Update of the U.S. DOE CCSI² Projects

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National Energy Technology Laboratory/AristoSys, LLC

CSLF Technical Group Meeting

April 26, 2019

CCSI²: 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

Berkeley Lab
Pacific Northwest National Laboratory
National Energy Technology Laboratory
Los Alamos National Laboratory
Lawrence Livermore National Laboratory

Academia

Carnegie Mellon
Princeton University
West Virginia University
Boston University
The University of Texas at Austin
CAER

Industry

Google
ADA Environmental Solutions
Alstom
B&W
GE
CO2 Technology Centre Mongstad
Fluor
Phillips 66
AEP American Electric Power
EPRI Electric Power Research Institute
Southern California Edison
Southern Company
ExxonMobil
Chevron
URS
Air Products
Eastman
aspentech
ANSYS
Schneider Electric
PSE
NCCC National Carbon Capture Center

Carbon Capture Simulation for Industry Impact

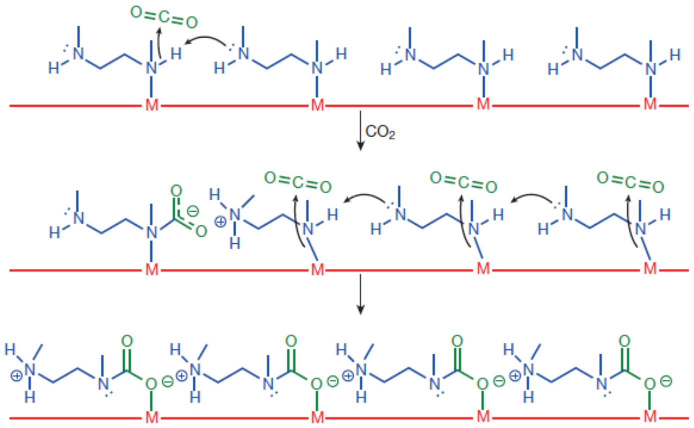
- **Overview**
  - **50+ personnel** accelerating CCS technology understanding and development
  - Engagement with International Test Center Network (ITCN) and **~50 Industrial/Academic Stakeholders**

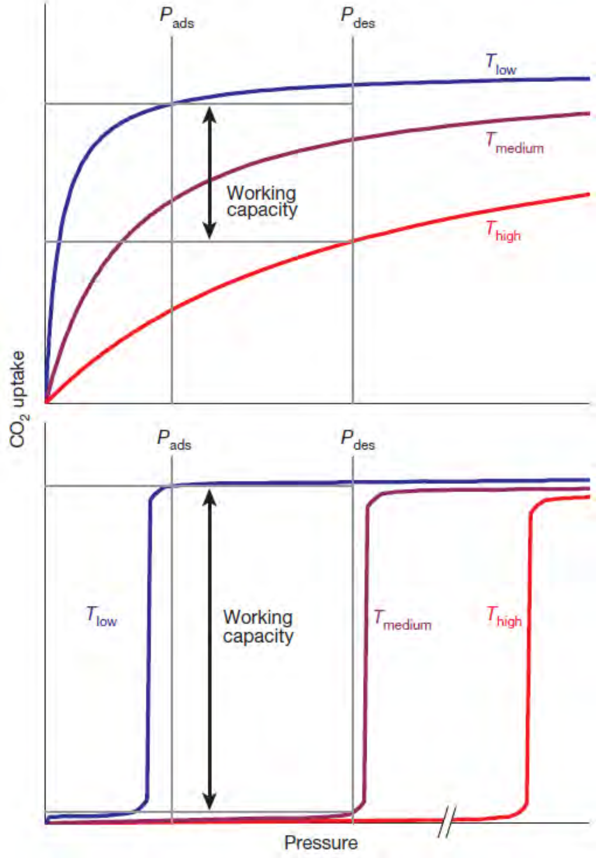
- **Industrial Collaborations**
  - CCSI[2] Supports **10 CO_2 Capture Program projects $60MM+** in total project value (TRL 3-7)
    - Three DOCCSS projects, four Developers Testing at TCM, LLNL MECS Technology, UT Austin AFS, UKy Process Control, ORNL Advanced Manufacturing
  - Additional external industrial agreements (executed or in progress)
    - GE, ADA-ES, Test Centre Mongstad (TCM), SINTEF

- **CCSI[2] 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 CO_2 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**

Siegelman, R.L., McDonald, T.M., Gonzalez, M.I., Martell, J.D., Milner, P.J., Mason, J.A., Berger, A.H., Bhown, A.S., Long, J.R. Controlling Cooperative Adsorption in Diamine-Appended Mg_2(dobpdc) Metal-Organic Frameworks. Journal of the American Chemical Society. 2017; 139, 10526-10538

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

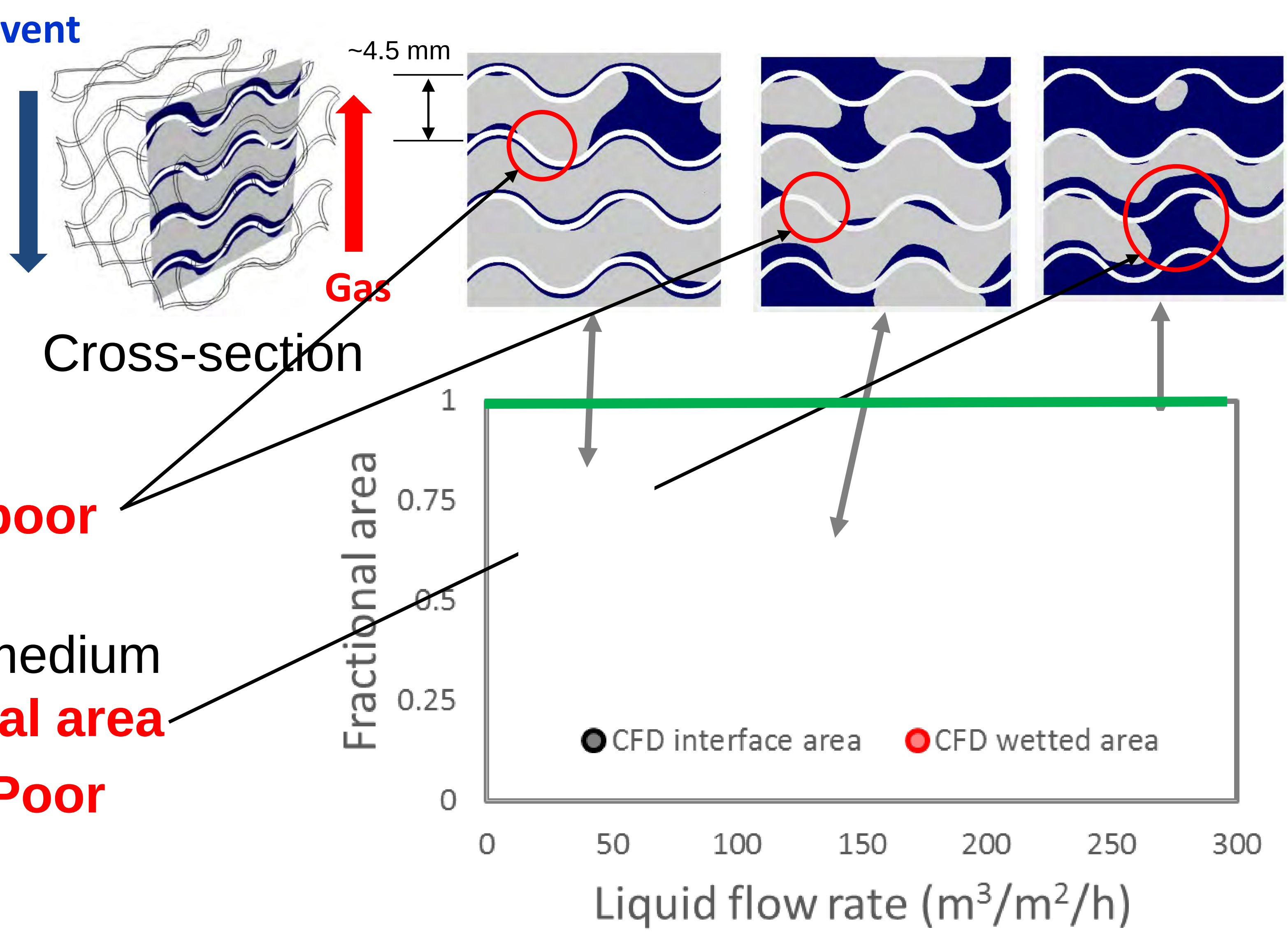
- Techno-economic analysis shows potential to improve when compared to traditional MEA system
  - **Fixed bed system**: cooling during adsorption can improve EAOC by about 10% in comparison to adiabatic adsorption
  - **Fixed bed system**: cooling during adsorption and 35% heat recovery result in similar 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



