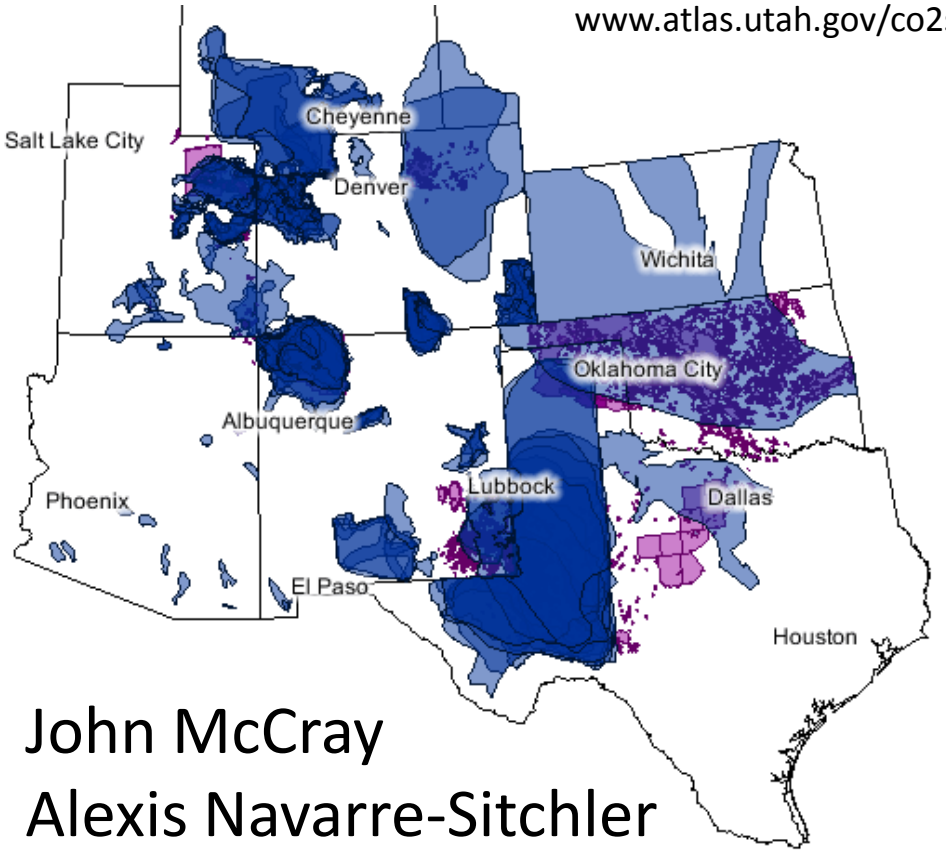
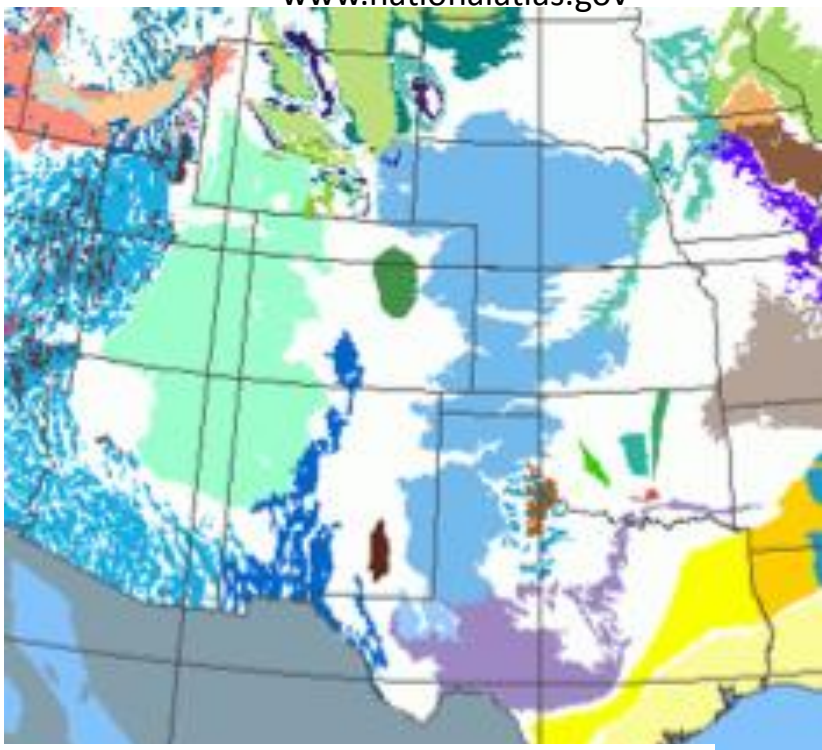
Risk-Based Decision Making for Assessing Potential Impacts of Geologic CO2 Sequestration on Drinking-Water Sources

DoE/EPA Collaborative Review,
Pittsburgh, 23 Mar 2010

www.atlas.utah.gov/co2sw



www.nationalatlas.gov



John McCray
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COLORADO SCHOOL OF MINES
EARTH • ENERGY • ENVIRONMENT

UNIVERSITY OF WYOMING

Carbon Sequestration Research at Mines

Carbon Management Center
Carbon Collaboratory
(CSM, CU, CSU, NREL)

Risks associated with leakage into aquifers:

Funded by U.S. EPA STAR

Project Manager Barbara Klieforth

US DoE-NETL (Training)

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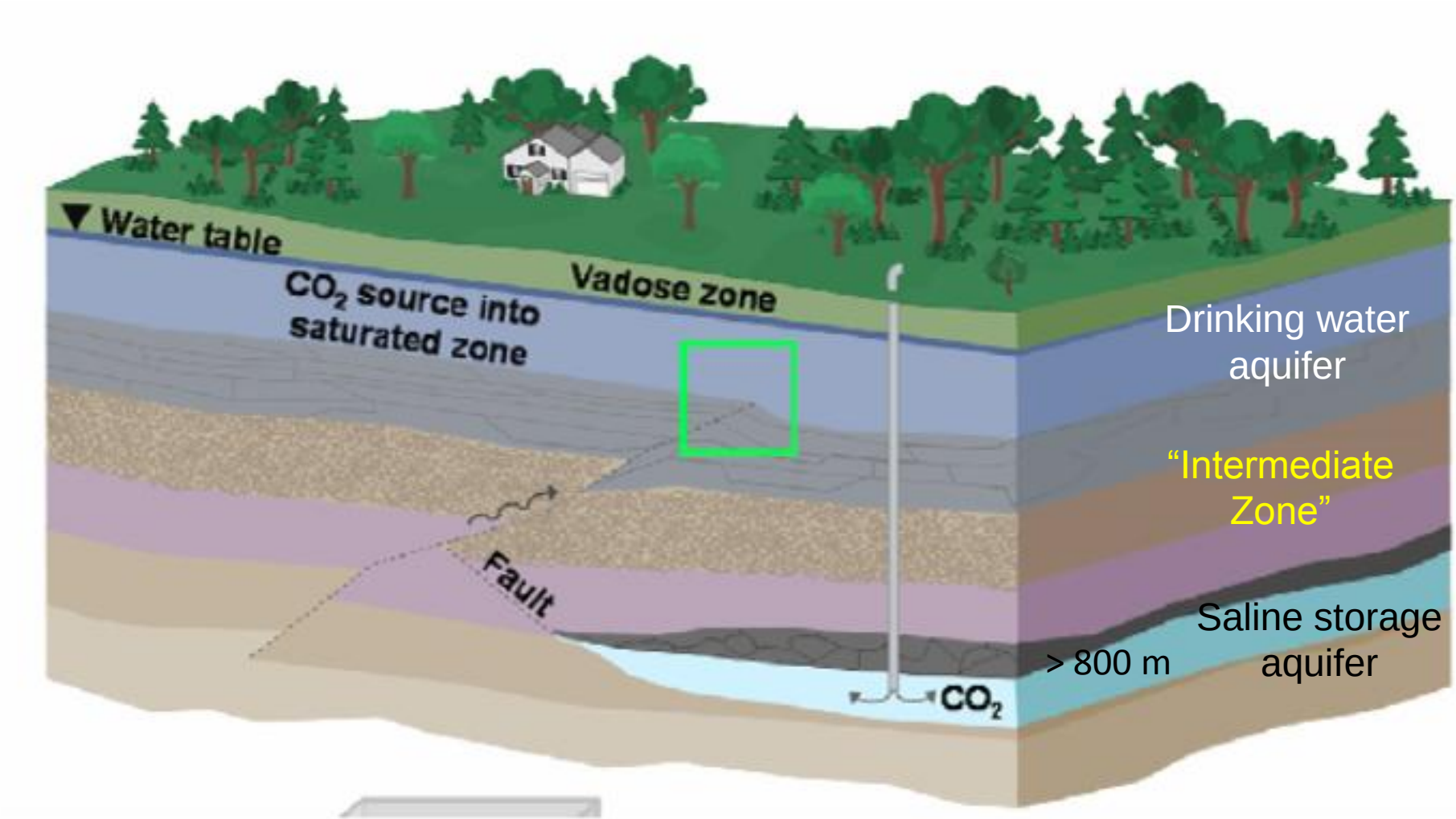
The Aquifer Susceptibility Problem



Darby et al. 9th International Conference on Greenhouse Gas Control (2008)

What risks are associated with CO2 leakage into the "shallow" subsurface?

Change in aquifer water chemistry due to introduction of CO_2 react with aquifer minerals…..

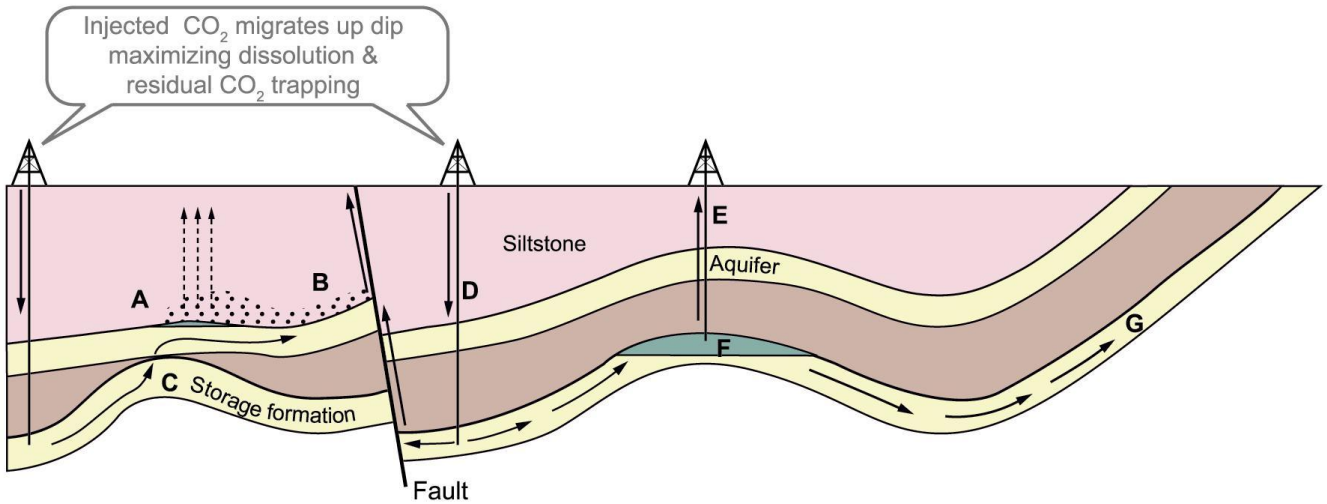
decrease pH
increase metal concentrations
increase salinity
increase TDS
Introduce organic vapors

