Uncertainty Quantification for Geological Carbon Sequestration

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Workshop on "Opportunities and Challenges in Uncertainty Quantification for Complex Interacting systems"
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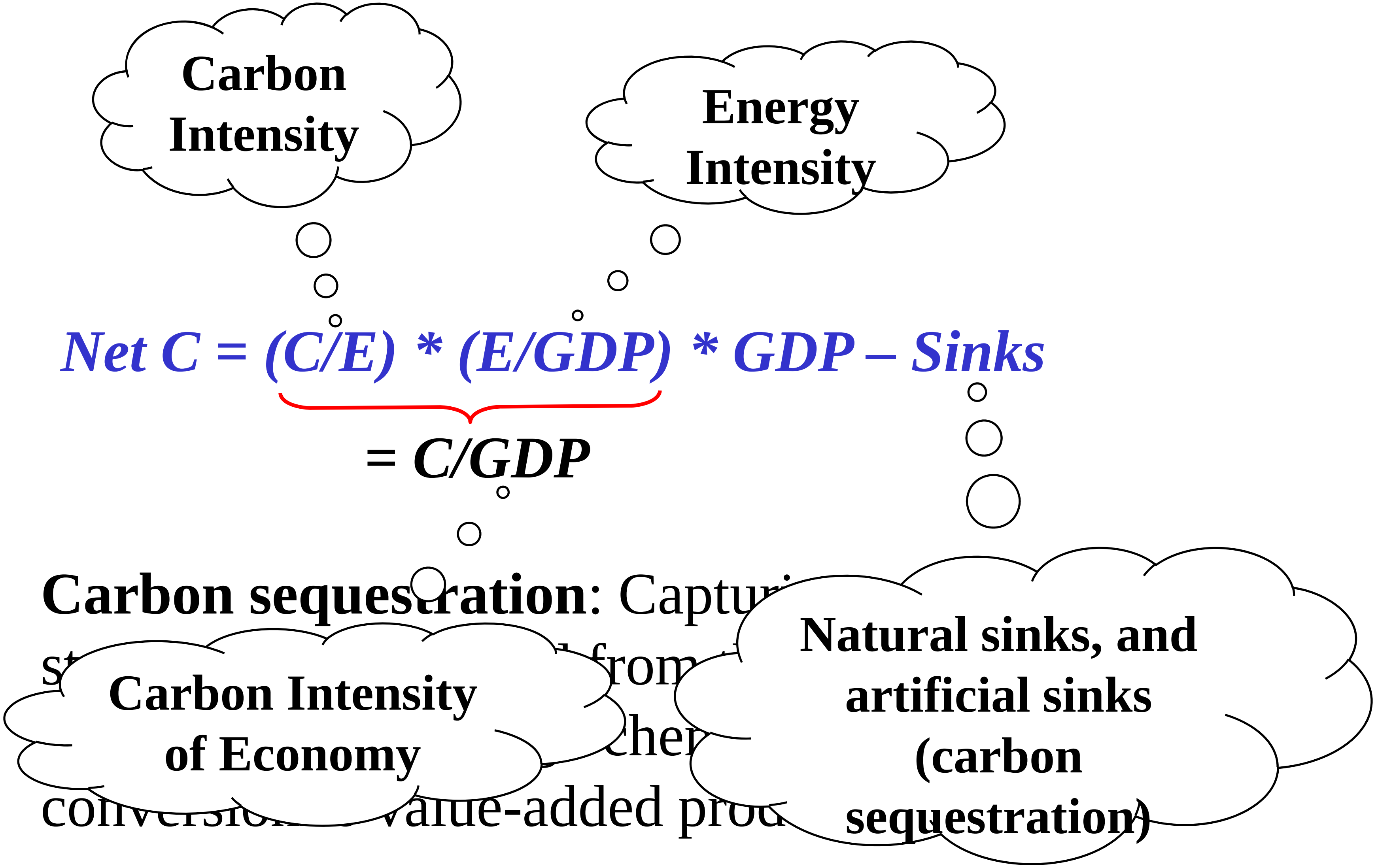
Carbon Management



Carbon Intensity

Energy Intensity

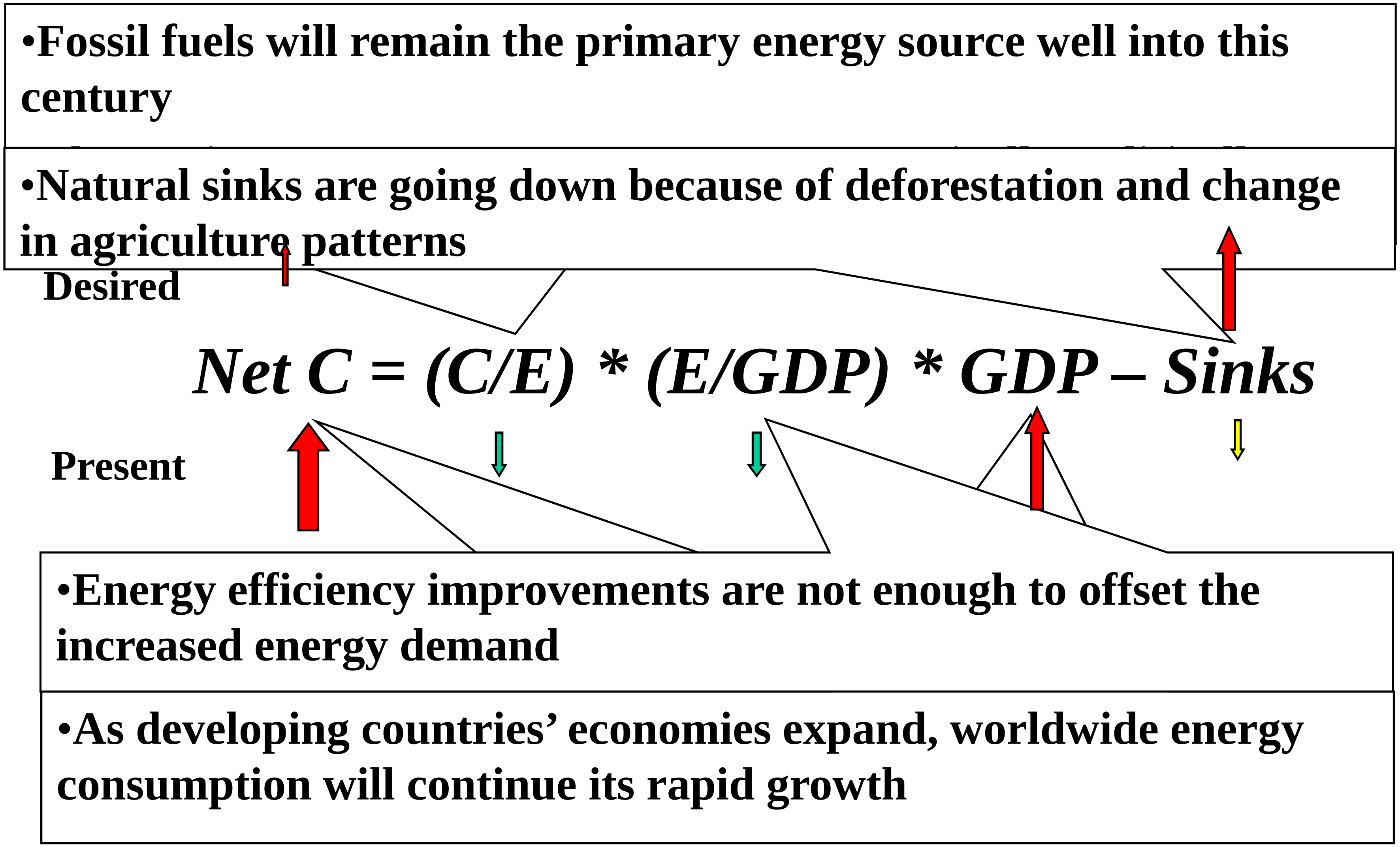
$$\text{Net C} = \underbrace{(C/E) * (E/GDP)}_{= C/GDP} * GDP - \text{Sinks}$$

Carbon sequestration: Captur
st from
chem
conversion value-added prod

Carbon Intensity of Economy

Natural sinks, and artificial sinks (carbon sequestration)

Carbon Sequestration is a MUST



- Fossil fuels will remain the primary energy source well into this century

- Natural sinks are going down because of deforestation and change in agriculture patterns

Desired

$$Net\ C = (C/E) * (E/GDP) * GDP - Sinks$$

Present

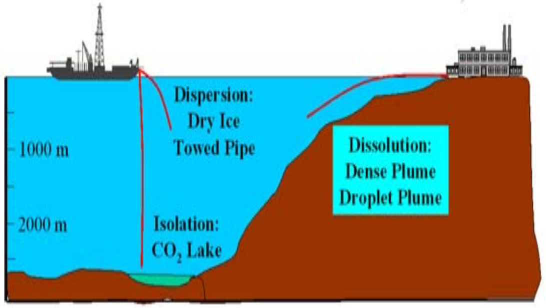
- Energy efficiency improvements are not enough to offset the increased energy demand

