriers, cells on the order of 0.5 meters might be needed. For simulations on the scale of even 10000 meters, this is currently not computationally feasible. If we want to account for reactions with minerals, then we would need to know the distribution of the minerals down to the 1 m scale to have any hope of accurately predicting the reactions, and we will never know the mineralogy in a larger aquifer anywhere approaching that scale.

An example related to CO2 storage

- **Some of the physics are not as well known as many people think e.g. the density of CO2 saturated brine is widely thought to be greater than brine under typical aquifer conditions of temperature, pressure and salinity. The actual experimental data under these conditions are sufficiently uncertain that it is hard to tell when this is true and when it is not true. The literature indicates that CO2 saturated brine will sink rather than rise due to buoyancy and thus not be at risk for leakage, so this very small but uncertain density will make reliable predictions very difficult indeed. It is possible to make such measurements with sufficient accuracy, but no one is doing it in practice and it is expensive to make such accurate measurements.**

Some partial answers to the prediction problem

- Look for strategies that are less subject to known uncertainties
- Look for strategies that are adaptable to new data
- Don't rely on history matching or inverse modeling
- Do more and better experiments and put more emphasis on the physics and chemistry
- Apply mathematical uncertainty analysis in a much broader sense than typically done
  - Don't limit analysis to the PDEs that you assume describe the flow and transport
  - Don't assume the physical property models include all of the physics or have been adequately tested

Some very well known examples of physics often omitted from flow and transport models (there are a lot of better but less well known examples)

- **Flow above parting pressure that very commonly (almost always?) occurs near injection wells in the oil field**
- **The spatial and temporal variations of permeability due to the interactions between the aqueous phase and minerals (clays in particular)**
- **Hysteresis in capillary pressure and relative permeability**
- **Almost all colloidal and surface chemistry except for linear, uncoupled adsorption and the like**
- **Non-Darcy flow**
- **Dependence of relative permeability on capillary number (even with no fancy stuff like surfactant)**

Some examples of what the oil industry does to cope with uncertain EOR predictions

- Enhanced oil recovery with carbon dioxide
  - Adjust the water-alternating-gas (WAG) ratio as the flood progresses over a period of 20 years
  - Adjust the amount of CO2 injected into individual well patterns depending on performance
  - Make changes in the well completions, injection profiles, or even in extreme case replace old wells or infill with new wells--watch and fix things
  - Continuously use a reservoir simulator tuned to field data during the entire flood to help understand and quantify all of the coupled effects
  - Identify and fix weak links e.g. reservoir description, simulation model, wells,....

Question

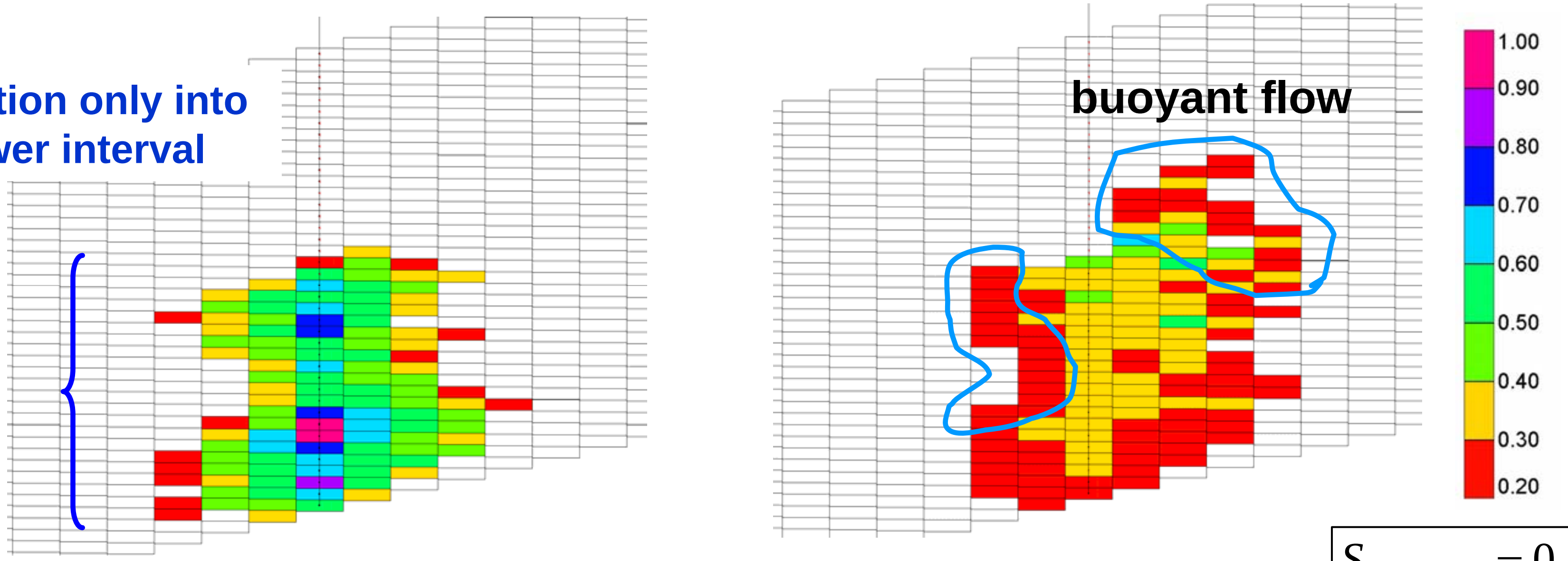
Do any of you incorporate that dynamic approach into your modeling framework?

An example CO2 injection strategy to reduce risk of CO2 escape

Saturation Profiles of CO_2-rich Phase

(vertical slice through the injection well in X-Z direction)

Injection only into lower interval

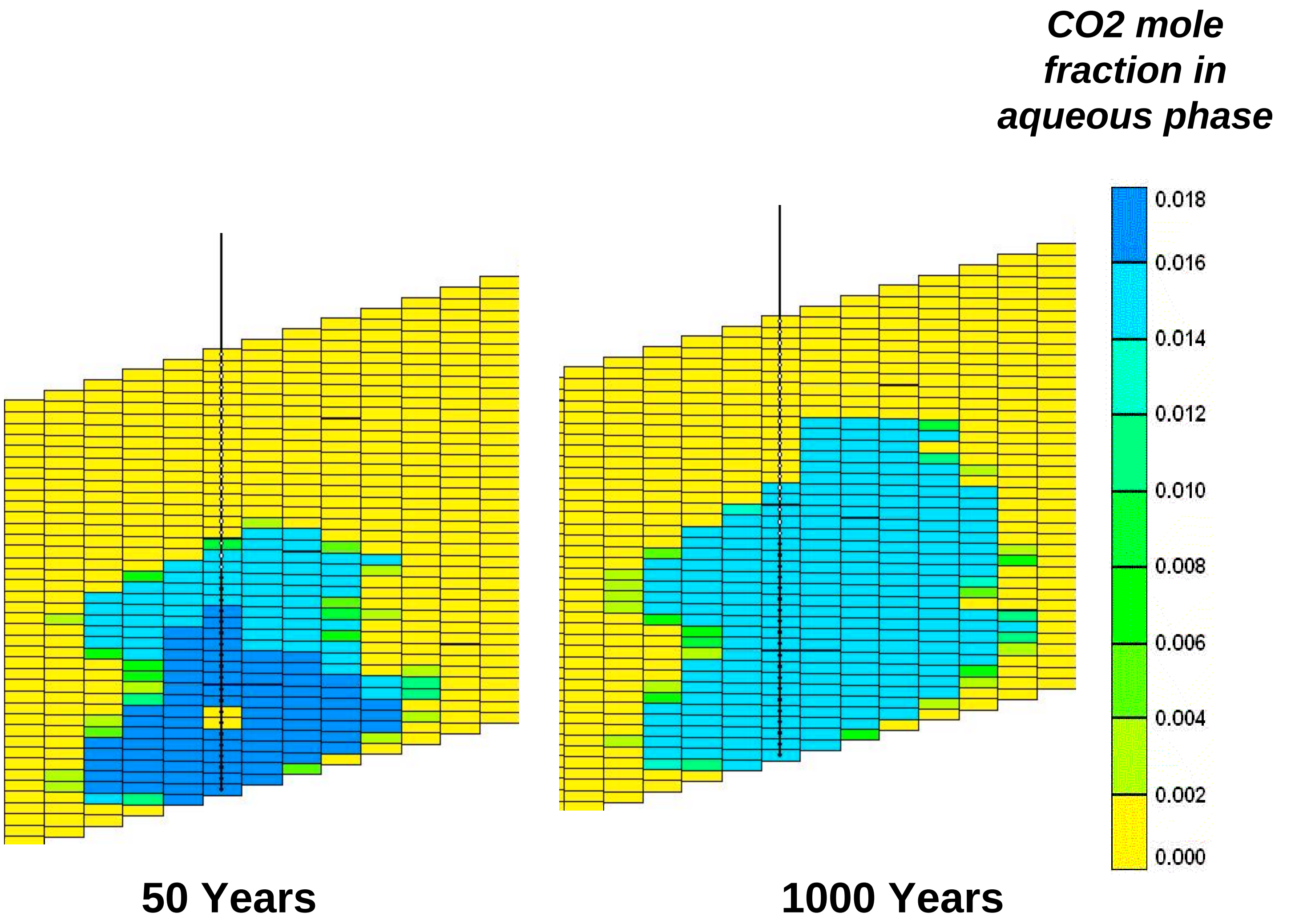


$$S_{g,residual} = 0.25$$

50 Years

1000 Years

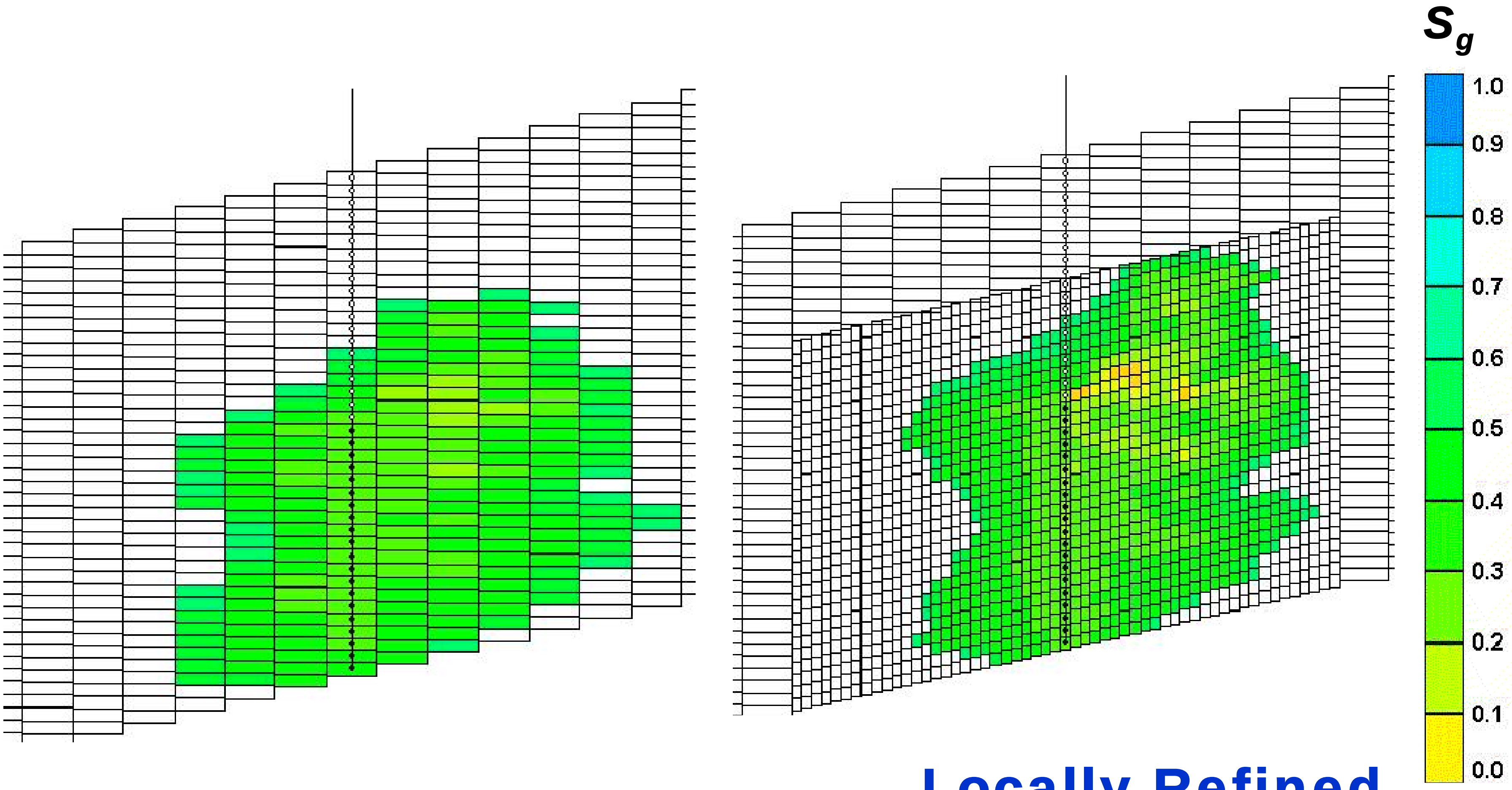
Brine Dissolution Traps Significant CO_2 Volume



50 Years **1000 Years**

CPGE

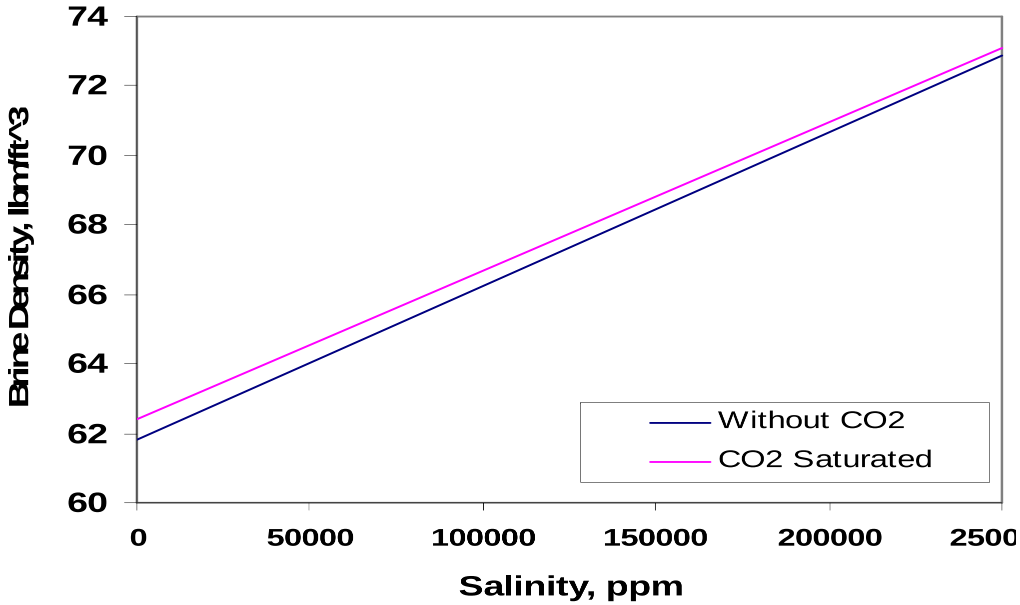
Gas (Supercritical CO2) Saturation Computed with Coarse and Fine Grid--notice the physics can be used to minimize the sensitivity to the grid



Coarse Grid

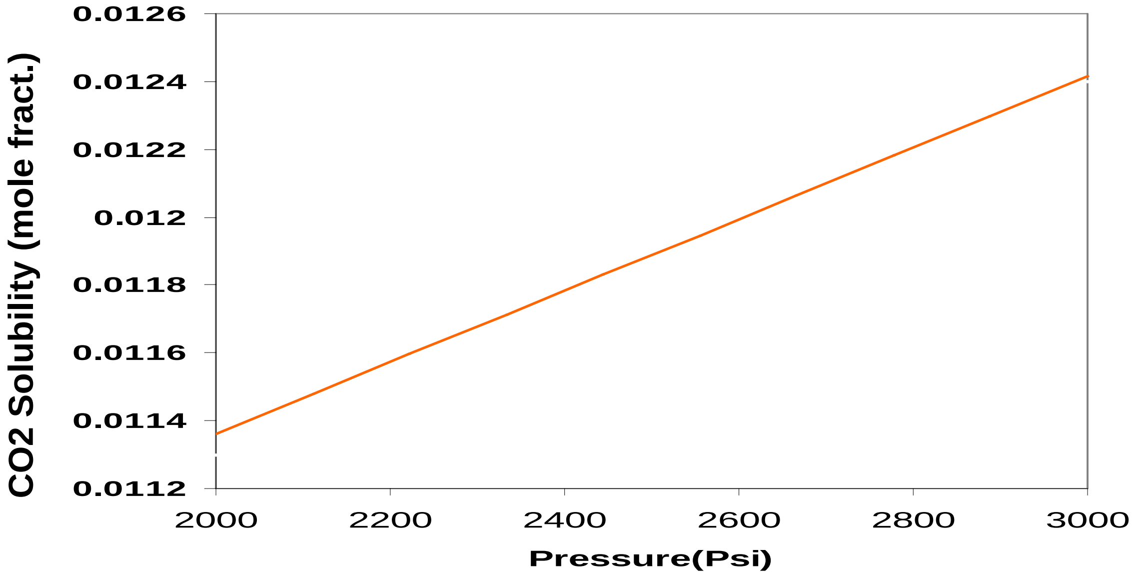
Locally Refined Grid (5x5x1)