CO_2 gas in the vadose zone may diffuse into basements

CO_2 gas is lighter than water but denser than air,
High leakage pressures, shallow aquifers

Insufficient Storage – cost and regulatory implications

Leakage Pathways into Aquifers



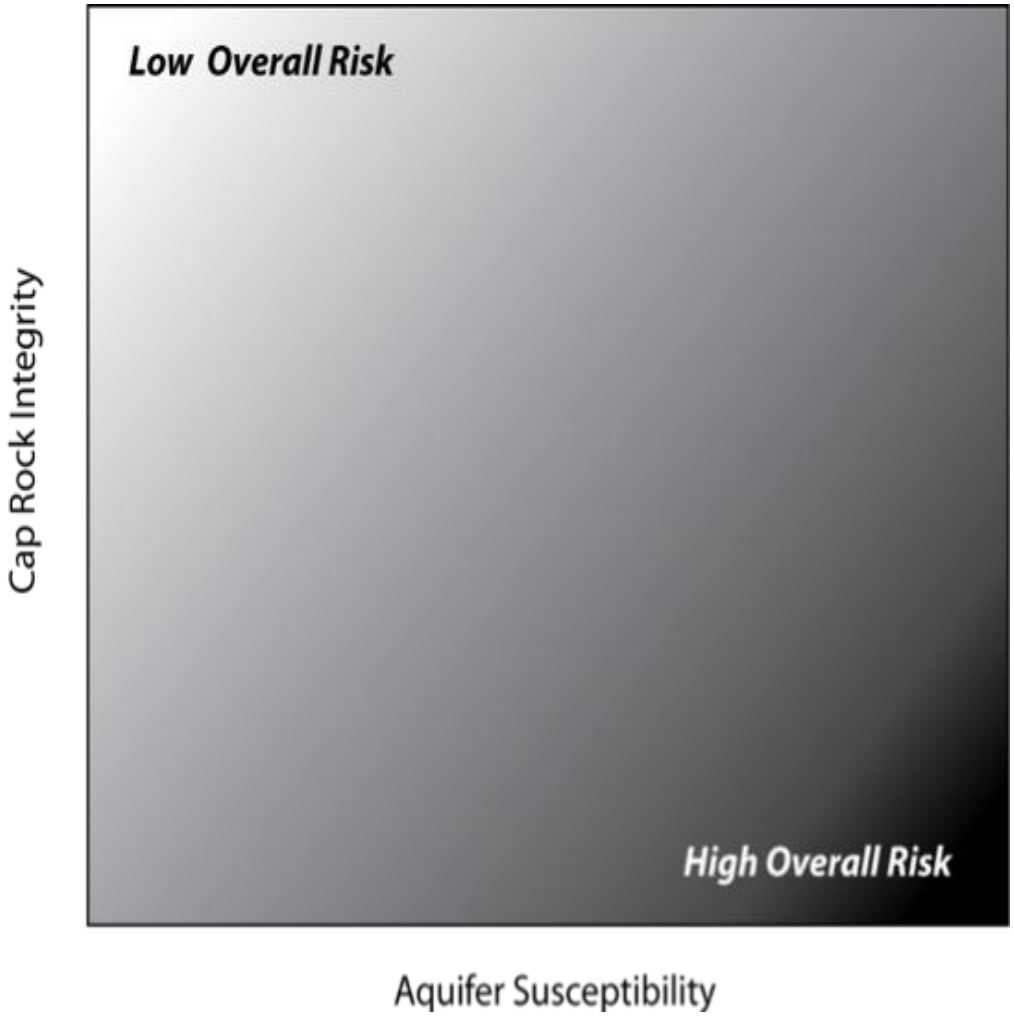
Potential Escape Mechanisms

A. CO_2 gas pressure exceeds capillary pressure & passes through siltstone	**B.** Free CO_2 leaks from A into upper aquifer up fault	**C.** CO_2 escapes through 'gap' in cap rock into higher aquifer	**D.** Injected CO_2 migrates up dip, increases reservoir pressure & permeability of fault	**E.** CO_2 escapes via poorly plugged old abandoned well	**F.** Natural flow dissolves CO_2 at CO_2 / water interface & transports it out of closure	**G.** Dissolved CO_2 escapes to atmosphere or ocean

Remedial Measures

A. *Extract & purify ground-water*	***B.*** *Extract & purify ground-water*	***C.*** *Remove CO_2 & reinject elsewhere*	***D.*** *Lower injection rates or pressures*	***E.*** *Re-plug well with cement*	***F.*** *Intercept & reinject CO_2*	***G.*** *Intercept & reinject CO_2*

Risk to Aquifers from CO_2 Sequestration
Our focus: Aquifer Susceptibility



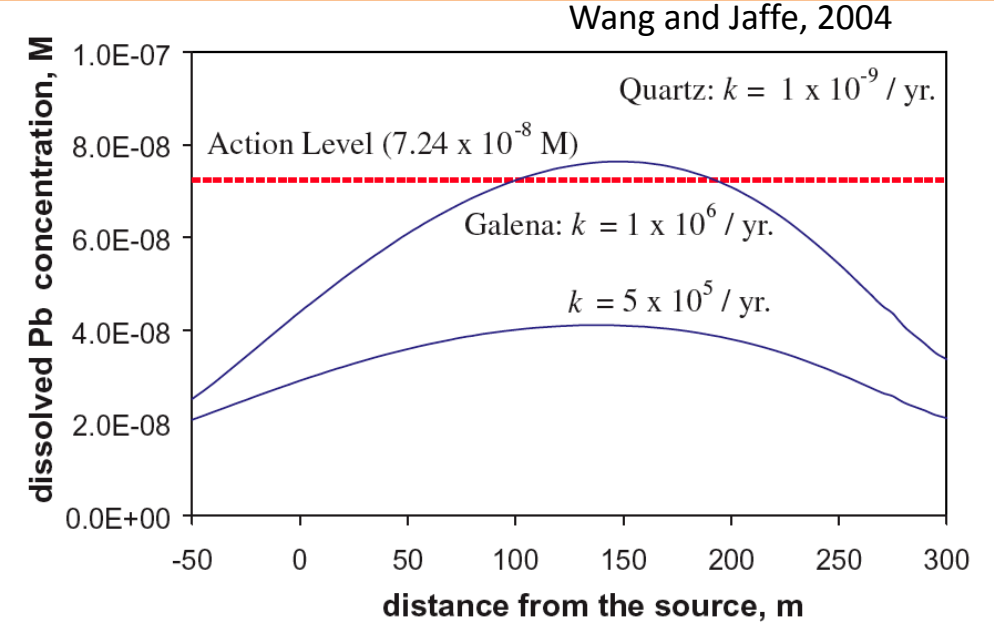
Caprock or Wellbore Integrity vs. Aquifer Susceptibility

If Caprock /well Integrity is high, the risk of leakage is low, and the overall risk of sequestration is low.

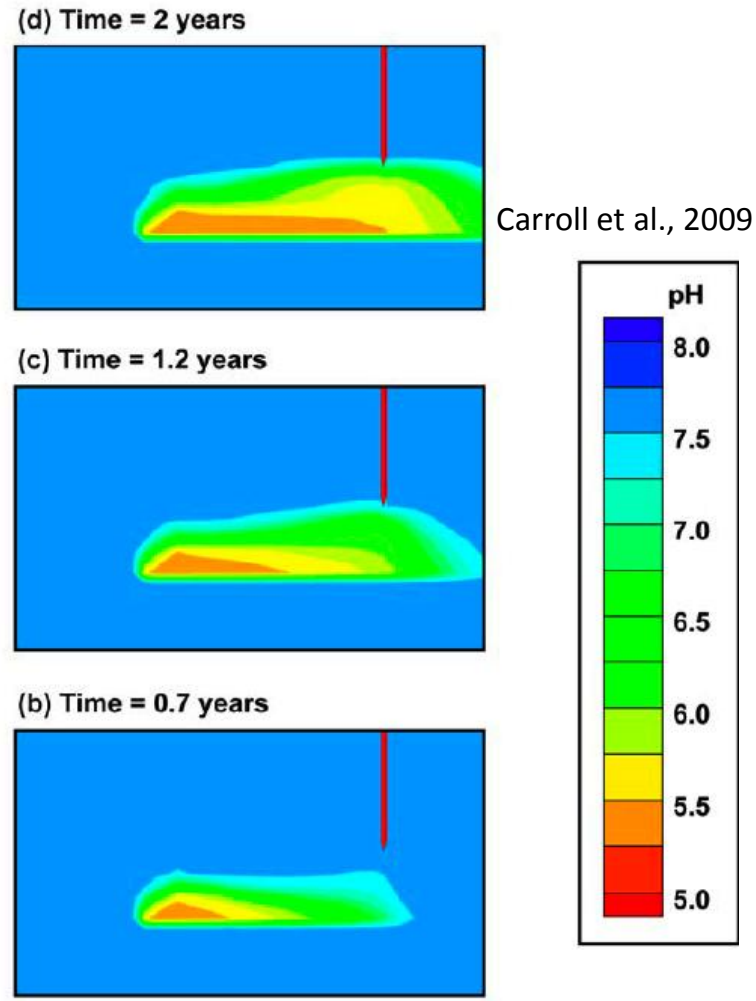
If Caprock Integrity is low, the risk of leakage is high – must quantify the risk associated with the aquifer susceptibility to impacts from the CO_2 to evaluate the overall risk of the project.

We are proposing a method to evaluate aquifer susceptibility from common aquifer parameters, such as mineralogy, water quality, and hydrologic properties.

Very little work to date on leakage rates or impacts of leakage on aquifers



Very low leakage rates lead to exceedence of MCL for Pb in simplified aquifer mineralogy (equal parts galena and quartz.