- As developing countries' economies expand, worldwide energy consumption will continue its rapid growth

Carbon Sequestration Approaches

- Ocean **(>1400 Gt Est. Capacity)**
  - Direct injection
  - Enhancement of natural processes
  - Largest capacity, but least understood

NEHLA Project at
Keahole Point, Hawaii



- Terrestrial **(>10 Gt Est. Capacity)**
  - Crops & land management
  - Soil improvement
  - C-species selection

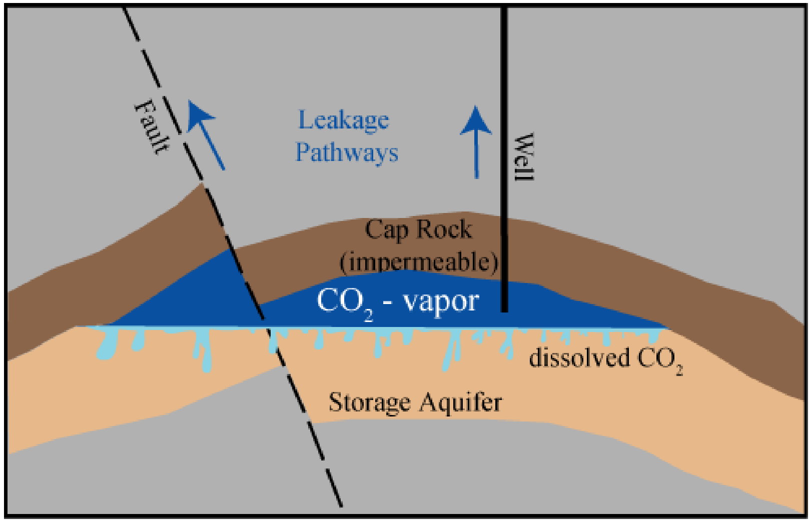
- Geologic **(>1000 Gt Est. Capacity)**
  - Oil & gas reservoirs
  - Deep saline aquifers
  - Unmineable coal beds

Geological Sequestration Presents a Viable Option

- Past experience
  - Recent: Natural gas storage, groundwater remediation
  - Century-long: Oil/gas production, groundwater resources management
  - Geological time: Natural CO_2 reservoirs (e.g., Bravo Dome, NM)
- Economic benefits that offset the cost of sequestration
  - Enhanced oil recovery from oil reservoirs
  - Increased gas production from natural gas reservoirs
  - Enhanced methane production from coal beds
- Worldwide availability and in close proximity of geological media to CO_2 sources

Basic Research Questions

- The science of geological sequestration is just starting
- Many R &D questions remain:
  - Capacity
  - Injectivity
  - Impact to reservoir
  - Caprock integrity
  - Leakage pathway and rate
  - Monitoring
  - Performance assessment
  - Risk assessment



EOR/EGR vs. Sequestration

- Although industrial EOR experiences exist, there are major differences between EOR and Sequestration:
  - The current EOR minimizes the amount of CO_2 used while the goal of seq. is to store as much CO_2 as possible
  - EOR is a short term process (of several years) while seq. is at the scale of 100s to 1000s years
  - Long term performance assessment required for sequestration --- EOR has an industrial experience of 40 years (still a short timeframe for seq.)
  - Higher-confidence predictive and monitoring tools are needed for sequestration
- New EOR strategies are needed if sequestration is the goal

Saline Aquifers

Features:

Viscous fingering

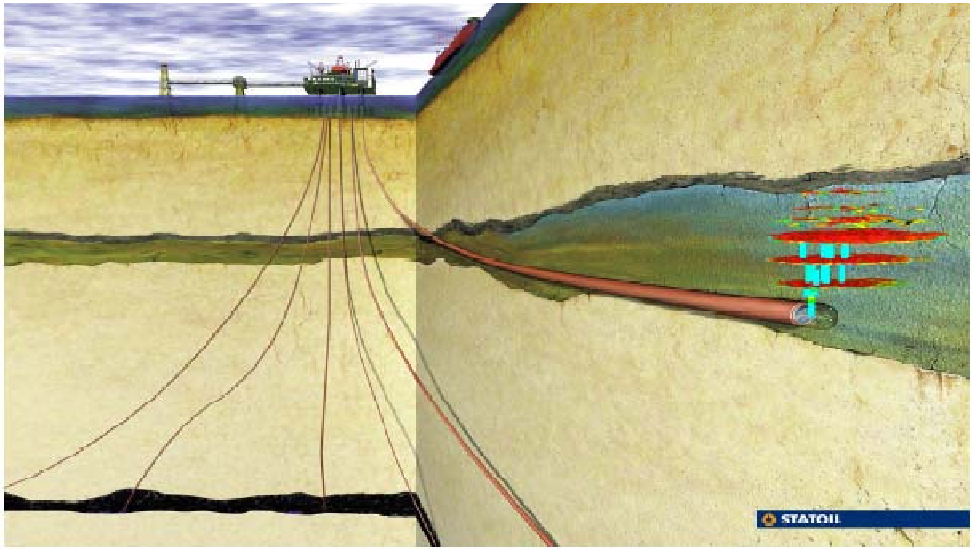
Gravity segregation

Capillary entrapment

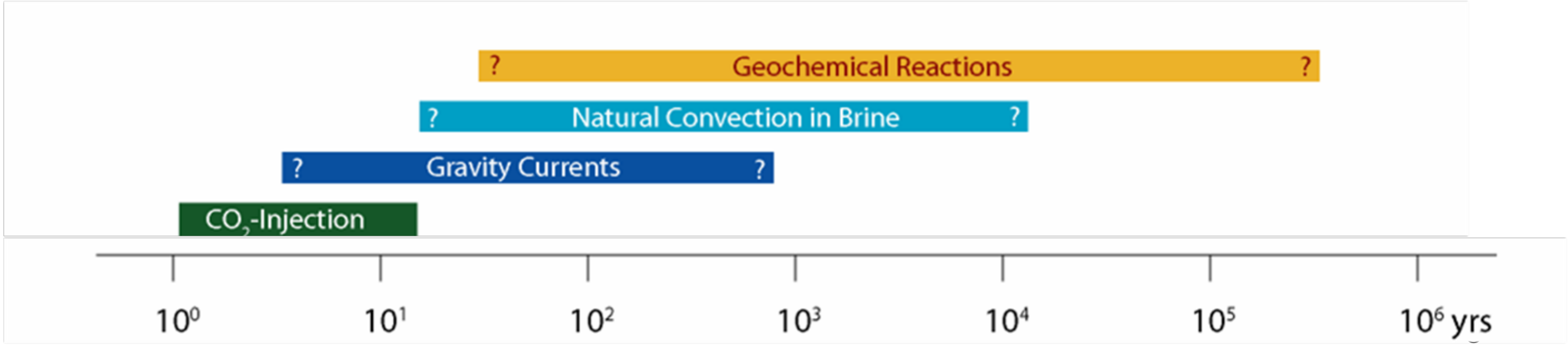
Convective mixing

Geochemistry

Sleipner CO2 Injection

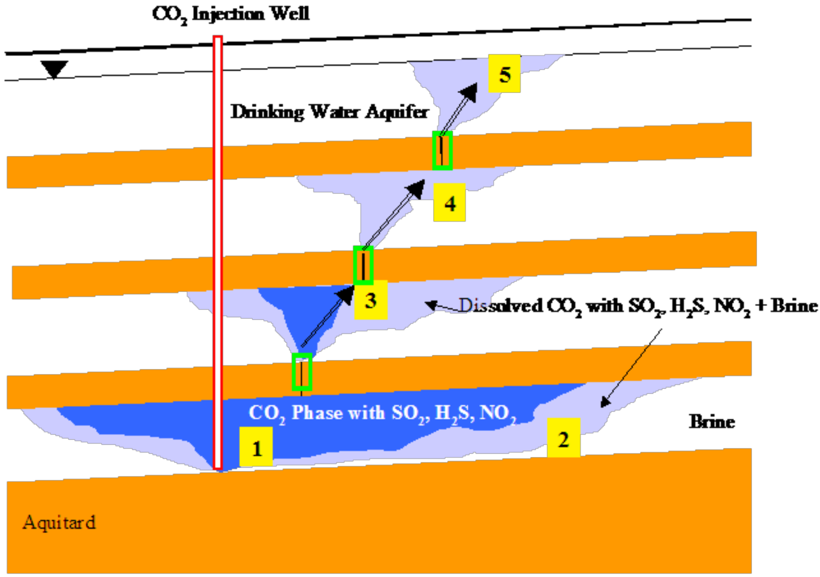


Time scale estimates



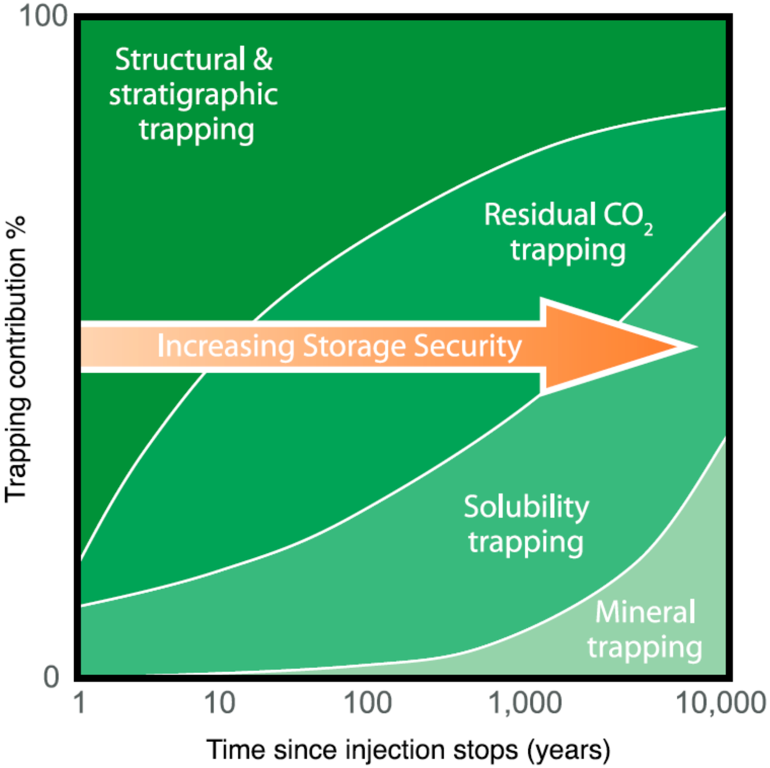
Complexities and Uncertainties

- A multiplicity of length scales
  - From atomistic and microscopic, to macroscopic and to field-scale
- Large timescale range of interest
  - From picoseconds to millennia
- Coupled processes
  - Fluid flow, geomechanics, geochemistry, and heat transfer