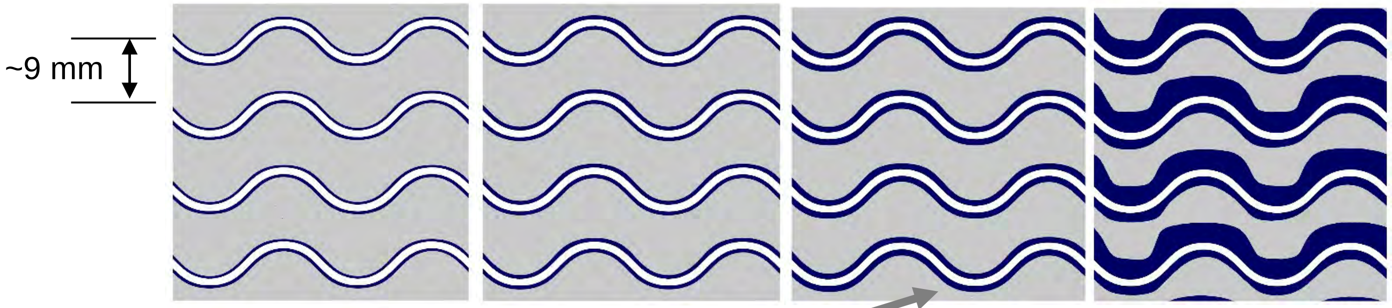
Findings:

- Rivulet flow at low flowrates – **poor wetted area**
- Solvent blocks the channel at medium /high flow rate – **poor interfacial area**
- Geometry/solvent mismatch – **Poor CO_2 absorption**

Improvement via Geometry Manipulation

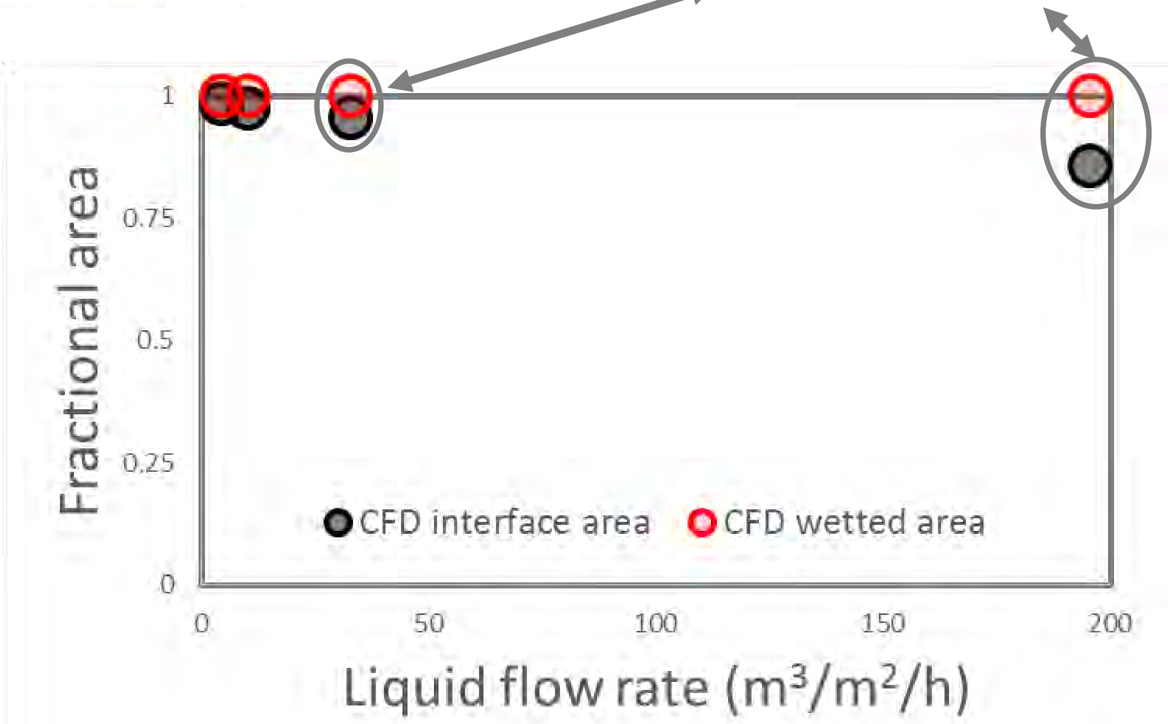
Modified gyroid geometry

- Channel size: ~9 mm
- Surface volume ratio: 307 1/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 $m^3/m^2/h$)



TCM: Bayesian Inference Continues to Improve Model

Sample No. represents variation in input variables:

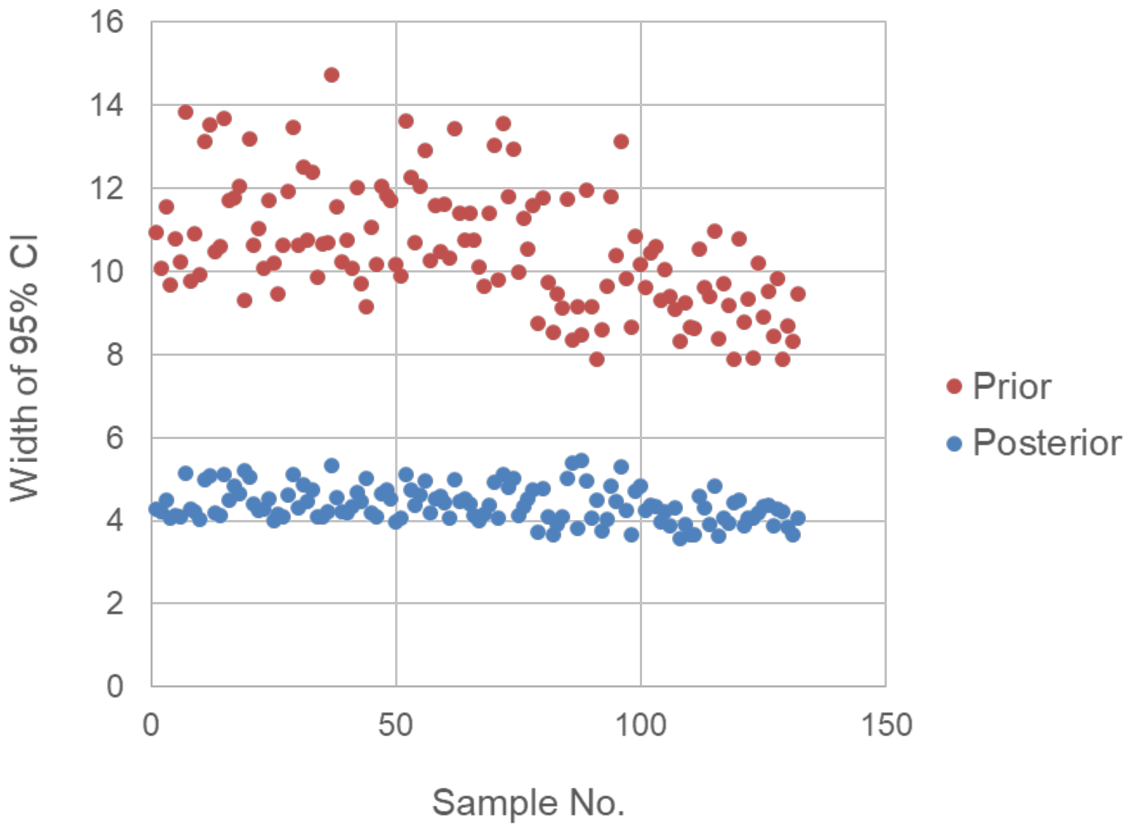
- Liquid Flowrate
- Flue Gas Flowrate
- Lean Loading
- CO_2 Percentage in Flue Gas

