Update of the U.S. DOE CCSI\textsuperscript{2} Projects

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CSLF Technical Group Meeting
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CCSI$^2$: Accelerating Rate of RD&D

Rapidly synthesize optimized processes to identify promising concepts → Better understand internal behavior to reduce time for troubleshooting → Quantify sources and effects of uncertainty to guide testing & reach larger scales faster → Stabilize the cost during commercial deployment

National Labs

Academia

Carnegie Mellon

Industry
Carbon Capture Simulation for Industry Impact

• **Overview**
  • 50+ personnel accelerating CCS technology understanding and development
  • Engagement with International Test Center Network (ITCN) and ~50 Industrial/Academic Stakeholders

• **Industrial Collaborations**
  • CCSI² Supports 10 CO₂ Capture Program projects $60MM+ in total project value (TRL 3-7)
    - Three DOCCSS projects, four Developers Testing at TCM, LLNL MECS Technology, UT Austin AFS, UKy Process Control, ORNL Advanced Manufacturing
  • Additional external industrial agreements (executed or in progress)
    - GE, ADA-ES, Test Centre Mongstad (TCM), SINTEF

• **CCSI² Operational Strategy and Mission**
  • Integrates National Lab Expertise, Industrial Perspective and advanced modeling and optimization for most effective R&D guidance
LBNL Metal Organic Framework (MOF)

- **Material: Step Isotherm**
  - Amine Functionalization results in cooperative CO₂ adsorption
  - **Extremely rapid adsorption** – step change in loading
  - **Extremely rapid heat liberation**

- **Equipment Design Conclusions**
  - Heat accumulation undermines performance
  - Bed breakthrough times can be increased by ~4X with ideal design
  - LBNL MOF competitive with MEA

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Conclusions: LBNL MOF Sorbent

• Isothermal operation of the fixed bed system can reduce the capital cost by about 3-4 times in comparison to the adiabatic operation.

• Techno-economic analysis shows potential to improve when compared to traditional MEA system:
  – **Fixed bed system**: cooling during adsorption can improve EAOC by about 10% in comparison to adiabatic adsorption.
  – **Fixed bed system**: cooling during adsorption and 35% heat recovery result in similar EAOC as the MEA system.
  – **Moving bed system**: 13.8% decrease in EAOC compared to the MEA system under nominal cost calculation.
  – Different contactor technology with rigorous optimization is expected to reduce costs further.

• **Thermal management is the key to achieve the optimal performance out of the MOF technology**.
Solvent capture mechanism: Gyroid geometry

**Original LLNL gyroid geometry**
- Channel size: ~4.5 mm
- Surface/volume: 614 1/m
- Low viscosity solvent: 2.5 cp

**Findings:**
- Rivulet flow at low flowrates – **poor wetted area**
- Solvent blocks the channel at medium/high flow rate – **poor interfacial area**
- Geometry/solvent mismatch – **Poor CO₂ absorption**
Improvement via Geometry Manipulation

Modified gyroid geometry
- Channel size: ~9 mm
- Surface volume ratio: 307 m^3/m
- Highly viscous solvent: 25 cp

Findings:
- Higher viscosity results in film flow, better for mass transfer
- No solvent blockage observed
- Geometry induced film thickness fluctuation begins at high flow rate (~200 m^3/m^2/h)
Sample No. represents variation in input variables:

- Liquid Flowrate
- Flue Gas Flowrate
- Lean Loading
- CO₂ Percentage in Flue Gas

**Capture Range**

- 80-95% CO₂

**DoE Results**

- Precision shown at 2\textsuperscript{nd} iteration – ~2 weeks
- Remaining uncertainty attributed to thermodynamic model

**50-70% Reduction in CO₂ Capture Prediction Uncertainty**
Maximize the learning at each stage of technology development

- **Early stage R&D**
  - Screening concepts
  - Identify conditions to focus development
  - Prioritize data collection & test conditions

- **Pilot scale**
  - Ensure the right data is collected
  - Support scale-up design

- **Demo scale**
  - Design the right process
  - Support deployment with reduced risk
Complete Toolset Available at: github.com/CCSI-Toolset

**FOQUS** - Framework for Optimization and Quantification of Uncertainty and Surrogates

**CFD Models**: High fidelity device scale Computational Fluid Dynamics (CFD) models

**Oxy-Combustion Models**: Boiler model and a suite of equation-based models

**Process Models**: A suite of process models implemented in gPROMS, Aspen Custom Modeler, Aspen Plus and Aspen Plus Dynamics

Many more...
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CCSI²
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- Dr. David Heldebrant

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- Dr. Josh Stolaroff
For more information:
https://www.acceleratecarboncapture.org/

For Toolset:
github.com/CCSI-Toolset

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Objective: Building tools and improving the science base to address key questions related to environmental impacts from potential release of CO$_2$ or brine from the storage reservoir, and potential ground-motion impacts due to injection of CO$_2$. 