Brine Density and CO2 Solubility



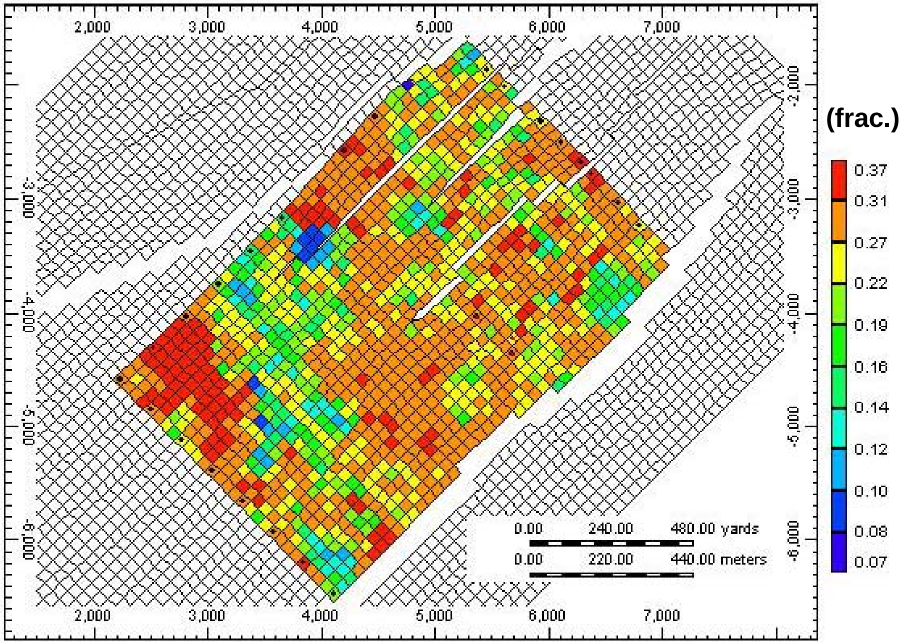
Brine Density at T=134ºF, P=2200 psi

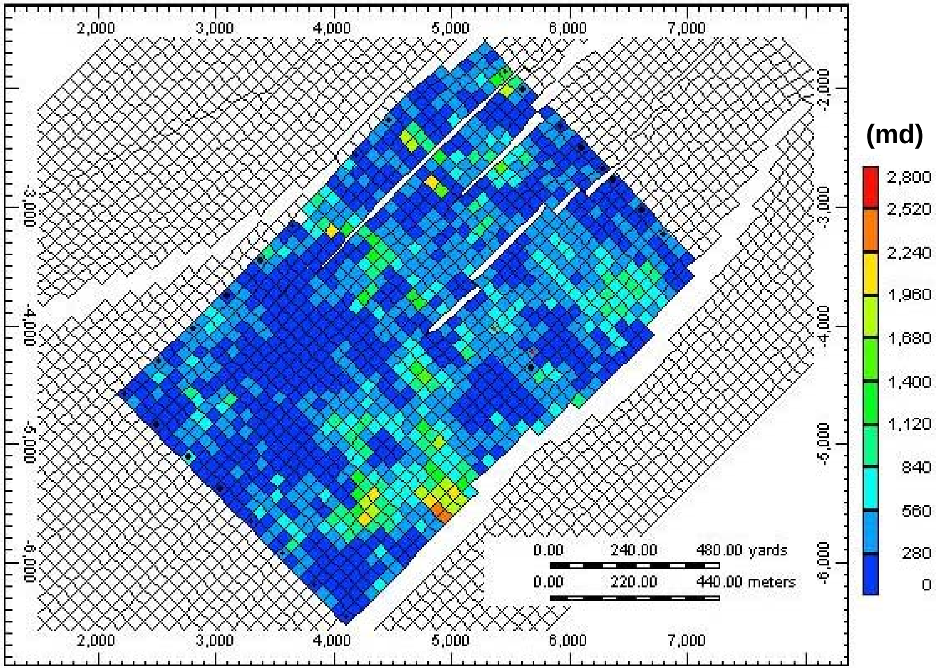
CO2 Solubility at T=134ºF, and 100,000 ppm Salinity



Frio example

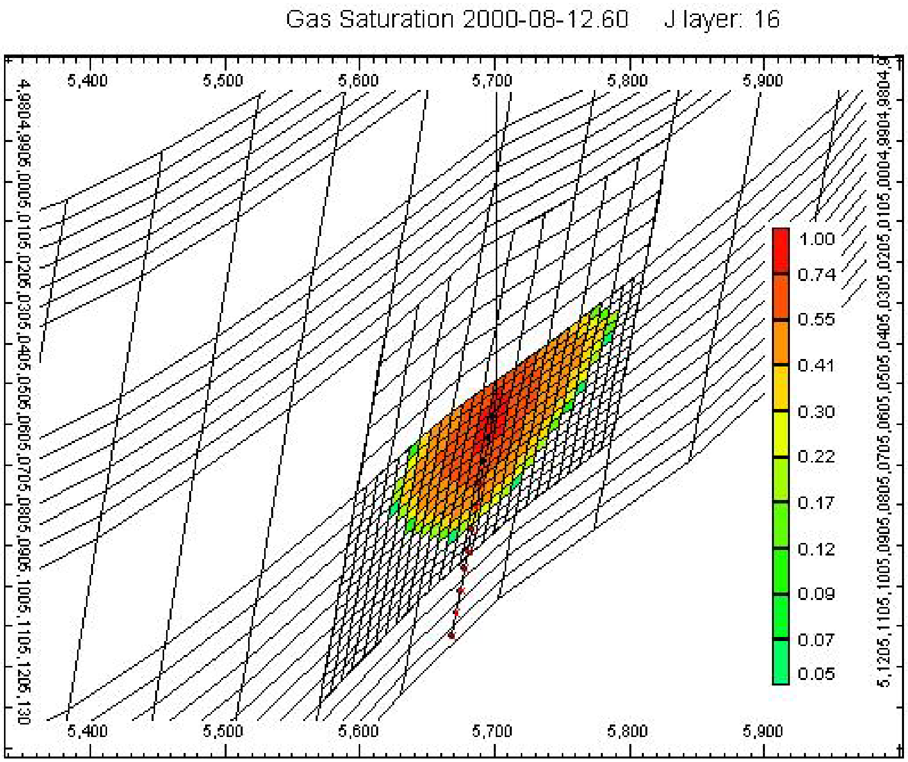
Porosity Field



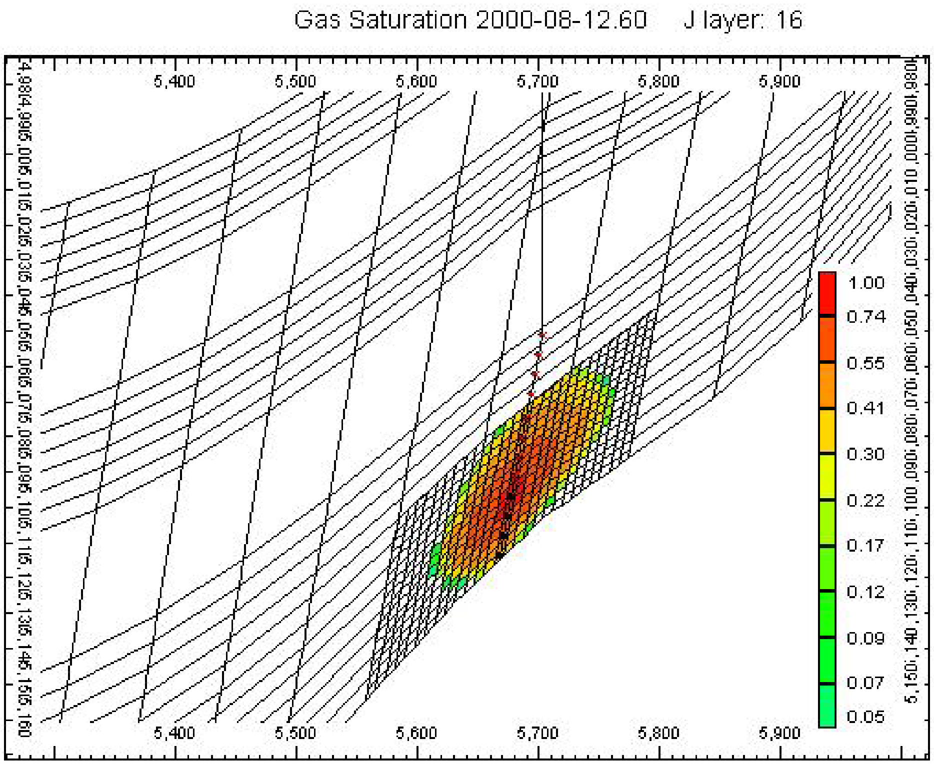


Permeability Distribution

Comparison of Predicted Gas Saturation for Alternative Well completions



Injection at the top



Injection a the Bottom

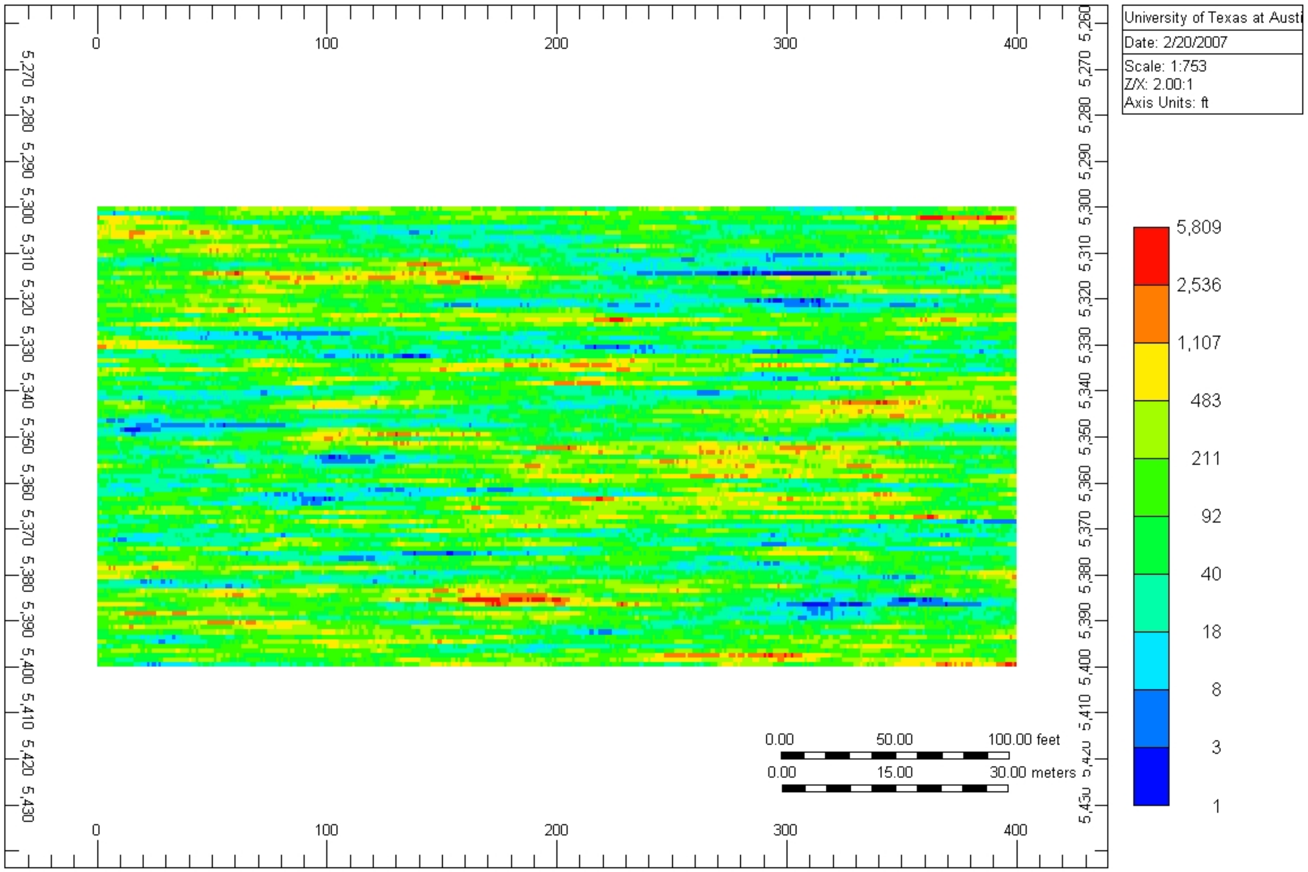
Conclusion:

Change the CO2 injection strategy to reduce uncertainty, reduce the need for complete and accurate data of the aquifer and most importantly reduce the need to accurately model phenomena associated with unstable flow at the top of the aquifer that are extremely difficult to predict

Effect of Capillary Pressure Heterogeneity on Buoyancy Driven Flow of CO_2

- **Permeability Field**
- **Correlation length = 50 ft in x-direction, 1 ft in z-direction**
- **Average permeability = 190 md**

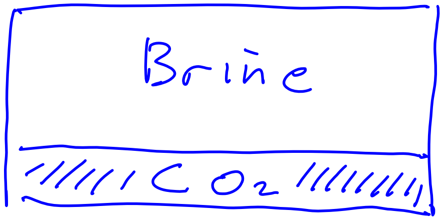
Permeability I (md) 2006-01-01 J layer: 1



No Capillary Pressure

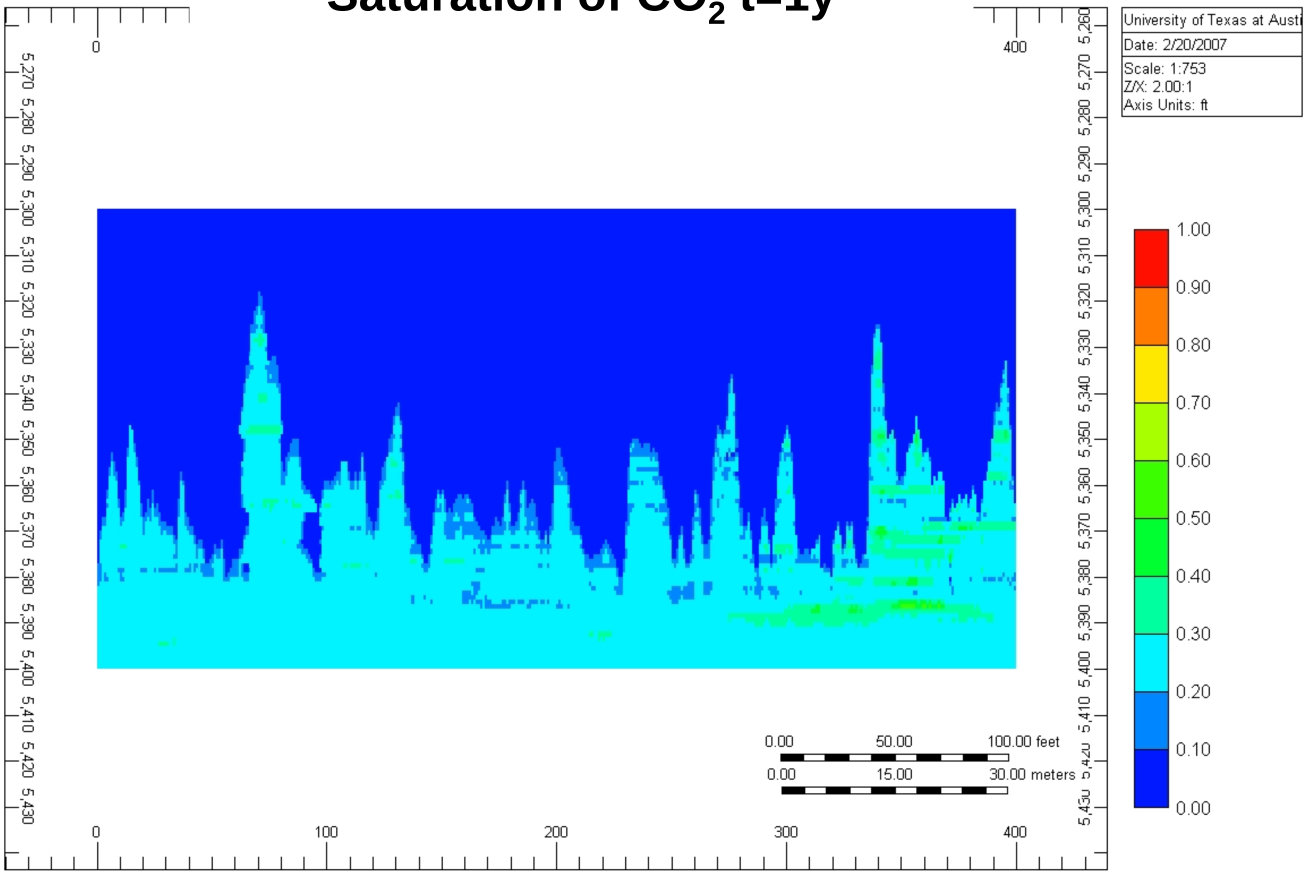
- **Without considering Pc (At the end of first year)**