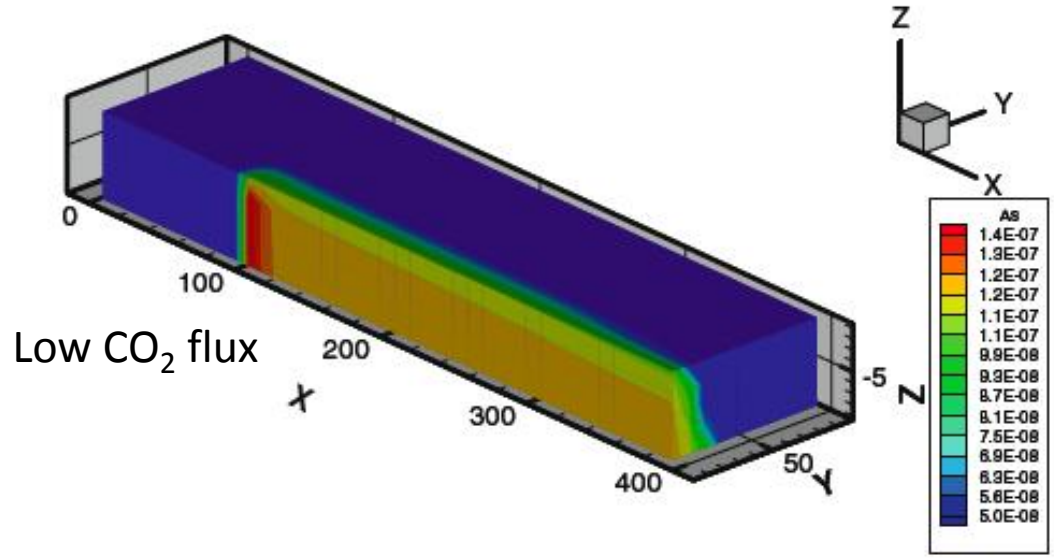


Carroll et al., 2009

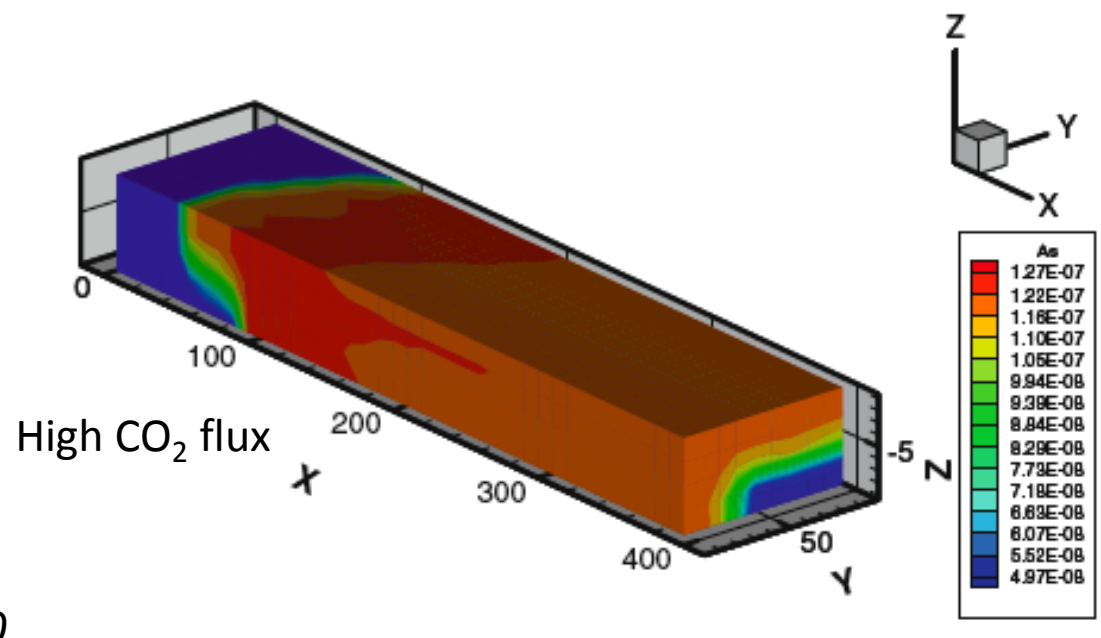
Leakage rates 1000 to 2 million tonnes CO_2 per year: 0.01% to 1% of CO_2 injected from 1 GW coal fired power plant. Tracked pH as an indicator of impact

As concentrations in simulated groundwater

CO_2 in aquifers can liberate metals into groundwater



Computationally expensive and require small model domains



Apps et al., 2010

Research Goals and Objectives:

1) Understand the geochemical processes and scales associated with CO_2 & brine leakage into aquifers.

2) Understand how heterogeneous aquifer physicochemical properties are related to aquifer susceptibility

1) Develop a methodology to assess the probabilistic *aquifer-scale* risk associated with CO_2 leakage into a potential drinking water source

Overview of EPA-funded Research Project on Aquifer Risk (1)

- Identify & rank potentially leaky aquifers over GCS targets
  - Characterize aquifer hydrogeology, water quality and mineralogy
  - Characterize leakage potential of cap rock/intermediate zones (IZ)

- Identify potential toxic constituents

- Multiphase and geochemical modeling to understand the CO_2 source in the aquifer, and the aquifer-solid reactions downgradient

- High P & T geochemical experiments to evaluate metals released into brine, may leak to aquifers via fractures under hydraulic gradients.

- 2-Dimensional, Intermediate Scale Experiments:
  - Understand mass-transfer within CO_2 source zone
  - Evolution of products from the CO_2/ brine source zones
  - Verify ability to model geochemical reaction processes in heterogeneous media at a more realistic scale

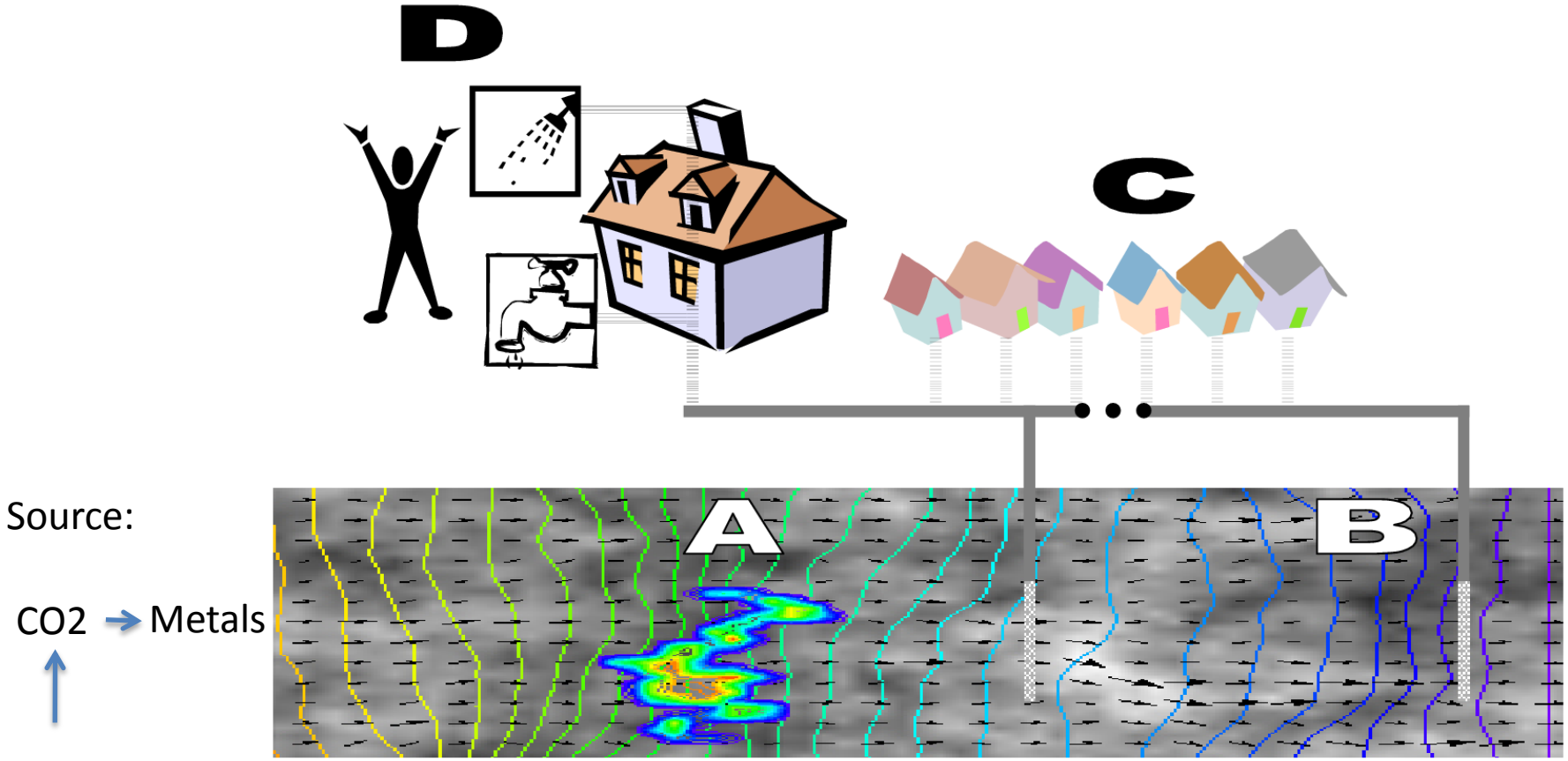
Overview of EPA-funded Research Project on Aquifer Risk (2)

- Develop <u>particle tracking models</u> to assess the probability of contamination for different aquifer conditions
- Extract and simplify important geochemical processes from full reactive transport models to particle tracking models

- Develop <u>stream-tube models</u> to assess critical complex geochemical reactions between CO2 and aquifer minerals in aquifers of interest at aquifer scales (for rapid simulations)

- Define the <u>risk framework</u>
- Conduct probabilistic risk simulations, create risk-surface maps

This Risk Framework



A: Heterogeneous subsurface flow and contaminant transport of metals

B: Possible capture in one or more downgradient receptors (wells)

C: Water delivery system to many different households (C)

D: Household exposure and health risk via multiple pathways to varying individuals

Maxwell et al. WRR34(4), 1998; Maxwell and Kastenberg, SERRA 13(1-2), 1999

Risk and Exposure

- What do we mean by Risk?
  - probability of adverse health effects (cancer, over background) for an individual due to some exposure to contaminants

  Risk = *f*(Dose, Dose Response)

  Dose=*f*(Exposure)
- What do we mean by Exposure?
  - the delivery of some contaminant to an individual via a specific pathway (i.e., drinking water)

  Exposure = *f*(concentration, physiology, pathway, duration time, frequency)
  - Exposure Pathways
    - direct ingestion (drinking)
    - dermal contact (washing)
    - inhalation (showering)

Uncertainty and variability

- Parameters can be variable, uncertain or both
  - variable parameters may be well known, but vary spatially, temporally, or between individuals (e.g. exposure parameters)
  - uncertain parameters are not well known (e.g. transport parameters)

- Variable parameters

  *distributions of certain values often expressed as **fractiles** of frequency*

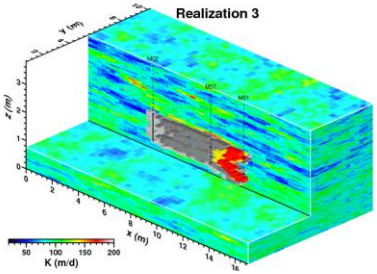
- Uncertain parameters

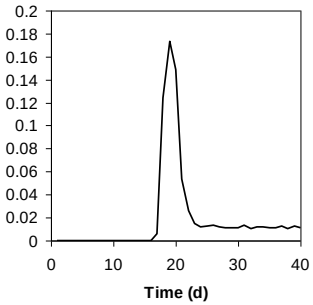
  *confidence in knowledge of parameters expressed as **percentiles** in uncertainty*

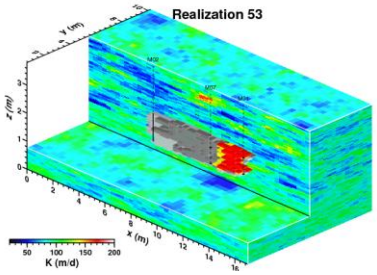
- Risk=*f*(U,V)
- Nested Monte Carlo procedure: transport => exposure => risk