Technical Team

Stakeholder Group

BP

University of Utah

Battelle

USGS

Southern Company

NRDC

Global CCS Institute

United Carbon Sequestration Council
NRAP Phase I Accomplishments

Assessing environmental risk and quantifying uncertainties in risk performance at CO₂ storage sites

- Generated the first publicly available quantitative, site-specific risk profiles for a complete CO₂ storage system
- Created the first comprehensive risk model for induced seismicity
- Characterized the behavior of key risk metrics associated with pressure and plume sizes for a wide variety of reservoir conditions
- Developed a toolset used to address leakage impacts and ground motion from underground storage of CO₂
- Developed and applied a novel approach for using reduced-order modeling to quantify uncertainty in subsurface systems
- Identified no-impact thresholds for groundwater quality
- Reduced uncertainty in understanding leakage pathways through experimental studies
NRAP Phase I Products

Virtual Special Issue of International Journal of Greenhouse Gas Control with 54 articles considering aspects of:

- Reservoir response and plume evolution.
- Fluid migration through leakage pathways.
- Groundwater impacts.
- Atmospheric leakage.
- System integrated assessment.
- Strategic monitoring.
- Ground motion/induced seismicity.

Using Science-Based Prediction to Probe Reservoir Behavior

NRAP Tools Available at: www.edx.netl.doe.gov/nrap
NRAP Phase II Technical Focus

Managing environmental risk and reducing uncertainties in risk performance at CO₂ storage sites

- Containment assurance
- Induced seismicity risk
- Strategic monitoring for better system design
- Applying and validating risk assessment tools and methodologies using synthetic and field data
Containment Assurance

Developing robust, science-based workflows and software tools to:

• *predict* containment effectiveness and leakage risk
• *evaluate* the effectiveness of leakage risk monitoring, management, and mitigation.

• NRAP OpenIAM now in Beta testing.
• Workflows release target August 2019.
Next-generation Integrated Assessment Model (NRAP-OpenIAM)

Combined ensemble and statistical visualization of system model output

Graphic representation of system model parameter/output correlations

Building confidence in GCS Conformance using robust decision analysis

Building confidence in PISC by plume stability analysis

Constraining system model output and reducing uncertainty by model updating using MCMC

Evaluating the uncertainty of plume stability through ensemble analysis

Plume mobility

Plume spreading
Developing practical tools to assess and manage induced seismicity risk at carbon storage sites and identify site characteristics and operational approaches to lower seismic risk.

- Probabilistic seismic risk forecasting tool generated.
- State of Stress tool available.
Induced Seismicity Risk Tool Catalog

State-of-Stress Assessment Tool

Joint probability for $\sigma_H$ and $\sigma_h$

Probability of activating critically-oriented fault

Probabilistic Seismic Risk Assessment Tool

Short Term Seismic Forecasting (STSF) Tool
Developing insights, methods, and tools to understand the ability of monitoring technologies to detect system behavior, in the context of uncertainties in system features, events, and processes.

• Version 2 monitoring design tool DREAM (beta) released.
- DREAM v2 ERT module Beta released
- Considers both remote and point source monitoring parameters
- More flexible user input including compatibility with NRAP-OpenIAM output

Risk-Based Monitoring Network Design

Probability of detection using monitoring response

Proposed monitoring well locations

Two-stage monitoring design solution

Toward an adaptive monitoring design for leakage risk – Closing the loop of monitoring and modeling

Yu-Mei Yang\(^{1,2}\), Robert M. Dilmire\(^3\), Grant S. Bromhal\(^3\), Mitchell J. Small\(^3\)
Validation and Use of Risk Assessment Tools and Methodologies

Enabling the adoption of NRAP tools and methods for large-field demonstration projects and validating the tools and the science-based risk assessment approach.

• Tools used in >15 planned or existing projects
  – 7 CarbonSAFE projects; CaMi, IBDP, Farnsworth, OK water injection, ITRI, and more
Using a risk-based approach to justify closure at a GCS site

**Purpose:** To provide a technical basis for a cost-effective and safe closure of GCS projects, using a risk-based approach as opposed to a default monitoring period.