INITIAL STATE



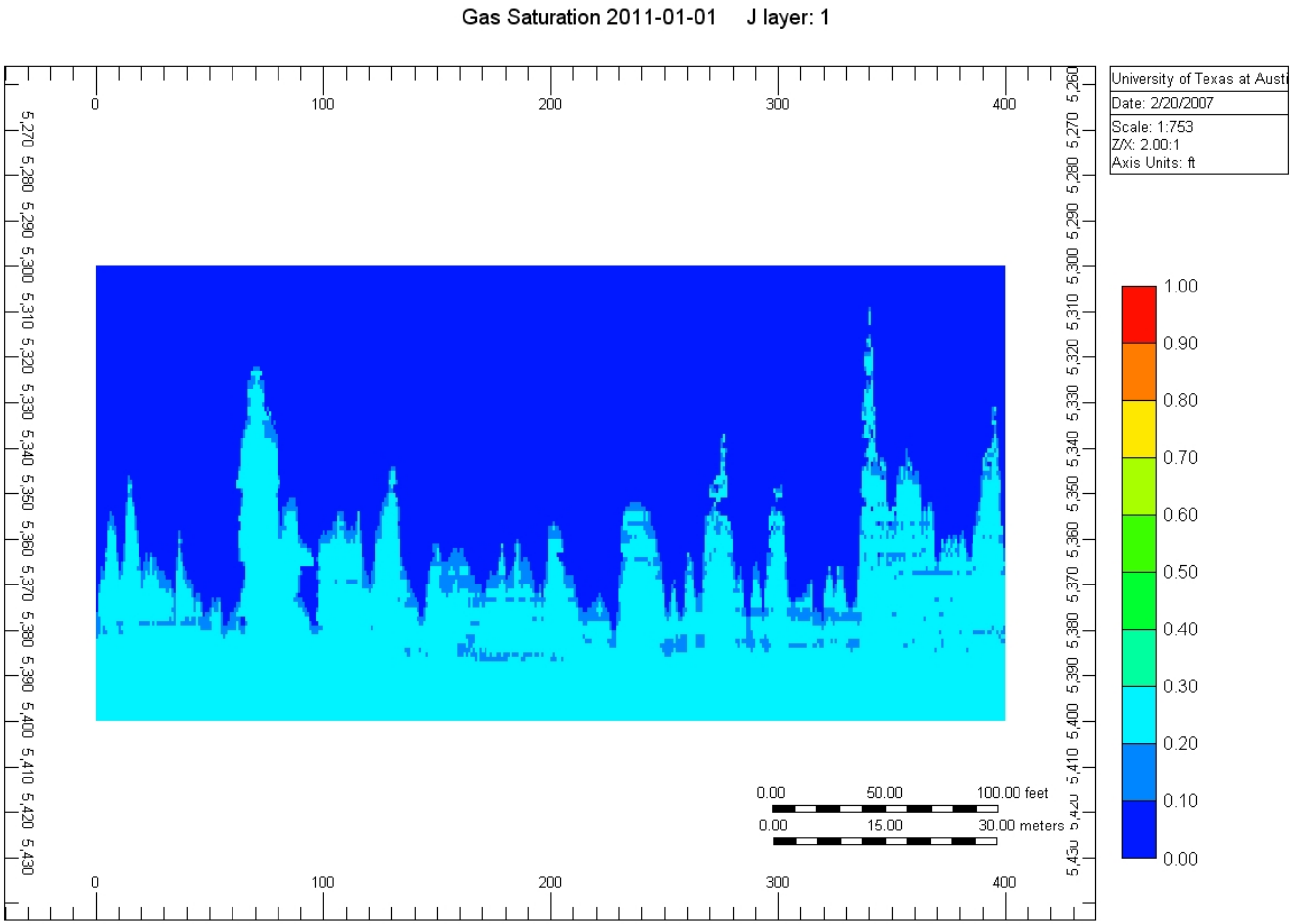
no flow boundaries

Saturation of CO_2 t=1y



Effect of Capillary Pressure Scaling on Buoyancy Driven Flow of CO_2

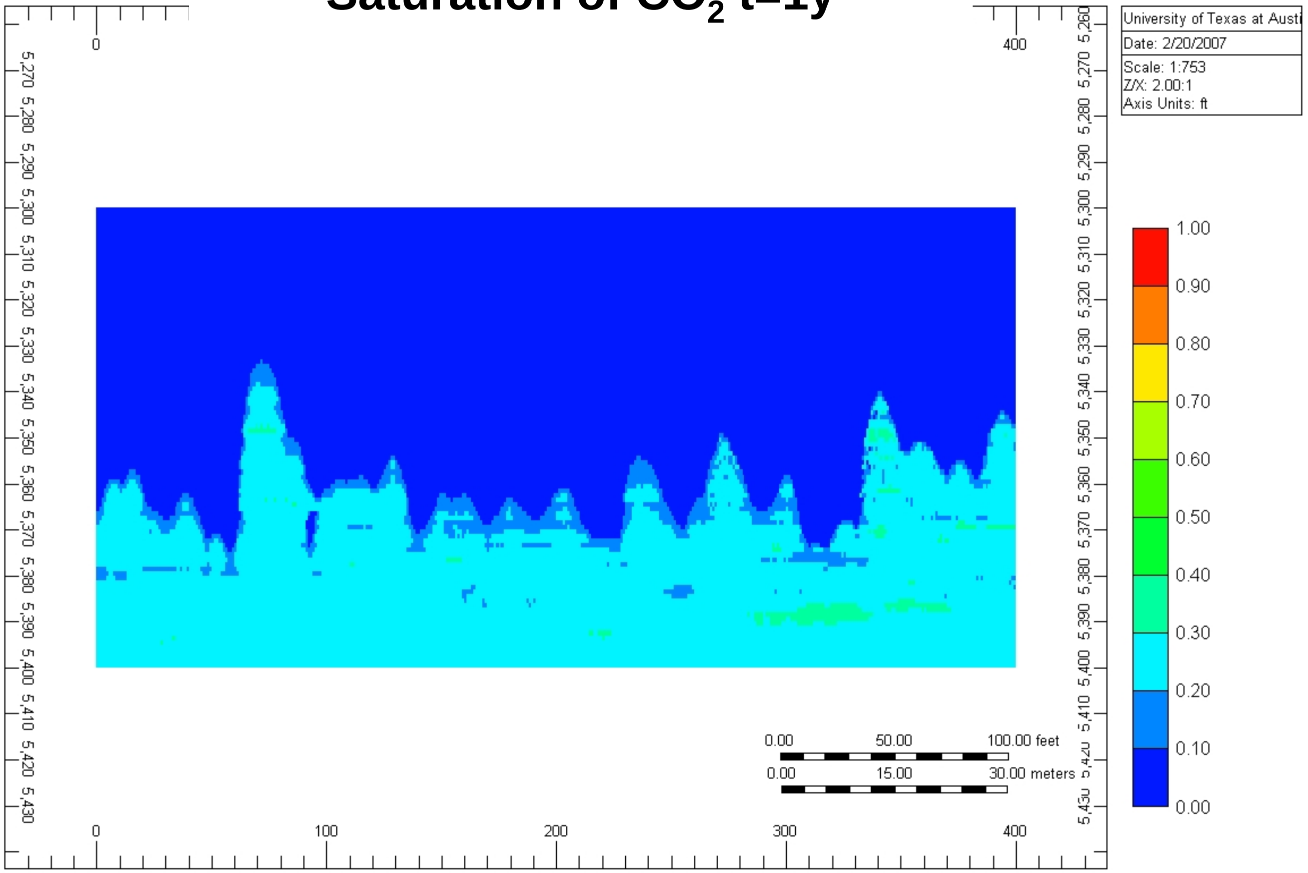
- **Without considering Pc (At the end of 5th year)**



Single Capillary Pressure Curve

- **Considering a single Pc curve (At the end of first year)**

Saturation of CO_2 t=1y



Effect of Capillary Pressure Scaling on Buoyancy Driven Flow of CO_2

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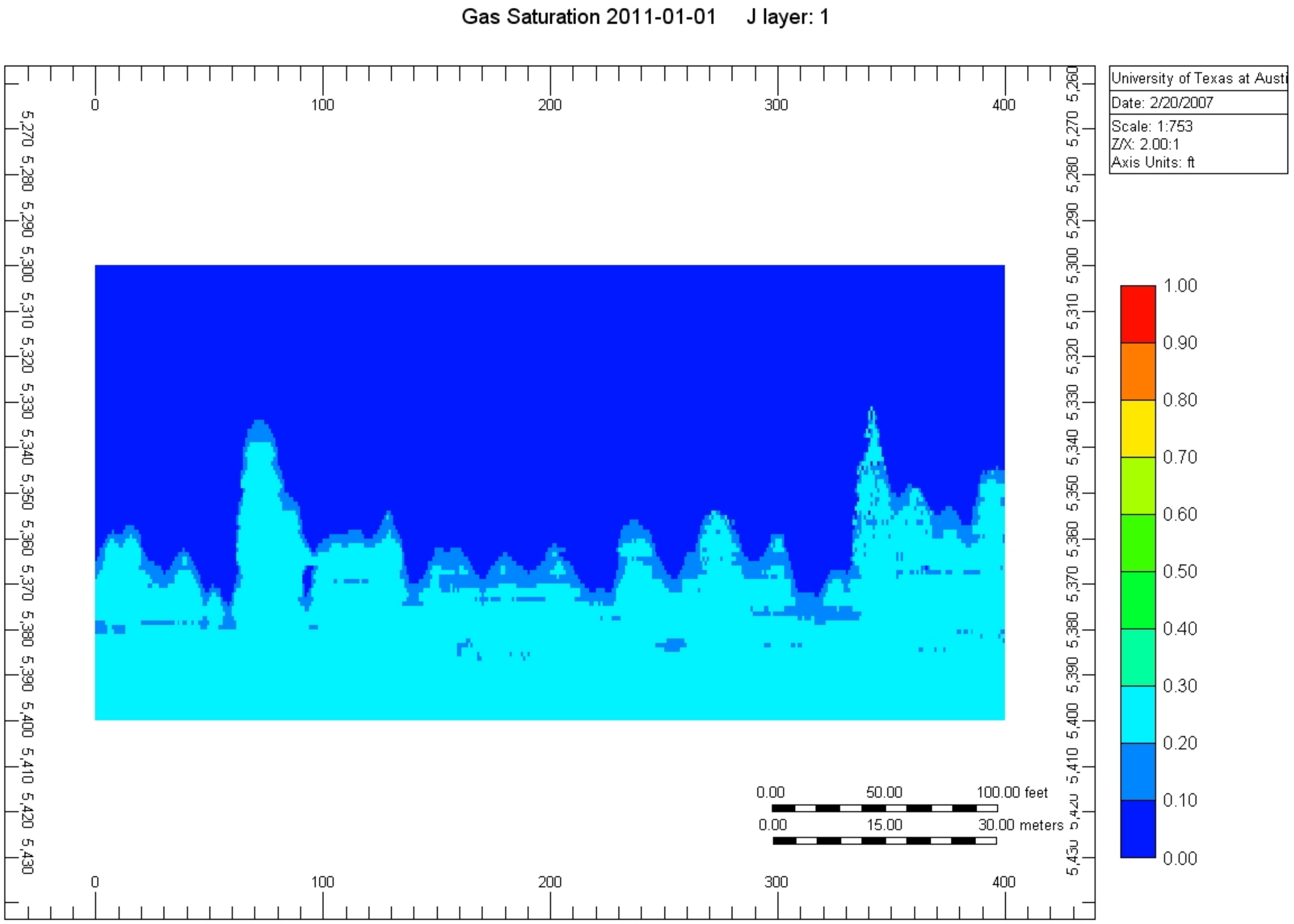
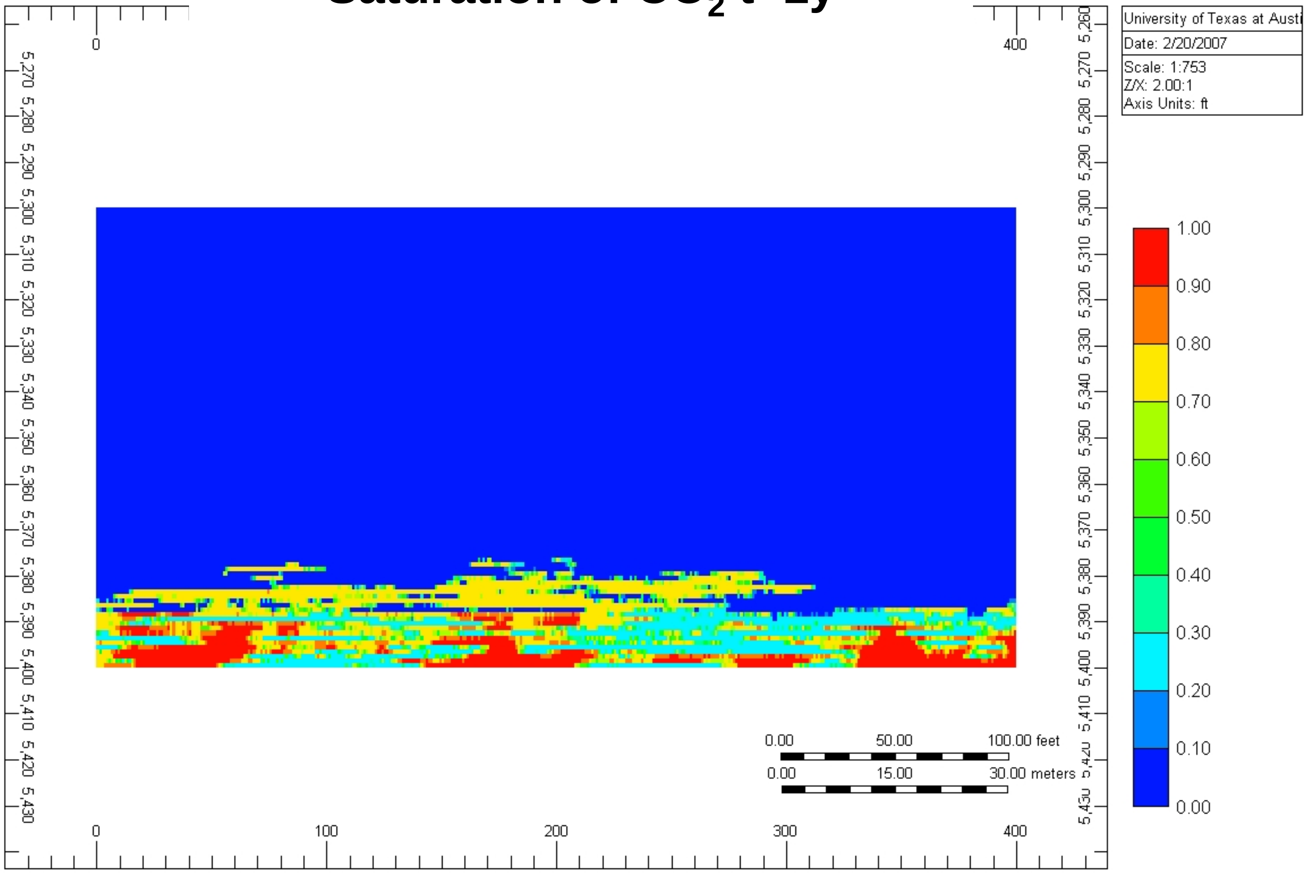