Capture Range

- 80-95% CO_2

DoE Results

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



50-70% Reduction in CO_2 Capture Prediction Uncertainty

CCSI Toolset: New Capabilities for Modeling

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

2016 R&D 100 Awards

Complete
Toolset Available at:
github.com/CCSI-Toolset

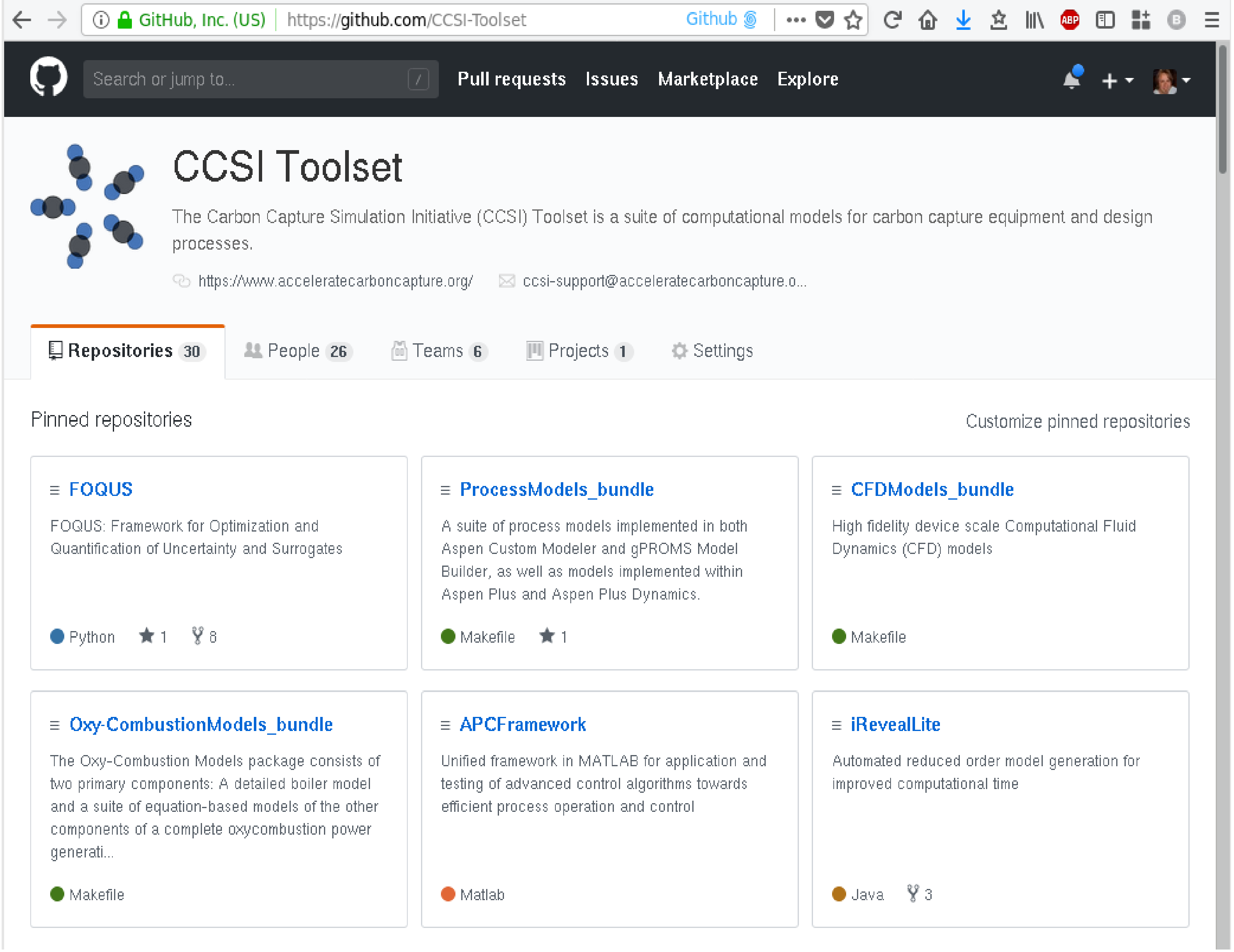
FOQUS - Framework for Optimization and Quantification of Uncertainty and Surrogates

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...



Acknowledgements

CCSI^2

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- Dr. Justin Finn
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- Dr. Jay Xu
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- Dr. Rebecca Siegelmann
- Dr. Tom MacDonald

PNNL DOCCSS

- Dr. Charles Freeman
- Dr. David Heldebrant

LLNL DOCCSS

- Dr. Josh Stolaroff

CCSI^2 Carbon Capture Simulation for Industry Impact | NATIONAL ENERGY TECHNOLOGY LABORATORY | BERKELEY LAB | Lawrence Livermore National Laboratory | Los Alamos NATIONAL LABORATORY EST. 1943 | Pacific Northwest NATIONAL LABORATORY | West Virginia University | THE UNIVERSITY OF TEXAS AT AUSTIN | U.S. DEPARTMENT OF ENERGY

CCSI²
Carbon Capture Simulation for Industry Impact

For more information:
https://www.acceleratecarboncapture.org/

For Toolset:
github.com/CCSI-Toolset

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National Risk Assessment Partnership (NRAP)