**Key Learnings:**
- Monitoring during injection yields a better understanding of reservoir performance and builds confidence in safe, long-term storage.
- Drivers for leakage decrease once injection stops.
- PISC period can be reduced for many storage reservoir systems.
Additional Workflows
**State-of-Stress Assessment Tool (SoSAT)**

<table>
<thead>
<tr>
<th><strong>Input data available</strong></th>
<th><strong>Joint probability for $\sigma_H$ and $\sigma_h$</strong></th>
<th><strong>Probability of activating critically-oriented fault</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>• Pore pressure</td>
<td><img src="image1" alt="Joint probability graph" /></td>
<td></td>
</tr>
<tr>
<td>• Overburden density</td>
<td><img src="image2" alt="Joint probability graph" /></td>
<td></td>
</tr>
<tr>
<td>• Regional stress indicators</td>
<td><img src="image3" alt="Joint probability graph" /></td>
<td></td>
</tr>
<tr>
<td>• Geodetic data</td>
<td><img src="image4" alt="Joint probability graph" /></td>
<td></td>
</tr>
<tr>
<td>• Local measurement of $\sigma_h$</td>
<td><img src="image5" alt="Joint probability graph" /></td>
<td></td>
</tr>
</tbody>
</table>

Probabilistic Seismic Risk Assessment Tool (RiskCat)

## MISSION

Ensure Permanence – Protect Environment – Facilitate Awareness – Improve Storage Efficiency – Commercial-Readiness by 2030

### Program Approach & Technical Accomplishments

<table>
<thead>
<tr>
<th>ADVANCED STORAGE</th>
<th>STORAGE INFRASTRUCTURE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monitoring, Verification, and Accounting</td>
<td>Regional Carbon Sequestration Partnership</td>
</tr>
<tr>
<td>Geologic Storage, Simulation, and Risk Assessment</td>
<td>Onshore and Offshore Characterization, Brine Extraction Storage Tests (BEST), and CarbonSAFE – NETL – Industry – Universities – National Labs–</td>
</tr>
</tbody>
</table>

For more information, please visit the Carbon Storage Program web page at: https://www.netl.doe.gov/coal/carbon-storage
Using Science-Based Prediction to Probe Reservoir Behavior and the Reservoir Evaluation and Visualization (REV) tool

- **Size of CO₂ plume injection**
  - Rate of growth for early phase
  - Rate of growth for long-term phase
  - Plume radius at end of injection

- **Size of pressure plume**
  - Maximum size of plume
  - Various pressure thresholds, relevant
    - Brine rise
    - Fault-slip criteria

- **Pressure at a location**
  - Maximum pressure increase

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**Size of CO₂ Plume**
- Injection period
- Post-injection period
- \( R_i \) — plume size (radius) at end of injection
- \( m_1 \) — growth rate for early phase
- \( m_2 \) — growth rate for long-term phase

**Size of Pressure Plume**
- Injection period
- Post-injection period
- \( R_{\text{max}} \) — maximum size of plume for a specific pressure increase

**Pressure at a Location**
- Injection period
- Post-injection period
- \( \Delta P_{\text{max}} \) — maximum pressure increase
- \( t_{0.5} \) — time for pressure to decay to 0.5\( \Delta P_{\text{max}} \)
GCS Site Closure Products

- Bacon, Yonkofski, Brown, Demirkanli, Whiting. Risk-based Post Injection Site Care and Monitoring for Commercial-Scale Carbon Storage: Reevaluation of the FutureGen 2.0 Site using NRAP-IAM-CS v2 and DREAM. submitted to IJGGC
- Yang, X., Buscheck, T. A., Mansoor, K., Carroll, S. A. Assessment of Geophysical Monitoring Methods for Detection of Brine and CO2 Leakage in Drinking Aquifers. submitted to IJGGC
- Carroll, Yang, Mansoor, Buscheck, Wang, Huang, Appriou, “Integration of monitoring data to reduce risk uncertainty and to define site closure. International J. Greenhouse Gas Control, planned submission
- Harp, D., Oldenburg, C., Pawar, R. A metric for evaluating conformance robustness during geologic CO2 sequestration operations. accepted by IJGGC
- Pawar, R., Chu, S., Makedonska, N., Onishi, T., Harp, D. Assessment of relationship between post-injection plume migration and leakage risks at geologic CO2 storage sites. submitted to IJGGC
- Harp, D., Ohishi, T., Chu, S., Chen, S., Pawar, R. Development of quantitative metrics of plume migration at geologic CO2 storage sites. submitted to Greenhouse Gas Science
- Doughty, C. and Oldenburg, C.M. CO2 Plume Evolution in a Depleted Natural Gas Reservoir: Modeling of Conformance Uncertainty Reduction Over Time. in preparation to be submitted to IJGGC
- Dilmore, R.; Bacon, D; Bromhal, G.; Brow, C.; Carroll, S.; Doughty, C.; Harp, D; Huerta, N.; Oldenburg, C.; Pawa, R.; Toward Robust and Resilient Geologic Carbon Storage: Insights from System Modeling and Integrated Risk Assessment Supporting Safe Site Closure. in preparation to be submitted to PNAS
CCSI² Sequential Experimentation: Optimal Test Conditions