- Various components
  - Reservoir/aquifer, caprock, overburdens, faults, and wells
- Spatial variabilities and poor knowledge of them

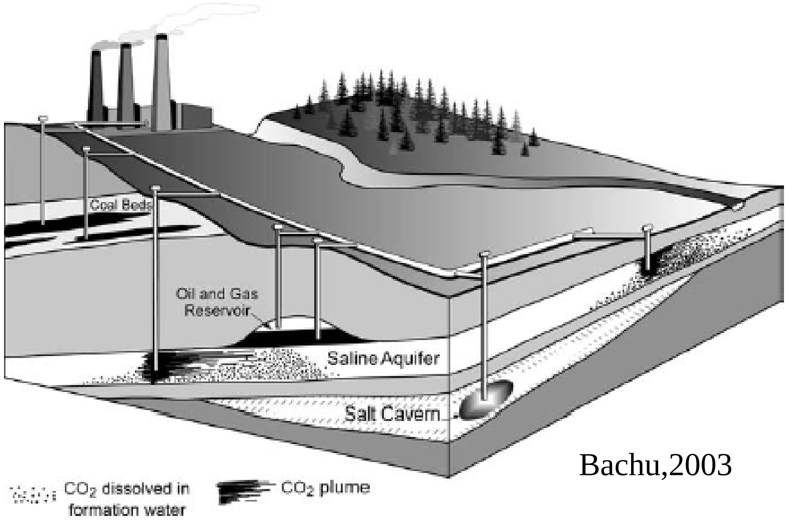


CO_2 Trapping Mechanisms

- Structural trapping
- Residual gas trapping
- Solubility trapping
- Mineral trapping



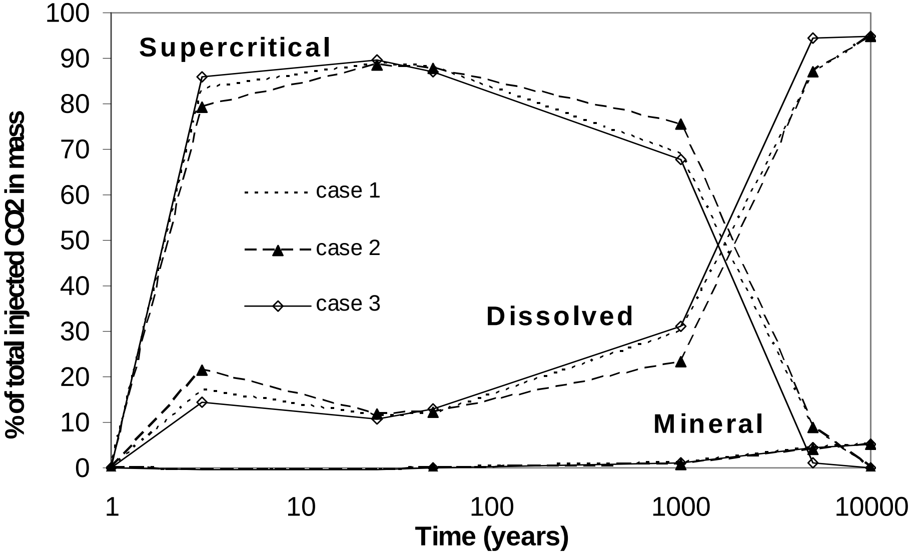
(2005 IPCC Special Report on Carbon Dioxide Capture and Storage; http://www.ipcc.ch/activity/srccs/index.htm)



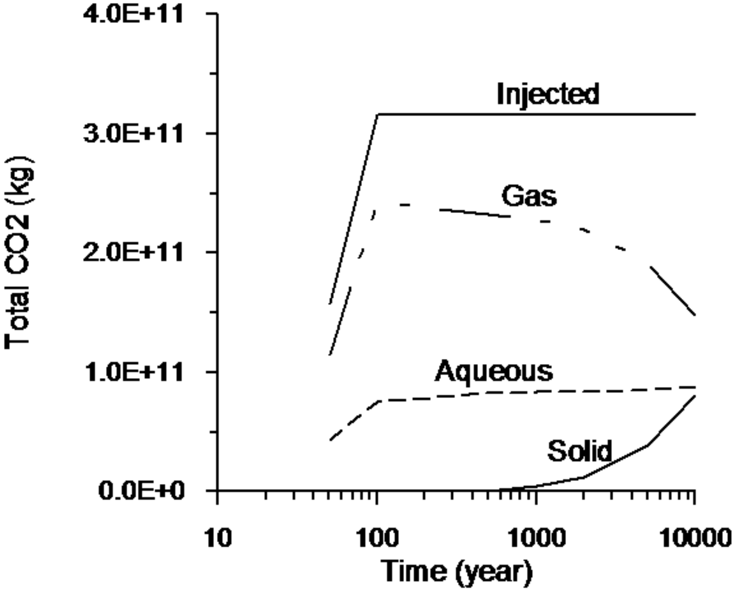
Bachu,2003

Fate of Injected CO_2

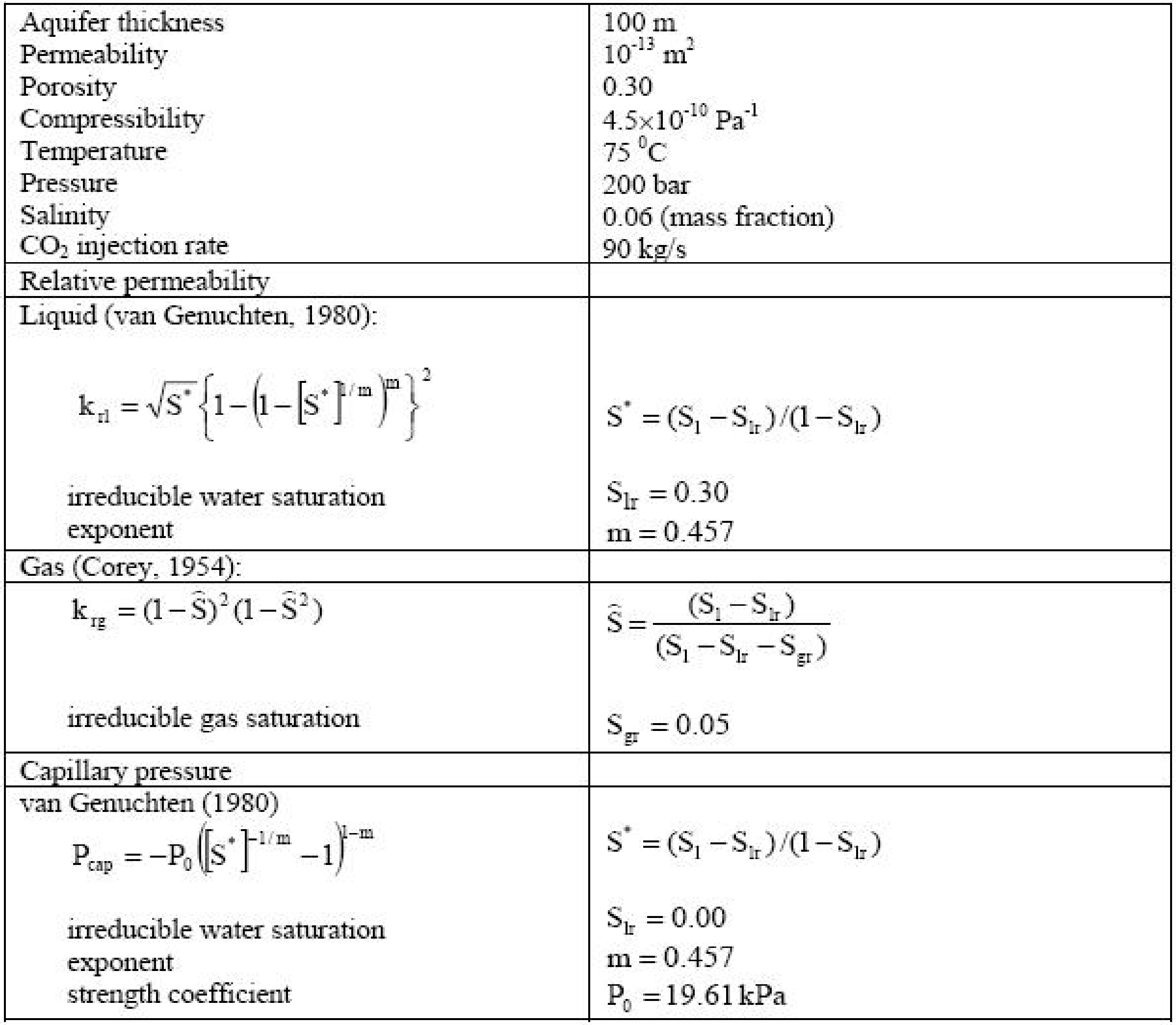
Sleipner (Audigane et al, 2007)



