Maximization of Permanent Trapping of CO<sub>2</sub> in the Highest-Porosity Formations of the Rock Springs Uplift Project Number: FE0004832

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## **Presentation Outline**

- Benefit to the Program
- Project Overview
- Technical Status
  - $_{\odot}$  Experimentation: core-flooding and IFT/CA
  - Pore-scale modeling modeling
- Accomplishments to Date
- Summary

## Benefit to the Program

### • Program goal:

 'Develop technologies that will support industries' ability to predict CO<sub>2</sub> storage capacity in geologic formations to within ±30 percent.'

### • Benefits statement:

 The research project is focused on performing reservoir conditions experiments to measure steady-state relative permeabilities, residual saturations, interfacial tensions, and contact angles to inform models at pore, core, and reservoir scales. These can then be used to develop improved understanding of displacement mechanisms leading to design of strategies to maximize trapping.

## **Project Overview**: Goals and Objectives

#### • Goal:

 The overall goal of this project is to provide information that will assist in maximizing the permanent trapping of supercritical CO<sub>2</sub> (scCO<sub>2</sub>), and co-contaminants (referred to as 'mixed scCO<sub>2</sub>') in deep saline aquifers.

#### • Objectives:

- Measurement of reservoir conditions drainage and imbibition relative permeabilities, irreducible brine and residual mixed scCO<sub>2</sub> saturations and relative permeability scanning curves (hysteresis).
- Characterization of wettability through measurements of contact angles and interfacial tensions under reservoir conditions.
- o Development of physically-based dynamic core-scale pore network model.
- Development of new, improved high-performance modules for the UW-team simulator to provide new capabilities to the existing model in order to include hysteresis in the relative permeability functions, geomechanical deformation and an equilibrium calculation (for mixed scCO<sub>2</sub>).
- Validation of the compositional reservoir model against well-characterized unsteady-state coreflooding experiments.
- Numerical study of long term permanent trapping of mixed scCO<sub>2</sub>, through high-resolution numerical experiments taking into account reservoir heterogeneity, saturation history, dissolution, capillary trapping and geomechanical deformation.

## **Technical Status**

Project includes two major groups of tasks (6 UW faculty members):

- 1. Experimentation and Modeling: Pore and Core Scales
- Task 2: Relative permeability measurements at reservoir conditions
- Task 3: IFT and CA measurements at reservoir conditions
- Task 4: Dynamic pore-scale modeling to predict k<sub>r</sub> and P<sub>c</sub> functions
- 2. Modeling and Simulation: Core and Field Scales
- Task 5: Reservoir modeling activities
- Task 6: Development of the UW-team compositional simulator
- Task 7: Geomechanics model development
- Task 8: Field-scale numerical experiment

## Experimentation and Modeling Pore and Core Scales

- Measurement of relative permeability functions
- Measurements of IFT and CA
- Development dynamic, parallel pore-scale network models





Vertical positioning system

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## Core samples (Category A)

#### Nugget sandstone

- Core length: 14.8 cm
- Core diameter: 3.8 cm
- Porosity: 14.3 %
- Permeability (Brine): 312 mD
- Pore volume: 24.0 cc

#### **Berea sandstone**

- Core length: 15.0 cm
- Core diameter: 3.8 cm
- Porosity: 20.1 %
- Permeability (Brine): 50 mD
- Pore volume: 34.19 cc



### Core samples (Porosity)



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## Core-flooding conditions (Category A)

### **Gaseous Condition (group 1)**

- Pressure: 3.46 MPa
- Temperature: 20 ° C
- Overburden pressure: 4.82 5.86 MPa

#### **Supercritical Condition (group 2)**

- Pressure: 11.0 MPa
- Temperature: 55 ° C
- Overburden pressure: 12.7 13.1 MPa
- ➤ Typical capillary number: 1.03 × 10<sup>-5</sup>
- Sleeve: Viton (Teflon+ Aluminum foil)
- Wetted material: Hastelloy
- O-rings: Ultra High Molecular Weight (UHMW)- AFLAS
- Core-holder: Hassler type

10.0 wt% Nal
Brine composition: • 5.0 wt% NaCl
0.5 wt% CaCl

## Fluid properties (Category A)

Fluid	Pressure MPa	TemperatureViscosity°CcP		Density gr/cm <sup>3</sup>	CO <sub>2</sub> /Brine IFT mN/m <sup>*</sup>
Supercritical CO <sub>2</sub>	11.0	55	0.044	0.393	38.15
Gaseous CO <sub>2</sub>	3.46	20	0.016	0.081	51.24
Brine	11.0	55	0.91	1.126	-
Brine	3.46	20	1.57	1.125	-

## Flow rates (Category A)

Experimental flow rates for  $CO_2$  and chase brine injections

#### 1- $CO_2$ injection

2- Chase brine injection

Sample	NWP	WP	0.125	0.25	0.5	1.0	2.5	5	10	15	20	30	60	100	120
			$\mathrm{cm}^3/\mathrm{min}$												
01-Berea SS	$scCO_2$	Brine		•	•	•	•	•	•	•	•				
01-Berea SS	$gCO_2$	Brine	•	•	•		•		•			•	•	•	•
02-Nugget SS	$scCO_2$	Brine		•	•	•	•	•	•						

