

Coupled Reactive Flow and Transport Modeling of CO₂ Sequestration in the Mount Simon Sandstone Formation, Midwest, USA*

Faye Liu¹, Peng Lu², Chen Zhu², and Yitian Xiao³

Search and Discovery Article #80169 (2011)

Posted July 18, 2011

*Adapted from oral presentation at AAPG Annual Convention and Exhibition, Houston, Texas, USA, April 10-13, 2011

¹Geological Sciences, Indiana University, Bloomington, IN (liu60@indiana.edu; eefaye0728@hotmail.com)

²Geological Sciences, Indiana University, Bloomington, IN

³ExxonMobil Upstream Research Company, Houston, TX

Abstract

Multi-phase reactive flow and transport modeling is an effective tool for monitoring, verification, and accounting of CO₂ sequestration in deep geological formations. In the current study, modeling is performed to simulate large scale CO₂ injection (a million tons per year for 100 years) into Mt. Simon sandstone, a major candidate saline reservoir in the Midwest of USA. The long term fate of CO₂ was simulated by extending the modeling period to 10,000 years. The results indicate that most of the injected CO₂ remains within a radius of 3300 m lateral distribution. Four major trapping mechanisms and their spatial and temporal variations are evaluated in our simulations: hydrodynamic, solubility, residual, and mineral trapping. A strongly acidified zone (pH 3-5) forms in the areas affected by the injected CO₂ (0 - 3300 m), and consequently causes extensive mineral precipitation and dissolution. The predicted long-term fate of CO₂ is closely linked to the geochemical reactions conceptualized in the models. In our model, the replenishing upstream water continues to dissolve CO₂ long after the injection, which results in total dissolution of hydrodynamically trapped CO₂ at the end of 10,000 years. In contrast, most previous models neglected the regional flow after injection and hence artificially limited the extent of geochemical reactions as if in a batch system. Consequently, a supercritical CO₂ plume (hydrodynamic trapping) would persist after 10,000 years. The continued supply of acidified water from interaction between replenishing water and CO₂ also results in extensive dissolution of feldspars and precipitation of secondary clay minerals, to a much more extent than what predicted in models without including regional flow. However, the prediction of complete dissolution of feldspars in 10,000 years can also result from the artifact that the linear rate laws are used in our model (as well as all previous work), which overestimates the rates of feldspar dissolution near equilibrium. Nevertheless, our simulations indicate the prolonged existence of an acidic brine plume, which suggests long-term risk assessment should transfer from the primary risk of CO₂ leakage to secondary risk of acidic plume leakage after all CO₂ is dissolved.

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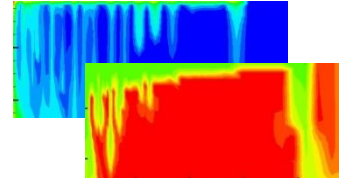
Liu, F.Y., P. Lu, C. Zhu, and Y.T. Xiao, 2011, Coupled reactive flow and transport modeling of CO₂ sequestration in the Mt. Simon sandstone formation, Midwest USA: International Journal of Greenhouse Gas control, v. 5/2, p. 294-307.

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AAPG, 2011



Coupled Reactive Flow and Transport Modeling of CO₂ Sequestration in the Mt. Simon Sandstone Formation, Midwest, U.S.A.

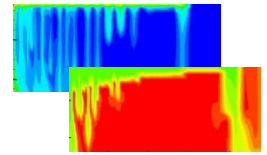
Faye Liu, Peng Lu, Chen Zhu, Indiana University

Yitian Xiao, ExxonMobil

April 13rd, 2011



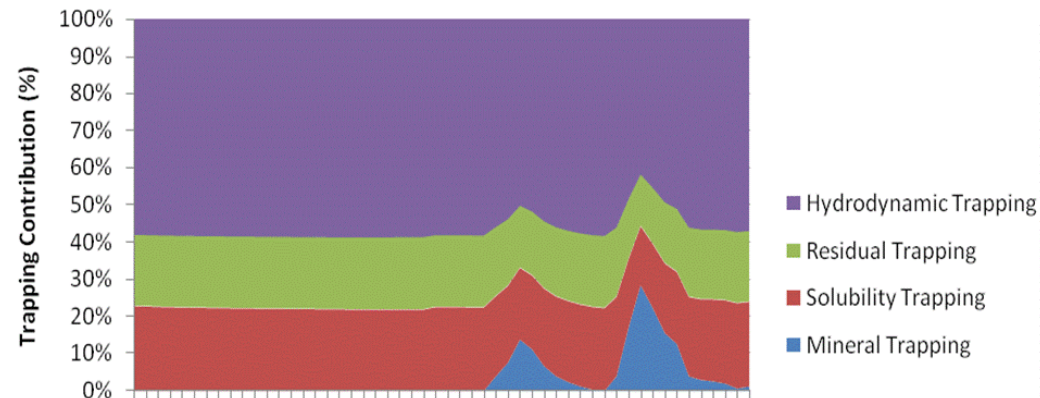
Overview



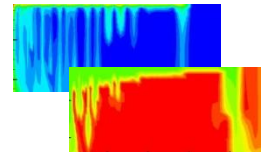
Objective: Evaluate & quantify the competing roles of various trapping mechanism in terms of long-term CO₂ fate in deep saline formation using RTM.

Effectiveness, Capacity, Safety

1. Background
2. Method
3. Geological Settings
4. Simulation Results
5. Conclusions
6. Current Studies



Background

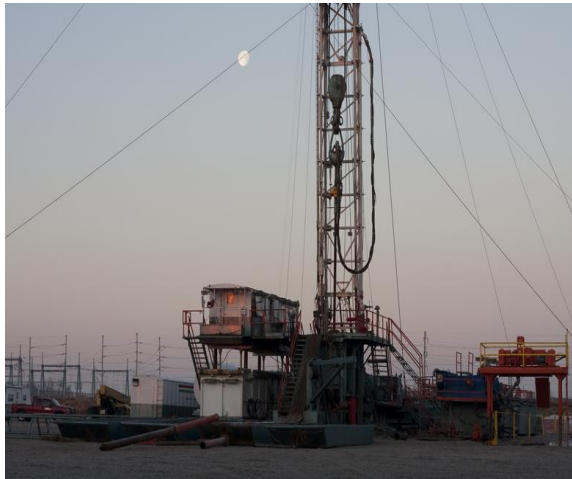


Midwest Geologic Sequestration Conso



Underlies one of the largest concentrations of coal-fired power plants in the world: **~280 million tons of CO₂/yr** from stationary emission, about 10% of total CO₂ emission of the U.S.

Midwest Geological Sequestration Consortium
1 million tons/ 3 yrs

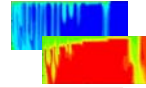


Illinois Basin-Decatur project: Feb. 2010 ~ Feb. 2013

(<http://sequestration.org/>)



Method



Reactive Transport Model (RTM): upscale the capability in both **time & space** to predict the results of a complex interplay of **multi-phase flow, mass transport, and geochemical processes** induced by large-scale injection of CO₂

$$\frac{\partial}{\partial t}(\phi C_i) = \frac{\partial}{\partial x} \left(\phi D \frac{\partial C_i}{\partial x} \right) - q \frac{\partial C_i}{\partial x} + \phi \sum_k \left(\frac{\partial C_i}{\partial t} \right)_k$$

Model features:

- Multi-phase (supercritical CO₂ and brine) flow
- Advective, diffusive transport
- Fully accounting chemical reactions
 - Aqueous speciation
 - Reaction kinetics
- Density – dependent flow
- Allow changes in porosity and permeability;
- Consider the impact of regional flow (0.3 m/yr)



Presenter's notes: CS becomes more attractive in the MW region where not much renewable energies such as wind or solar resources are available as in TX or CA to mitigate the C emission and climate change.