Gulf Coast Sandstone (Xu et al., 2003)



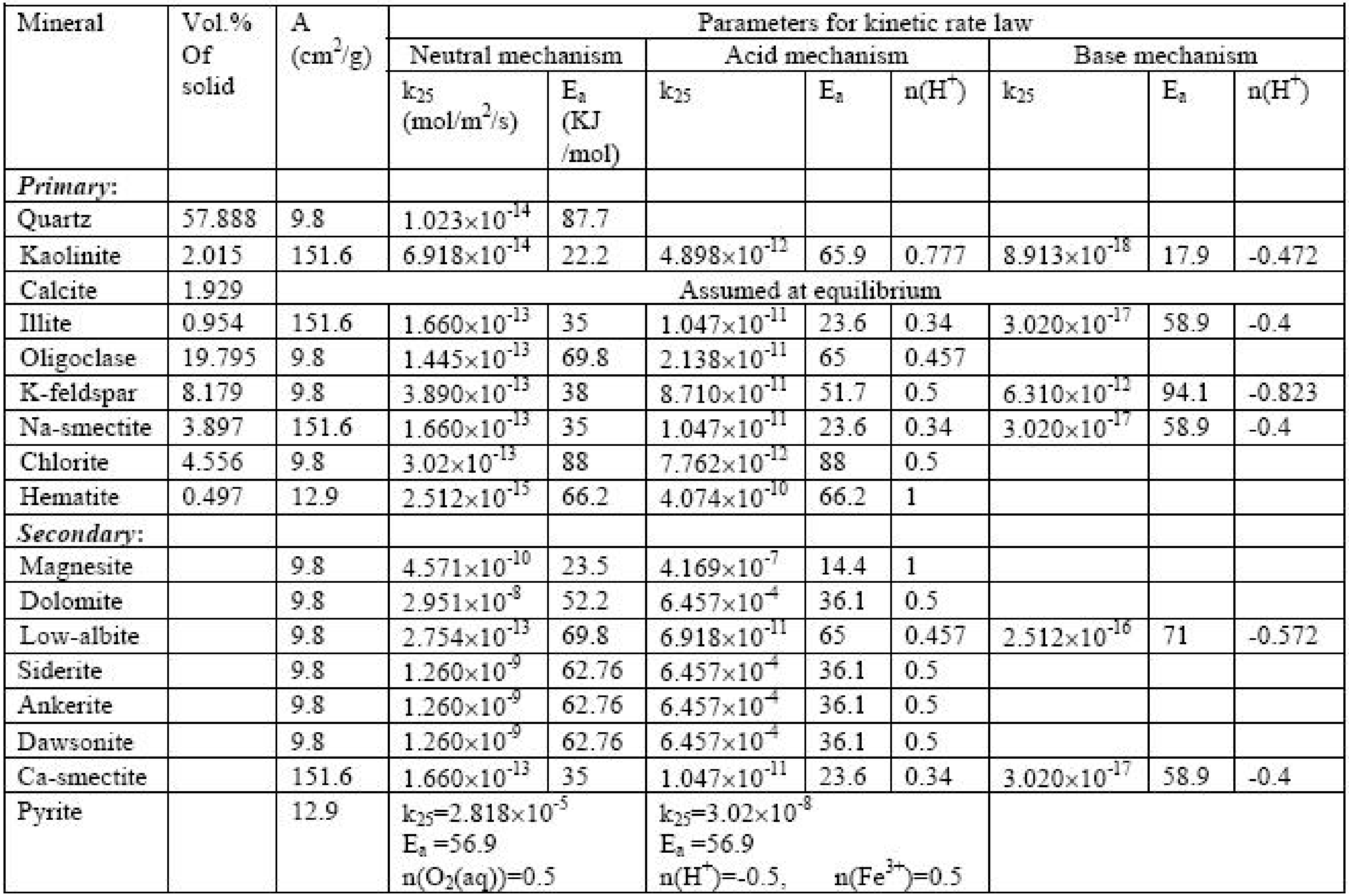
Hydrologic Properties



Aquifer thickness	100 m
Permeability	10^{-13} m^2
Porosity	0.30
Compressibility	4.5×10^{-10} Pa^{-1}
Temperature	75 ^{0}C
Pressure	200 bar
Salinity	0.06 (mass fraction)
CO_2 injection rate	90 kg/s
Relative permeability	
Liquid (van Genuchten, 1980):	
$k_{rl} = \sqrt{S^*}\left\{1-\left(1-\left[S^*\right]^{1/m}\right)^m\right\}^2$	$S^* = (S_l - S_{lr})/(1 - S_{lr})$
irreducible water saturation	$S_{lr} = 0.30$
exponent	$m = 0.457$
Gas (Corey, 1954):	
$k_{rg} = (1-\hat{S})^2(1-\hat{S}^2)$	$\hat{S} = \frac{(S_l - S_{lr})}{(S_l - S_{lr} - S_{gr})}$
irreducible gas saturation	$S_{gr} = 0.05$
Capillary pressure	
van Genuchten (1980)	
$P_{cap} = -P_0\left(\left[S^*\right]^{-1/m} - 1\right)^{1-m}$	$S^* = (S_l - S_{lr})/(1 - S_{lr})$
irreducible water saturation	$S_{lr} = 0.00$
exponent	$m = 0.457$
strength coefficient	$P_0 = 19.61$ kPa

Similar to Gulf Coast Sandstone (Xu et al., 2003)

Geochemical Properties



Mineral	Vol.% Of solid	A (cm^2/g)	Parameters for kinetic rate law							
			Neutral mechanism		Acid mechanism			Base mechanism		
			k_{25} ($mol/m^2/s$)	E_a (KJ /mol)	k_{25}	E_a	$n(H^+)$	k_{25}	E_a	$n(H^+)$
Primary:										
Quartz	57.888	9.8	1.023×10^{-14}	87.7						
Kaolinite	2.015	151.6	6.918×10^{-14}	22.2	4.898×10^{-12}	65.9	0.777	8.913×10^{-18}	17.9	-0.472
Calcite	1.929	Assumed at equilibrium								
Illite	0.954	151.6	1.660×10^{-13}	35	1.047×10^{-11}	23.6	0.34	3.020×10^{-17}	58.9	-0.4
Oligoclase	19.795	9.8	1.445×10^{-13}	69.8	2.138×10^{-11}	65	0.457			
K-feldspar	8.179	9.8	3.890×10^{-13}	38	8.710×10^{-11}	51.7	0.5	6.310×10^{-12}	94.1	-0.823
Na-smectite	3.897	151.6	1.660×10^{-13}	35	1.047×10^{-11}	23.6	0.34	3.020×10^{-17}	58.9	-0.4
Chlorite	4.556	9.8	3.02×10^{-13}	88	7.762×10^{-12}	88	0.5			
Hematite	0.497	12.9	2.512×10^{-15}	66.2	4.074×10^{-10}	66.2	1			
Secondary:										
Magnesite		9.8	4.571×10^{-10}	23.5	4.169×10^{-7}	14.4	1			
Dolomite		9.8	2.951×10^{-8}	52.2	6.457×10^{-4}	36.1	0.5			
Low-albite		9.8	2.754×10^{-13}	69.8	6.918×10^{-11}	65	0.457	2.512×10^{-16}	71	-0.572
Siderite		9.8	1.260×10^{-9}	62.76	6.457×10^{-4}	36.1	0.5			
Ankerite		9.8	1.260×10^{-9}	62.76	6.457×10^{-4}	36.1	0.5			
Dawsonite		9.8	1.260×10^{-9}	62.76	6.457×10^{-4}	36.1	0.5			
Ca-smectite		151.6	1.660×10^{-13}	35	1.047×10^{-11}	23.6	0.34	3.020×10^{-17}	58.9	-0.4
Pyrite		12.9	$k_{25}=2.818\times10^{-5}$ $E_a=56.9$ $n(O_2(aq))=0.5$		$k_{25}=3.02\times10^{-8}$ $E_a=56.9$ $n(H^+)=-0.5$, $n(Fe^{3+})=0.5$					