1- Brine flow rate: Q<sub>b</sub>=0.05-0.5 cm<sup>3</sup>/min 2- Gradual increase in flow rate

1-46 unsteady-state drainage and imbibition experiments

2- Full recirculation condition for all the experiments regardless of flow rate

## **Results** (Effect of S<sub>CO2</sub><sup>max</sup> on S<sub>CO2r</sub> – Berea SS)



## **Results** (Effect of S<sub>CO2</sub><sup>max</sup> on S<sub>CO2r</sub> – Berea SS)



## **Results** (Effect of S<sub>CO2</sub><sup>max</sup> on S<sub>CO2r</sub> – Nugget SS)



### Core sample (Category B)

#### **Berea sandstone**

- Core length: 15.4 cm
- Core diameter: 3.76 cm
- Porosity: 21.2 %
- Permeability (Brine): 612 mD
- Pore volume: 36.3 cc



#### **Experimental Conditions**

- Temperature: 55.0 ° C
- Pressure: 11 MPa
- •Overburden Pressure: 13.1 MPa
- $scCO_2$  flow rate: 0 5.0 cc/min
- •Brine flow rate: 0.45 0.0 cc/min (Drainage)
- •Brine flow rate: 0 0.25 cc/min (Imbibition)
- •Typical capillary no.  $\leq 2.5 \times 10^{-6}$





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### Results (Dissolution or in-situ re-saturation)



## **Results** (Dissolution relative permeability)



### Core sample (Category C)

#### **Madison limestone**

- Core length: 17.4 cm
- Core diameter: 3.76 cm
- Porosity: 19.03 %
- Permeability (Brine): 13.6 mD
- Pore volume: 36.77 cc



#### **Experimental Conditions**

- Temperature: 60.0 ° C
- Pressure: 19.6 MPa
- •Overburden Pressure: 21.37 MPa
- scCO<sub>2</sub> flow rate: 0 0.1 cc/min
- •Brine flow rate: 0.03 0.2 cc/min (Drainage)
- •Brine flow rate: 0.03 0.16 cc/min (Imbibition)
- •Typical capillary no.  $\leq 7.5 \times 10^{-7}$  (Cap.dom.)
- •Typical capillary no. > 10<sup>-5</sup> (Visc.-dom.) 25

## Madison limestone (Porosity)



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## Fluids and materials (Category C)

#### Fluids:

- Pure CO<sub>2</sub>
- Pure SO<sub>2</sub>: 1200 ppm
  - 50000 ppm Nal
- Brine:
- 36500 ppm NaCl

#### Material:

- Sleeve: AFLAS<sup>\*</sup> (Teflon+ Aluminum foil)
- Wetted material: Hastelloy
- •O-rings: AFLAS
- •Core-holder: Hassler type
- The AFLAS materials specifically designed for SO<sub>2</sub>+CO<sub>2</sub> experiments

Fluid	Pressure MPa	Temperature °C	Viscosity cP	Density gr/cm <sup>3</sup>	CO <sub>2</sub> /Brine IFT mN/m <sup>*</sup>
scCO <sub>2</sub> -rich phase	19.16	60	0.0692	0.70	28.1
Brine-rich phase	19.16	60	0.635	1.05	-

## Results (Steady-state relative permeability-Half cycle)



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## **Results** (Steady-state relative permeability-1/4 cycle)



## **Results** (Steady-state relative permeability–1/4 cycle)



## Results (Steady-state relative permeability-Both cycles)



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## **Results** (Effect of $S_{CO2}^{max}$ on $S_{CO2r}$ - Trapping efficiency)



### **Results** (Dynamic effects exp.- Category C-3)



## Accomplishments to Date

- 1. Milestones 1-6 were completed:
  - o Update Project Management Plan Hold kickoff meeting of Pls with govt. partners
  - o Acquisition of rock samples and micro-CT images for pore-level network model
  - o Measurement of unsteady-state core-flooding experimental data required for code validation
  - o Measurement of steady-state relative permeabilities for code validation
- 2. A new state-of-the-art IFT and contact angle apparatus was built from scratch and validated
- 3. Development of fully parallel dynamic pore-scale network model is nearing completion
- 4. Development of hysteresis model was completed
- 5. Development of phase equilibrium calculation module for scCO<sub>2</sub>, SO<sub>2</sub>, and brine is nearing completion
- 6. Development of compositional simulator was completed
- 7. Code validation for the UW-Team simulator (Milestones 5) is on track for completion in September
- 8. Active dissemination of findings through publications and presentations in scientific meetings

## Summary

- Key findings
  - Significant fractions of initial CO<sub>2</sub> in place can be stored through residual trapping
  - Lower initial  $CO_2$  saturation leads to higher trapping efficiency (R=S<sub>CO2r</sub>/S<sup>max</sup><sub>CO2</sub>)
  - Trapping efficiency between 49 to 83% of CO<sub>2</sub> in place
  - o Accurate numerical approximation of transport problems with hysteresis
- Future Plans
  - o Develop a fully parallel version of the phase equilibrium module
  - o Dynamic pore-scale modeling of imbibition in large networks
  - o Completion of geomechanics module
  - o Compositional reservoir simulations on large computer clusters, UQ studies