The target reservoir of the current simulation is the Mt. Simon Sandstone formation, which is recognized as a highly promising host reservoir targeted for CS in the MW region. It underlies much of the Illinois Basin that includes most of IL, western IN & western KY.

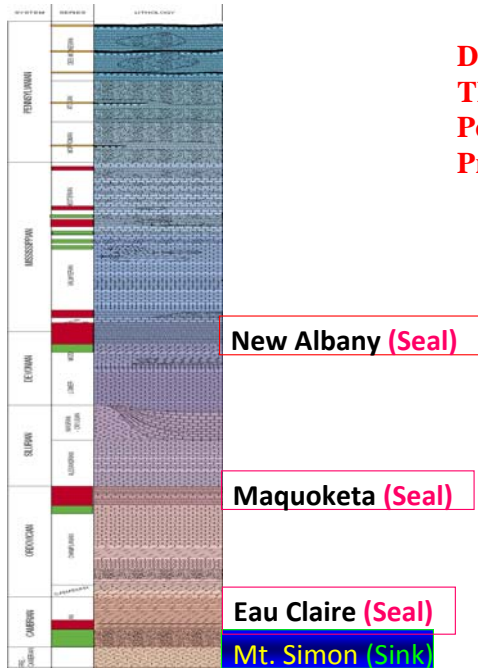
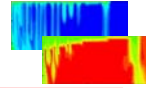
The formation underlies much of the Illinois Basin=most of IL, western IN & western KY.

Underlies one of the largest conc. of coal-fired power plants in the world and may provide one **of the most significant target for CS purpose**.

Carbon Monitoring for Action (CARMA)

As part of the initiative of Midwest (Illinois Basin) Geologic Sequestration Consortium, 1m t CO₂ will be injected over 3 yrs into the M.S. formation to demonstrate that the formation will be available as the predominant storage reservoir in the region.

Geological Settings



Depth ~ 2000 m at the injection point
Thickness ~520 m
Permeability ~100 mD
Presence of containment layers

Capacity: 22 to 89 Gt of CO₂ --- 100 year of carbon emission in the region



[\(http://sequestration.org/\)](http://sequestration.org/)

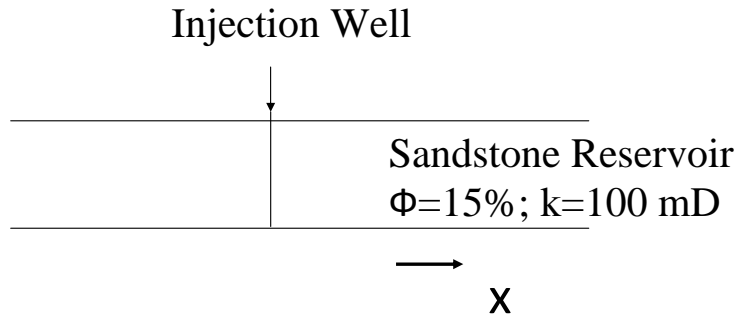
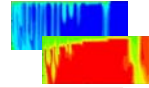
Presenter's notes: Mt. Simon sandstone is favored due to its favorable depth, thickness, permeability, and presence of caprock with low permeability.

The Eau Claire formation, which overlies the Mt. Simon sandstone, will provide the vertical containment needed to prevent movement of CO₂ out of the Mt. Simon formation and into shallower geologic formations, ground water, and the atmosphere. There are also several other low permeability layers that provide secondary containment.

The Mt. Simon formation and the containment layers are laterally extensive

The seismic survey verified the Eau Claire and Mt. Simon are laterally extensive through the study area with no discernible faults.

Model Set-up



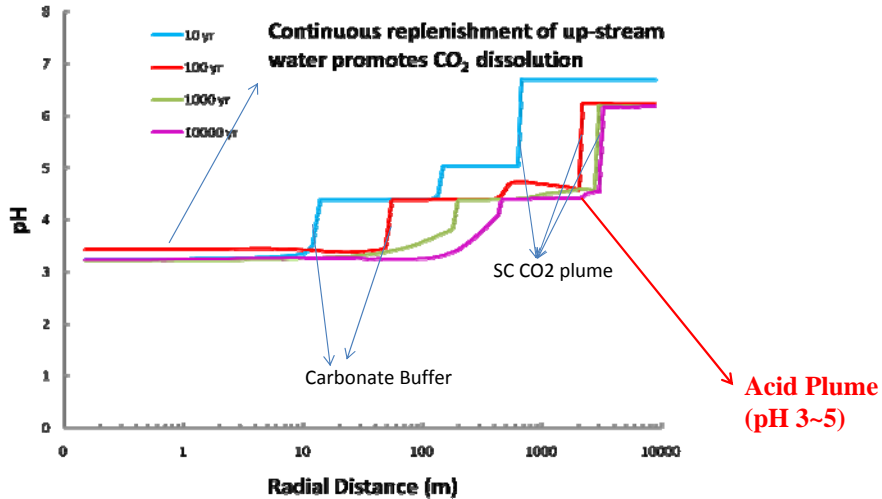
Reservoir condition: 2 km deep, 75 °C, 200 bars
0-10,000 m; 0- 10,000 yr (100 yr injection)

Regional Groundwater Flow of about 0.3m/yr



Presenter's notes: The model is conceptually set-up in a Mt. Simon-like scenario with reservoir properties of the formation.

pH Evolution



Regional Groundwater Flow of about 0.3m/yr



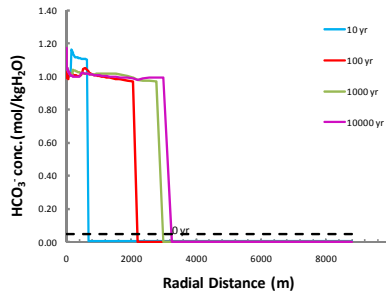
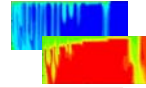
Liu *et al.* 2011

Presenter's notes: The focus of this study is on the ensued geochemical reactions which is best represented by the pH profiles. Injection of CO₂ results in acidified zones adjacent to the wellbore, causing progressive water-rock interactions in the surrounding region. The step-wise pH fronts are caused by buffer reactions, either modifications of the solute or solid phase. Low pH: promotes the dissolution of minerals, e.g. K-feldspar and oligoclase

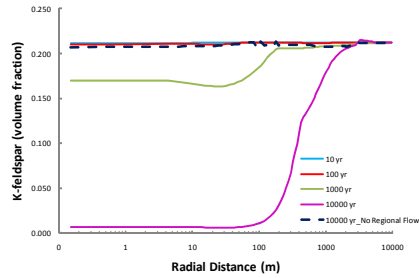
Including the replenishment of upstream groundwater after injection ceases greatly increase the predicted sandstone reactivity and plume migration

Another valuable alert from this diagram is the acidic plume migration, which could cause potential long-term risk both to the integrity of the reservoir and caprock. And this is also one of my current project relating to CO₂ leakage risk.