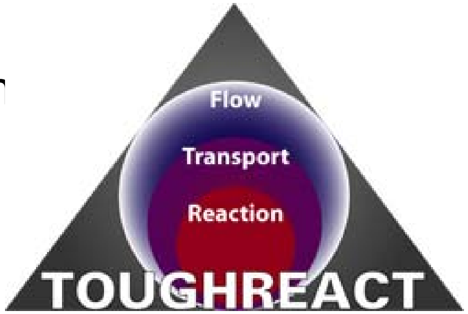
LBNL Simulator TOUGHREACT

Processes:

- Multiphase fluid and heat flow: TOUGH2 V2 (Pruess, et al., 1999)
- Transport: advection and diffusion in both liquid and gas phases
- Chemical reactions:
  - Aqueous complexation
  - Acid-base
  - Redox
  - Mineral dissol./precip. (equilibrium and/or kinetics)
  - Gas dissol./exsol.
  - Cation exchange
  - Surface complexation
  - Linear Kd adsorption
  - Decay

Features:

- Changes in porosity and permeability, and unsaturated zone properties due to mineral diss./ppt. and clay swelling
- Gas phase and gaseous species are active in flow, transport, and reaction
- General: Porous and fractured media; 5 ϕ-k models; rate laws; any number of chemical species
- Wide range of conditions: P, T, pH, Eh, Salinity
- http://esd.lbl.gov/TOUGHREACT/
- (Xu et al., 2004)



TOUGHREACT (2)

Equations for fluid and heat flow, and chemical transport.

General governing equations: $\frac{\partial M_\kappa}{\partial t} = -\nabla F_\kappa + q_\kappa$

Water: $M_w = \phi(S_l \rho_l X_{wl} + S_g \rho_g X_{wg})$ $\quad F_w = X_{wl}\rho_l u_l + X_{wg}\rho_g u_g$ $\quad q_w = q_{wl} + q_{wg}$

Air: $M_a = \phi(S_l \rho_l X_{al} + S_g \rho_g X_{ag})$ $\quad F_a = X_{al}\rho_l u_l + X_{ag}\rho_g u_g$ $\quad q_a = q_{al} + q_{ag}$

Heat: $M_h = \phi(S_l \rho_l U_l + S_g \rho_g U_g) + (1-\phi)\rho_s U_s$ $\quad F_h = \sum_{\beta=l,g} h_\beta \rho_\beta u_\beta - \lambda \nabla T$ $\quad q_h$

where $u_\beta = -k \frac{k_{r\beta}}{\mu_\beta}(\nabla P_\beta - \rho_\beta g)$ $\quad \beta = l, g$ (Darcy's Law)

Chemical components in the liquid phase ($j = 1, 2, \ldots, N_l$):

$M_j = \phi S_l C_{jl}$ $\quad F_j = u_l C_{jl} - D_l \nabla C_{jl}$ $\quad q_j = q_{jl} + q_{js} + q_{jg}$

Chemical components in the gas phase ($k = 1, 2, \ldots, N_g$):

$M_k = \phi S_l C_{kl}$ $\quad F_k = u_{gl} C_{kg} - D_g \nabla C_{kg}$ $\quad q_k = -q_{jg}$

where $C_{kg} = f_{kg}/RT$ (gas law)

Example of chemical reaction equations

General dissociation reactions $\quad S_i^s = \sum_{j=1}^{N_C} \nu_{ij} S_j^p$

(1) General mass action equations: $\quad K_i a_{S_i^s} = \sum_j^{N_C} (a_{S_j^p})^{\nu_{ij}}$

Aqueous dissociation: $HCO_3^- = CO_3^{2-} + H^+$ $\quad K_{HCO_3^-} \gamma_{HCO_3^-} c_{HCO_3^-} = \gamma_{CO_3^{2-}} c_{CO_3^{2-}} \gamma_{H^+} c_{H^+}$

Mineral dissolution: $CaCO_3(s) = CO_3^{2-} + Ca^{2+}$ $\quad K_{CaCO_3(s)} = \gamma_{Ca^{2+}} c_{Ca^{2+}} \gamma_{CO_3^{2-}} c_{CO_3^{2-}}$

Gas dissolution: $CO_2(g) = CO_2(aq)$ $\quad K_{CO_2(g)} f_{CO_2(g)} = \gamma_{CO_2(aq)} c_{CO_2(aq)}$

(2) Rate expressions: $\quad R_m = \sigma_m k_m (1 - \Omega_m^q)^p$ $\quad$ negative for precipitation

Calcite dissolution rate (first order): $\quad r_{CaCO_3(s)} = k_{CaCO_3(s)} A \left(1 - \frac{Q_{CaCO_3(s)}}{K_{CaCO_3(s)}}\right)$

$Q_{CaCO_3(s)} = \gamma_{Ca^{2+}} c_{Ca^{2+}} \gamma_{CO_3^{2-}} c_{CO_3^{2-}} = K_{CaCO_3(s)}$ at equilibrium

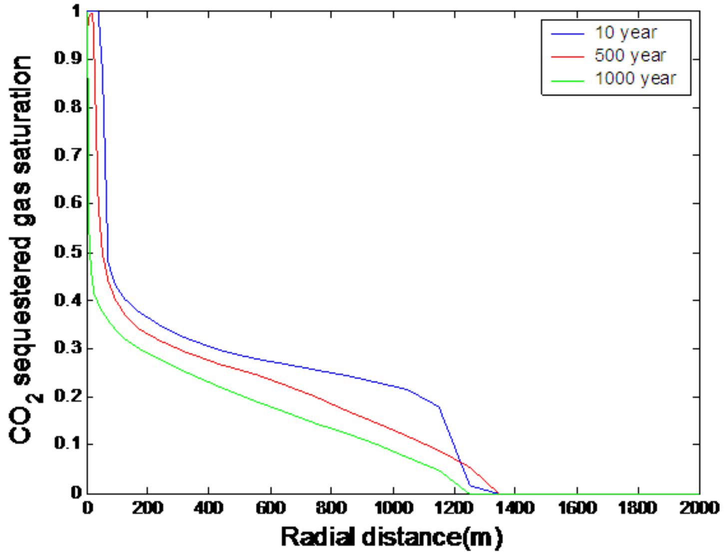
(3) Conservation of chemical component in a closed chemical system:

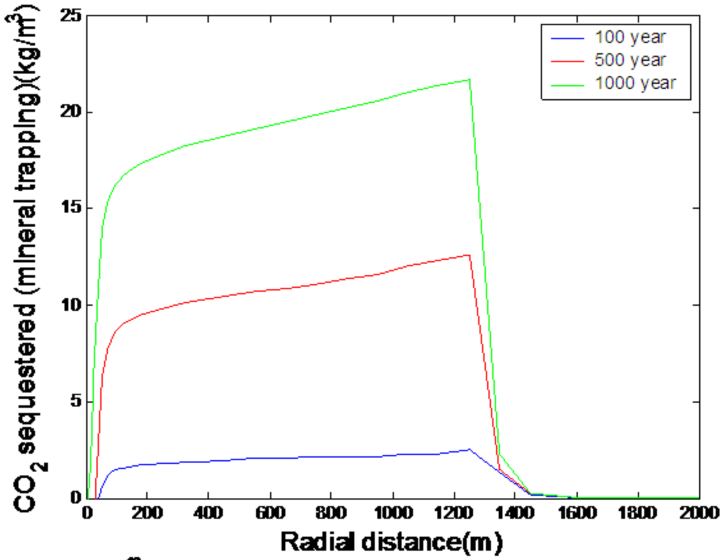
Carbonate component CO_3^{2-}: $\quad T_{CO_3^{2-}} = C_{CO_3^{2-}} + c_{CO_2(g)} + c_{CaCO_3(s)}$

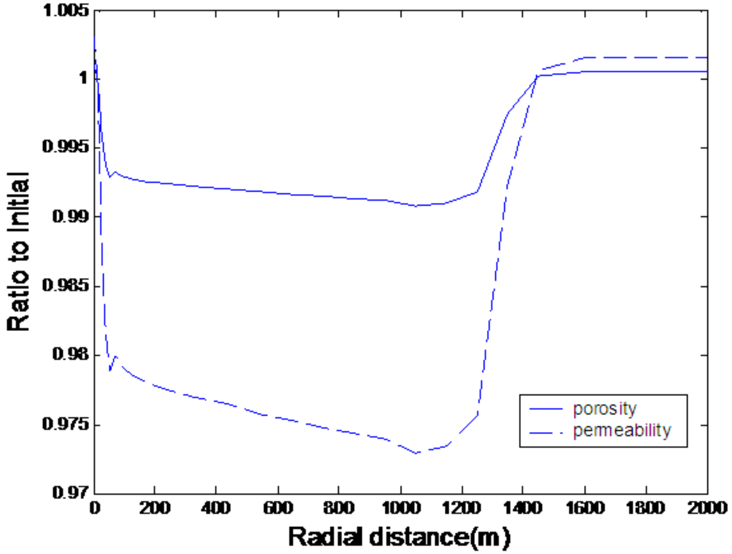
where $C_{CO_3^{2-}} = c_{CO_3^{2-}} + c_{HCO_3^{2-}} + c_{CO_2(aq)}$ (total dissolved, subject to transport)