Grant Bromhal, Senior Fellow, NETL
Robert Dilmore, Technical Lead, NETL

NATIONAL ENERGY TECHNOLOGY LABORATORY

CSLF Technical Group Meeting

April 26, 2019

Champaign, Illinois

Solutions for Today | Options for Tomorrow

U.S. DEPARTMENT OF ENERGY

National Risk Assessment Partnership

NRAP National Risk Assessment Partnership

NATIONAL ENERGY TECHNOLOGY LABORATORY

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

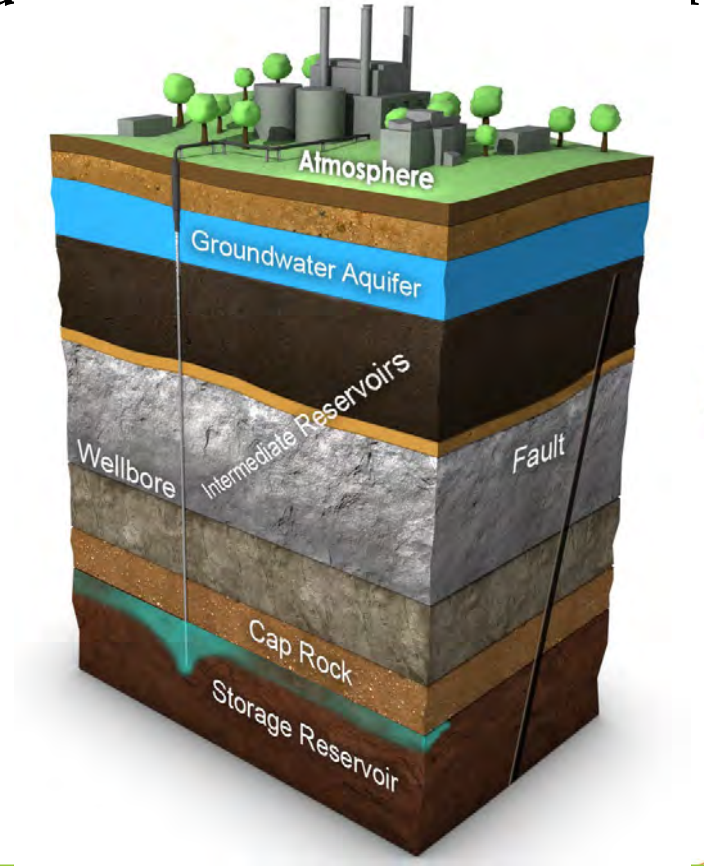
Technical Team

NATIONAL ENERGY TECHNOLOGY LABORATORY

BERKELEY LAB Lawrence Berkeley National Laboratory

Los Alamos NATIONAL LABORATORY EST.1943

Pacific Northwest NATIONAL LABORATORY



Stakeholder Group

PRINCETON UNIVERSITY

THE UNIVERSITY OF UTAH

ILLINOIS

BATTELLE

USGS science for a changing world

bp

GLOBAL CCS INSTITUTE

Southern Company

ieaghg

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

NRDC

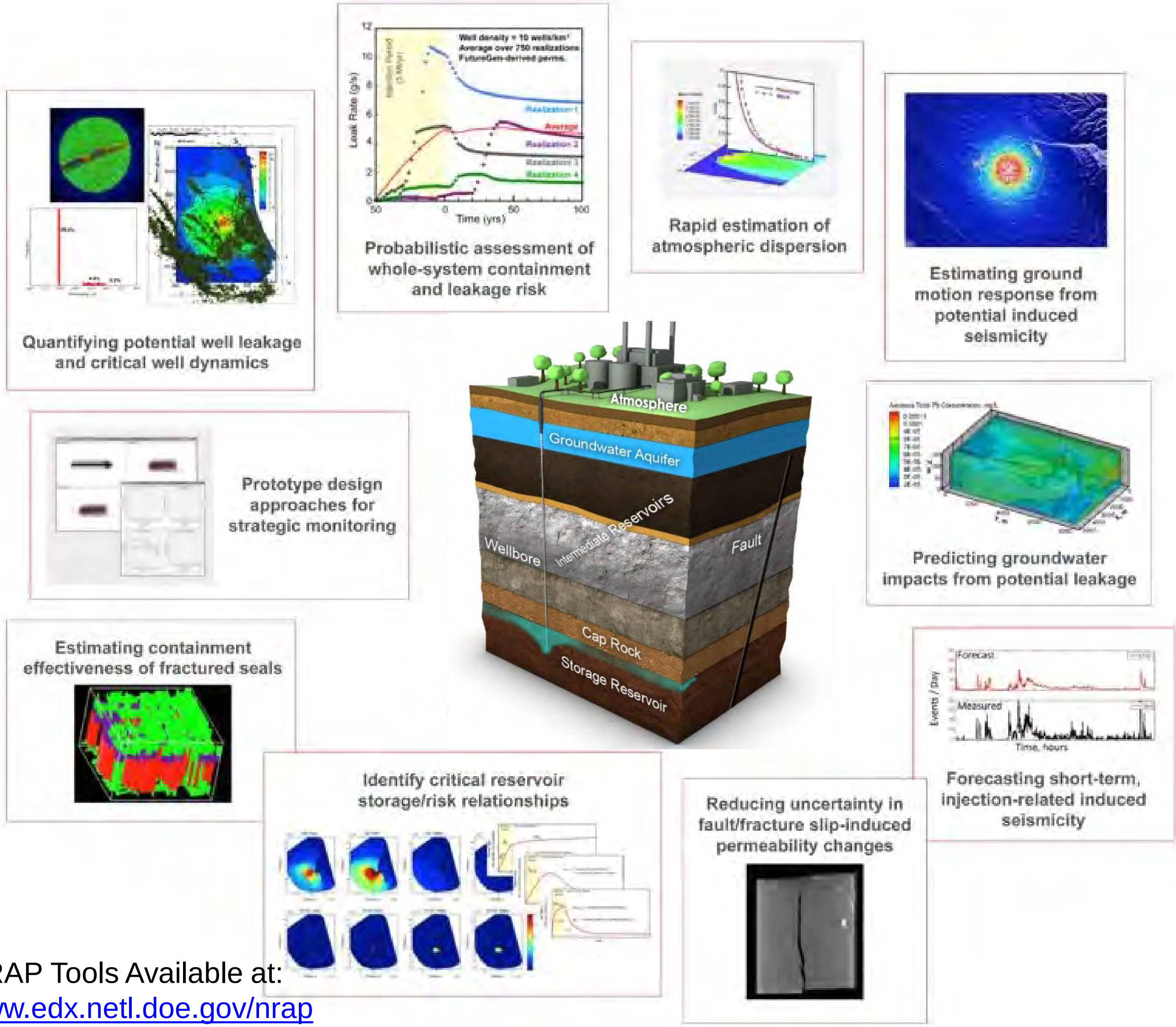
UNITED STATES Carbon Sequestration Council

NRAP Phase I Accomplishments

Assessing environmental risk and quantifying uncertainties in risk performance at CO_2 storage sites

- Generated the first publicly available quantitative, site-specific risk profiles for a complete CO_2 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 CO_2
- 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

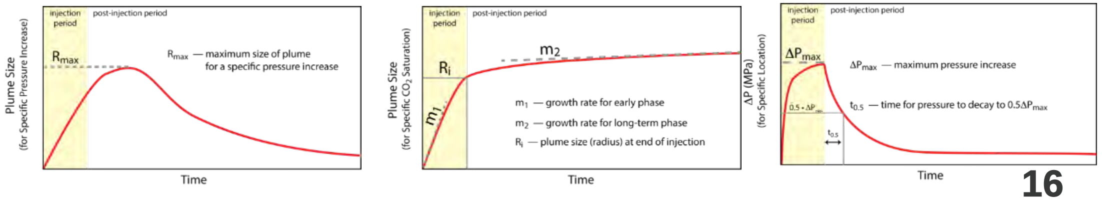
NRAP Phase I Products



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 CO_2 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**

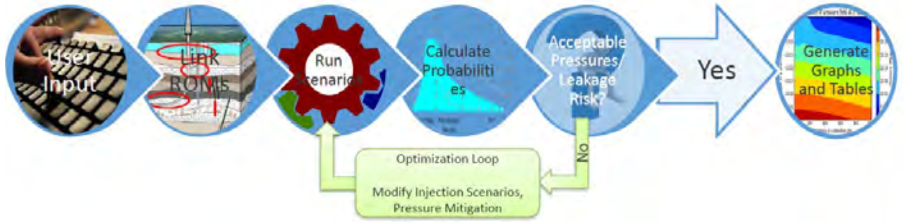
Containment Assurance

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

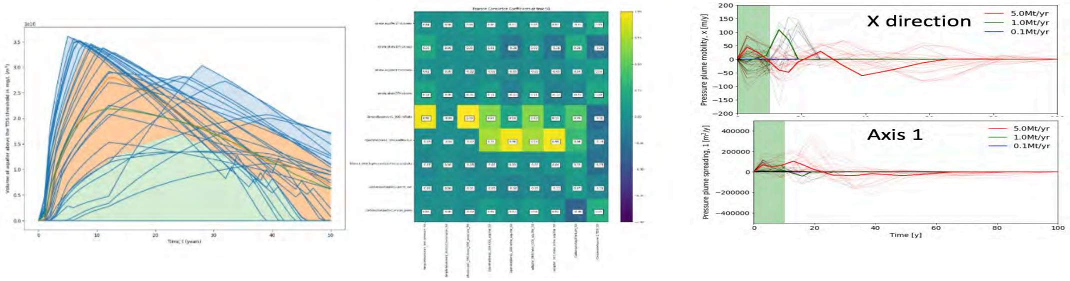
- *predict* containment effectiveness and leakage risk
- *evaluate* the effectiveness of leakage risk monitoring, management, and mitigation.