Capillary Pressure Curves Scaled by (Permeability)$^{1/2}$

- **Considering a spatially varying Pc curve (At the end of first year)**

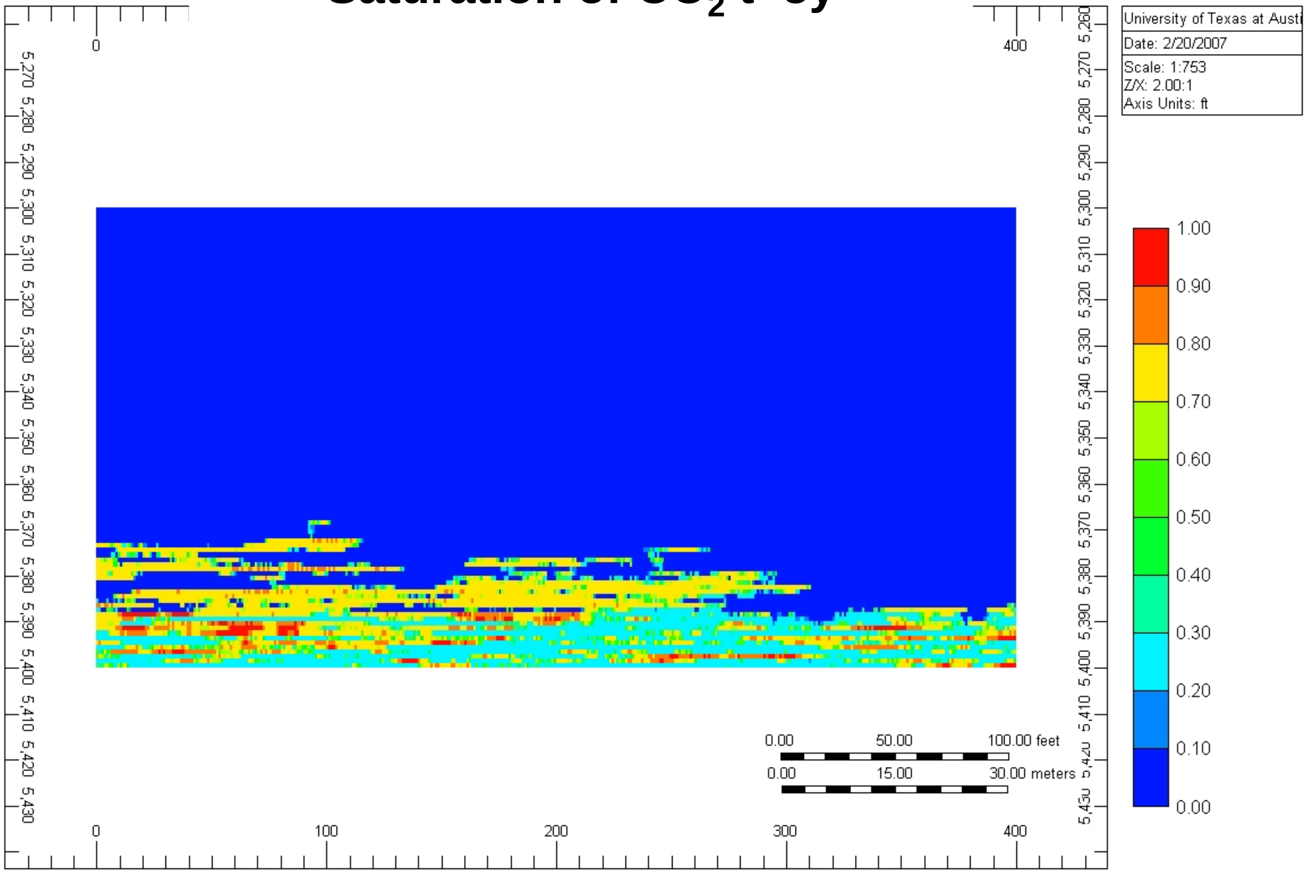
Saturation of CO_2 t=1y



Capillary Pressure Curves Scaled by (Permeability)$^{1/2}$

- **Considering a spatially varying Pc curve (At the end of 5th year)**

Saturation of CO_2 t=5y



Conclusion:

If capillary pressure is not modeled properly using Leverett scaling, then the model predictions can be so far off as to be misleading and useless despite the fact that capillary pressure is often considered a second order effect and either not included in the model or included without Leverett scaling

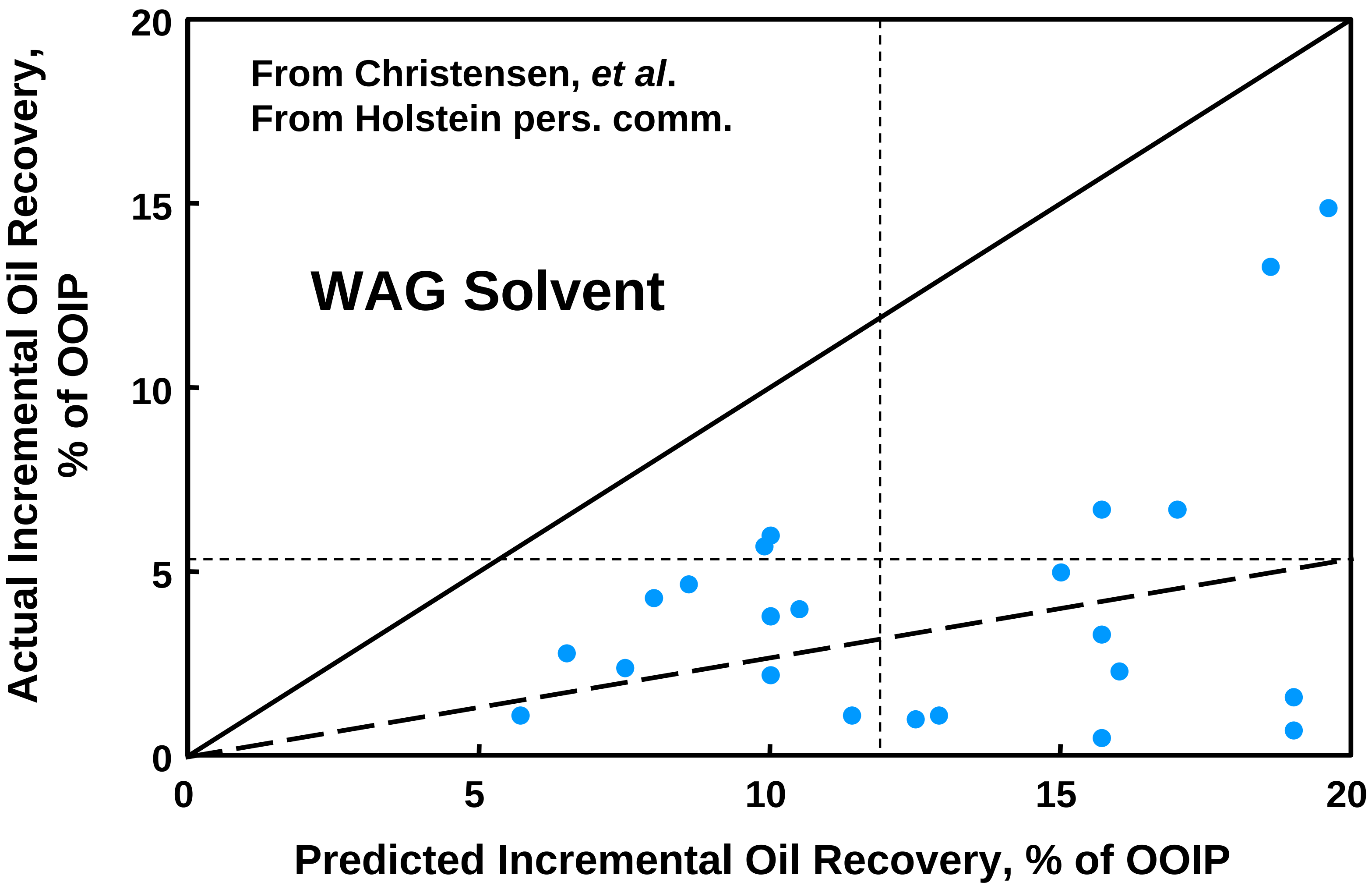
So do I think geological storage of CO2 can be done with a reasonably low risk and should be done if done prudently using good engineering judgment?

yes

Still not convinced predictions are difficult?

There are many examples from 40 years of experience trying to predict the performance of EOR of which time permits me to show only one related to CO2 EOR

Predicted vs. Actual Oil Recovery from CO2



Moving right along....

Examples of physical phenomena that completely dominate over most well known phenomena such as dispersion under certain circumstances

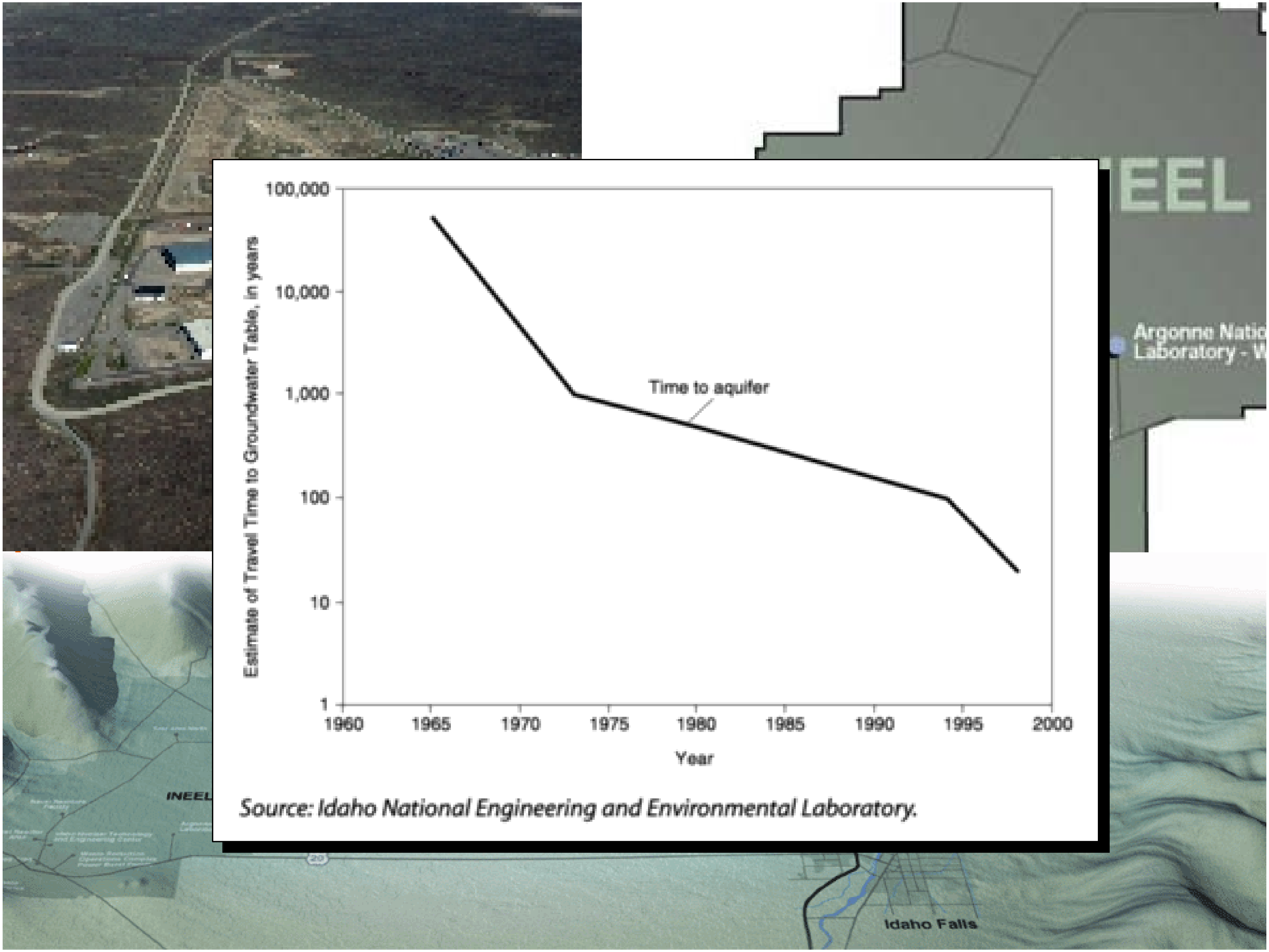
- Phase changes such as steam condensing in a steam drive in an oil reservoir
- Surfactant adsorption when a small amount of surfactant is injected for EOR
- Gas trapping during miscible EOR with WAG
- Viscous polymer solutions attenuate heterogeneity if sufficiently viscous
- Precipitation of minerals or other solids

ORIGIN AND IMPLICATIONS OF A NEW MODE OF SUBSURFACE TRANSPORT

Steven Bryant
Dept of Petroleum and Geosystems Engineering
The University of Texas at Austin

Anomalously Rapid Transport

- Contaminants moving farther than expected
  - Pu at NTS
  - radionuclides at INEEL
  - radionuclides at ORR
- Possible mechanisms
  - colloid-facilitated transport
  - subsurface heterogeneity
  - dispersion-induced fronts
- Basis for “expected”



Source: Idaho National Engineering and Environmental Laboratory.

Anomalously Rapid Transport

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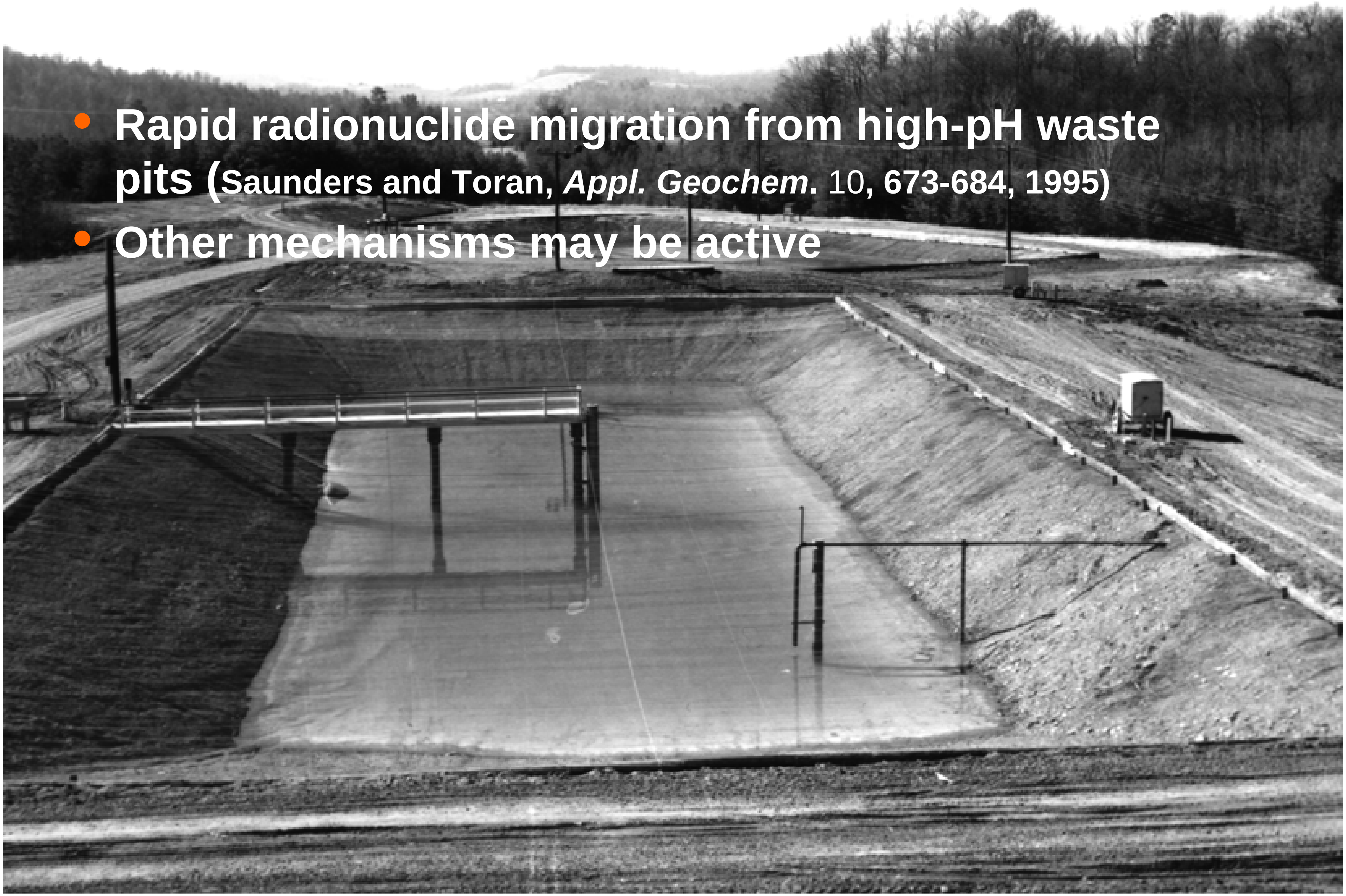
Oak Ridge observations

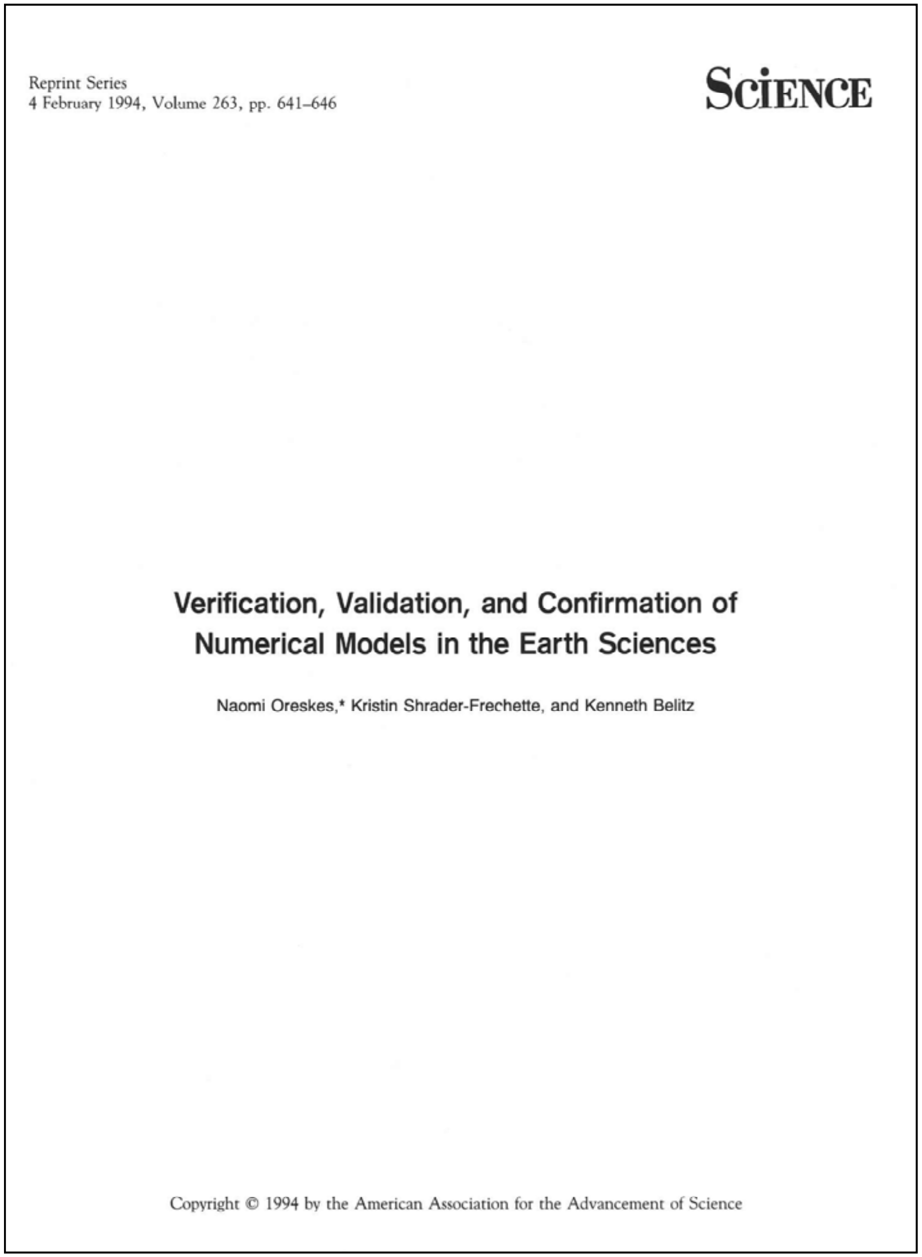


- **Rapid radionuclide migration from high-pH waste pits (Saunders and Toran, *Appl. Geochem*. 10, 673-684, 1995)**
- **Other mechanisms may be active**