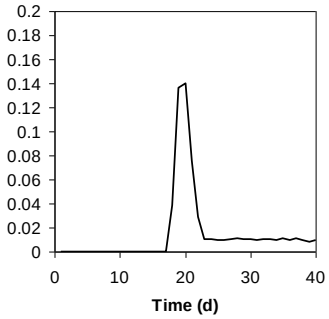
Monte Carlo Approach: Uncertain Transport to a Well

i=1

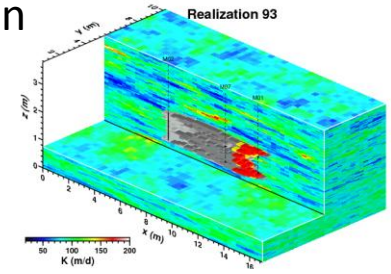


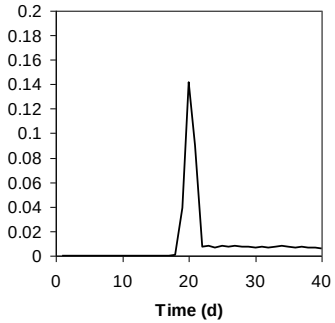


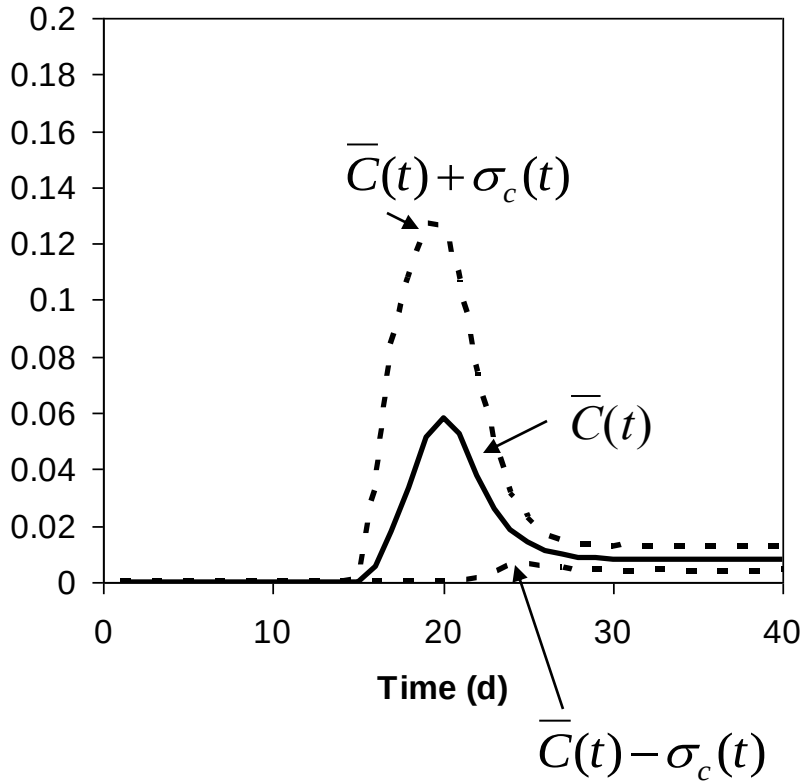




i=n





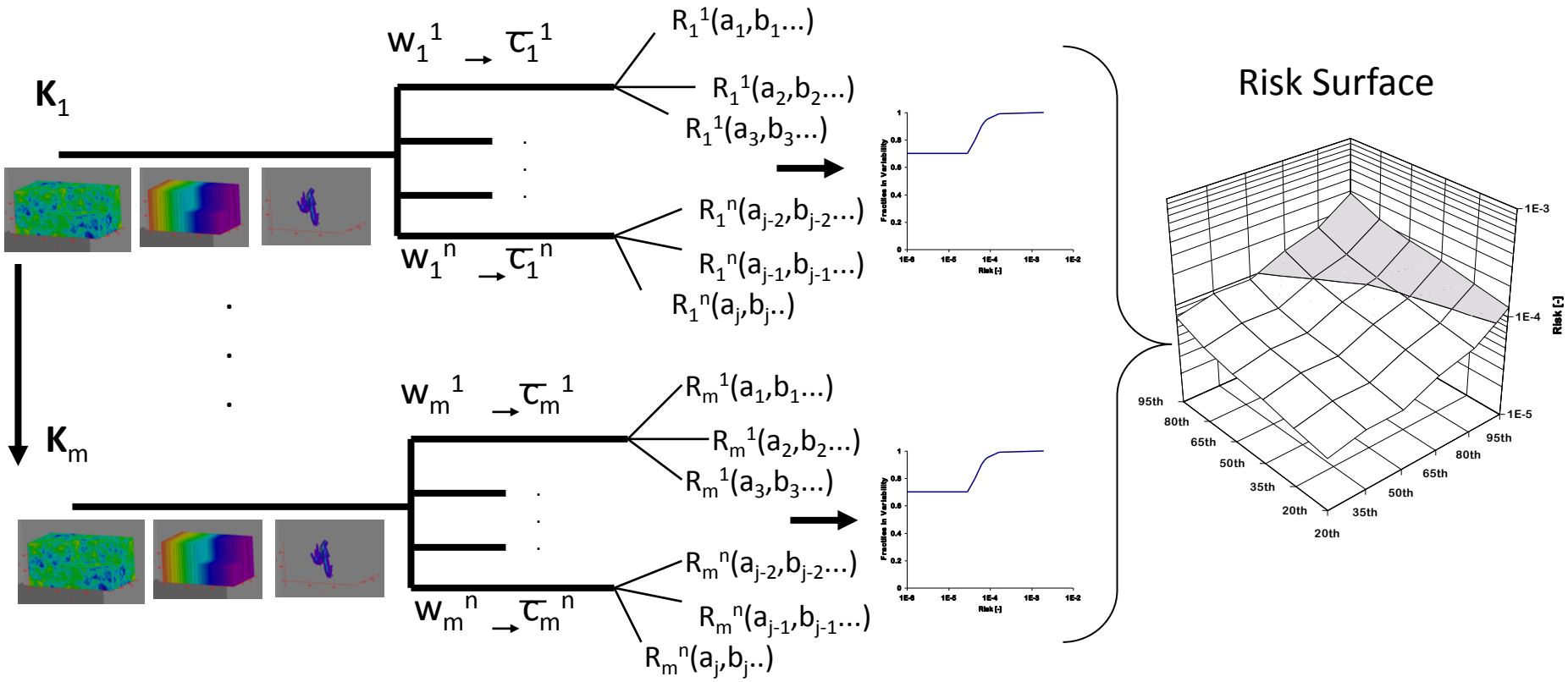


Uncertainty

Realizations of Aquifer Properties and transport

Variability

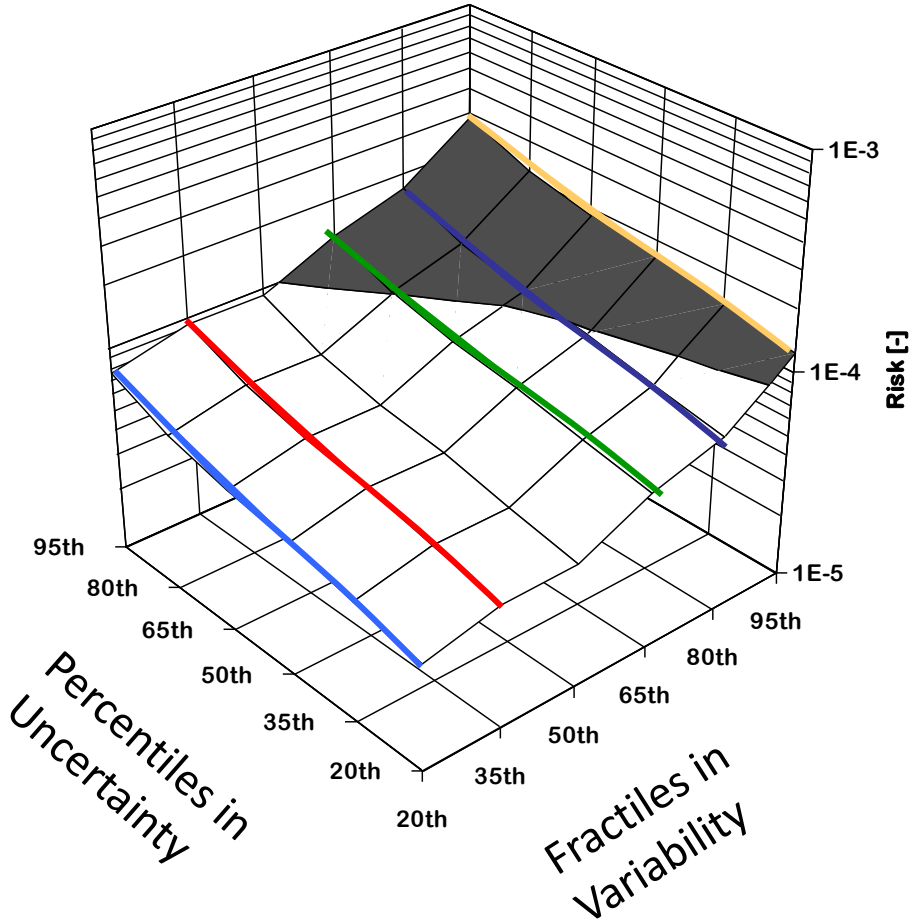
Exposure and Risk to individuals

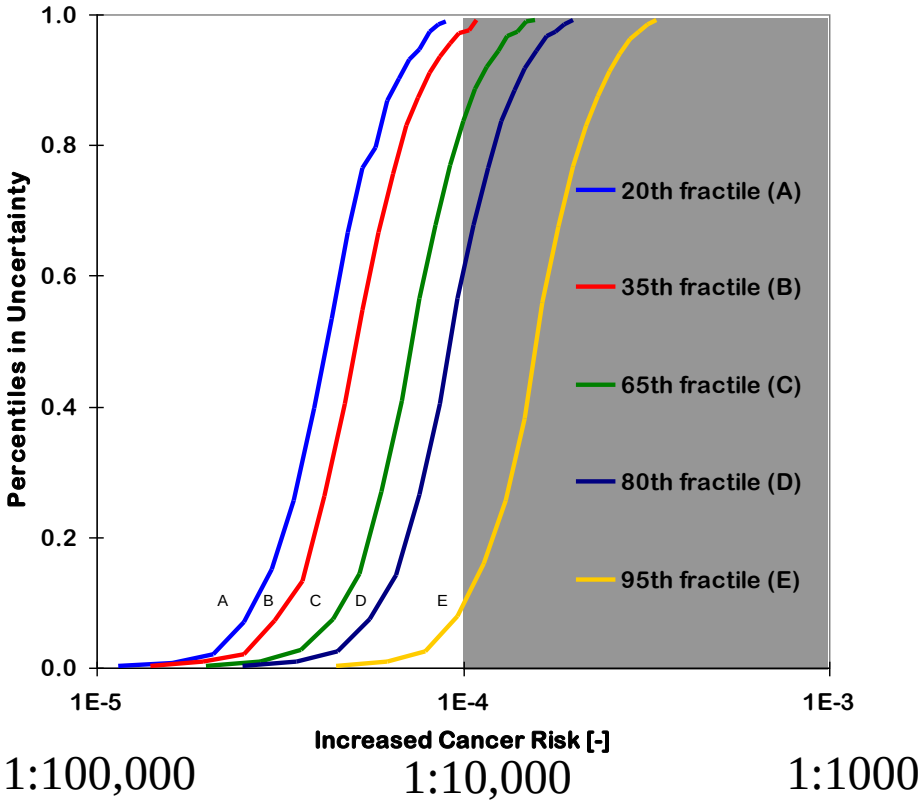


K is one or more hydrologic or geochemical variables influencing transport

Exposure variables include toxicity of a contaminant or dose that results in an increased risk, a persons' drinking rate, likelihood of receiving water from an impacted well, etc

Goal: Methodology that can produce a risk surface





Maxwell et al. WRR34(4), 1998

Probabilistic risk simulations cannot reasonably be conducted using complex, multiphase hydrochemical models

Use simpler streamline-based models for Monte Carlo risk simulations

- Particle tracking models with simplified reactions
- Stream tube models using more complex hydrochemistry

Computationally efficient (1-D), ideal for parallel simulation

Determine source-to-receptor stream lines for most important aquifer risk pathways (aquifer models/ existing data).