Geochemical Reactions

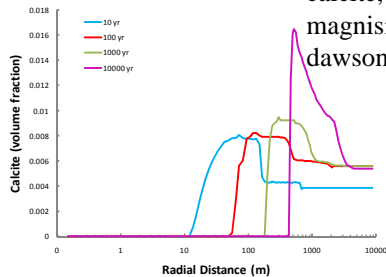


CO₂ Dissolution



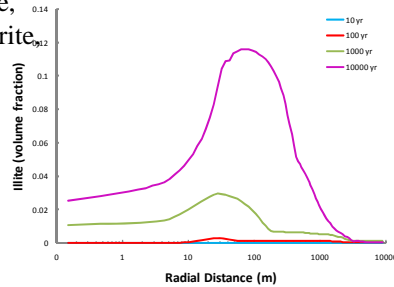
K-feldspar, oligoclase

Feldspar Dissolution



Carbonate Precipitation

calcite, dolomite,
magnisite, ankerite,
dawsonite



Alumino-silicate Precipitation

illite, Ca/Na-
smectite



Liu *et al.* 2011

Presenter's notes: In accordance with the extensive **dissolution of K-feldspar**, sequential **precipitations of secondary carbonates and clay minerals** are predicted in this zone causing porosity variations. Apart from the influence of cation activities in the brine, the profiles are closely related to the migration of CO₂ plume as the carbonates precipitate the dissolved CO₂ from the SC CO₂ dissolution.

Feldspar: k-feldspar, oligoclase

Carbonate: calcite, dolomite, magnisite, ankerite, dawsonite

A-S: Ca/Na-smectite, illite, alunite

Predicted Fate of Injected CO₂ at 100 & 1000 yr



Liu *et al.* 2011

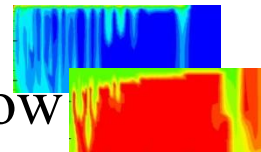
Presenter's notes: With these detailed analysis in mind, we come to the key question related to CO₂ storage, what is the fate of these injected CO₂? Where they will be and in what form?

There are four trapping mechanisms for the injected CO₂: xxx. The most desirable storage mechanisms are those that can permanently immobilize the CO₂

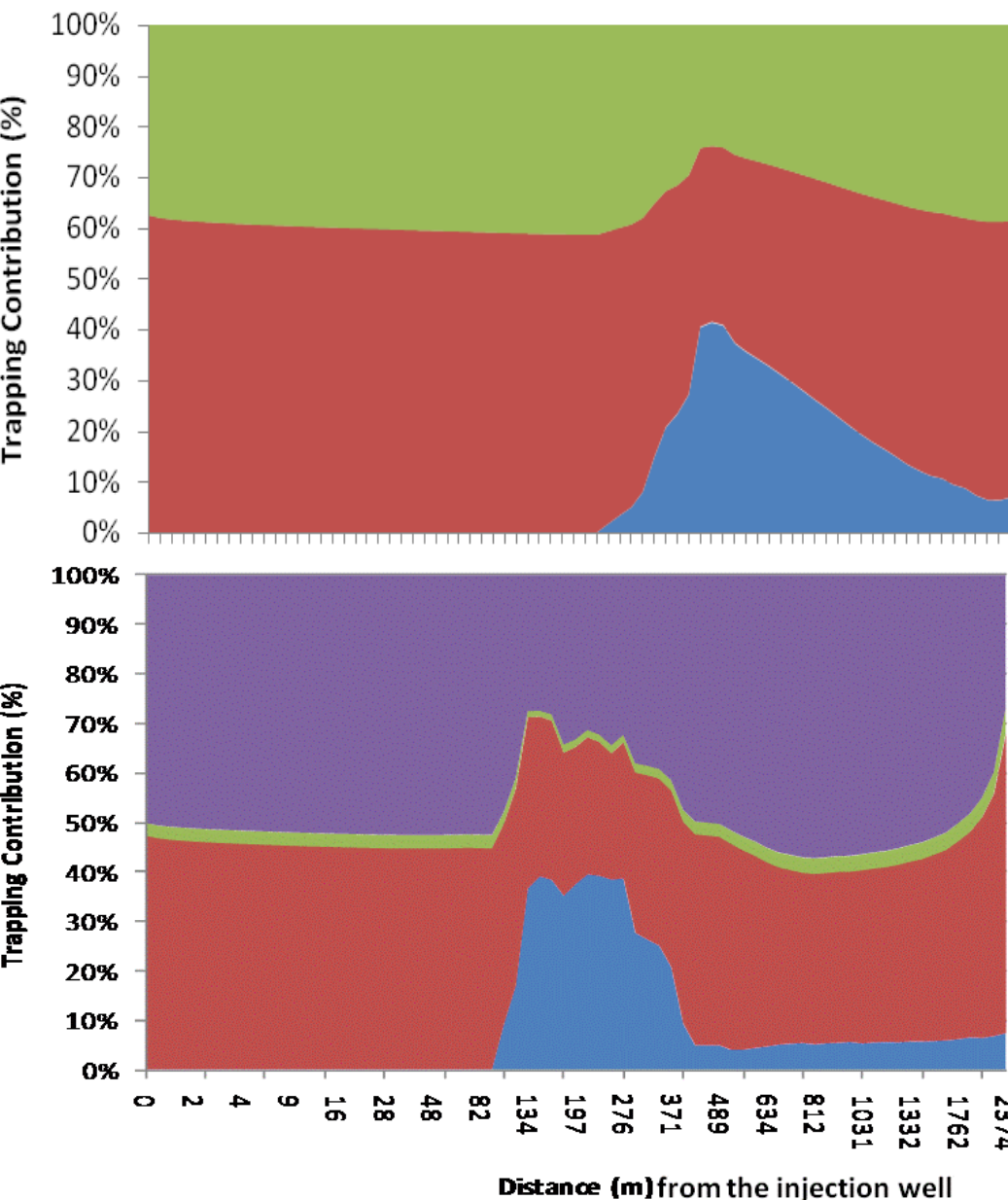
i.e., residual/solubility/mineral.

Hydrodynamic and solubility trapping are shown to be the dominant sinks for the injected CO₂ at both 100 yr and 10,000yr.

When supercritical CO₂ is injected into the Mt. Simon Sandstone, it forms a bubble around the injection wellbore, displacing the mobile formation brine in the pore space. Due to the buoyancy force, the injected CO₂ migrates upward and a significant amount is isolated in concentrated form as a distinct phase by hydrodynamic trapping. CO₂ remains mobile in hydrodynamic trapping and will continue to migrate. Before it reaches the caprock, it continues to spread out as a separate phase until it is trapped as residual CO₂ or in local structural traps within the sealing formation. CO₂ sequestered by the residual trapping mechanism is immobilized and will therefore **cause limited pressure perturbation to the reservoir seal**. In the long run, a large proportion of CO₂ react with the pore brine and dissolves into it. With appropriate mineralogy attained from the dissolution of minerals and those native to the formation brine, the dissolved CO₂ may eventually precipitate as secondary carbonate minerals.