Ground-Water Models Cannot Be Validated

Leonard F. Konikow
U.S. Geological Survey
Reston, VA

The University of Texas, Nov. 24, 2003



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4 February 1994, Volume 263, pp. 641–646

SCIENCE

Verification, Validation, and Confirmation of Numerical Models in the Earth Sciences

Naomi Oreskes,* Kristin Shrader-Frechette, and Kenneth Belitz

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Advances in Water Resources **15** (1992) 75–83

Ground-water models cannot be validated

Leonard F. Konikow
US Geological Survey, 431 National Center, Reston, Virginia 22092 USA

&

John D. Bredehoeft
US Geological Survey, 345 Middlefield Road, MS 439, Menlo Park, California 94025, USA

Ground-water models are embodiments of scientific hypotheses. As such, the models cannot be proven or validated, but only tested and invalidated. However, model testing and the evaluation of predictive errors lead to improved models and a better understanding of the problem at hand. In applying ground-water models to field problems, errors arise from conceptual deficiencies, numerical errors, and inadequate parameter estimation. Case histories of model applications to the Dakota Aquifer, South Dakota, to bedded salts in New Mexico, and to the upper Coachella Valley, California, illustrate that calibration produces a nonunique solution and that validation, *per se*, is a futile objective. Although models are definitely valuable tools for analyzing ground-water systems, their predictive accuracy is limited. The terms *validation* and *verification* are misleading and their use in ground-water science should be abandoned in favor of more meaningful model-assessment descriptors.

INTRODUCTION

The need to calibrate ground-water models has existed as long as ground-water models. In recent years, there has been an increased emphasis on the need to validate ground-water models, driven largely by those engaged in radioactive waste disposal. This has led to institutionalized and publicized programs for verification or validation of hydrogeological models, such as the INTRACOIN, HYDROCOIN, INTRAVAL, and GEOVAL projects. For example, two of the three stated objectives of the HYDROCOIN project are code verification and model validation (Swedish Nuclear Power Inspectorate[21]). The INTRAVAL project was established to evaluate the validity of mathematical models for predicting the potential transport of radioactive substances in the geosphere (Swedish Nuclear Power Inspectorate[22]). It is natural for people who apply ground-water models, as well as those who make decisions based on model results, to want assurance that the model is valid.

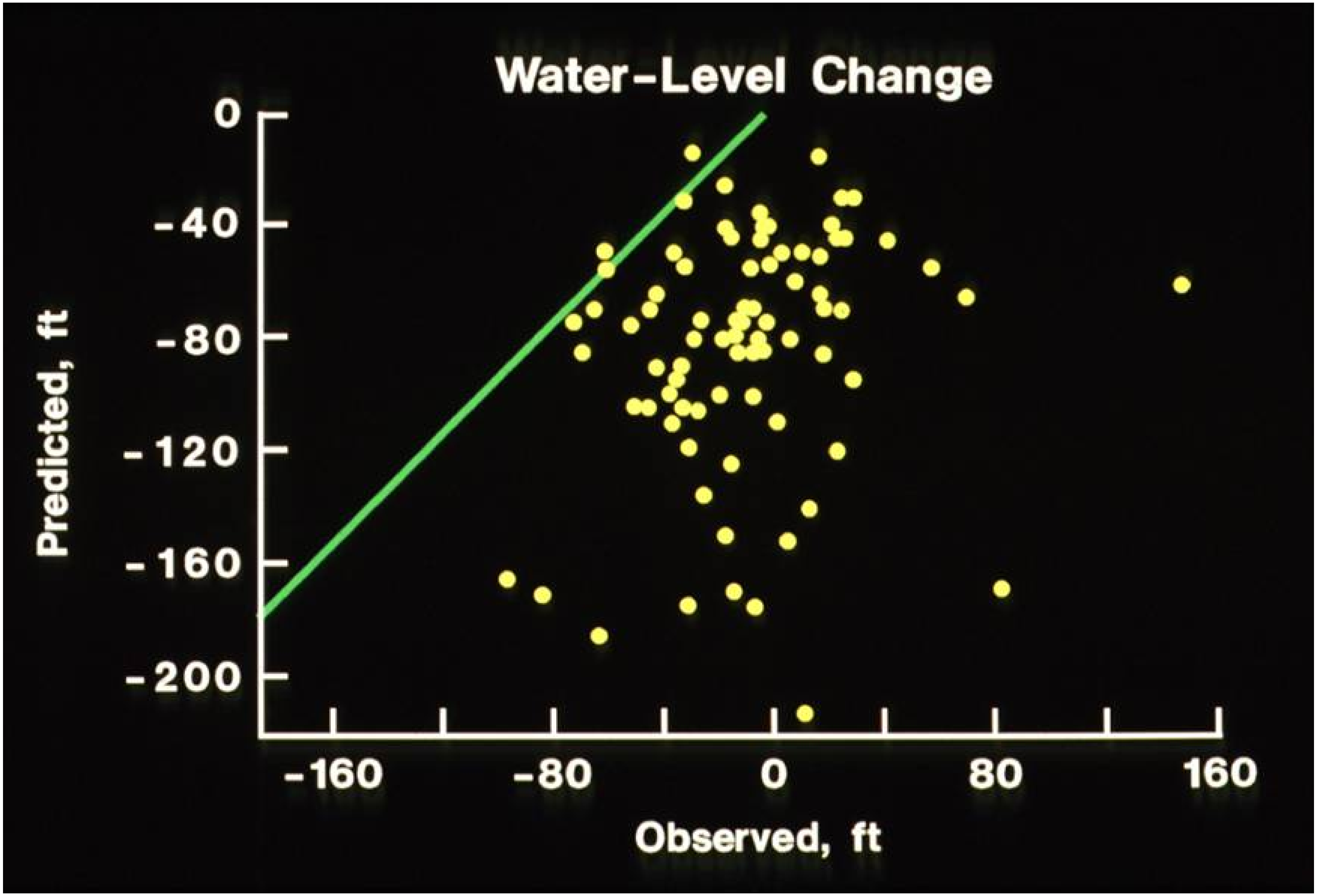
It is our intent to approach the question of validation on two levels: (1) the philosophical level, and (2) the practical level of validating a site-specific model. We will argue that, at both levels, validation has no place in hydrology. Although we focus on ground-water flow and transport models, the discussion is applicable to other types of ground-water models, such as geochemical models.

MODELS

The word *model* has so many meanings and is so overused that it is sometimes difficult to know what one is referring to. For this discussion, we define a *model* as a *representation of a real system or process*. To help clarify our discussion, we briefly discuss several types of ground-water models.

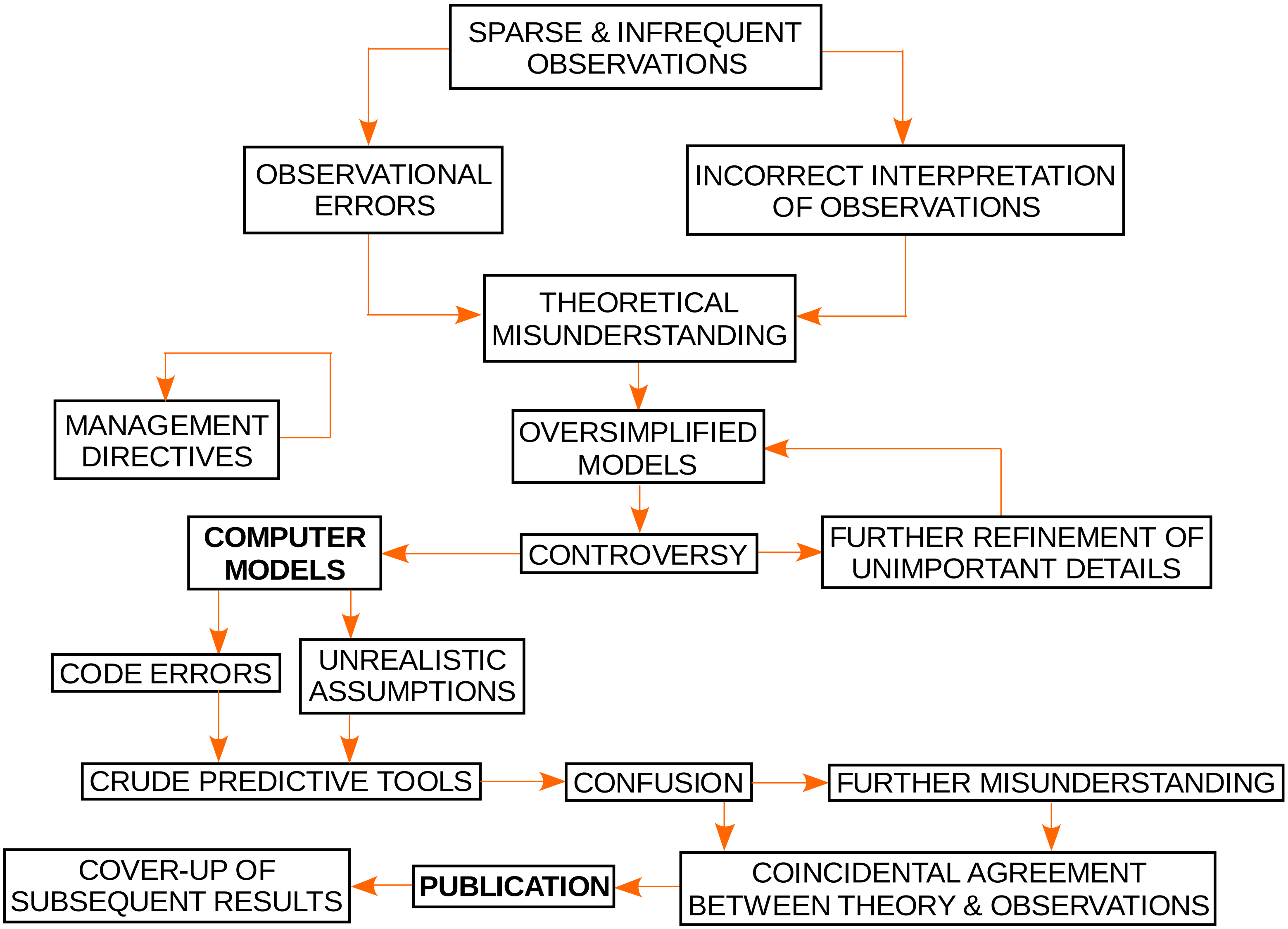
We define a *conceptual model* as a *hypothesis for how a system or process operates*. The idea can be expressed quantitatively as a mathematical model. *Mathematical models* are abstractions that replace objects, forces, and events by expressions that contain mathematical variables, parameters, and constants (Krumbein and Graybill,[13] p. 15).

Most ground-water models in use today are *deterministic* mathematical models. Deterministic models are based on conservation of mass, momentum, and energy — that is, on a balance of the various fluxes of these



Water-Level Change
Predicted, ft
0
-40
-80
-120
-160
-200
-160
-80
0
80
160
Observed, ft

Models and the Course of Science



SPARSE & INFREQUENT OBSERVATIONS

OBSERVATIONAL ERRORS

INCORRECT INTERPRETATION OF OBSERVATIONS

THEORETICAL MISUNDERSTANDING

MANAGEMENT DIRECTIVES

OVERSIMPLIFIED MODELS

COMPUTER MODELS

CONTROVERSY

FURTHER REFINEMENT OF UNIMPORTANT DETAILS

CODE ERRORS

UNREALISTIC ASSUMPTIONS

CRUDE PREDICTIVE TOOLS

CONFUSION

FURTHER MISUNDERSTANDING

COVER-UP OF SUBSEQUENT RESULTS

PUBLICATION

COINCIDENTAL AGREEMENT BETWEEN THEORY & OBSERVATIONS

CPGE

Source: Unknown

USING WORDS CAREFULLY

“Virtually all papers published in peer-reviewed journals contain language or jargon that may be misleading, ambiguous, or opaque to those not familiar with such discipline-specific usage. When the maintenance of confidence by a broad audience of stakeholders and the general public is essential, it becomes particularly important to communicate carefully and accurately …

… care needs to be taken … when using … phrases that may promise more than they can deliver.”

From: *“One Step at a Time: The Staged Development of Geologic Repositories for High-Level Radioactive Waste”* (2003) National Academy Press.

THAT'S LIFE *By* MIKE TWOHY

"You can do a lot with computer models, but at some point you have to use real animals."

Chemical Flooding: Lessons Learned from Groundwater Cleanup & EOR and Where Do We Go From Here

Gary A. Pope
Center for Petroleum and Geosystems Engineering
The University of Texas at Austin

Gordon Research Conference
Flow and Transport in Permeable Media
August 4-8, 2002

Objectives of Using Numerical Simulators

- **Establish the operating parameters**
- **Demonstrate to the regulators that hydraulic capture can be accomplished**
- **Predict the effluent contaminant and surfactant concentration for surface treatment**
- **Improve understanding of process mechanisms and feedback to laboratory experiments**
- **Optimization, risk reduction, and scaleup**
- **Assess performance of field data**

Design Variables

- Well pattern and well rates
- Hydraulic control well locations and rates
- Location of well screens
- Location of multilevel samplers and frequency of sampling
- Mass of injected surfactant/cosolvent
- Composition of surfactant solution
- Mobility control (i.e. polymer or foam)
- Surface treatment facilities

Model Output

- Effluent concentrations of contaminant, surfactant, and cosolvent are critical to the surface treatment program
- DNAPL saturation reduction within the well field
- Recovery of free-phase product
- Concentrations of contaminant, surfactant, and cosolvent at the monitoring locations
- Water level fluctuations due to the injected chemicals
- Recoveries of contaminant, surfactant, and cosolvent
- Final concentrations of contaminant and all the injected chemicals

Benefits of Modeling

- Understanding of aquifer characteristics
- Optimization of surfactant remediation design
- Assessment of problems and risks
- Guide to laboratory program
- Guide to field operations
- Aid in communication with regulators
- Guide to future research

Mass Conservation Equations

$$\frac{\partial}{\partial t}\left(\phi \tilde{C}_{\kappa} \rho_{\kappa}\right) + \vec{\nabla} \cdot \left[\sum_{\ell=1}^{n_p} \rho_{\kappa} \left(C_{\kappa\ell} \vec{u}_{\ell} - \vec{\tilde{D}}_{\kappa\ell} \right) \right] = R_{\kappa}$$

Overall concentration for species κ:

$$\tilde{C}_{\kappa} = \left(1 - \sum_{\kappa=1}^{n_{cv}} \hat{C}_{\kappa} \right) \sum_{\ell=1}^{n_p} S_{\ell} C_{\kappa\ell} + \hat{C}_{\kappa}$$

dispersive flux:

$$\vec{\tilde{D}}_{\kappa\ell,x} = \phi S_{\ell} \vec{\vec{K}}_{\kappa\ell} \cdot \vec{\nabla} C_{\kappa\ell}$$

Source term:

$$R_{\kappa} = \phi \sum_{\ell=1}^{n_p} S_{\ell} r_{\kappa\ell} + (1 - \phi) r_{\kappa s} + Q_{\kappa}$$