Particle tracking: Lagrangian Contaminant-Transport Approach

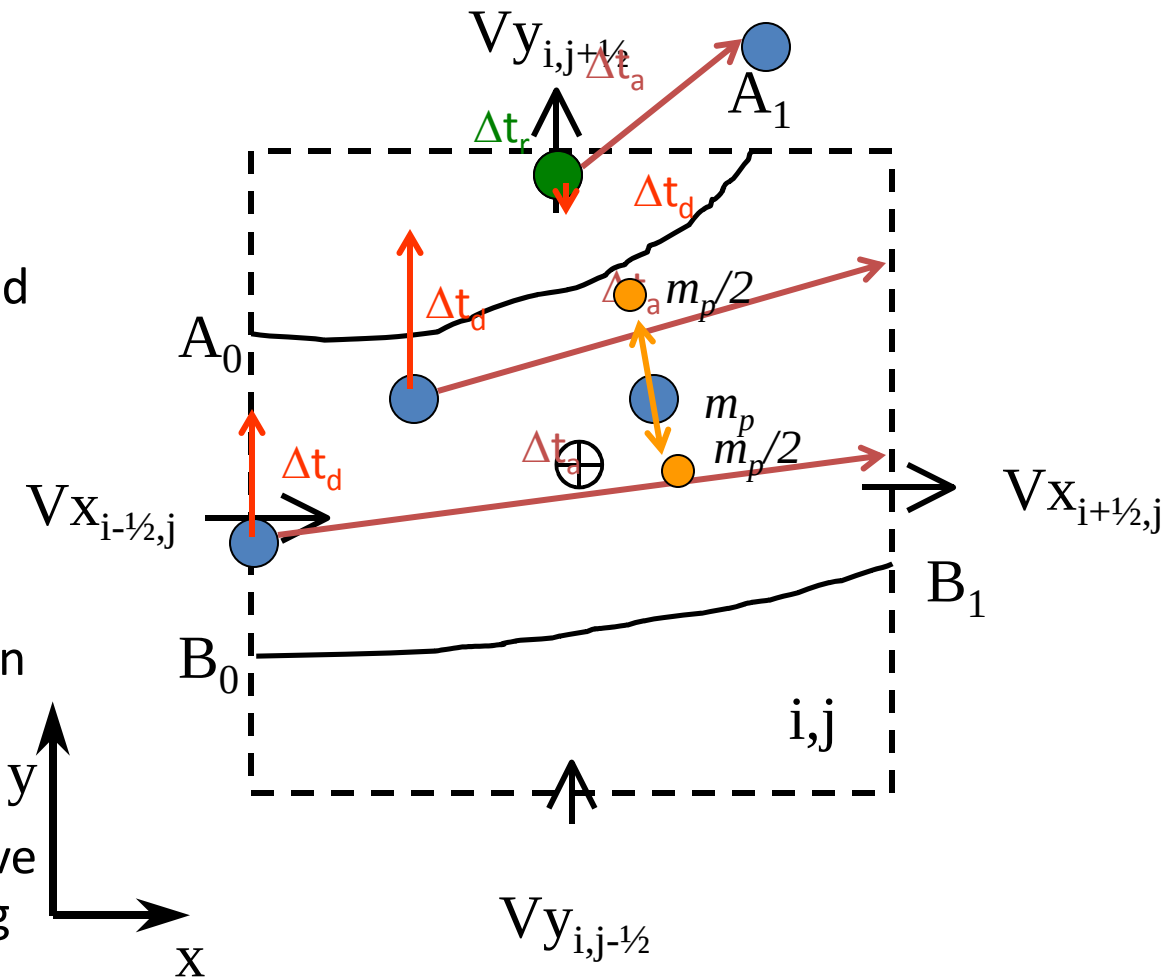
- Advection along streamlines calculated using

$$x = \frac{(a + bx_0)e^{b\Delta t} - a}{b}$$

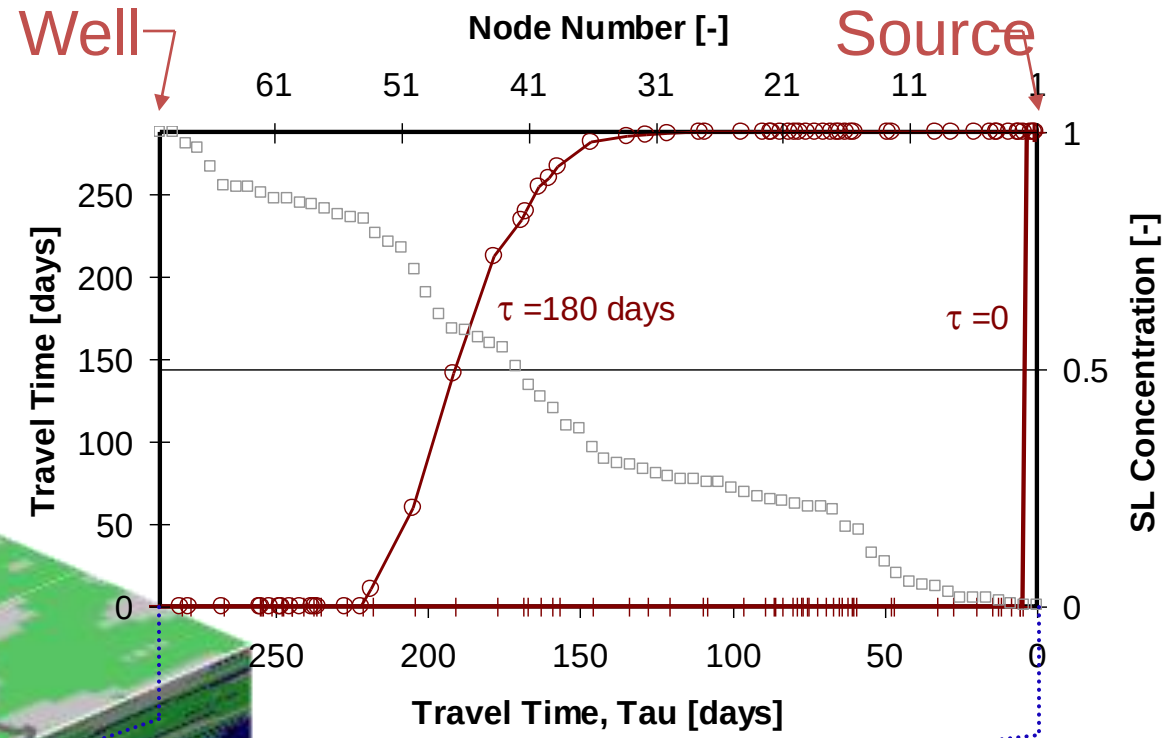
- Dispersion processes calculated numerically random walk algorithm

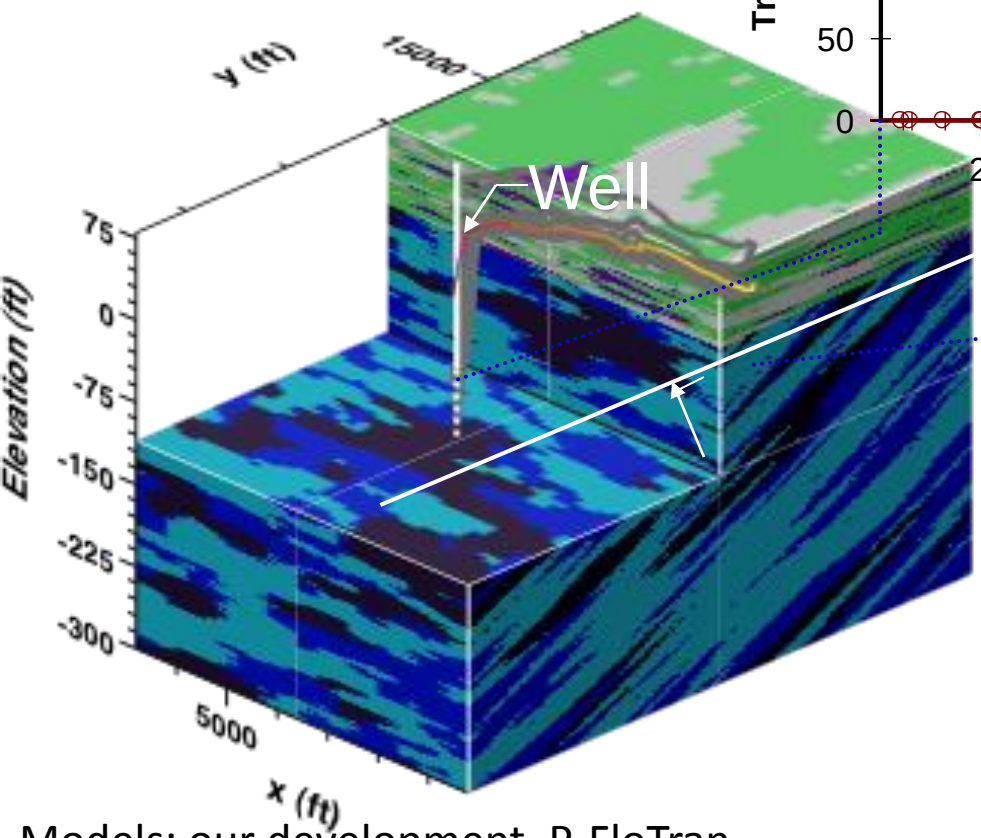
- Simple linear reactions. Use a probability approach to calculate transference between phases

- Use particle splitting to improve concentration resolution along fronts



Streamline Modeling Approach

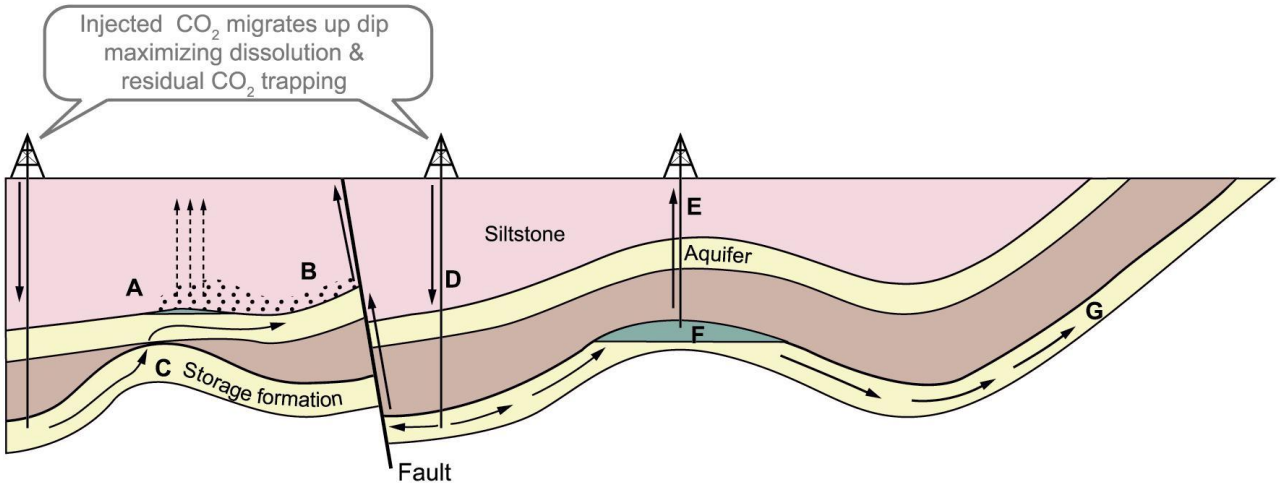




Models: our development, P-FloTran, Phreeqc, others.

- Streamlines are mapped and used to determine origin, travel time, travel pathway and flux of water entering a well screen
- Forward reactive transport simulated along each streamline using finite-difference 1-D grid: advection terms solved explicitly via high-order TVD algorithm, reaction terms solved implicitly
- Can incorporate complex, non-linear reactions
- Concentrations are mapped from each 1-D streamlines onto the 3-D grid
- Breakthrough curves at the well are flux-averaged across all streamlines

Simplify the source term….