Predicted Fate of Injected CO₂ at 10,000 yr w/wo Regional Flow

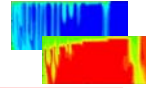


With Regional Flow

Without Regional Flow



Conclusions

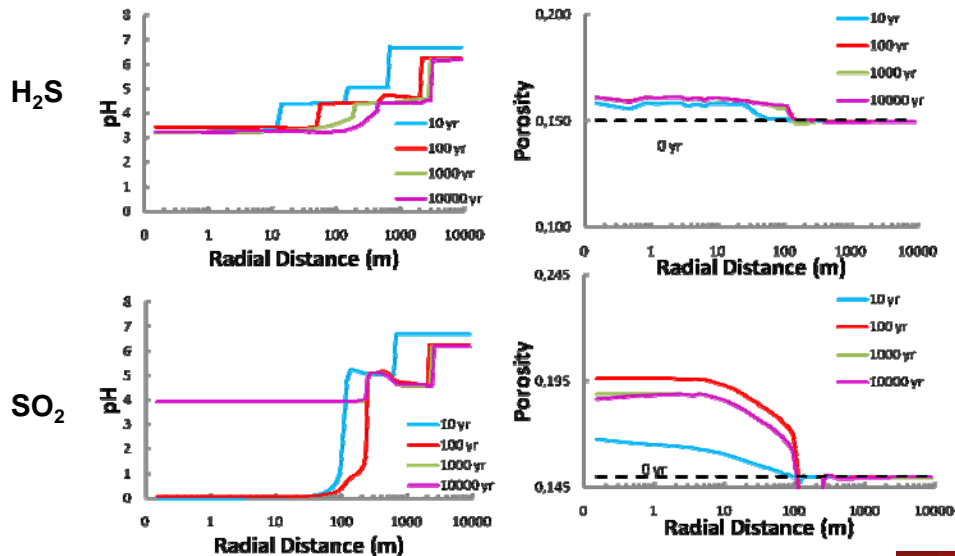


- The SC CO₂ plume within 3,300 m at 10,000 yr. However, **the acidic plume** remains after 10,000 yr.
- **Geochemical evolution** associated with CO₂ injection is controlled by the reactivity of the dissolved CO₂ with the host rock minerals.
- Four major mass partitioning mechanisms are identified and their spatial and temporal variations are qualified in our simulations. Hydrodynamic and solubility trappings sequester the largest percentage of the injected CO₂. With time, hydrodynamic trapping--> **solubility trapping --> mineral trapping (facilitate storage security)**.
- The **replenishment of upstream groundwater** by the regional flow promotes the continuous dissolution of CO₂ and facilitates the long-term storage of the injected CO₂.
- Our simulations indicate that the geochemical reactivity of the Mt. Simon Sandstone is relatively low in the simulated 10,000 yr. **Major chemical changes are very unlikely to occur to Mt. Simon as a consequence of CO₂ injection in the longer geological time scale.**



Presenter's notes: Most of the injected CO₂ remains within a radial distance of 3300m at the end of 10,000yr and is sequestered and immobilized by solubility and residual trapping; Hydrodynamic and solubility trapping are shown to be the dominant sinks for the injected CO₂ at both 100 yr and 10,000yr.

Risk Assessment of CCS with Flue Gas Co-injection

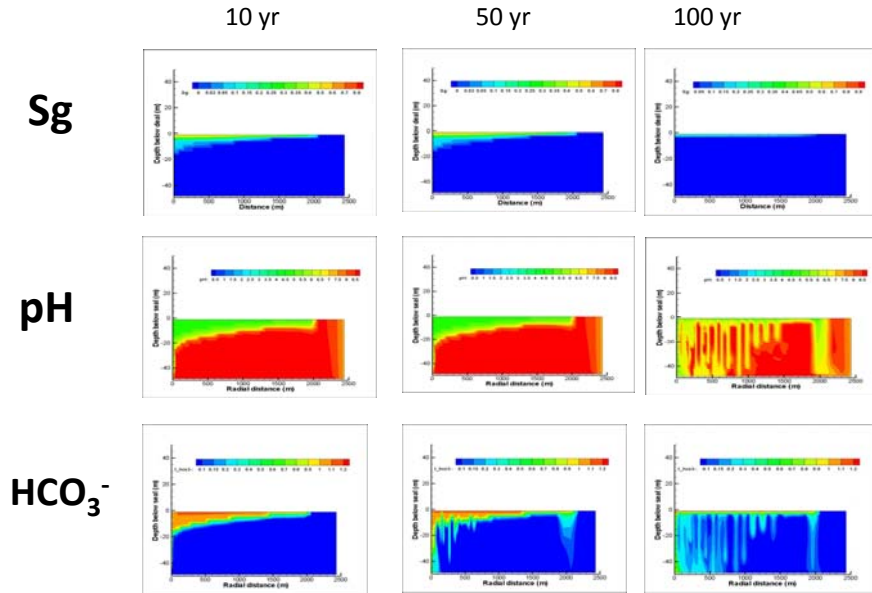
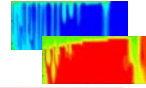


Presenter's notes: The IPCC estimated that as much as 30% of the energy created by coal plant would have to be spent on just pulling the CO₂ out of its flue gas.

SO₂: low pH, K-feldspar dissolution

Co-injection of H₂S causes relatively limited modification from the CO₂ alone case while significantly higher water-rock reactivity is associated with the SO₂ co-injection. Although co-injection of CO₂ with H₂S and SO₂ could potentially reduce separation and injection cost, it may lead to some uncertainty and risks and therefore require further investigation.

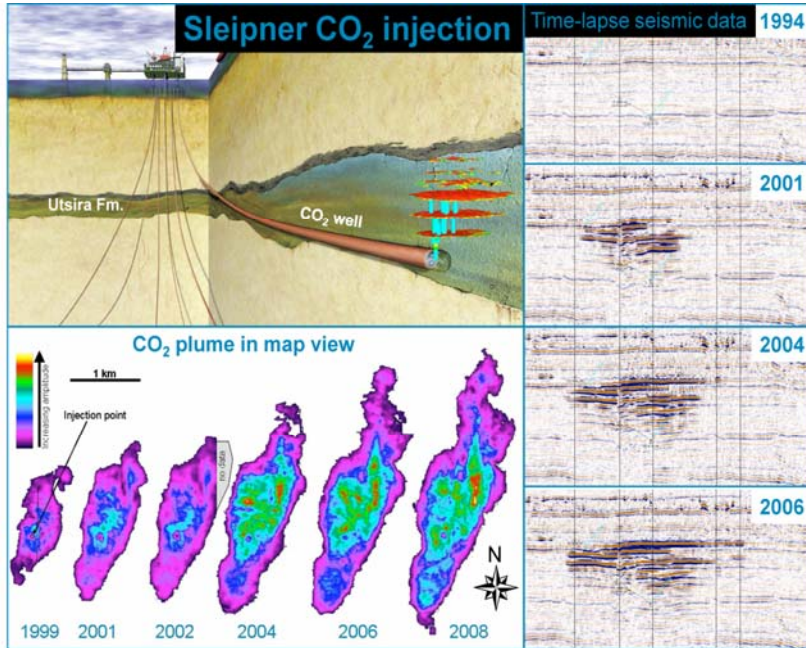
Preliminary 2-D model



Presenter's notes: Injection for 3 yr; 0.63 mt/yr; 50 x 2500m

The vertical profiles of CO₂ show fingering pattern from the top of the reservoir to the bottom due to the density variation of CO₂-impregnated brine, which facilitate the advection induced mixing and solubility trapping.