Pressure Equation

The pressure equation is developed by summing the mass balance equations over all volume occupying components, substituting Darcy's law for the phase flux terms, using the definition of capillary pressure, and noting that

$$\sum_{\kappa=1}^{n_{cv}} C_{\kappa\ell} = 1$$

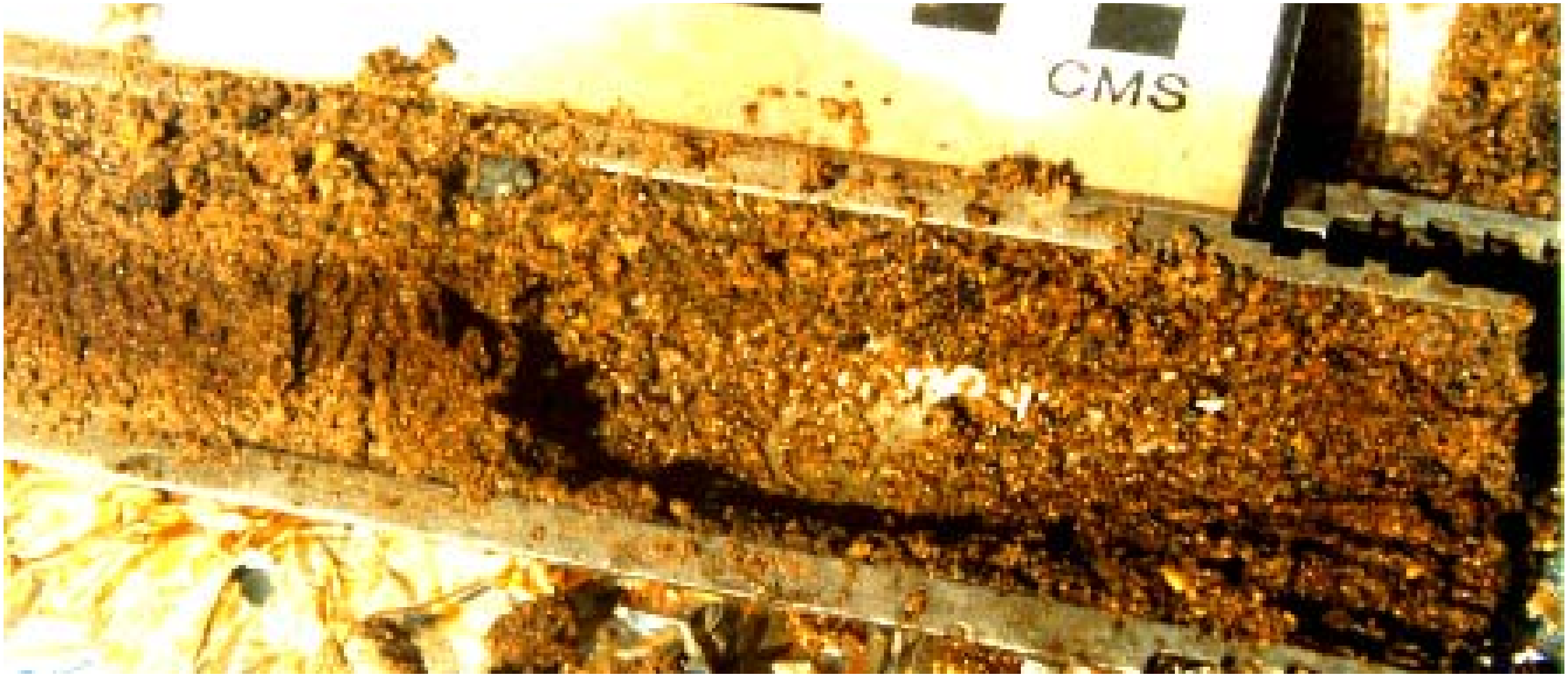
$$\phi C_t \frac{\partial P_1}{\partial t} + \vec{\nabla} \cdot \vec{\vec{k}} \cdot \lambda_{rTc} \vec{\nabla} P_1 =$$

$$- \vec{\nabla} \cdot \sum_{\ell=1}^{n_p} \vec{\vec{k}} \cdot \lambda_{r\ell c} \vec{\nabla} h + \vec{\nabla} \cdot \sum_{\ell=1}^{n_p} \vec{\vec{k}} \cdot \lambda_{r\ell c} \vec{\nabla} P_{c\ell 1} + \sum_{\kappa=1}^{n_{cv}} Q_\kappa$$

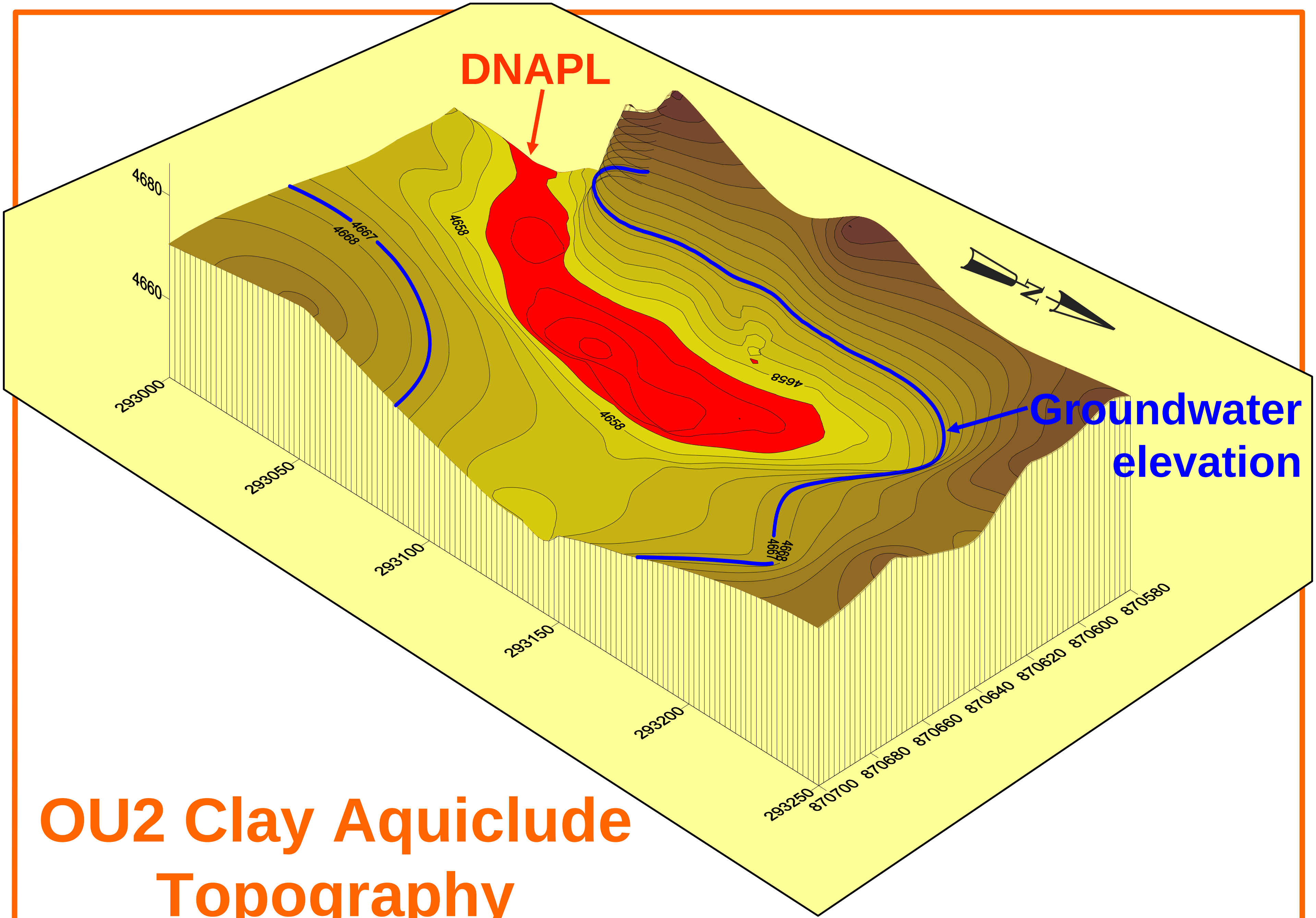
Total mobility is: $\lambda_{rTc} = \sum_{\ell=1}^{n_p} \frac{k_{r\ell}}{\mu_\ell} \sum_{\kappa=1}^{n_{cv}} \rho_\kappa C_{\kappa\ell}$

Hill Air Force Base, Utah
Operable Unit 2 (OU2)