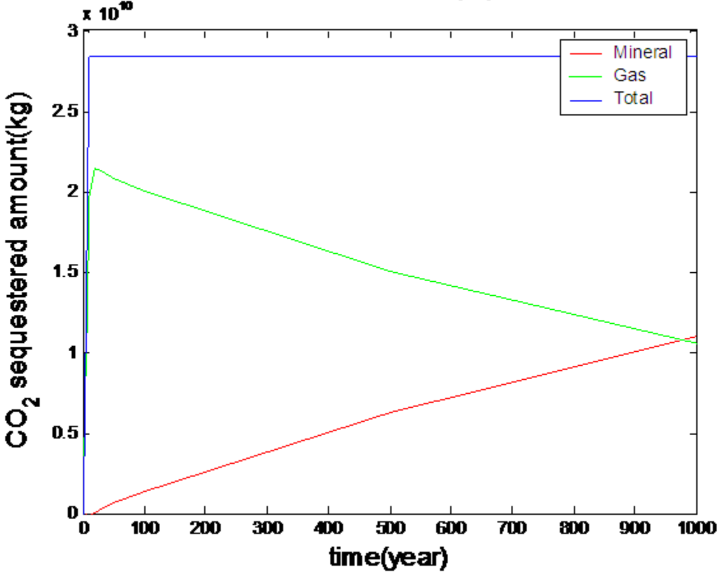
TOUGHREACT Simulation Results

Heli Bao, USC

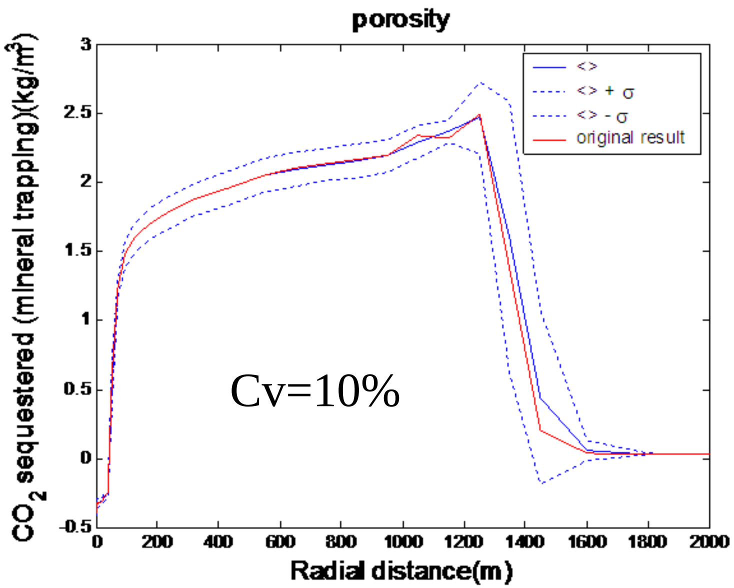


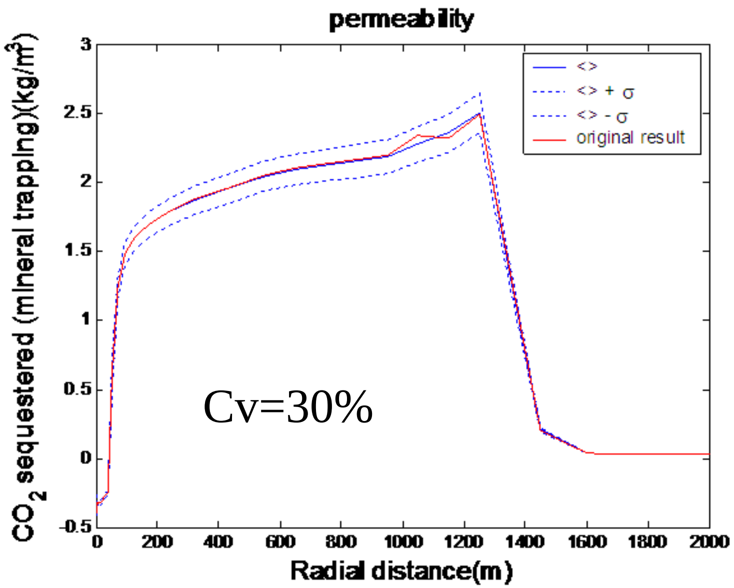


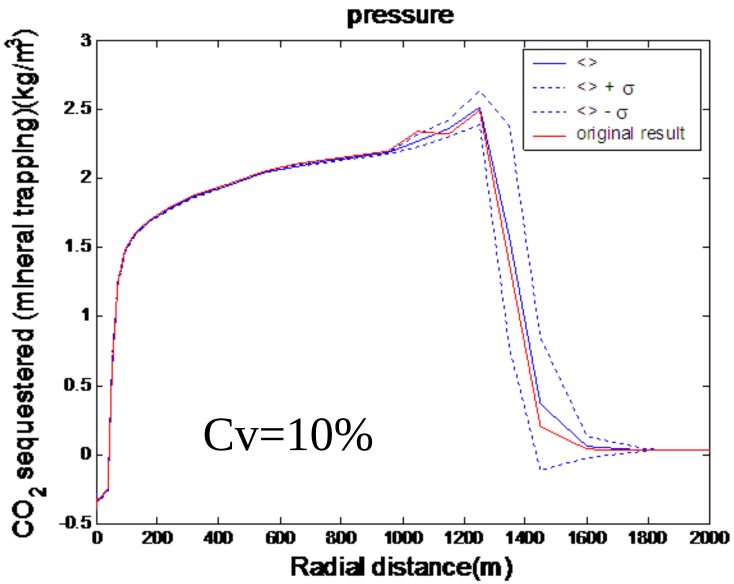


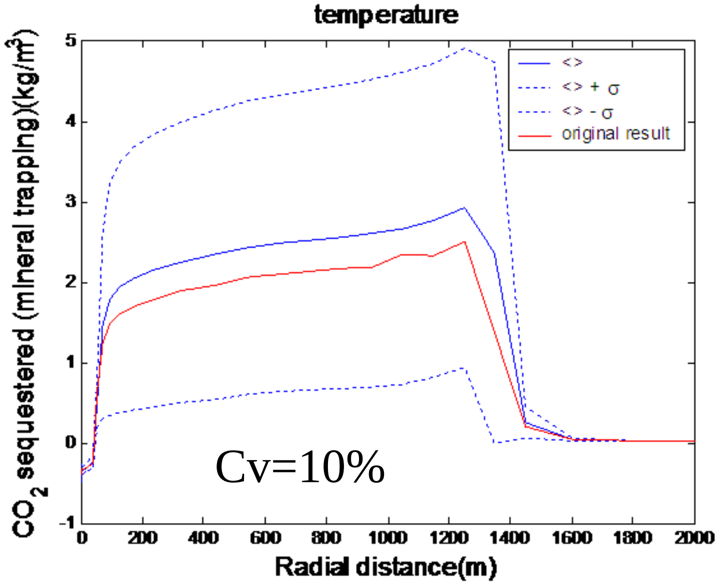


Effects of Variability: Single Parameter



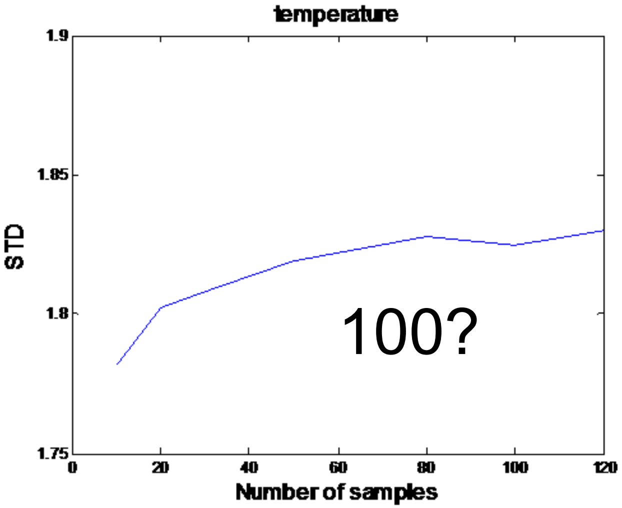


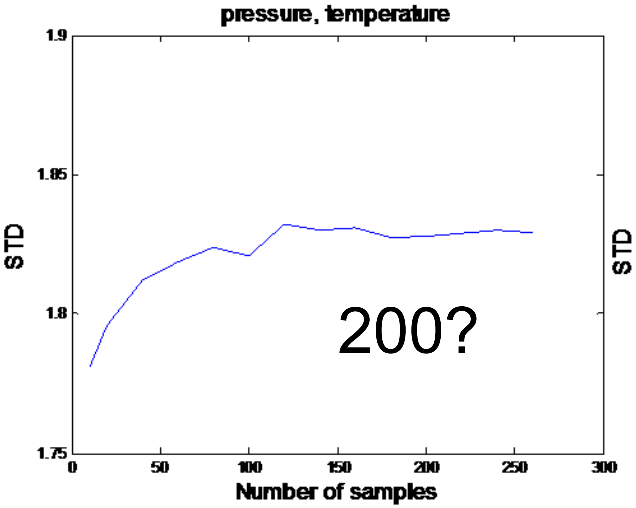


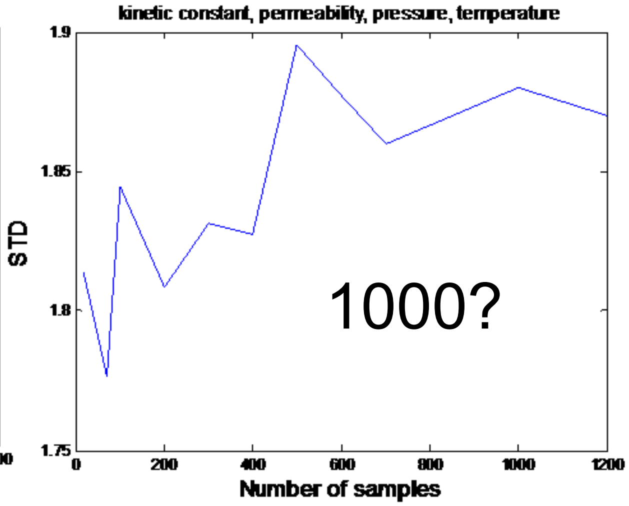


Effects of Variability: Multiple Parameters (1)

The number of Latin Hypercube samples needed to obtain stable variance of sequestered CO_2:



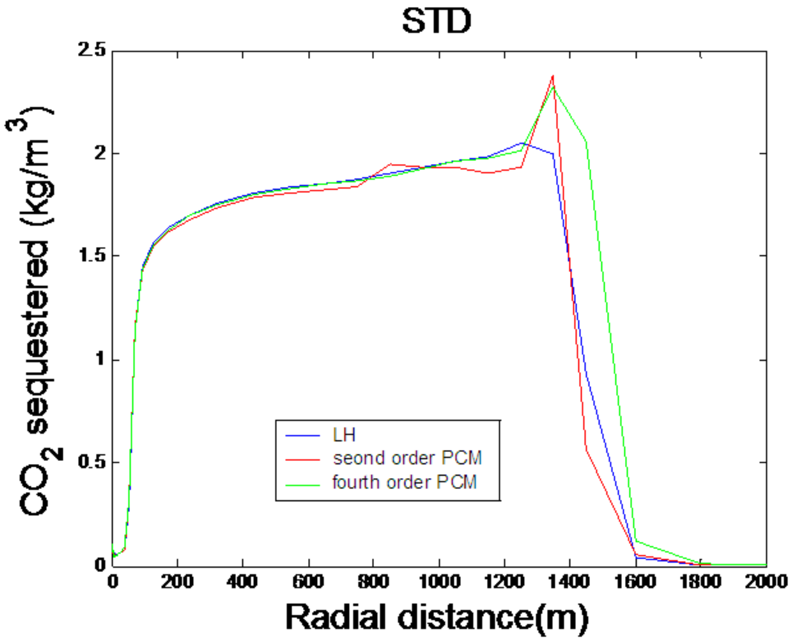




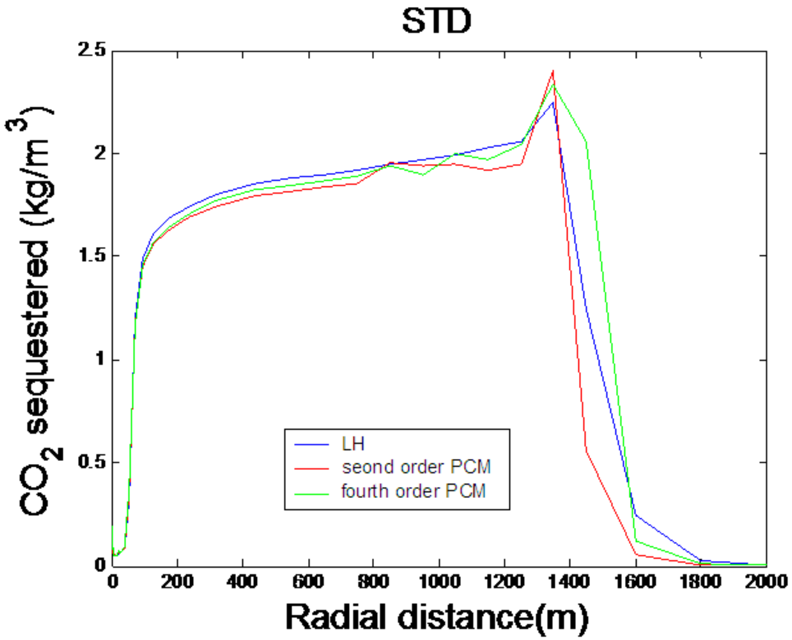
Questions:

How many samples are needed for 10s -100s parameters?
LHS or direct sampling MC?
How do the uncertainties interact among them?

Effects of Variability: Multiple Parameters (2)



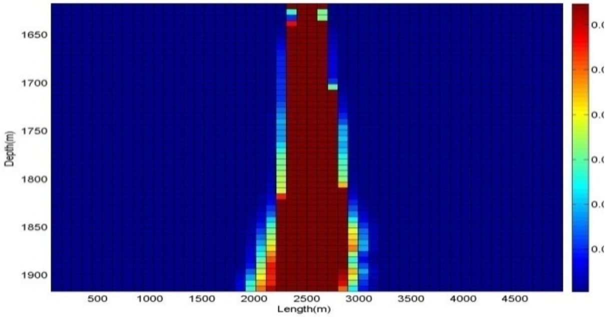
P, T: Cv=10%
LH: 200 runs
PCM-2nd: 6 runs
PCM-4th: 15 runs



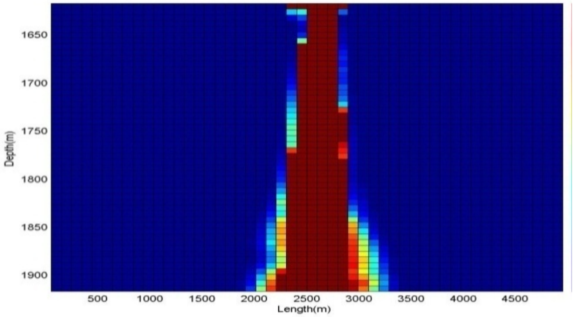
$K_{Chlorite}$, P, T, k: Cv=10%
LH: 1000 runs
PCM-2nd: 15 runs
PCM-4th: 70 runs

LH: Latin Hypercube sampling
PCM: Probabilistic Collocation Method (Li and Zhang, 2007)