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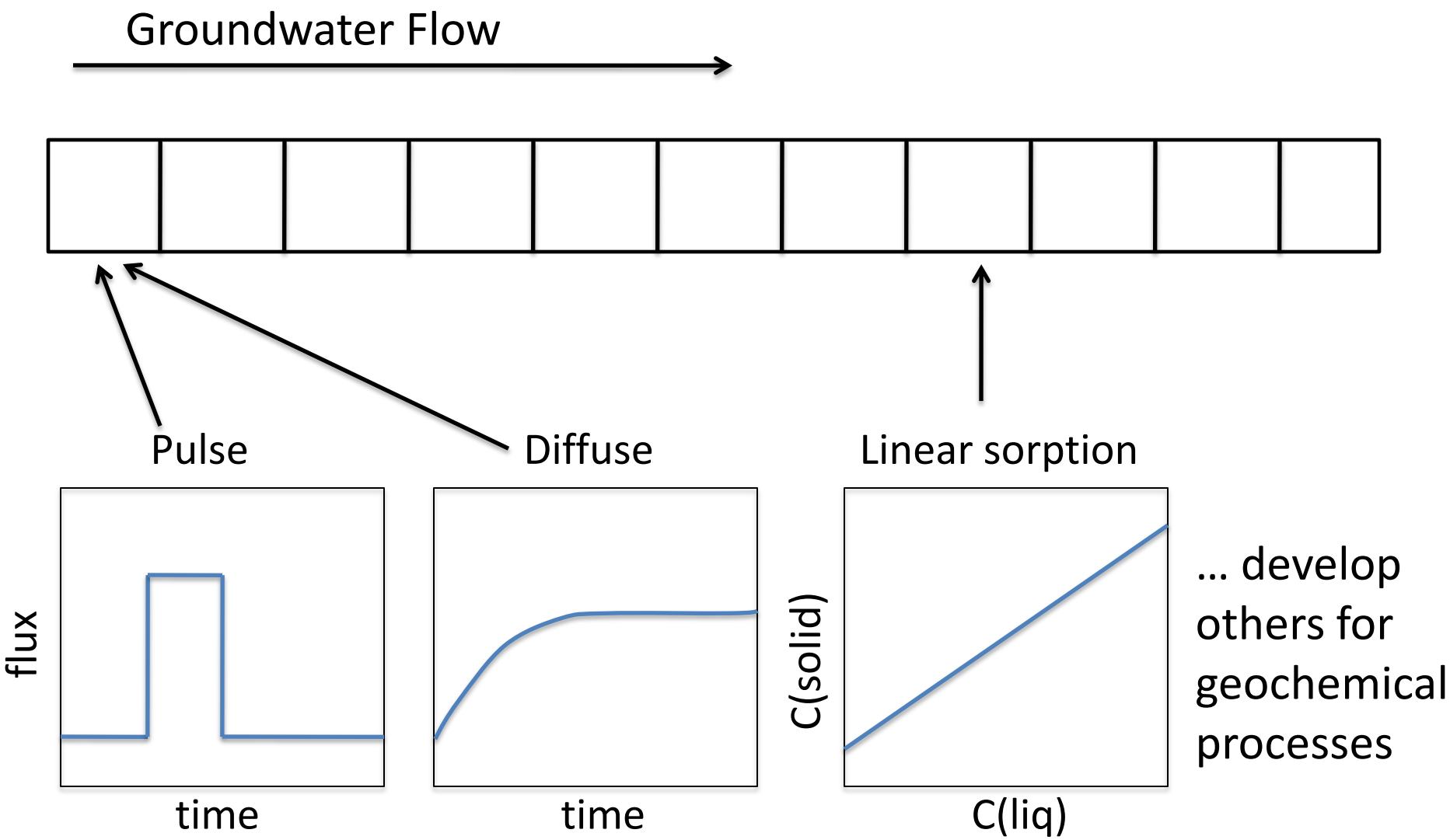
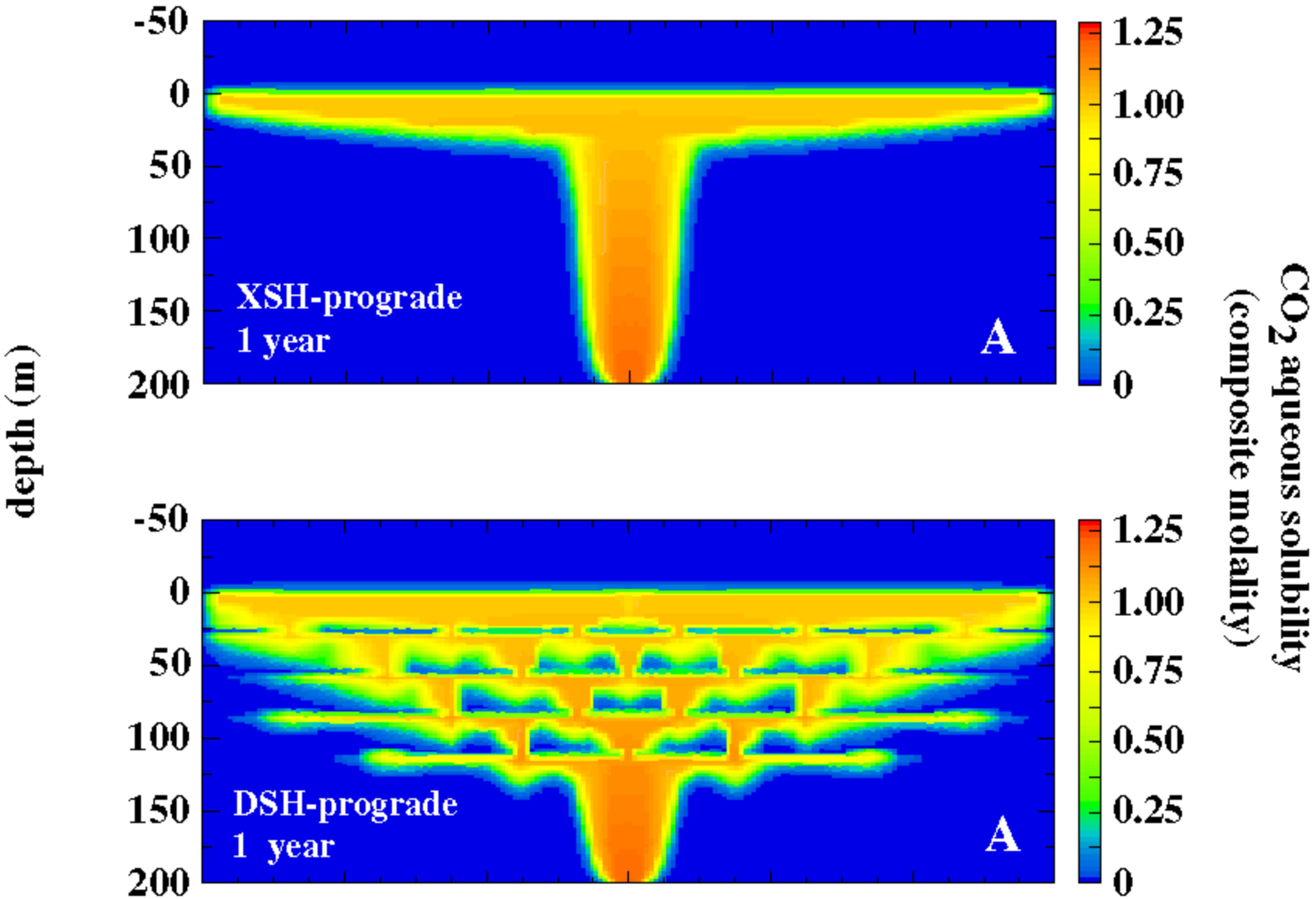
Simplified Source/Reaction Functions for Streamline Models: CO_2, H^+, M^{+b} ……



Diffuse Leakage



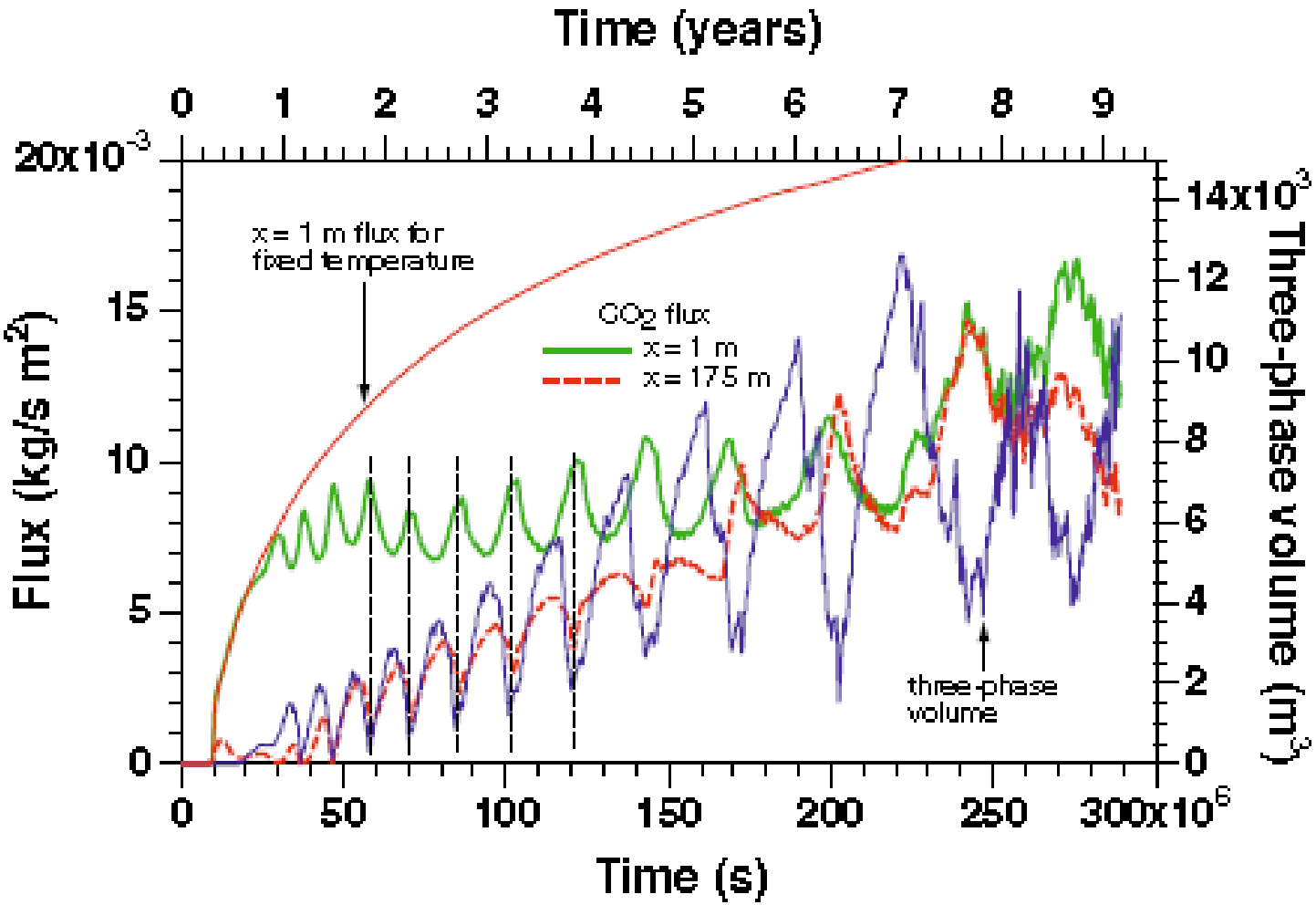
Johnson et al., 2001

Cyclic Leakage (Through A Fault)