Sleipner Project



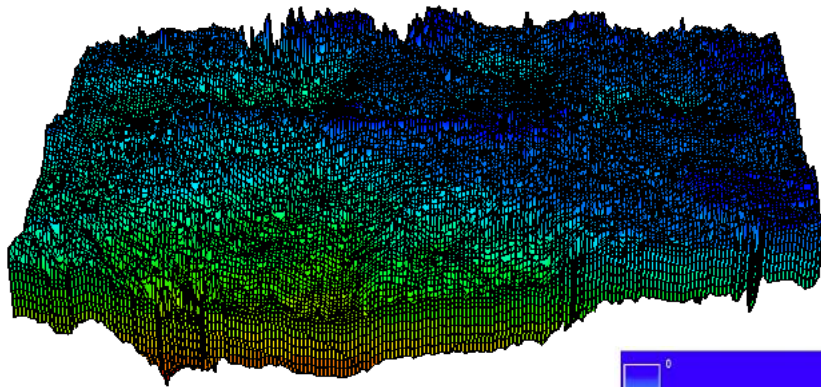
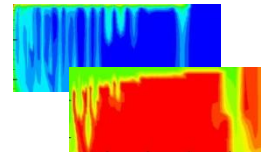
(Chadwick, 2010)

Presenter's notes: The injection started in August 1996. Approximately one million metric tons of CO₂ is injected each year, and by now, about 11 million tons CO₂ has been injected. So here is the cartoon. Natural gas is produced from a deeper formations. The natural gas contains about 9% CO₂. The CO₂ is separated on the platform. Then, it is captured and reinjected in a shallower Utsira sandstone formation through a single horizontal well. It is also cheaper for them to inject into this shallower formation and currently the cost is about \$12 per ton.

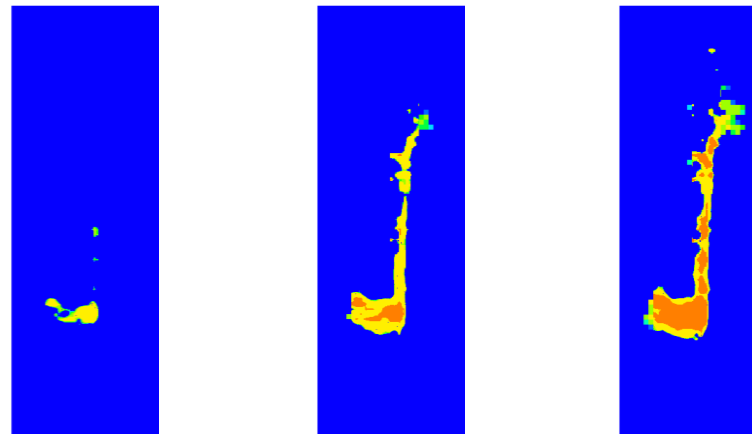
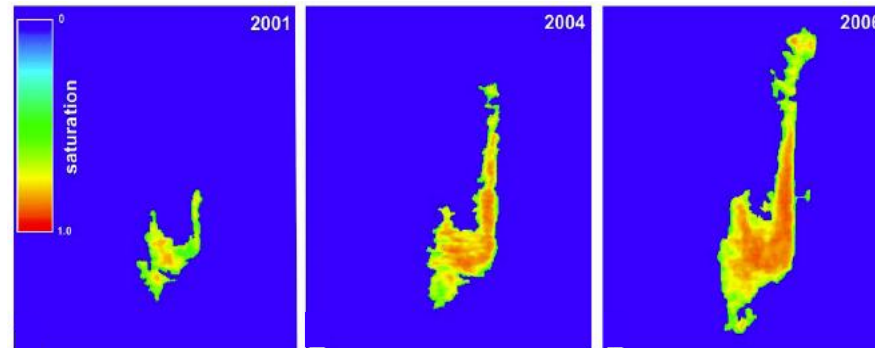
Statoil conducted seismic survey prior the injection (at 1994), which established the baseline, and then they repeated the survey every other year.

So this is the world's first industrial scale geological carbon sequestration. This is the only place in the world where we have up to 15 yrs of high quality 4D seismic data on the CO₂ plume migration in a real geological system.

Sleipner Project

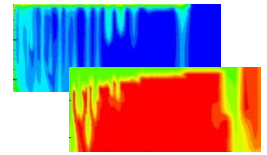


3-D reservoir model of the Sleipner Project



Upper: average saturation of the topmost layer through time from seismic data (Chadwick & Noy, 2010);

Lower: simulation results of gas saturation in the topmost layer in the same years.

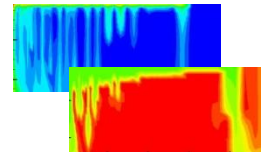


Faye Liu
liu60@indiana.edu



- **BACK-UP
SLIDES**

Mineral Assemblage

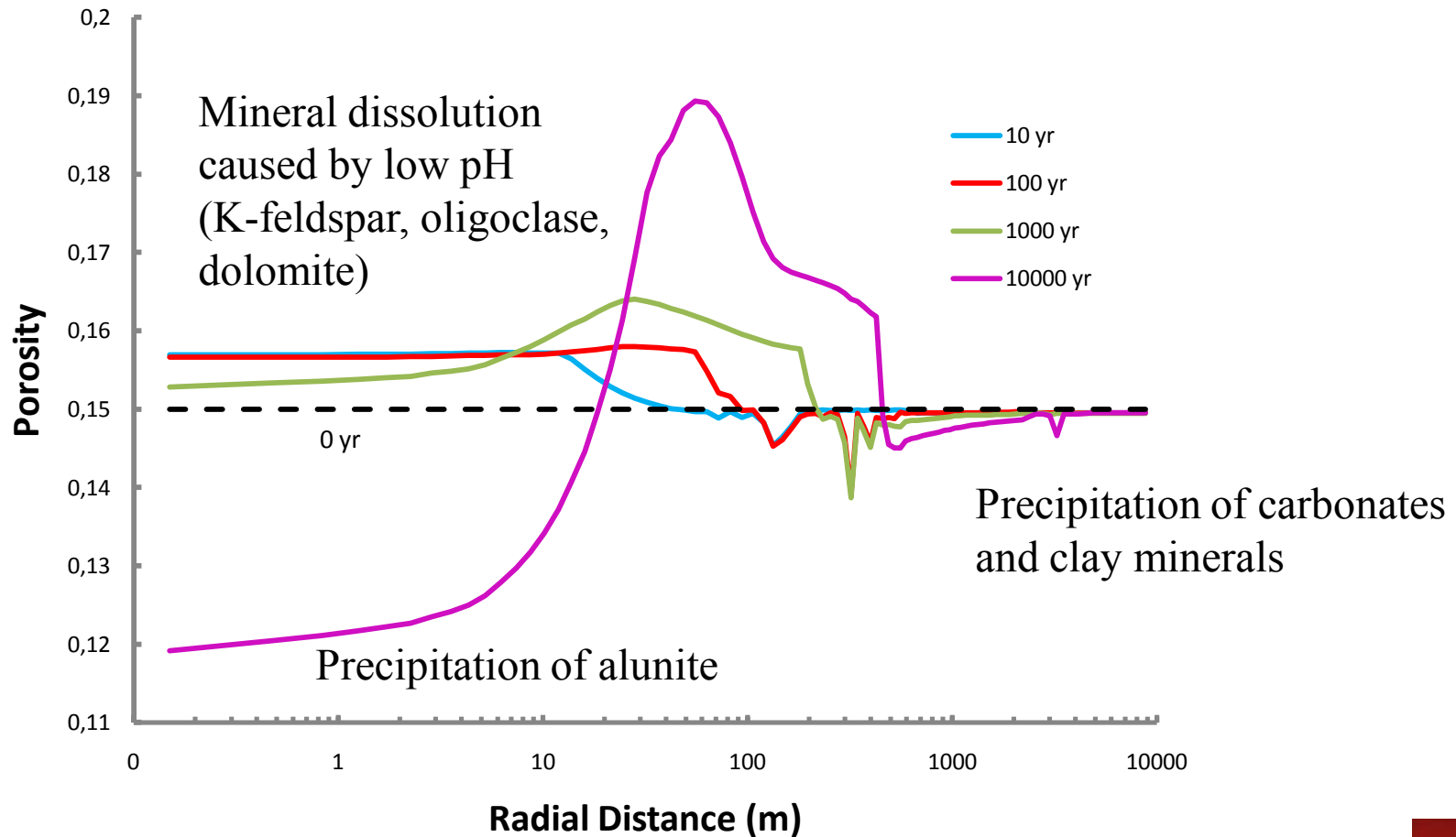
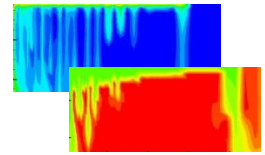