DNAPL in Soil from Hill AFB OU2



OU2 Clay Aquiclude Topography

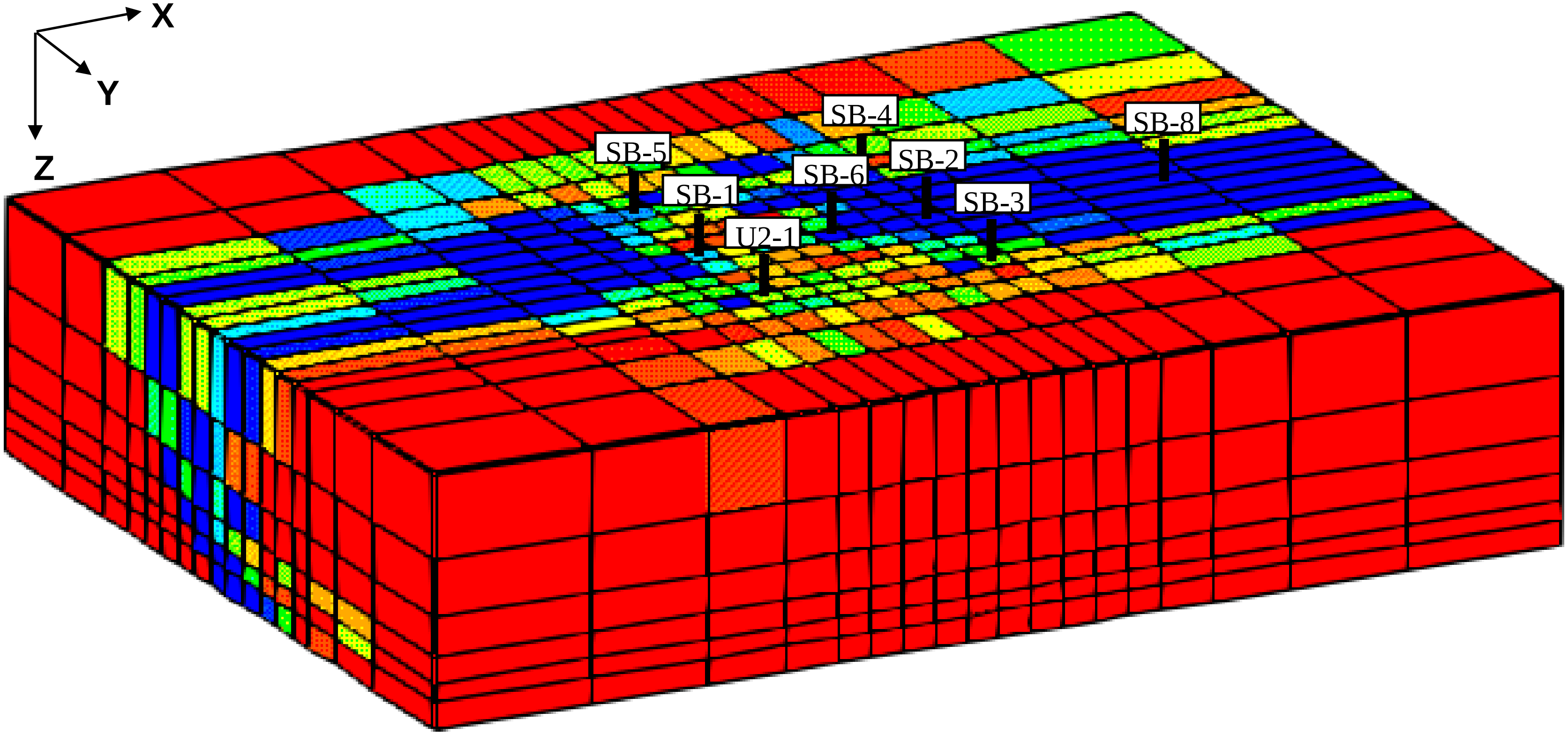


DNAPL

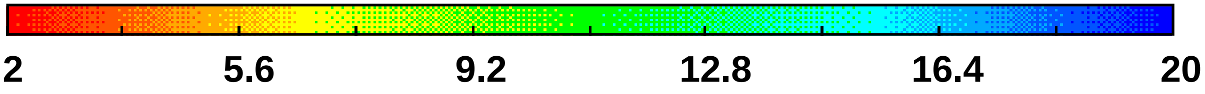
Groundwater elevation

CPGE

Horizontal Permeability Distribution Used in UTCHEM Simulations

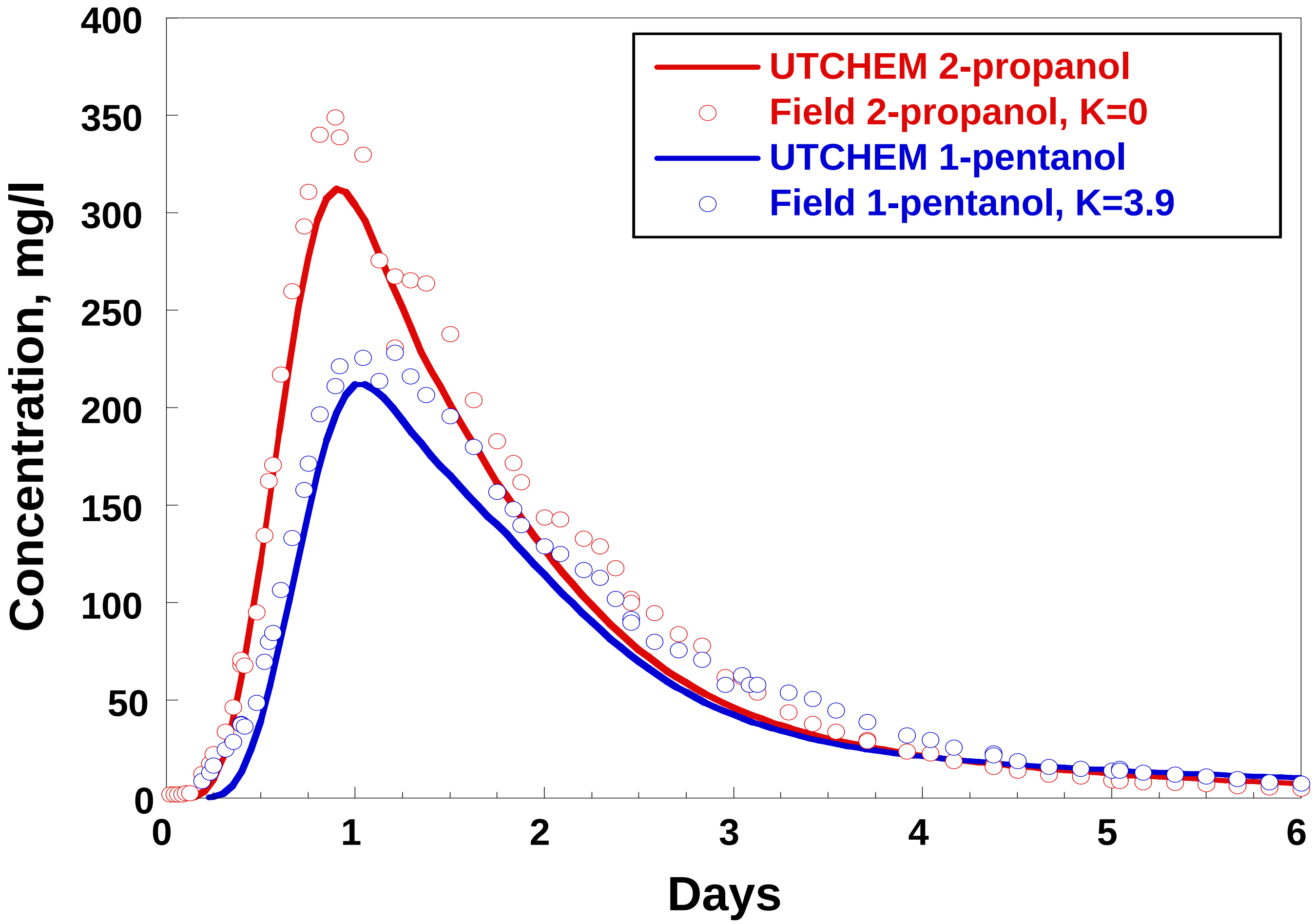


Permeability, Darcy

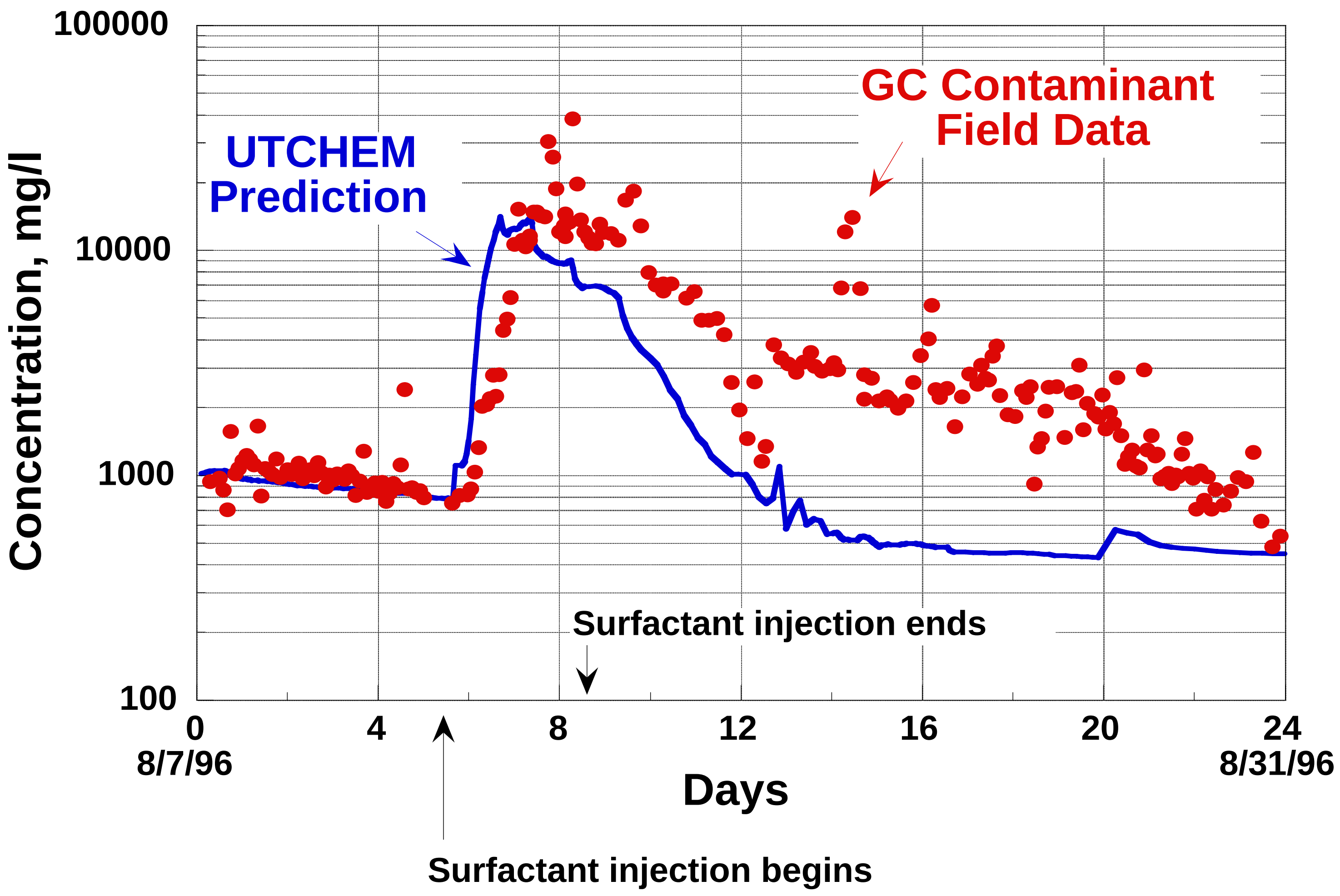


CPGE

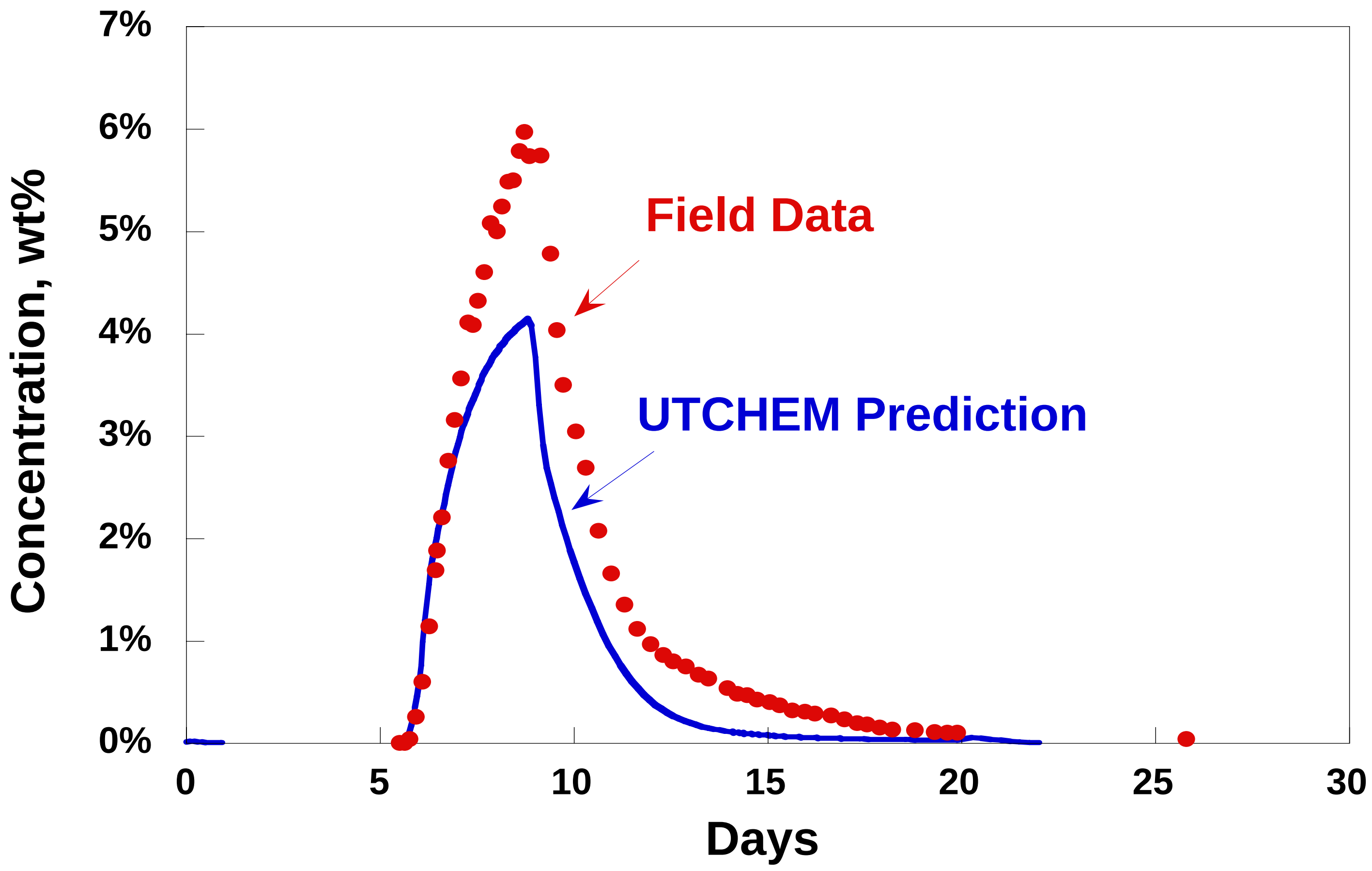
Actual and Predicted Tracer Concentrations



Comparison of UTCHEM Prediction with Field Contaminant Data During Phase II — Well SB-1



Comparison of UTCHEM Prediction with Field Surfactant Data During Phase II — Well SB-1



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Key Preparations and Precautions Before SEAR pilot

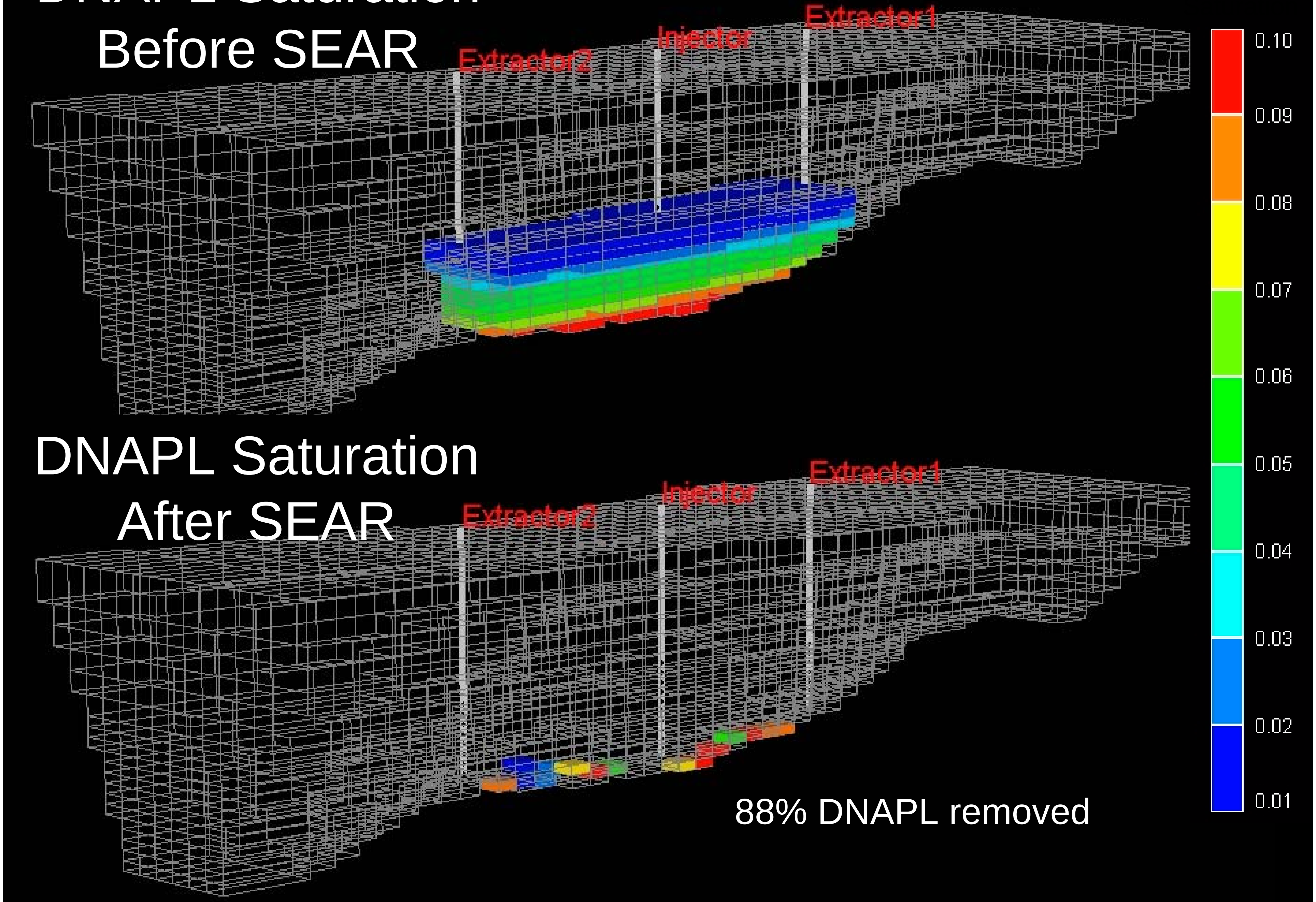
- Laboratory column tests
- Flow and transport modeling with UTCHEM
- Field tracers
- Small pretest with surfactant
- Monitoring well only 10 feet away and real time data analysis

3D Simulation of Contaminant Mass Flux Following Partial Mass Removal from a DNAPL Source Zone