Fixed Temperature

Flow and Heat Transfer

Volume of Fracture Occupied by Three CO_2 Phases



Pruess, 2008

Shapes of CO_2 Source Functions

Example in the injection-storage zone,
but relevant to aquifer sources

Aqueous CO_2 | **Residual GaseousCO_2** | **Mobile Gaseous CO_2**

Varying Brine Salinities

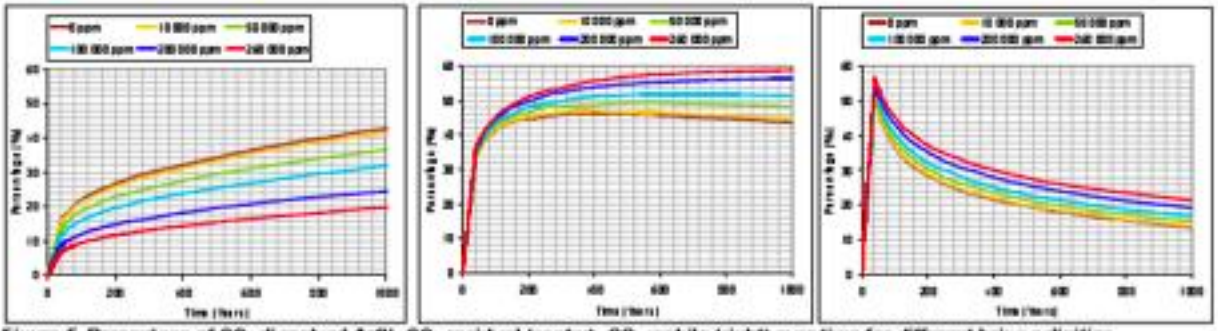


Figure 5. Percentage of CO_2 dissolved (left), CO_2 residual (center), CO_2 mobile (right) over time for different brine salinities.

Varying Horizontal Permeabilities

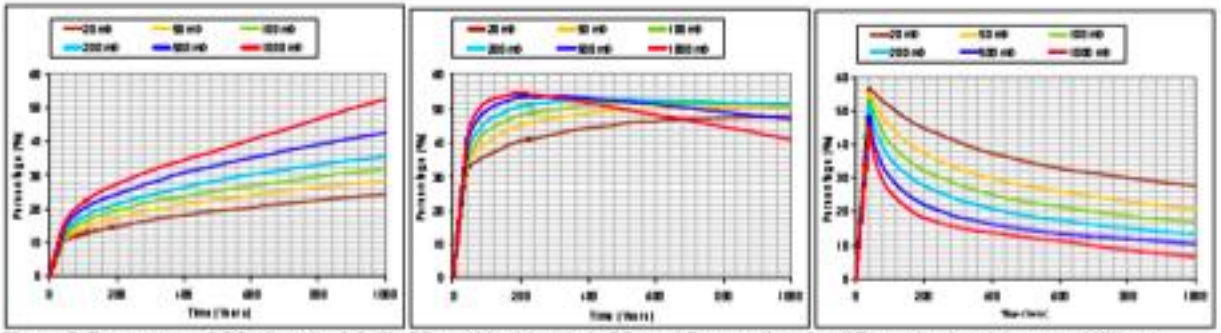
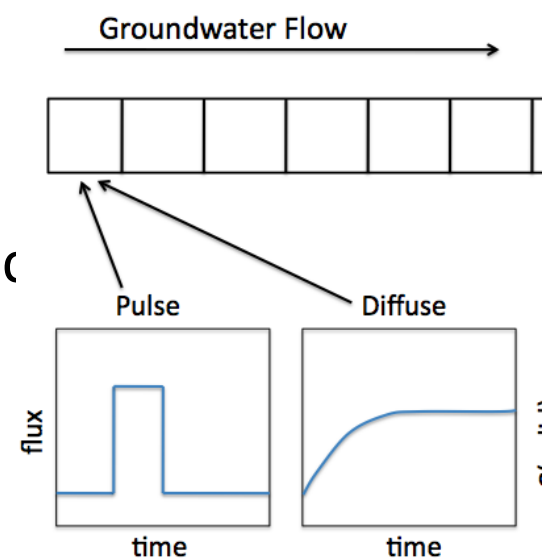


Figure 6. Percentage of CO_2 dissolved (left), CO_2 residual (center), CO_2 mobile over time for different horizontal permeabilities.

Sifuentes et al., 2009

Characterize the Source and Reaction Functions

Source functions for: CO_2, SO_x, H^+, metals…….



<u>Modeling</u> for:

- Geochemical transport of chemicals in aquifers….
- More realistic aquifer mineralogy
- Important liberated metals
- Various multiphase hydrologic conditions
  - TOUGH-React, Pflow-Trans, NUFT, etc
- Simplify into streamline models for risk simulations

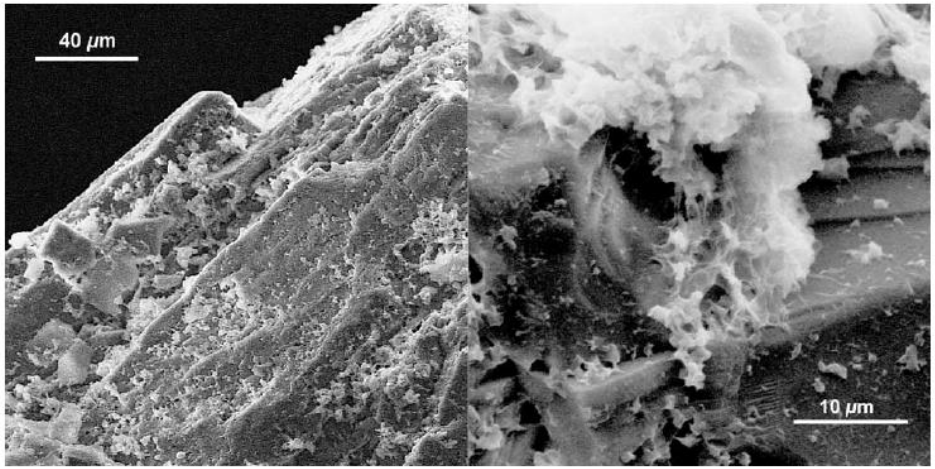
<u>2-D and Batch Experiments</u> to validate the source functions, determine appropriateness of geochemical models to simulate transport in heterogeneous media at a more realistic scale, evaluate stream-tube, particle tracking models.

Geochemical Experiments

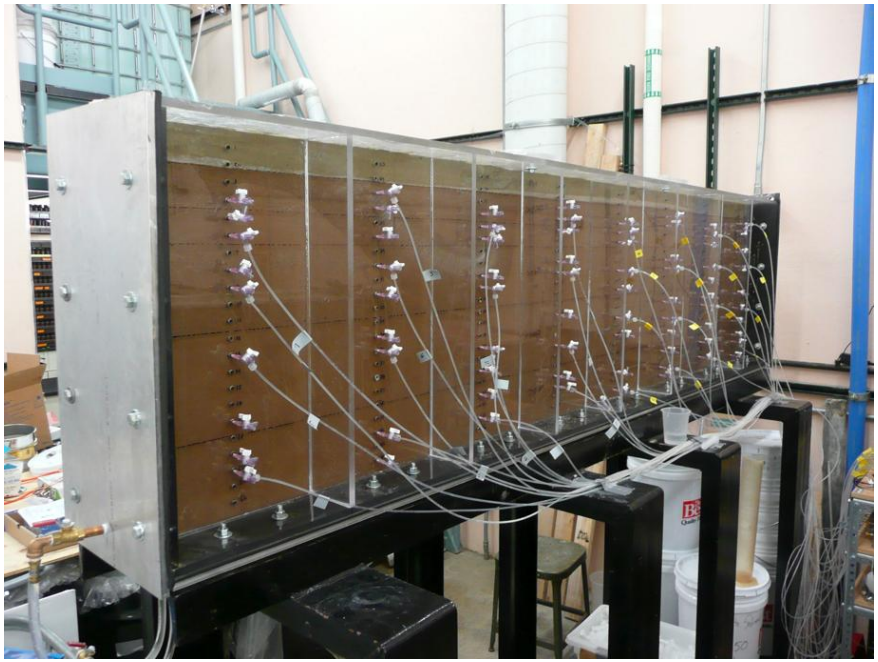
High Pressure and Temperature batch experiments to understand the potential liberation of metals into brine under high P & T in the injection or intermediate zones.

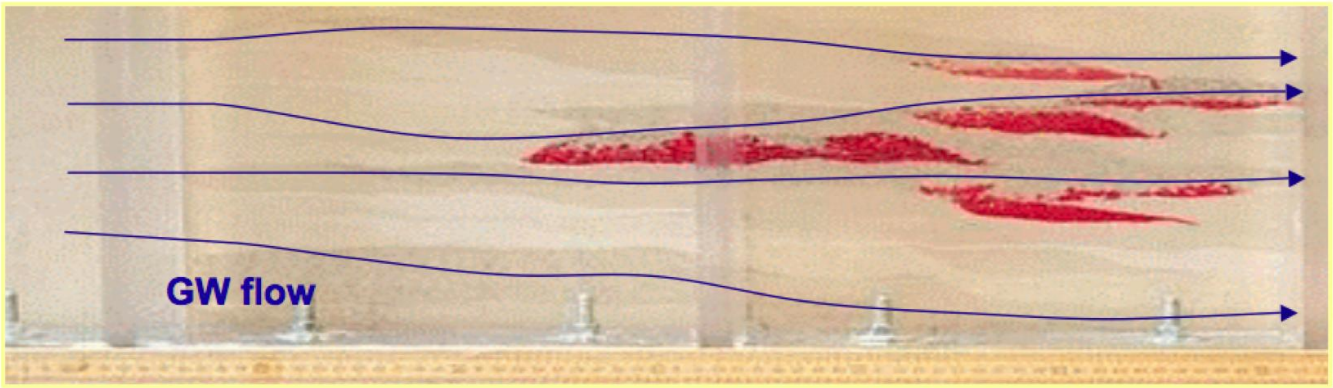
Environmental P & T column and batch experiments to understand chemical equilibria and rates for metal evolution for selected aquifer materials and water quality representative of heterogeneous aquifer conditions.