Mineral	Chemical formula	Volume percent (%)
Primary		
Quartz	SiO_2	62.61
K-feldspar	KAlSi_3O_8	21.20
Plagioclase	$\text{Ca}_{0.2}\text{Na}_{0.8}\text{Al}_{1.2}\text{Si}_{2.8}\text{O}_8$	0.44
Dolomite	$\text{CaMg}(\text{CO}_3)_2$	0.75
Porosity		15
Secondary		
Calcite	CaCO_3	
Magnesite	MgCO_3	
Ankerite	$\text{CaMg}_{0.3}\text{Fe}_{0.7}(\text{CO}_3)_2$	
Dawsonite	$\text{NaAlCO}_3(\text{OH})_2$	
Kaolinite	$\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4$	
Illite	$\text{K}_{0.6}\text{Mg}_{0.25}\text{Al}_{1.8}(\text{Al}_{0.5}\text{Si}_{3.5}\text{O}_{10})(\text{OH})_2$	
Low-albite	$\text{NaAlSi}_3\text{O}_8$	
Opal-A	SiO_2	
Na-smectite	$\text{Na}_{0.29}\text{Mg}_{0.26}\text{Al}_{1.77}\text{Si}_{3.97}\text{O}_{10}(\text{OH})_2$	
Ca-smectite	$\text{Ca}_{0.145}\text{Mg}_{0.26}\text{Al}_{1.77}\text{Si}_{3.97}\text{O}_{10}(\text{OH})_2$	

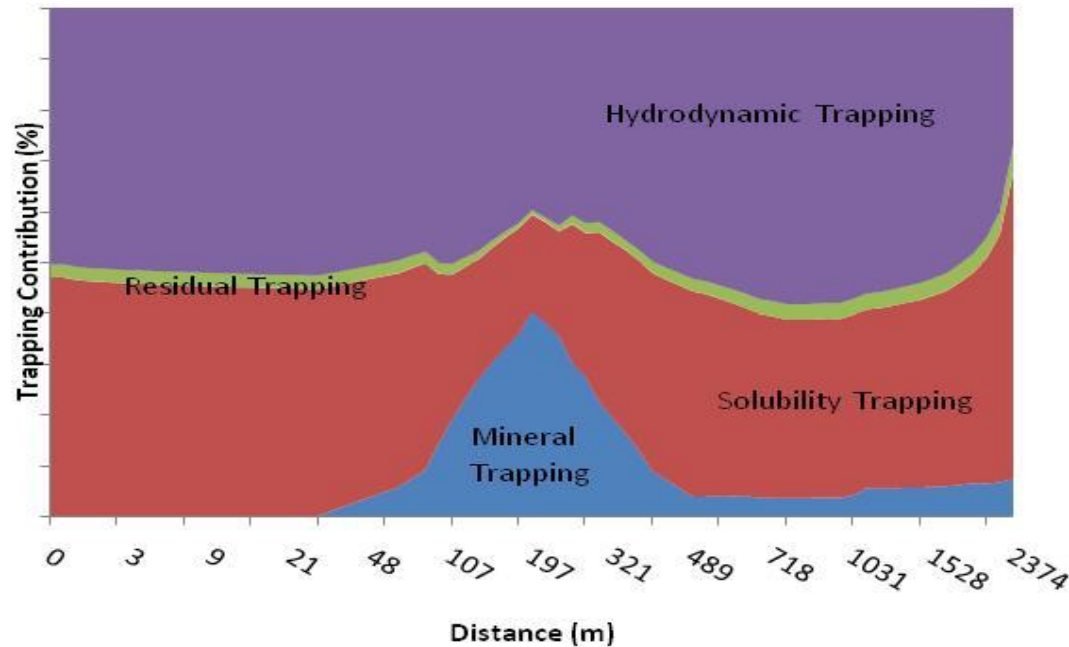
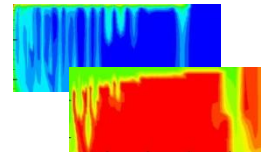
Initial mineral volume fractions and possible secondary mineral phases used in the simulations (ELIASSON et al., 1998)



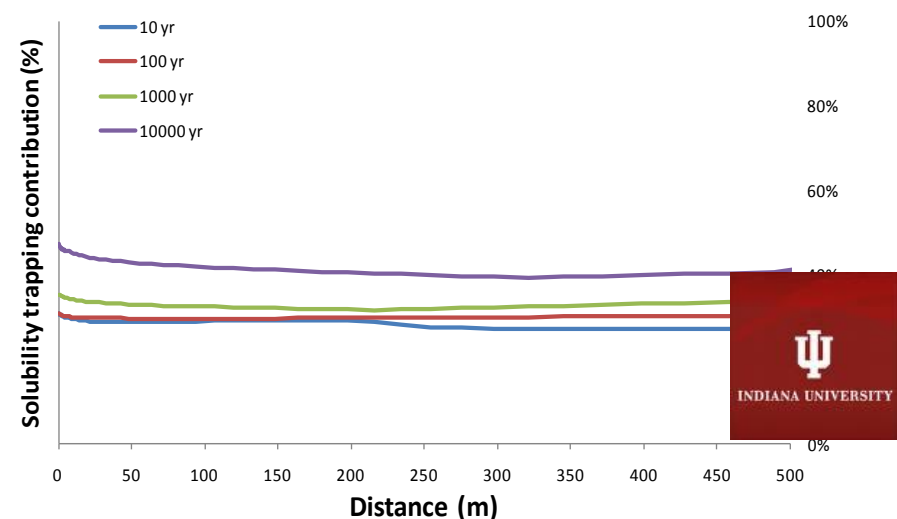
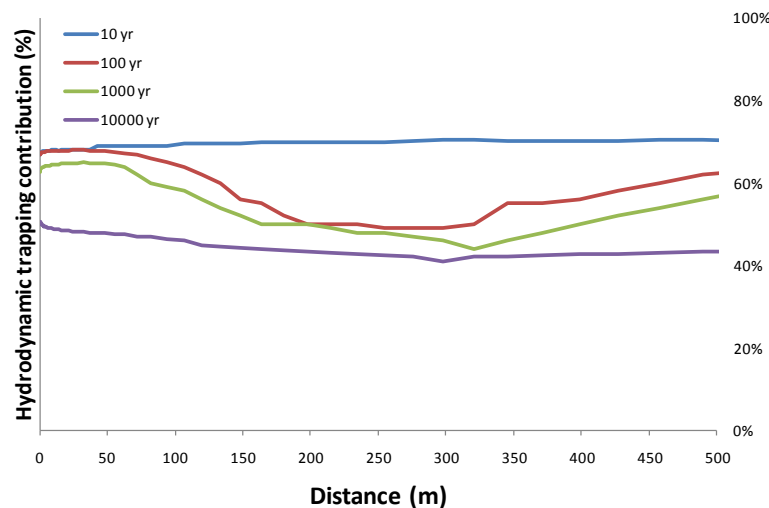
Reservoir Response - Porosity