- *NRAP OpenIAM now in Beta testing.*
- *Workflows release target August 2019.*

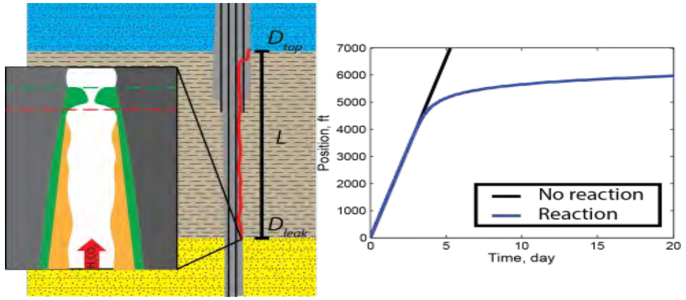
Workflows for risk assessment/risk management



NRAP OpenIAM: ***Developing next-generation Integrated Assessment Model***

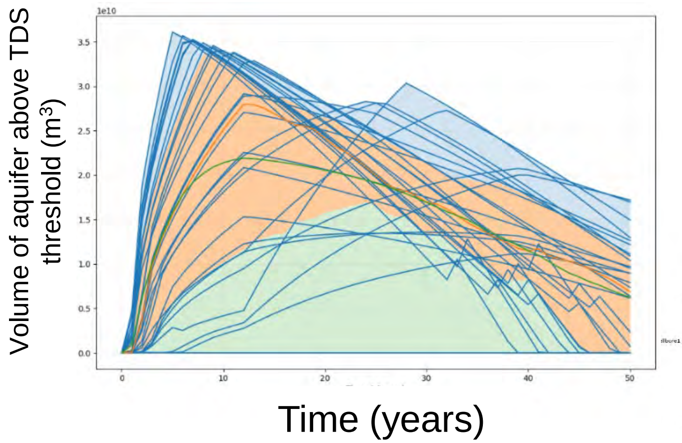


Developing improved characterizations of leakage behavior

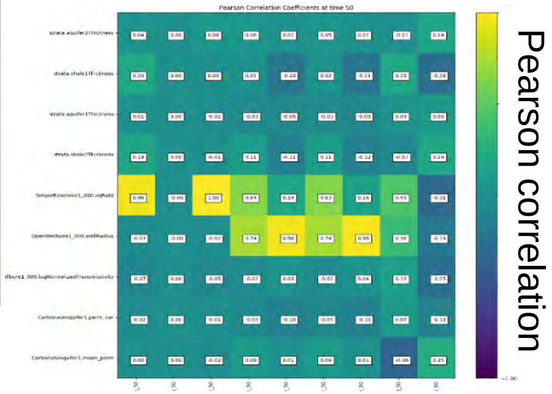


Next-generation Integrated Assessment Model (NRAP-OpenIAM)

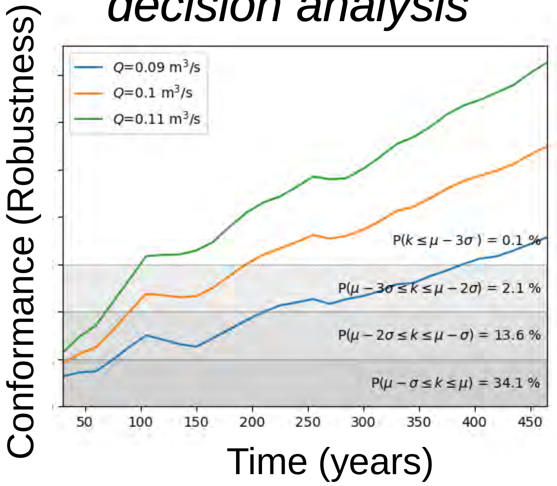
Combined ensemble and statistical visualization of system model output



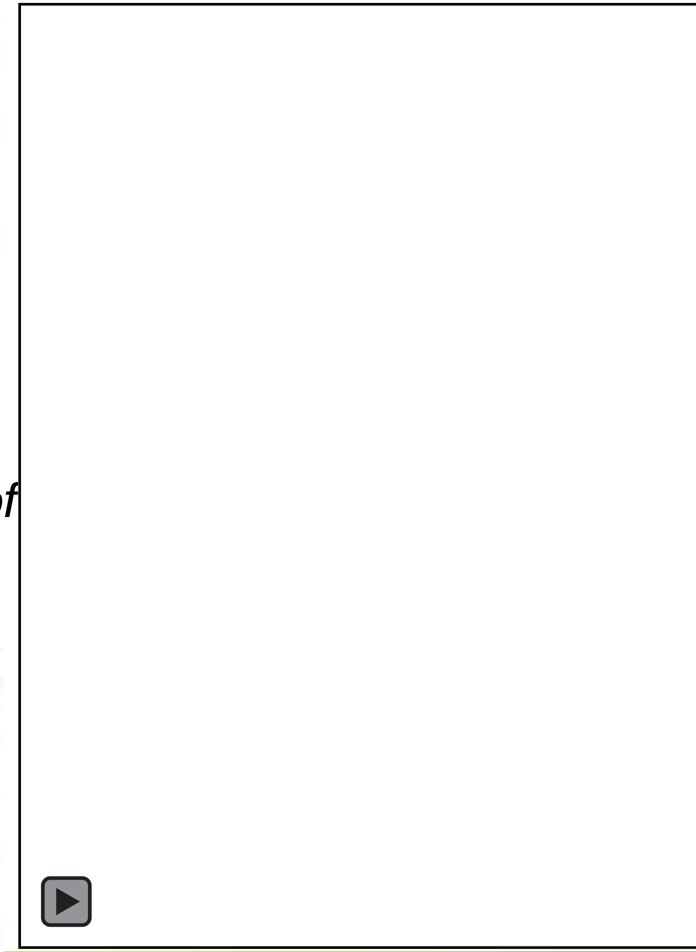
Graphic representation of system model parameter/output correlations



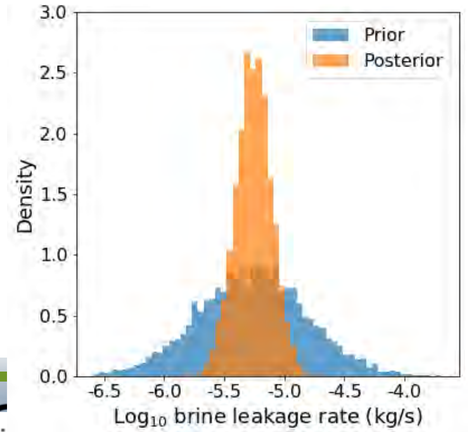
Building confidence in GCS Conformance using robust decision analysis

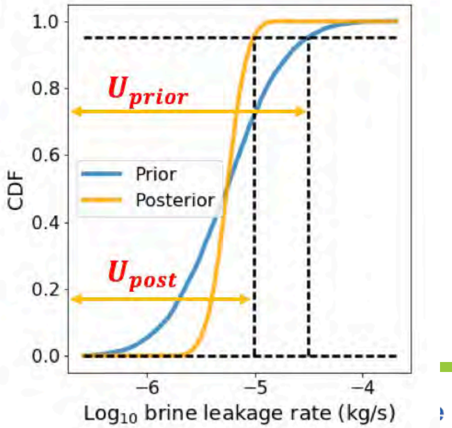


Building confidence in PISC by plume stability analysis

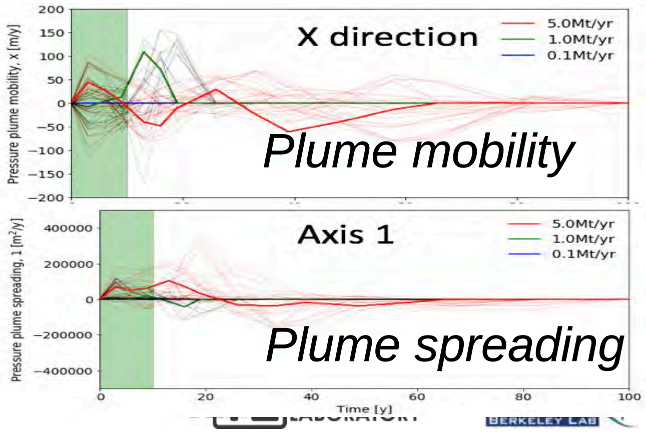


Constraining system model output and reducing uncertainty by model updating using MCMC