SEM of oligoclase with clay mineral on the surface after reaction with supercritical CO_2 (Kaszuba et al., 2003)



2-Dimensional Intermediate-Scale Experiments at CSM





Potential Leakage Pathways are Endless

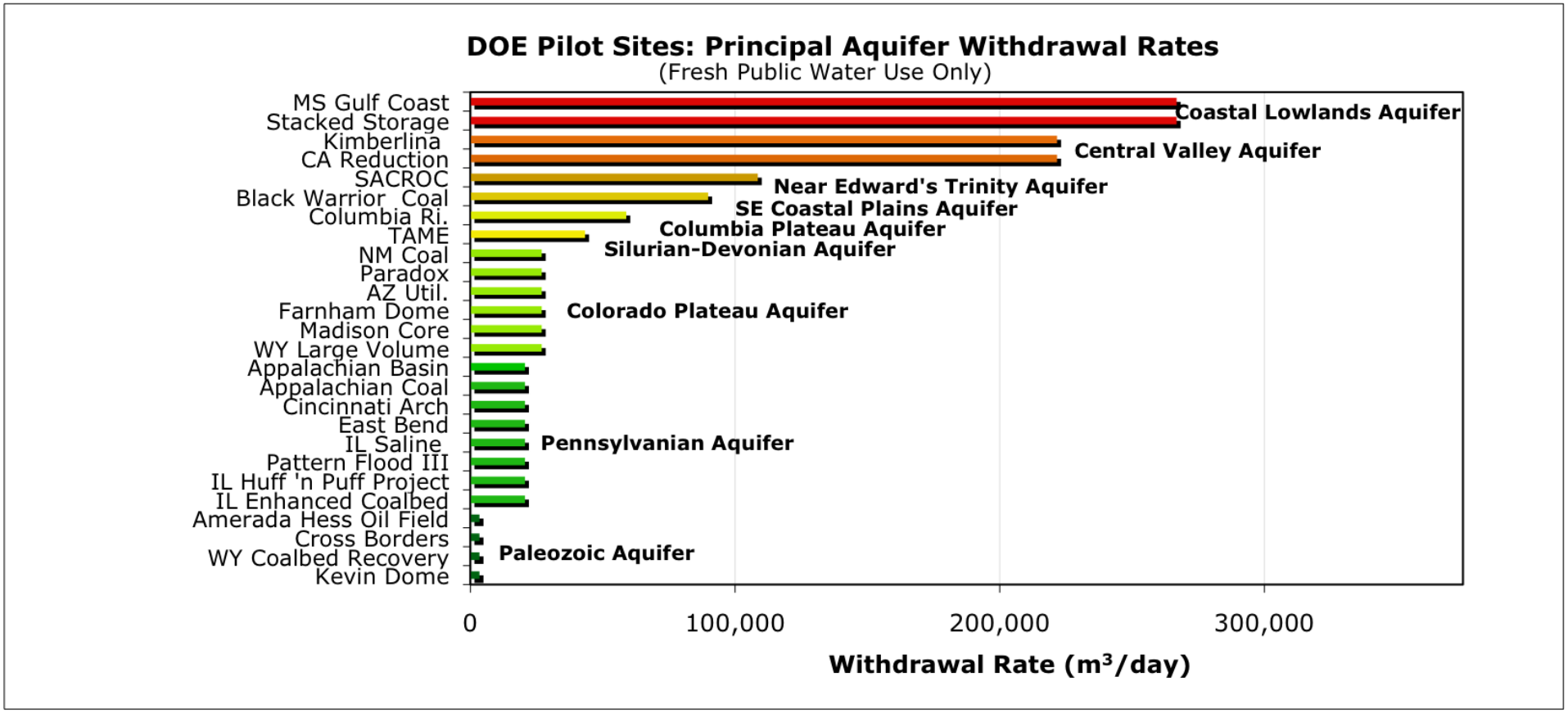
Screen current sequestration locations for risk, use these aquifer systems as basis for research (modeling and experimental porous media)

Screen for:

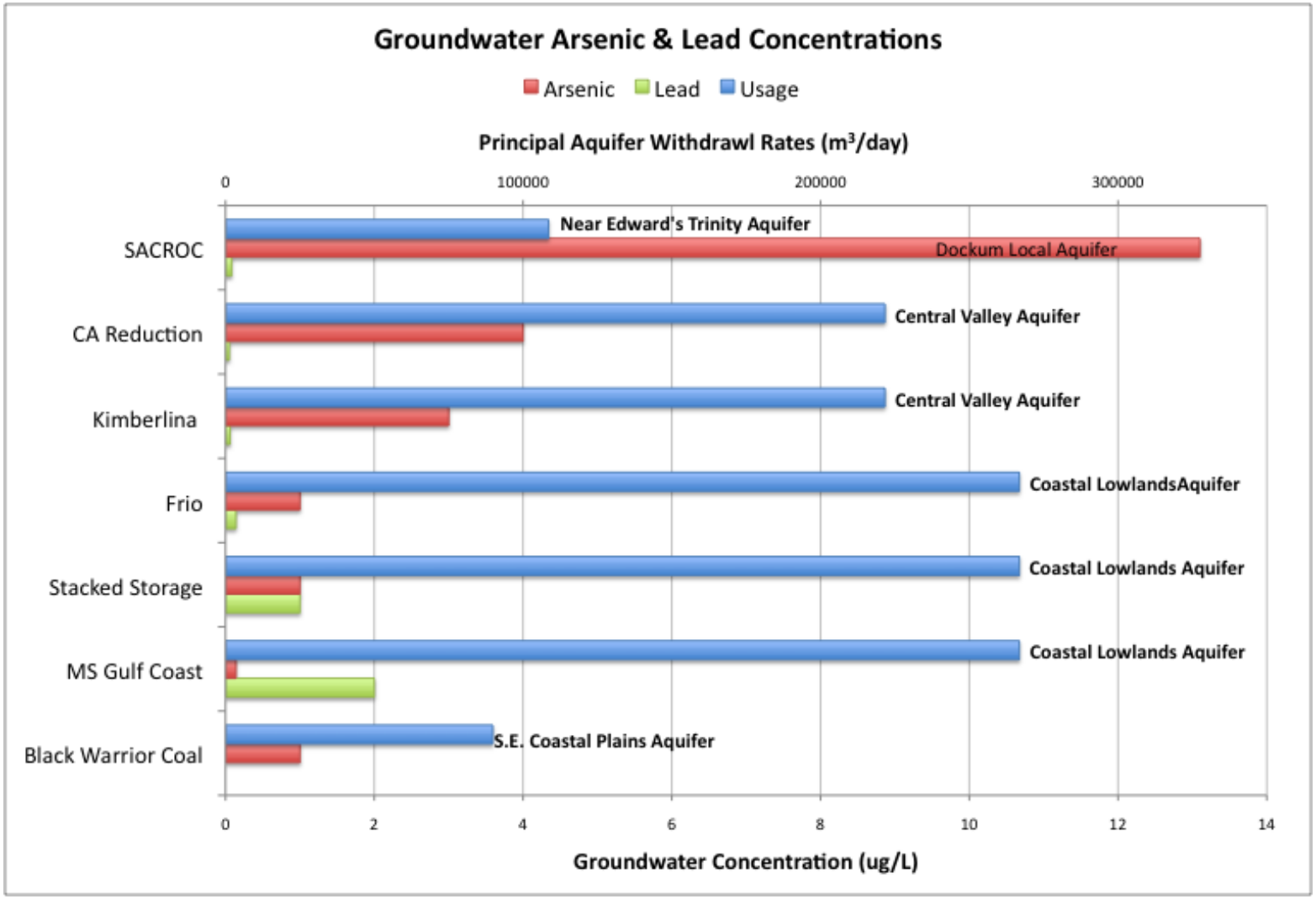
Aquifer usage
Indicator geochemistry
Mineralogy

IZ leakage pathways
Potential CO_2 reactions in IZ or caprock to release metals to brine

First Order Screening:
Principal Aquifer Withdrawals for Public Supply above Sequestration Pilot Sites

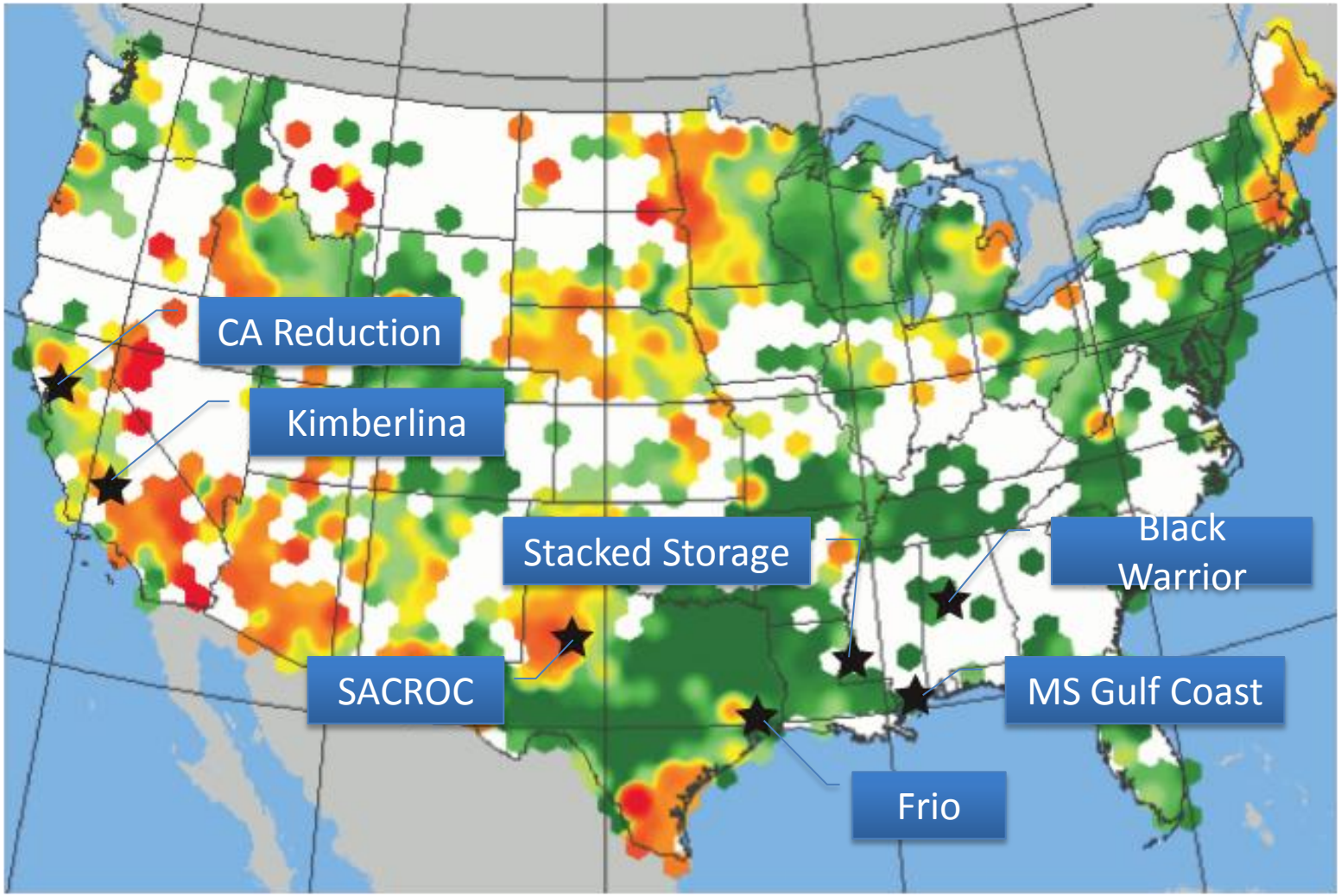


Second Order Screening:
Groundwater Metal Concentration as an Indicator of Availability



*Median groundwater concentrations from NWIS (USGS) data for wells within approximately 40km of the injection.

Sequestration + High Aquifer Use + Metals in Groundwater



Third Order Screening: Mineralogy

- Site specific mineralogy/geochemical studies from published literature

- Analysis of USGS National Geochemical Survey Database used to determine aquifer mineralogy from available surface sediment and grab samples. (Assumes reasonable correlation between subsurface source rock and surface weathered material).

Third Order Screening: Intermediate zone (IZ)

- Evaluate geology and structure of the IZ to assess potential for leakage.
- Specific geochemical/mineralogy studies in the literature
- Infer geochemical reaction potential and potential impacts on CO_2 stream from geologic descriptions.

What’s next?

- After screening, will choose aquifers to use as basis for modeling and experiments.
- Multiphase hydrochemical modeling to evaluate source zone and transport, and to inform 2 D experiments
- Batch experiments to quantifyrelevant reactions
- Confirmatory 2-D experiments in heterogeneous media.
- Identify important processes, incorporate into particle flow and stream tube models
- Develop risk assessment methodology
- Risk assessments should take some of the “fear” out of the potential impacts for GCS.

Questions?

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