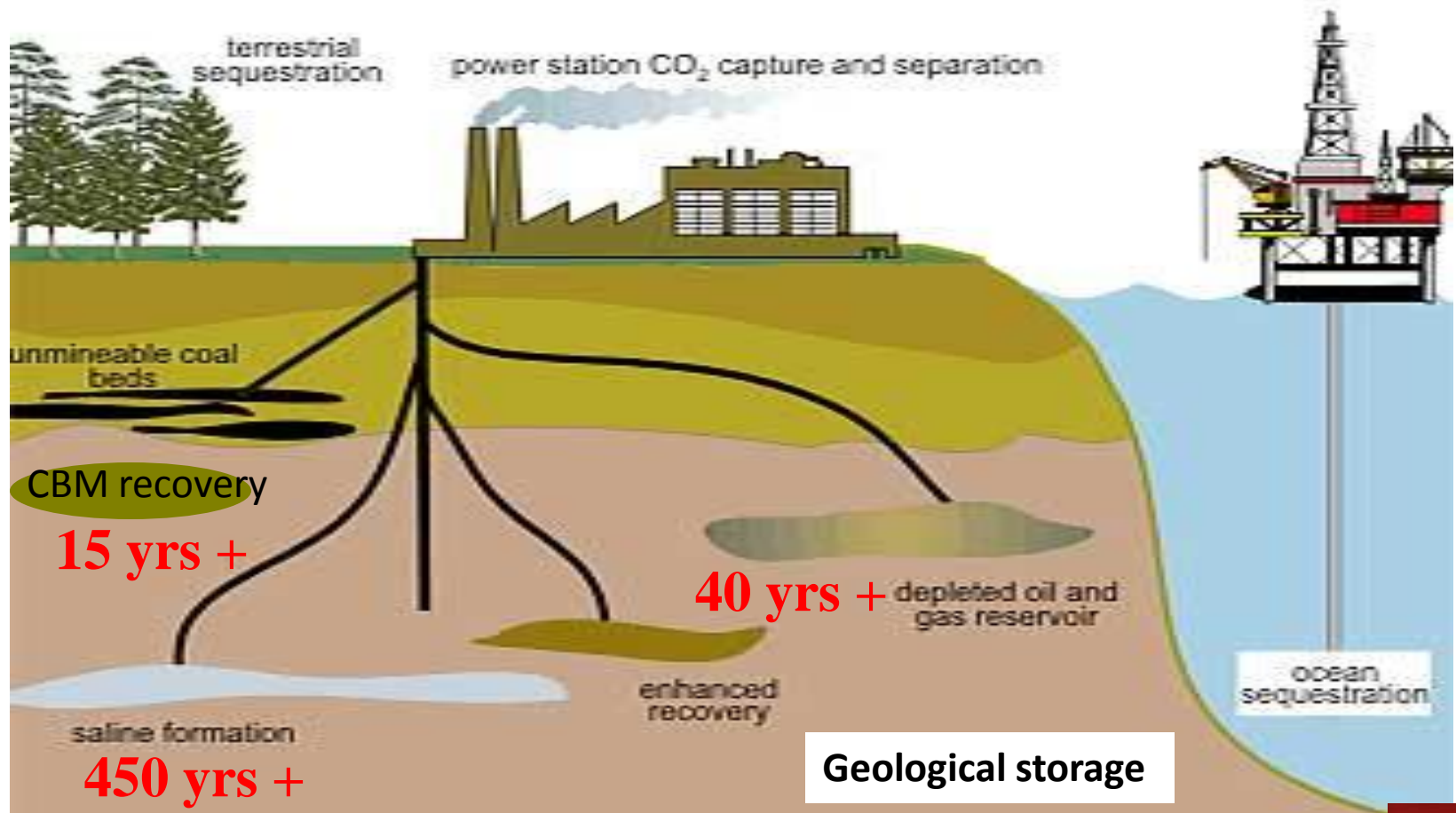
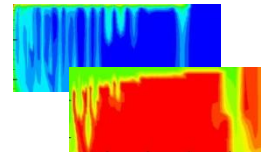
Fate of the injected CO₂



With time, **hydrodynamic trapping** contribution decreases with this part of CO₂ enters the formation brine, increasing the mass partitioning in the **solubility trapping**, and later, **mineral trapping**.

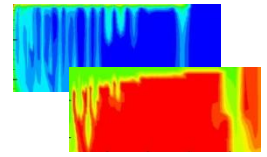


CCS Options & Storage Potential



~ carbon emission of North America at current emission rate

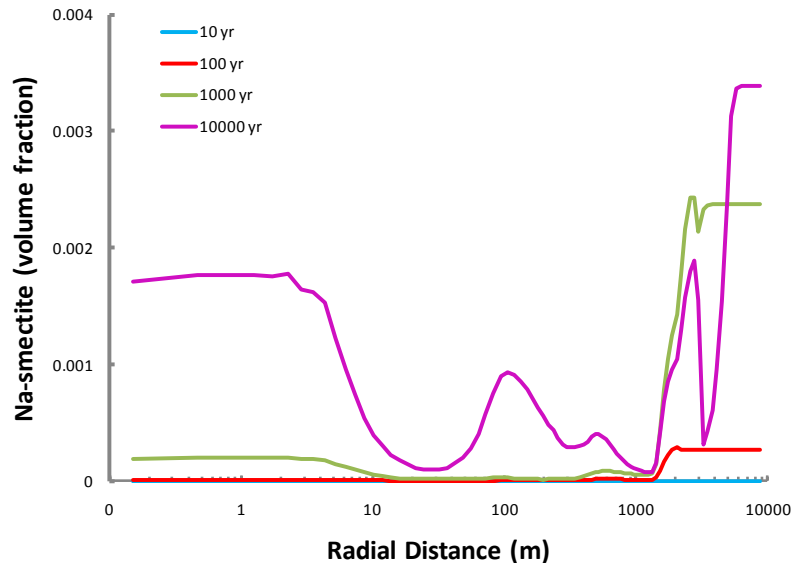
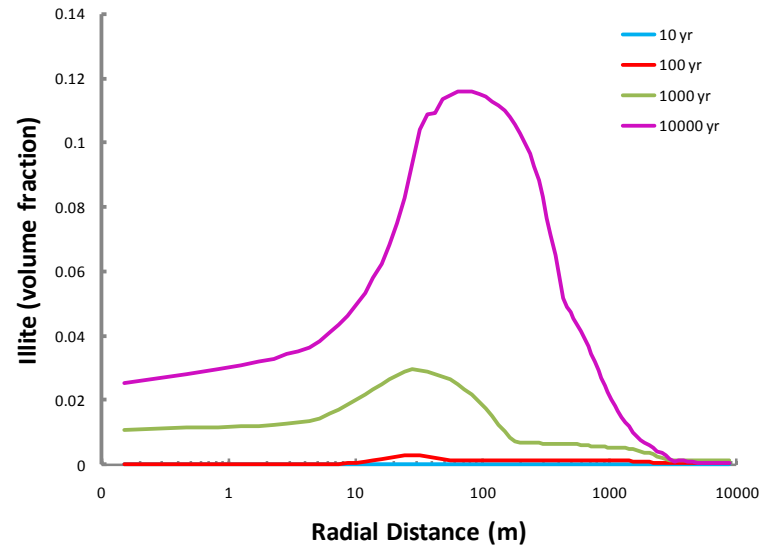
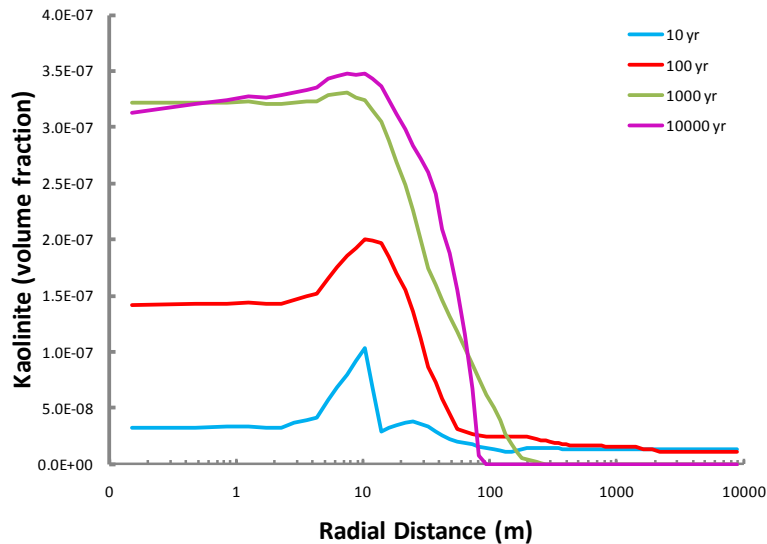
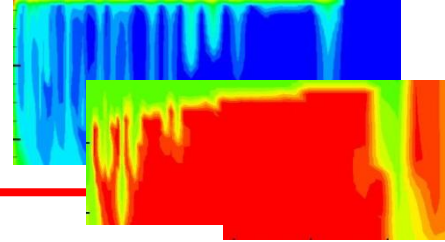
CO₂ Storage in Saline Aquifers: Key Geoscience (& Engineering) Issues