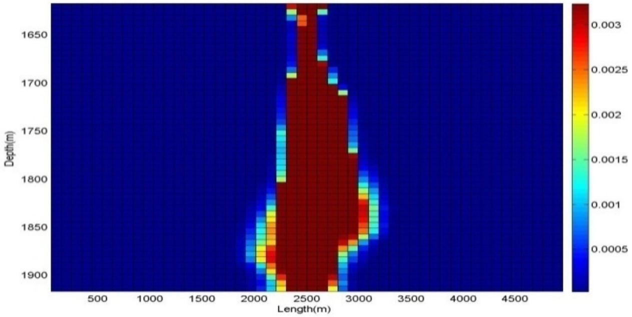
Plumes and Averages



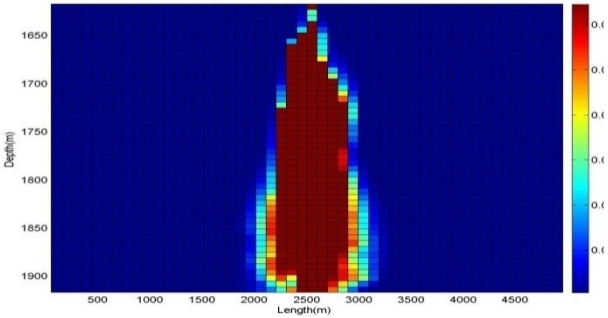
Sample 1



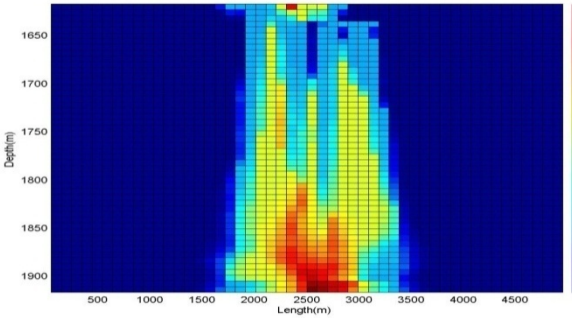
Sample 2



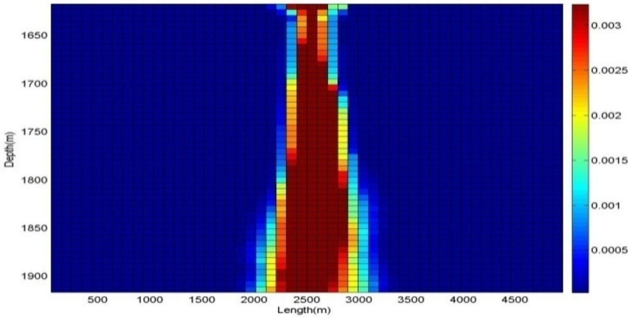
Sample 3



Sample 4



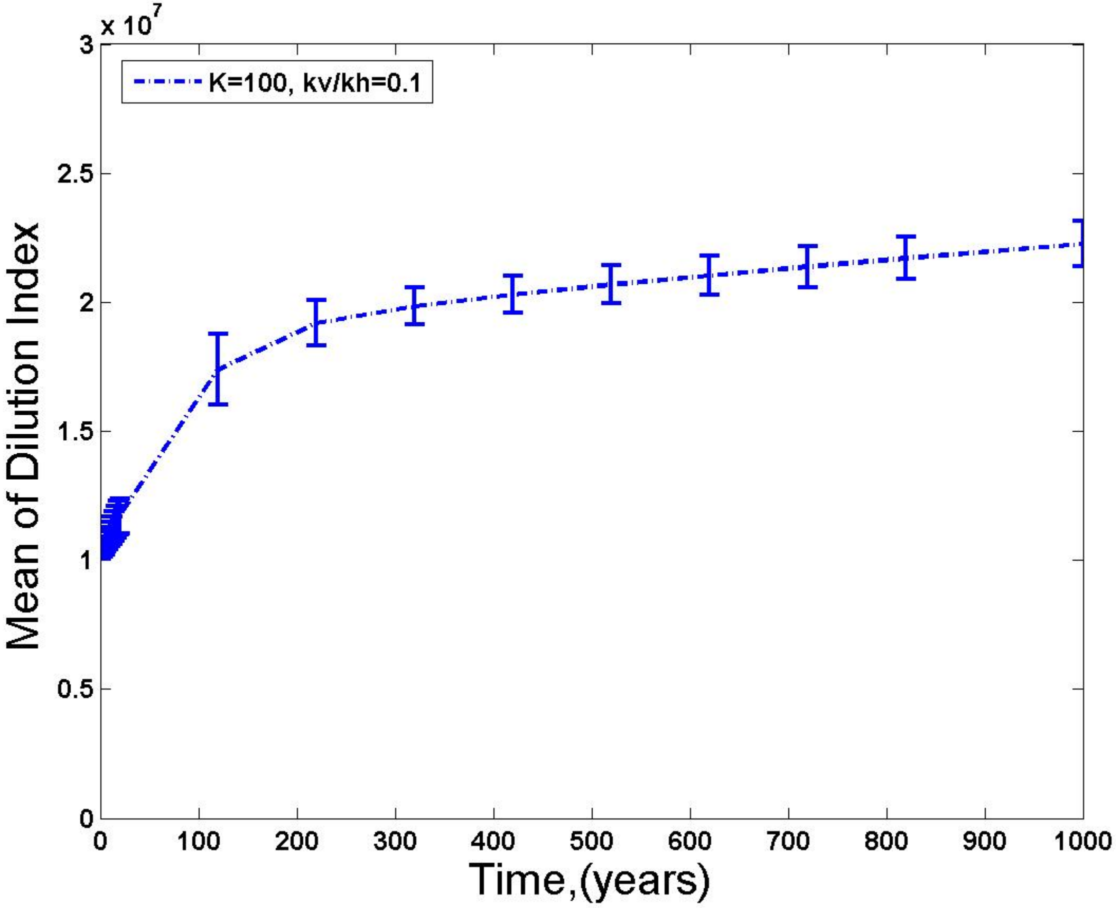
Absolute Dispersion Averaging



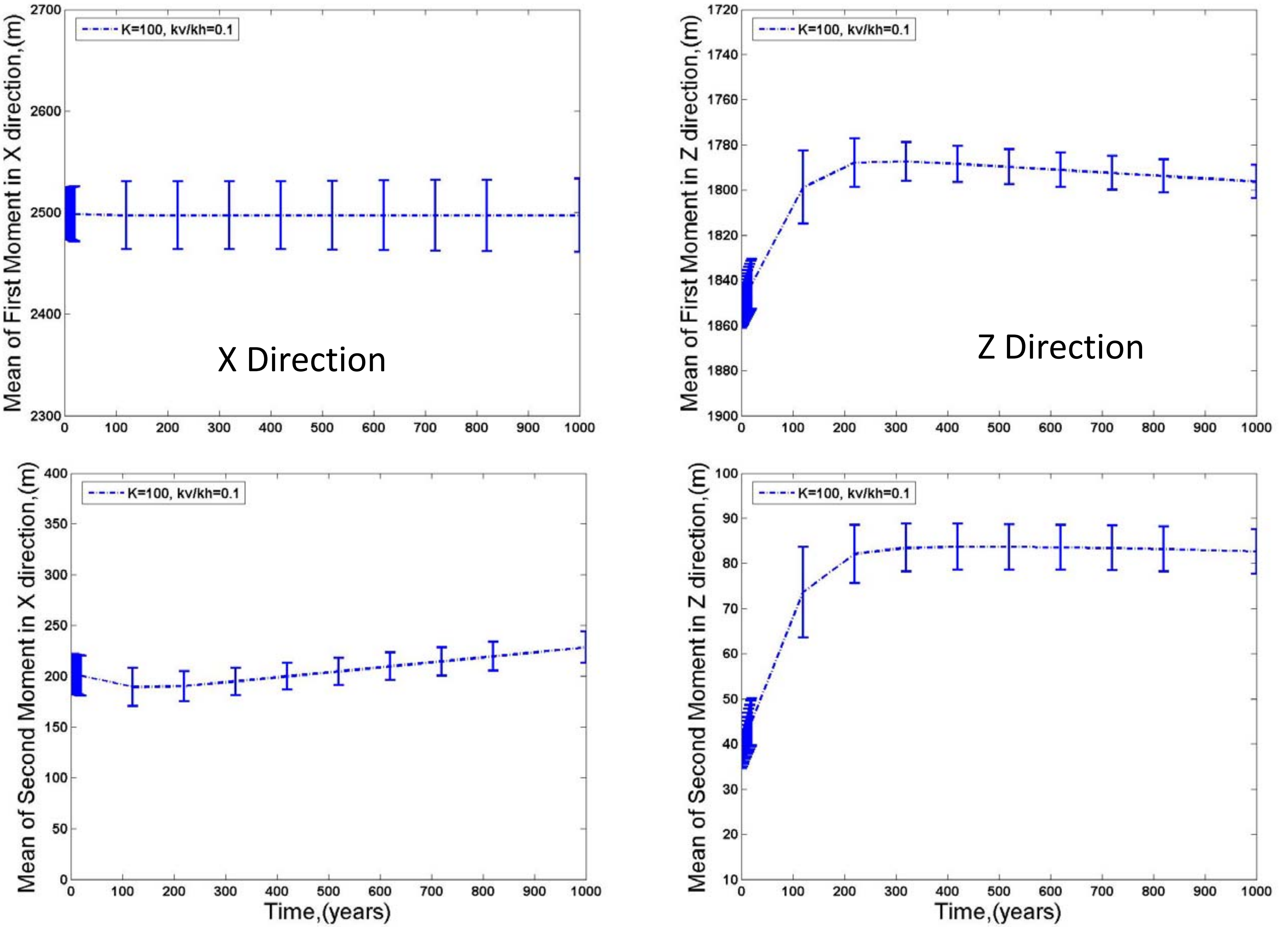
Relative Dispersion Averaging

Hamid Jahangiri, USC

Dilution Index



Spatial Moments



Challenges in Uncertainty Quantification for GCS

- Multiscale and multiphysics
- Highly nonlinear
- Time consuming for each simulation
  - **CPU: Several minutes to several days for each**
- Multiple parameters
  - 10s to 100s
  - Various distributions
  - Some being random fields
    - Approximations with finite dimensionality (N)
    - N could be 100s or 1000s (when with multiple fields)
    - MC or PCE: $M=(N+d)!/(N!\ d!)$ (d - order of polynomials)?

Key Ingredients for Viable UQ Approaches

- Accurate and robust
- Efficient, in particular, for large-scale problems
- Compatible with existing simulators
    - ✓ Non-intrusive

Summary

- Geological sequestration presents an **immediate, low-cost** option for carbon management.
- Carbon sequestration is an important measure for sustaining fossil fuel based economy.
- In spite of past experiences, many fundamental R&D issues are outstanding:
  - Prediction under uncertainties: Development, validation, and verification
  - Monitoring and verification technologies
  - Performance and risk assessment
  - Public awareness and acceptance
- The field of carbon sequestration is still in its infancy --- providing ample research opportunities