## Thank you

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## IFT/CA Experimental Setup



## Experimental Setup (cont.)



## **Contact Angle and IFT Measurements**



## Densities (CO<sub>2</sub>/Water system)



Hebach A., Oberhof A., Dahmen N., J. Chem. Eng. Data, 49, 950-953, 2004

## Densities (CO<sub>2</sub>/Water system)



Span R., and Wagner W., J. Phys. Chem. Ref. Data, 25 (6), 1509-1596, 1996

## IFT (CO<sub>2</sub>/Water)



Hebach, A., Oberhof A., Dahmen N., Kogez A., Ederer H., and Dinjus E., *J. Chem. Eng. Data*, 47, 1540-1546, 2002

IFT-CA (CO<sub>2</sub>/Water/Quartz system)



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## Results (Effect of P and T for sc-CO<sub>2</sub>)



Koschel D., Coxam J-Y, Rodier L., and Majer V.,, 2006, Fluid Phase Equilibria, 247, 107-120

## Results (Effect of P and T for sc-CO<sub>2</sub>)



## Results (Effect of P and T for sc-CO<sub>2</sub>)



## Results (Effect of Salinity)



Koschel D., Coxam J-Y, Rodier L., and Majer V., 2006, Fluid Phase Equilibria, 247, 107-120

## Results (Effect of Salinity)



## Results (Effect of Salinity)



## Results (Effect of SO<sub>2</sub>)

Emission stream from N.A. power plants has  $SO_2/CO_2$  ratio ranging between 0.02 to 8 wt% with an average of 0.6 wt%.



## Results (Effect of SO<sub>2</sub>)



T. Tarbuck and G. Richmond, *J. Am. Chem. Soc.*, 128, 10, 3256–3267, 2006. V. Shah, D. Broseta, G.Mouronval, and F.Montel, Int. J. Greenhouse Gas Control, 2, 4, 594–604, 2008.

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## Results (Effect of SO<sub>2</sub>)



D. Broseta, N. Tonnet, and V. Shah, *Geofluids*, vol. 12, no. 4, pp. 280–53 294, 2012.



Millions of pores and throats. They represent the size, distribution and connectivity of micro pores.

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Equivalent pore network constructed for Bentheimer Sandstone using high-resolution microtomography images.





## Modeling and Simulation Core and Field Scales

- Reservoir Modeling Activities
- Development of the UW-team Simulator

## Reservoir Modeling Activities (Task 5)

- Relative permeability hysteresis
  - Construction of a mathematical model of two-phase relative permeability hysteresis measured experimentally at deep reservoir conditions
  - Analysis of its wave structure, by solving the associated Riemann problem, and development of an appropriate numerical procedure for its simulation
  - o Code verification

## Reservoir Modeling Activities Relative Permeability Hysteresis

• Two-phase relative permeability functions constructed to fit the experimental data



Brine saturation (x) vs. permeabilities (y).

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## Reservoir Modeling Activities Relative Permeability Hysteresis

- Mathematical analysis (Riemann solutions) vs. numerical solutions
- Fully nonlinear system describing mass conservation and hysteresis effects
- o Example:
- Gravity points to the left
- Solution: Stationary discontinuity and a right-propagating shock

 Naive numerical schemes: incorrect answer



## Development of the UW-team simulator

(Tasks 6 and 7)

- Multi-phase, multi-component, compositional model for CO<sub>2</sub> injection development
- To be used both at the core scale (model validation) and field scale (prediction of injected CO<sub>2</sub> location)
- Educational tool: code development (graduate course developed and taught), HPC

## Development of the UW-team simulator Strategy for discretization

### • Operator splitting:

- The problem is decomposed into components representing relatively simple physics
- Accuracy: adequate numerical methods for distinct PDEs
- Computational efficiency: distinct time steps for distinct physical processes

Example: 2-phase flows



## Development of the UW-team simulator Numerical methods

- Locally conservative procedures:
- Hyperbolic systems: Explicit, high-resolution Central Schemes
  - o Riemann solvers not needed
  - Naturally parallelizable in CPU-GPU machines
  - Correct solutions: hysteresis

### • Elliptic and parabolic problems: Mixed finite elements

- Accurate velocity fields in the presence of rapidly varying coefficients
- Parallelization through multiscale mixed methods in CPU-GPU machines

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## Development of the UW-team simulator Model validation: Bayesian framework

### • Context

- o Characterization at the mm scale
- Prediction at the core scale
- Goal: validation of the compositional model at the Darcy scale against experimental data

### • The framework for UQ: MCMC/MC

- Static data: porosity field at the mm scale (perm. field unknown)
- Dynamic data: saturation fields at the mm scale, pressure drop, production curve

## Development of the UW-team simulator Model validation: Bayesian framework

Reservoir-conditions drainage experiment





### Simulation results



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