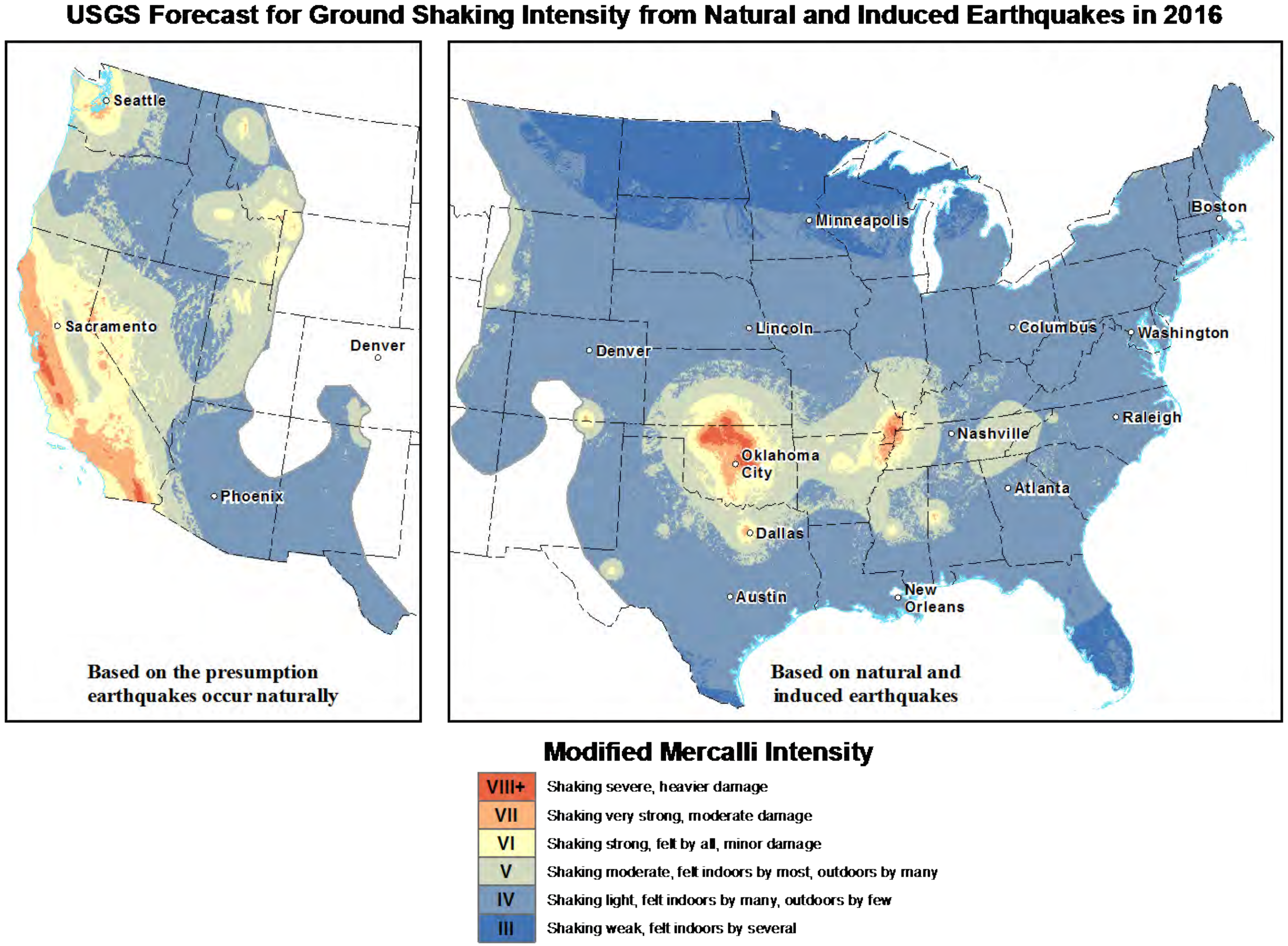
Evaluating the uncertainty of plume stability through ensemble analysis



Induced Seismicity Risk

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.*
- *IS Protocol Document for Carbon Storage target by 2020.*

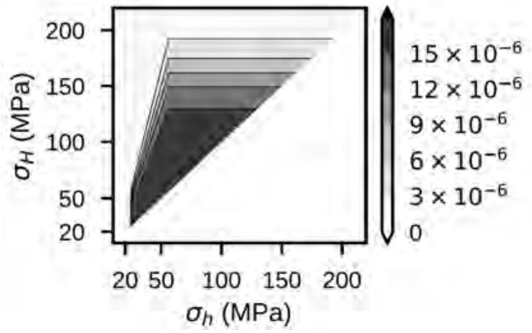


USGS map displaying intensity of potential ground shaking from natural and human-induced earthquakes. There is a small chance (one percent) that ground shaking intensity will occur at this level or higher. There is a greater chance (99 percent) that ground shaking will be lower than what is displayed in these maps.