Shekhar Jayanti and Gary A. Pope

The University of Texas at Austin

August 8, 2003

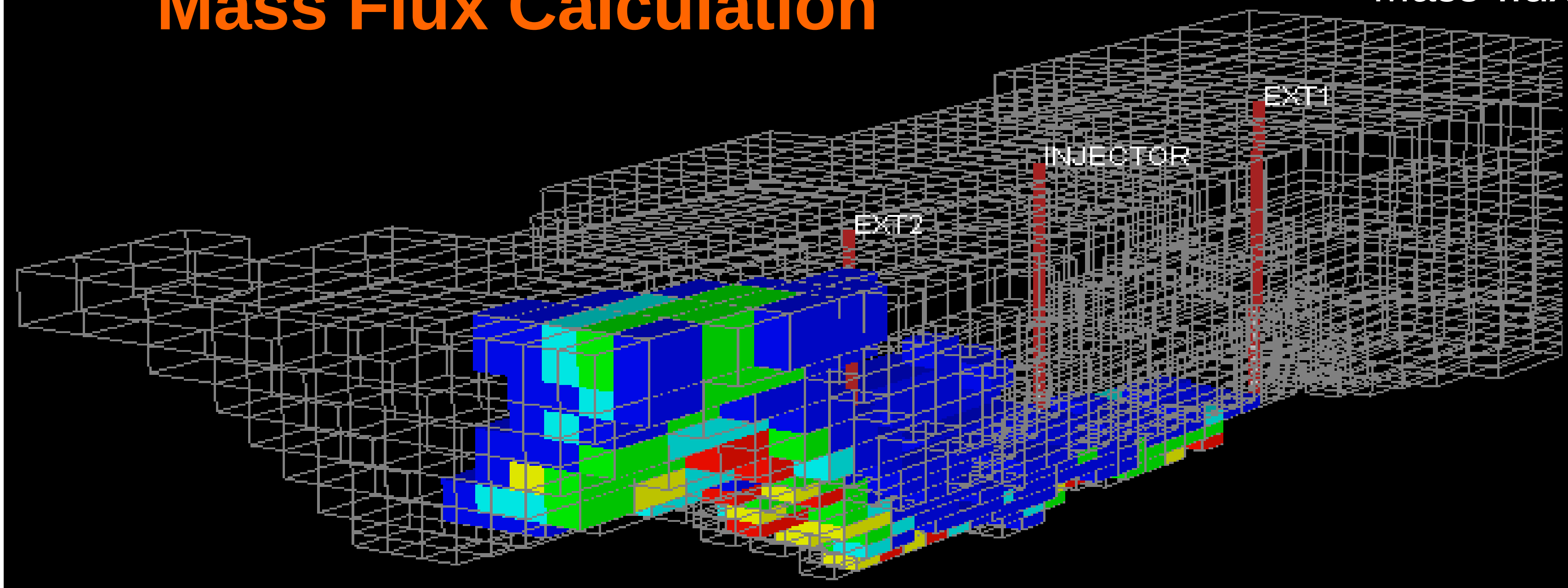


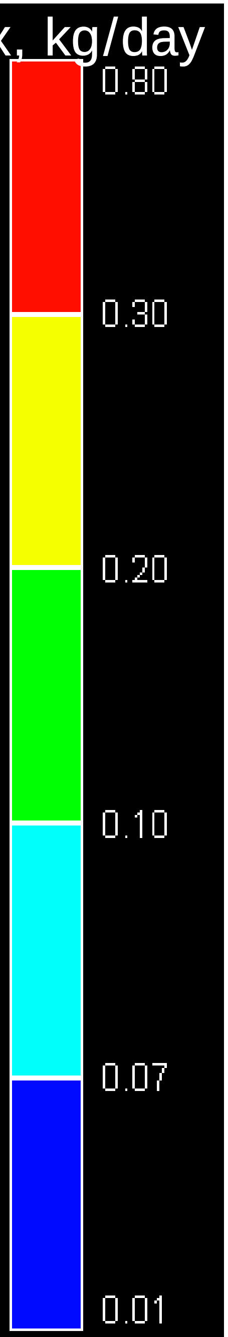
DNAPL Saturation
Before SEAR

DNAPL Saturation
After SEAR

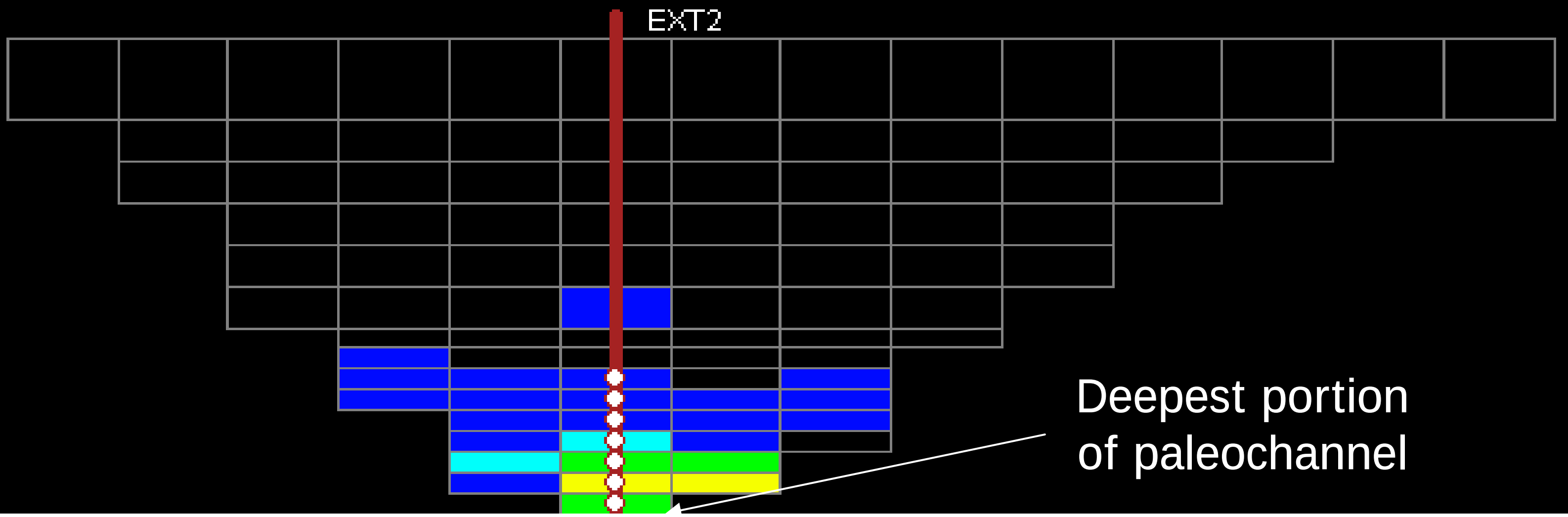
88% DNAPL removed

Mass Flux Calculation



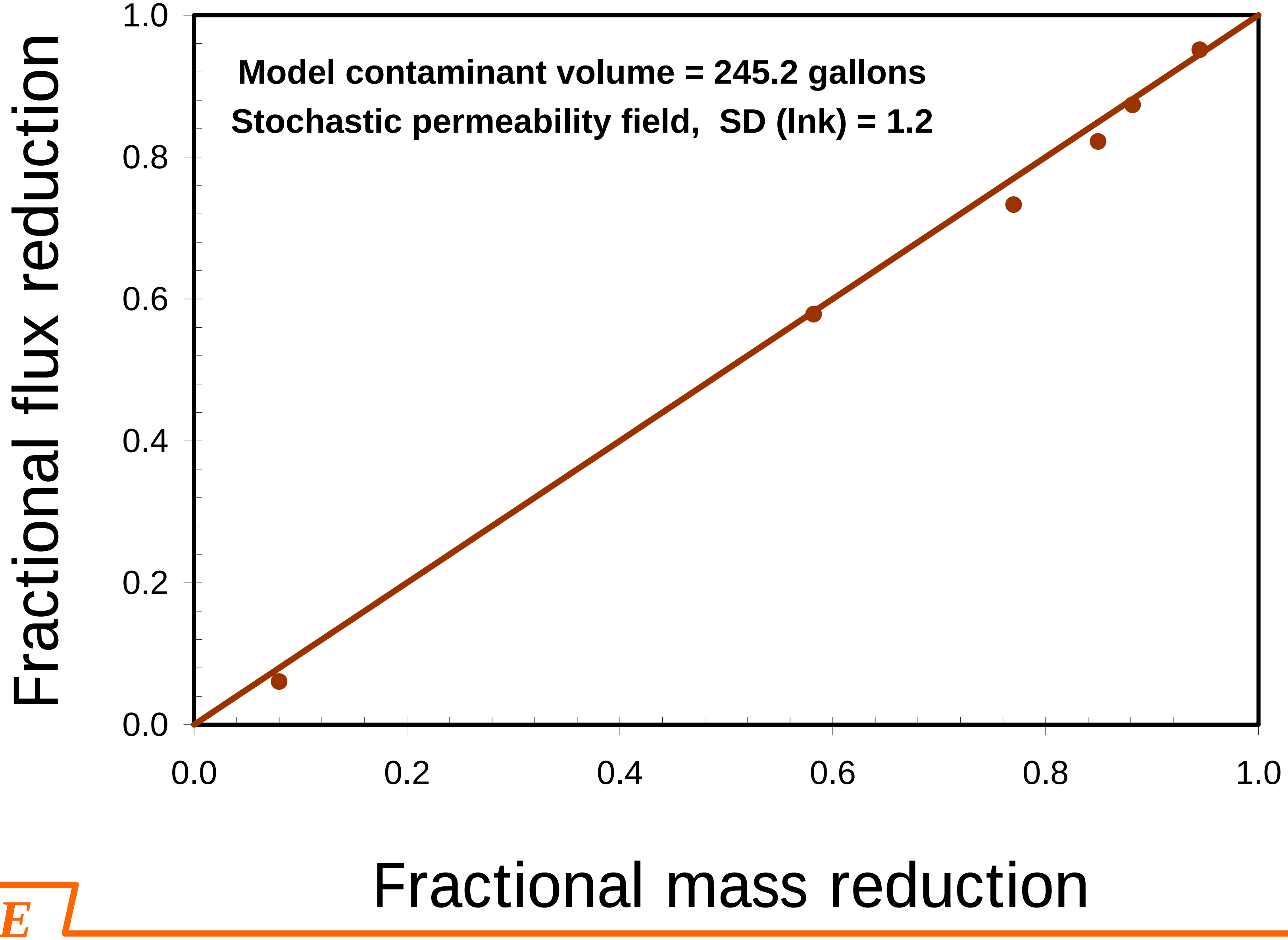


YZ cross-sectional view at control plane



Deepest portion
of paleochannel

SEAR + Natural Gradient Flow for 1 year



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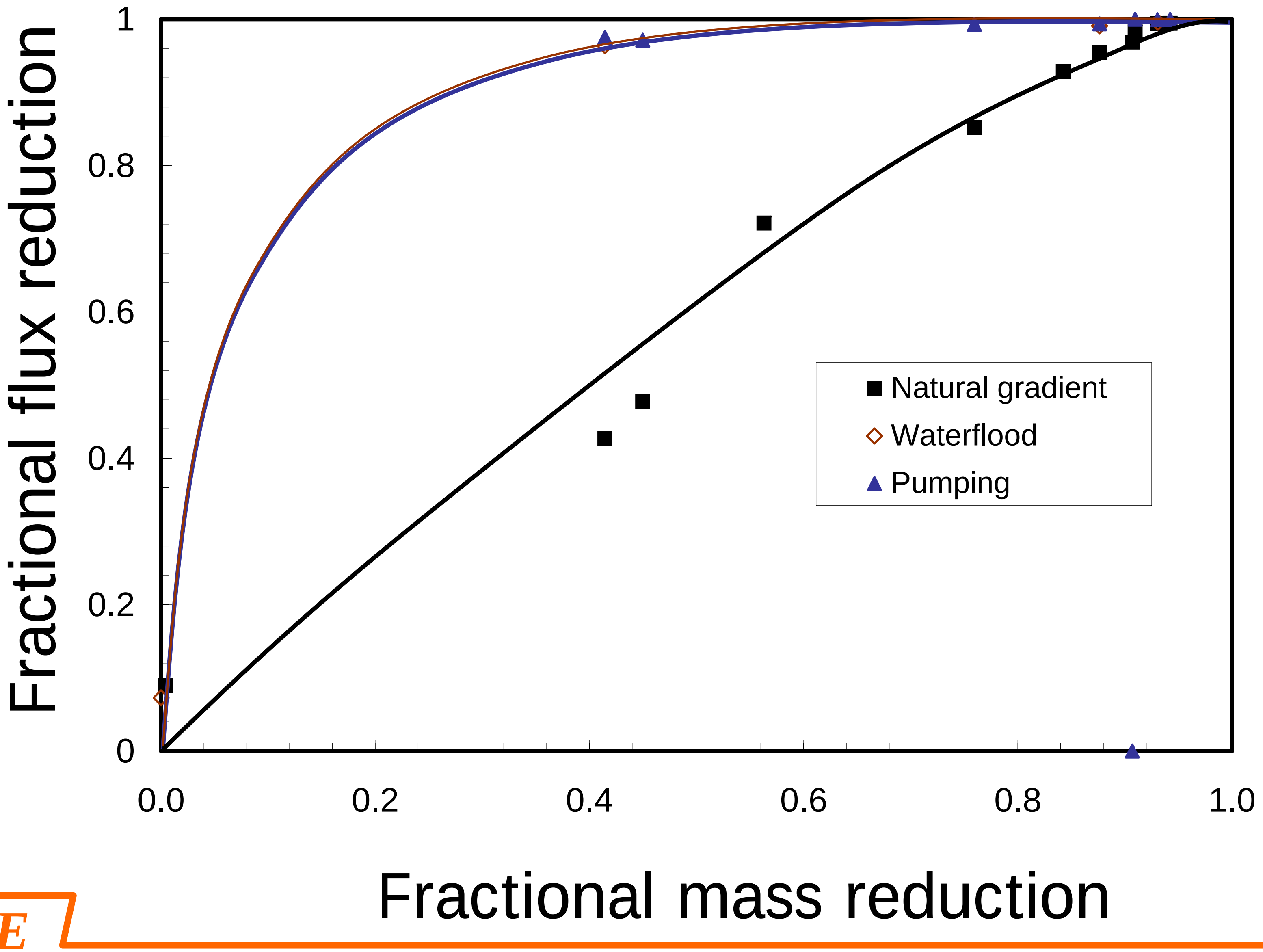
SEAR followed by waterflooding



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Conclusion:

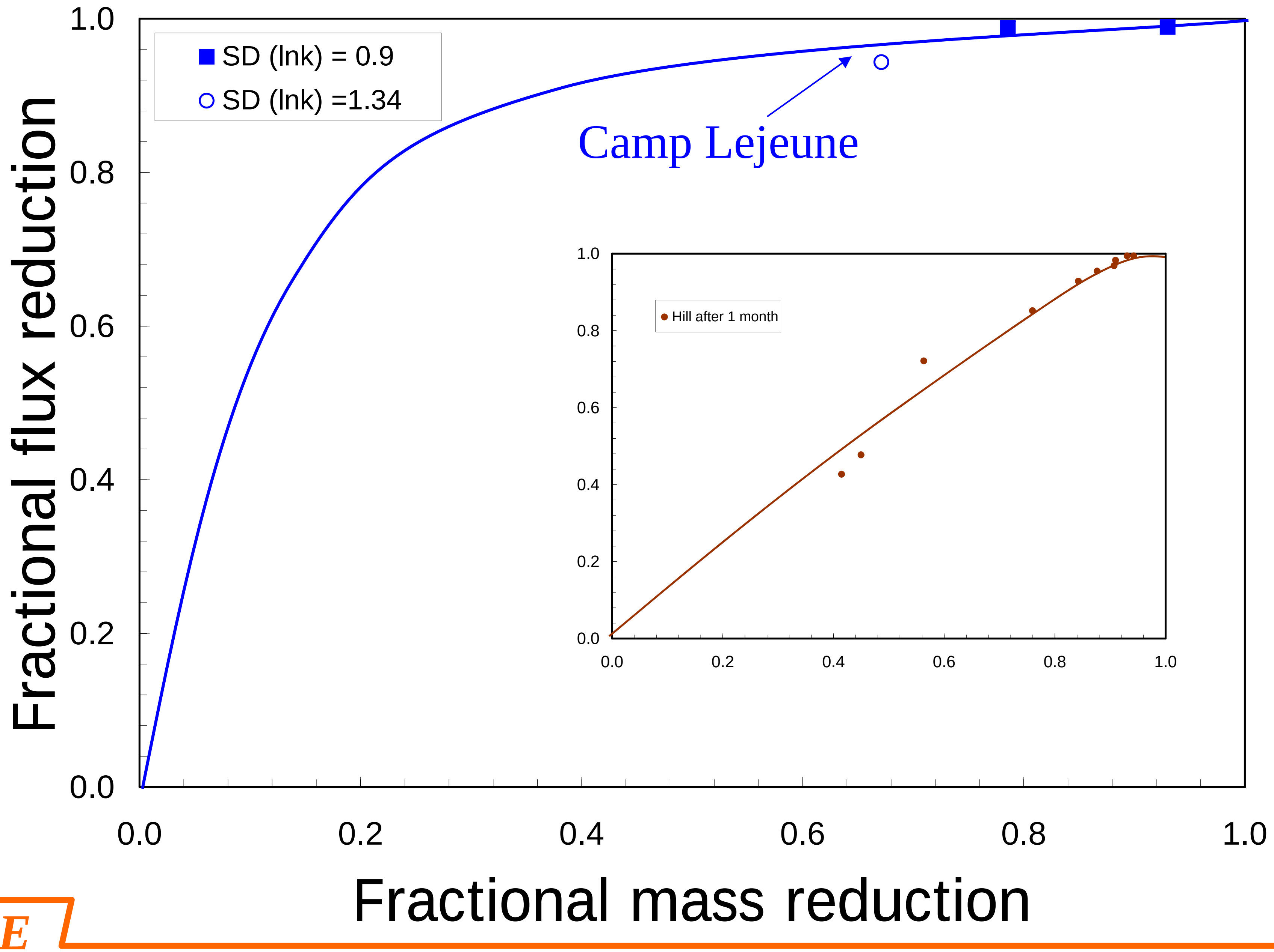
Change the problem!

Natural attenuation is very hard to predict, very uncertain and very slow whereas injecting water following SEAR is simple, easy to model and polishes off the contaminant in months rather than years

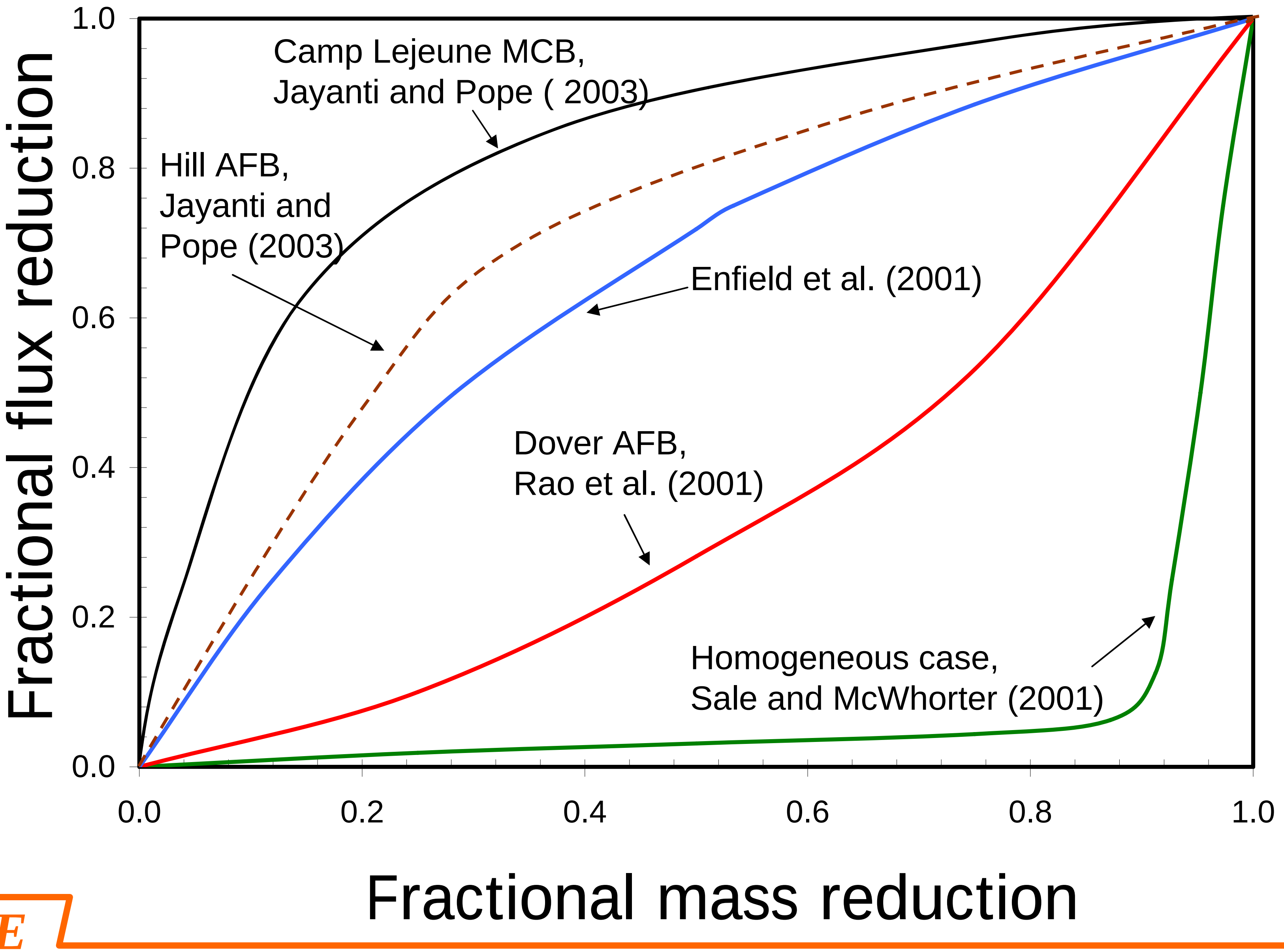
FIELD CASE 2

Camp Lejeune Marine Corps Base, North Carolina

Summary of two field cases
SEAR + natural gradient



Impact of Source Zone Reduction



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Conclusion:

The Sale and McWhorter model published in WRR is wrong and misleading due to several unrealistic assumptions.

They used it to make overly pessimistic predictions of the benefits of groundwater cleanup of toxic chemicals that had an unfortunate impact on government environmental policy.

Using Simulation Models to Predict Uncertainty

**(Just because we can run all those cells
doesn't mean we should.)**

Larry W. Lake

Center for Petroleum and Geosystems Engineering

The University of Texas at Austin

Closing Thoughts

- Distrust history-matched results
  - No outstanding record of prediction
  - Systematic changes required for history match
- Adding more data
  - Uncertainty reduction can lead to bias
  - Consider alternative scenarios
  - Honor the unexpected

Closing Thoughts (cont.)

- Use simplest model possible to
  - Interpret results
  - Pass results to higher scale
  - Use time efficiently
  - Find global optima in design
  - Investigate uncertainties
- Principle of parsimony

The Usual Surprises (cont.)

- **Must decrease vertical permeability for history match**
- **Other petrophysical properties scale-dependent**
- **Lab kr's require adjustment (straightening and endpoints)**
- **Injected fluids breakthrough early**

Closing Thoughts (cont.)

- Invest time in sensitivity analysis (seek understanding)
  - Distinguish between "ϕh" effect…aquifer size, net pay, primary recovery
  - "kh" effect...injectivity, productivity, sweep, secondary recovery, EOR
  - Dimensional analysis

Closing Thoughts (cont.)

- Interrogate gradients
  - Look for vertical equilibrium
  - Tank-type behavior
- Use simplest model possible (parsimony)

Conclusion:

Keep modeling for all of the usual reasons and for fun, but ....

Use all of that intelligence and imagination to do a better job of making predictions in the face of the real uncertainties, not just the ones easy to quantify, and change the strategy or the problem when appropriate!