- Initially-assumed parameter distributions
- G-optimality criterion
- Model Refinement
- FOQUS
- Outputs: Updated parameter distributions
- Batch Tests
- Outputs: Data

CCSI² Sequential Experimentation

G-optimality criterion

CCSI² Sequential Experimentation

G-optimality criterion
Conclusions: LLNL Reactor Geometry

• Gyroid geometry can be manipulated to improve solvent flow and interfacial area
• Solvent viscosity affects the interface area at different flow rates
• Higher viscosities $\rightarrow$ film flow $\rightarrow$ improved mass transfer

Future Work

• Geometry design to optimize countercurrent gas/solvent flow and heat transfer for MEA
• Apply framework to CO$_2$BOL
• Characterize performance as a function of geometry and solvent characteristics
Task 2.2: CFD Validation Effort

Packed column
- Column diameter: 100 mm
- Column height: 200 mm
- Number of rings: 160

Design of pall ring
- Diameter: 16 mm
- Height: 16 mm
- Thickness: 0.5 mm
- Specific Area: 282 m²/m³

Solvent Properties (30% MEA)

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m³)</td>
<td>1000</td>
</tr>
<tr>
<td>Viscosity (cP)</td>
<td>2.46</td>
</tr>
<tr>
<td>$D_{CO_2}[L]$ (m²/s)</td>
<td>1.0×10⁻⁹</td>
</tr>
<tr>
<td>$D_{CO_2}[S]$ (m²/s)</td>
<td>1.0×10⁻⁵</td>
</tr>
<tr>
<td>Reaction Rate</td>
<td>5.96</td>
</tr>
<tr>
<td>Henry's constant (Dimensionless)</td>
<td>1.228</td>
</tr>
</tbody>
</table>

Surface Tension (N/m) 0.065
Contact angle (°) 40

Dash Line: $A = 1.16\eta(u_lg^{1/2}a_p^{-3/2}\rho_l/\sigma)^{0.138}$

Optimal Design of Experiments: NCCC Trial

Candidate Points

Points with Experimental Data

Prior Distribution

Width of 95% CI

Sample No.

0 100 200 300 400 500

Next iteration

NEW PRIOR

Width of 95% CI

Sample No.

0 100 200 300 400 500

Posterior Distribution

Width of 95% CI

Sample No.

0 100 200 300 400 500

50-70% Reduction in CO₂ Capture Prediction Uncertainty (18 total runs)
Task 2.1: Fixed Bed Results

- Large temperature spikes due to high heat of adsorption and poor heat removal from the system
- Thermal management can considerably increase performance
  - $t_b$, non-intensified = 22.7 min
  - $t_b$, intensified = 80.4 min

Operating Conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure (bar)</td>
<td>1.1</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>25</td>
</tr>
<tr>
<td>Flow rate (mol/s)</td>
<td>120</td>
</tr>
<tr>
<td>$Y_{CO2}$</td>
<td>0.132</td>
</tr>
<tr>
<td>$Y_{H2O}$</td>
<td>0.055</td>
</tr>
<tr>
<td>$Y_{N2}$</td>
<td>0.813</td>
</tr>
<tr>
<td>Bed Length (m)</td>
<td>10</td>
</tr>
<tr>
<td>Bed Diameter (m)</td>
<td>3</td>
</tr>
</tbody>
</table>

High temperature = poor use of potential working capacity
Task 2.1: Moving Bed Results

- **Moving Bed**
  - More effective at cooling bed, lower cost

- **Practical Issues**
  - High heat recoveries required to compete with MEA
  - Sorbent attrition may offset cost savings in moving bed operation

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![Graphs showing Fixed Bed and Moving Bed Costs](image-url)

- **Fixed Bed Costs**
  - 85% Heat Recovery

- **Moving Bed Costs**
  - ~35% Heat Recovery (Practical)

- MEA Comparison: -9.8%

- MEA Comparison: -13.8%
Task 2.2: PNNL CO$_2$BOL Low Aqueous Solvent

- **Technology**
  - Low Aqueous Solvent
  - Polarity swing-assisted regeneration
  - Anti-solvent

- **Multi-scale modeling**
  - CO$_2$BOL Solvent
  - Equipment
  - System

- **Objective**
  - Elucidate solvent/packing interactions
  - Proper absorber optimization