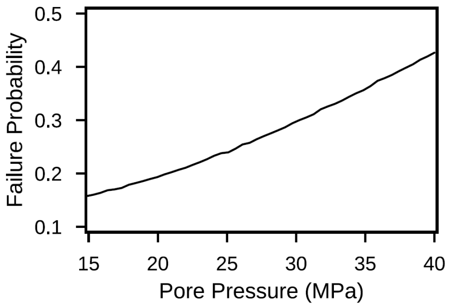
Induced Seismicity Risk Tool Catalog

State-of-Stress Assessment Tool

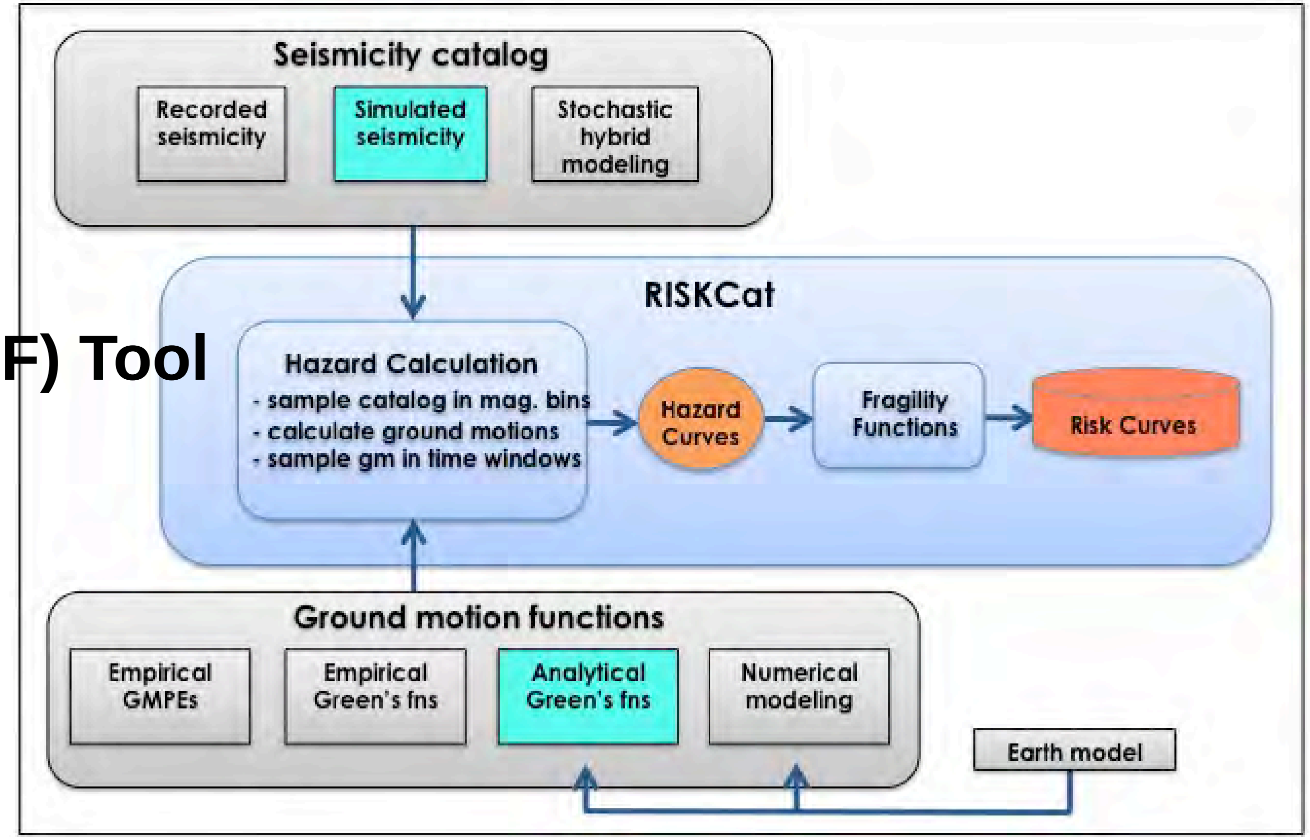
Joint probability for σ_H and σ_h



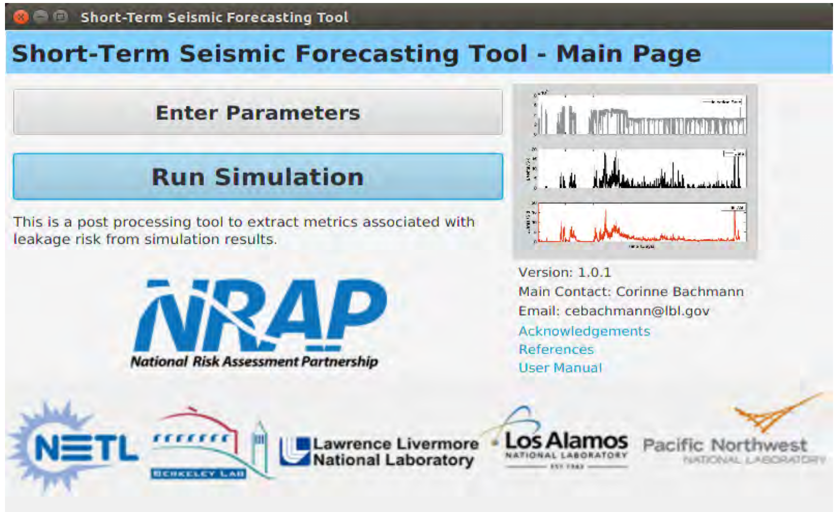
Probability of activating critically-oriented fault



Probabilistic Seismic Risk Assessment Tool



Short Term Seismic Forecasting (STSF) Tool

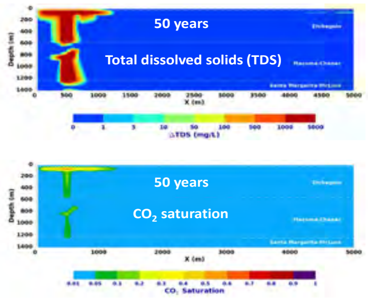


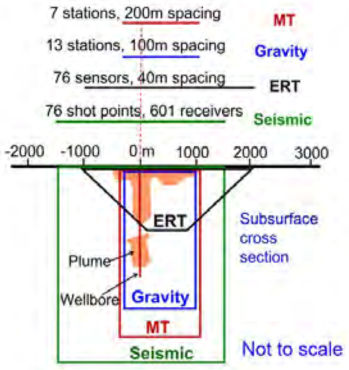
Strategic Monitoring for Uncertainty Reduction

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.

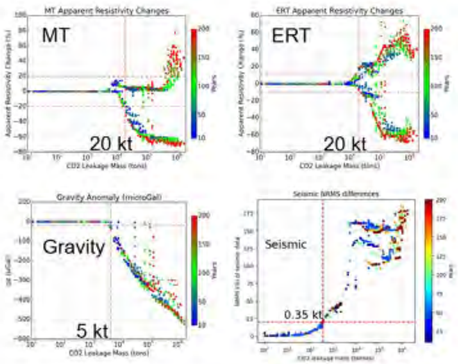
- *Version 2 monitoring design tool DREAM (beta) released.*

Modeling of Geophysical Monitoring

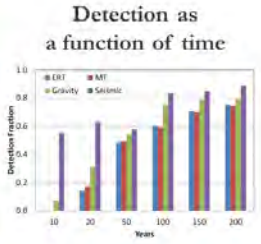




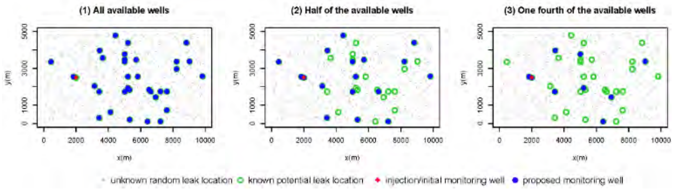
Layout of Surface Geophysical Methods

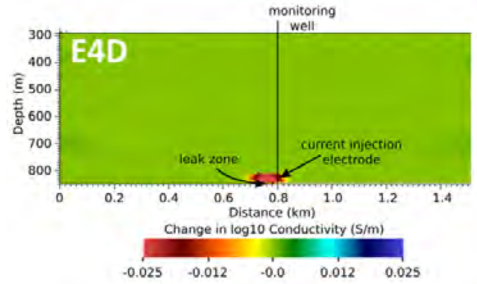


Geophysical signals versus CO_2 leakage mass

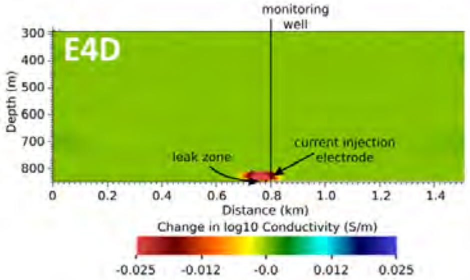


Risk-Based Monitoring Network Design Tools

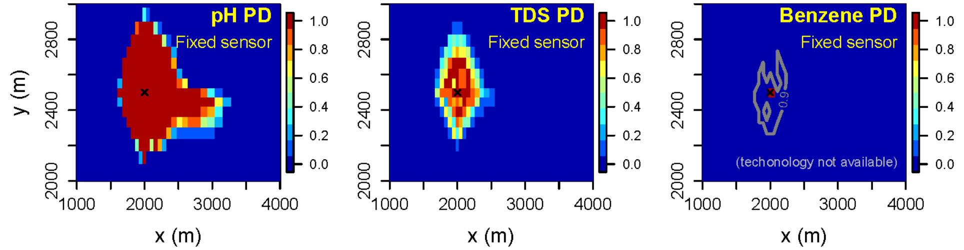




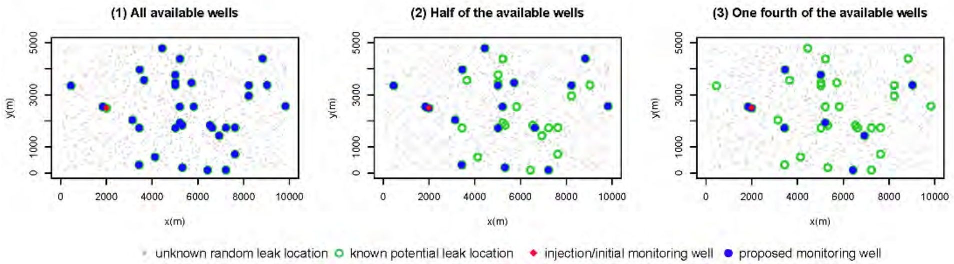
Risk-Based Monitoring Network Design



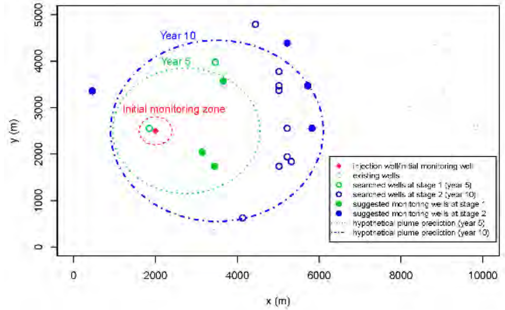
- DREAM v2 ERT module Beta released
- Considers both remote and point source monitoring parameters
- More flexible user input including compatibility with NRAP-OpenIAM output