Capacity, Integrity, Safety

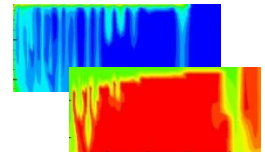
- Short/long-term fate of the injected CO₂
- What fraction of CO₂ is stored as a free phase (mobile or trapped), dissolved in the aqueous phase, or sequestered in solid minerals?
- Reservoir response?
- How do the relative proportions of CO₂ in these different storage modes change over time?
- Leakage of stored CO₂: Will it leak? How much? How?

Precipitation of alumino-silicate minerals



As $\log(aK^+/aH^+)$ and $\log a_{(SiO_2)}$ increase, a pathway of kaolinite to smectite and finally to illite can be predicted

Goal & Challenges



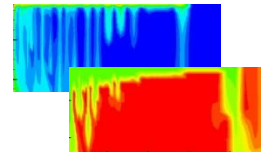
Goal: Full-scale demonstration & commercialization of CCS by 2020

	Challenges	Priority Activities
Storage Science	Modeling: Refinement, coupling of models, and validation of models at field project;	1. Develop appropriate & standard coupled models with capability to accommodate impurities in CO ₂ ; 2. Establish best practice for history matching; 3. Assess long-term performance & security using verified models.
	Fundamental Science: geochemistry	1. Use more accurate rate laws; 2. Advance knowledge on reactive surface area and surface reaction calculation; 3. Multi-component EOS; 4. Porewater chemistry in the caprock 5. Develop more extensive datasets targeted to CCS scenario



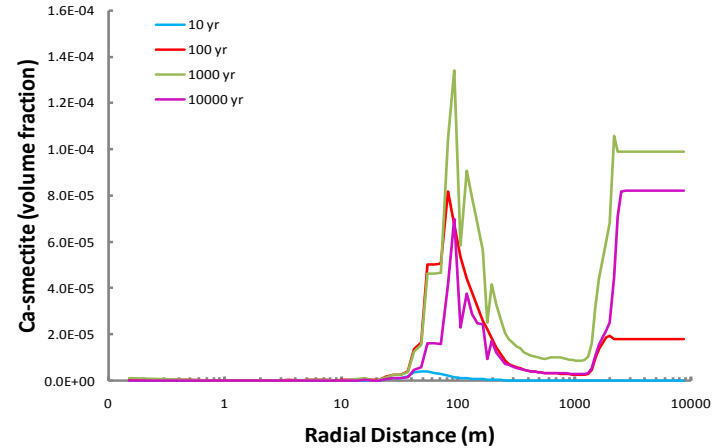
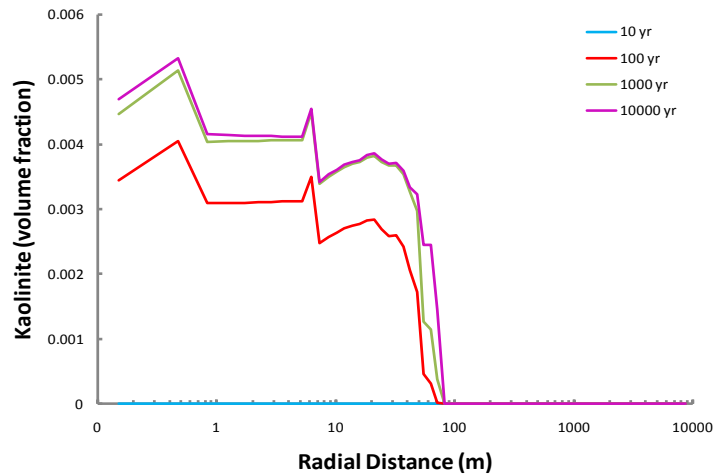
(NETL/DOE, IPCC, IEA, CSLF, ZEP)

Summary of Reservoir response and CO₂ fate



- When supercritical CO₂ is injected into the Mt. Simon Sandstone, it forms a bubble around the injection wellbore, **displacing** the mobile formation brine in the pore space as well as **dissolving** into it. The dissolved CO₂ results in **acidified zones** adjacent to the wellbore, causing **progressive water-rock interactions** in the surrounding region. In accordance with the extensive **dissolution of authigenic K-feldspar, sequential precipitations of secondary carbonates and clay minerals** are predicted in this zone causing porosity variations.
- Due to the buoyancy force, the injected CO₂ migrates upward and a significant amount is **isolated in concentrated form as a distinct phase by hydrodynamic trapping**. CO₂ remains mobile in hydrodynamic trapping and will continue to migrate. Before it reaches the caprock, it continues to spread out as a separate phase until it is trapped as **residual CO₂ saturation or in local structural traps within the sealing formation**. CO₂ sequestered by the residual trapping mechanism is immobilized and will therefore cause limited pressure perturbation to the reservoir seal. In the long run, a large proportion of CO₂ react with the pore brine and dissolves into it. With appropriate mineralogy attained from the dissolution of authigenic minerals and those native to the formation brine, the dissolved CO₂ may **eventually precipitate as secondary carbonate minerals**.

Alumino-silicate mineral alteration



3 progressive zoning: Kaolinite --- Smectite --- Illite