Probability of detection using monitoring response



Proposed monitoring well locations



Two-stage monitoring design solution

Contents lists available at ScienceDirect

International Journal of Greenhouse Gas Control

journal homepage: www.elsevier.com/locate/ijggc

ELSEVIER

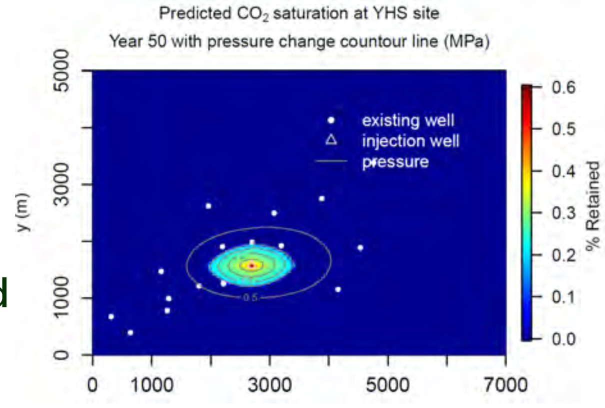
Toward an adaptive monitoring design for leakage risk – Closing the loop of monitoring and modeling

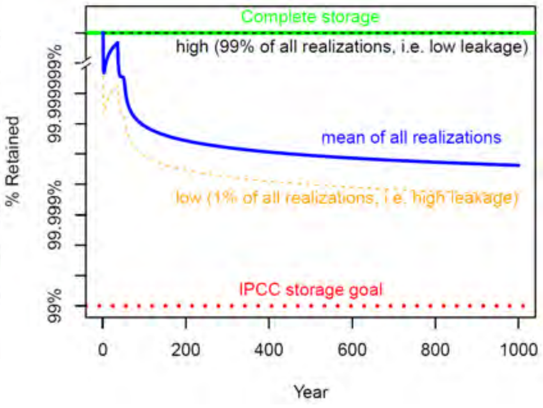
Ya-Mei Yang[a,c,*], Robert M. Dilmore[a], Grant S. Bromhal[a], Mitchell J. Small[b]

Validation and Use of Risk Assessment Tools and Methodologies

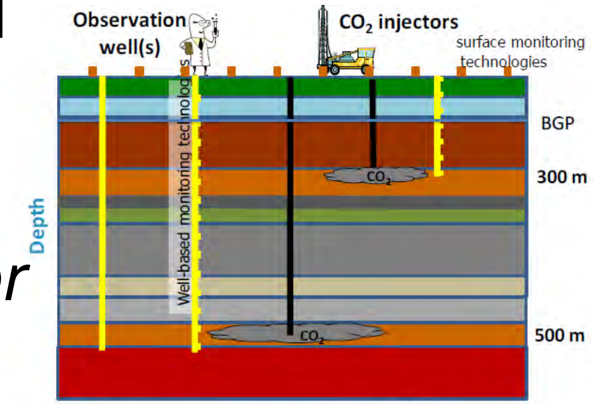
Enabling the adoption of NRAP tools and methods for large-field demonstration projects and validating the tools and the science-based risk assessment approach.

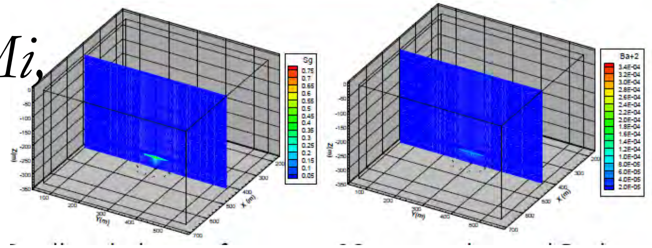
- *Tools used in >15 planned or existing projects*
  - *7 CarbonSAFE projects; CaMi, IBDP, Farnsworth, OK water injection, ITRI, and more*

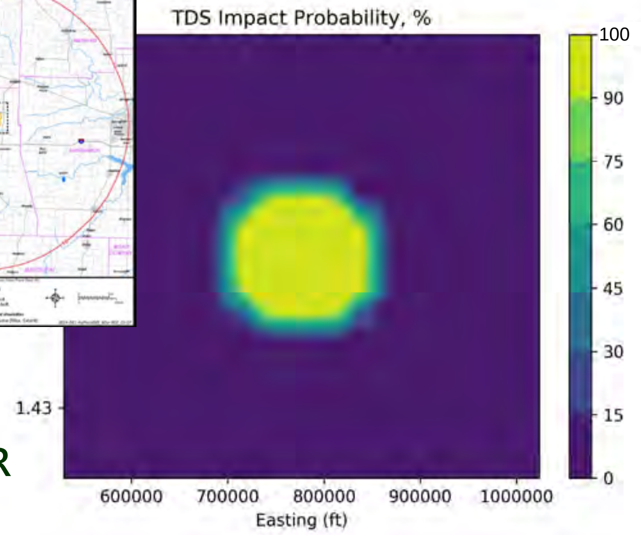




CaMI Field Test Site







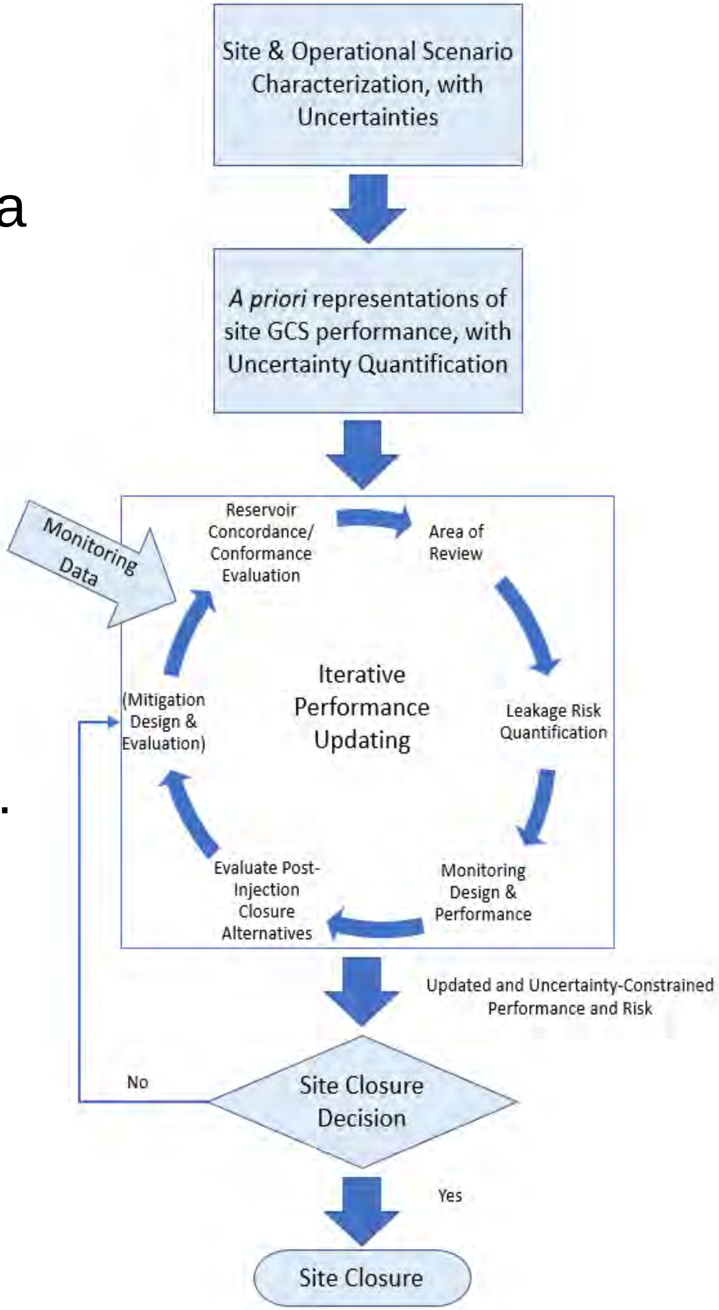
FutureGen 2.0 Risk-Based AOR

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:

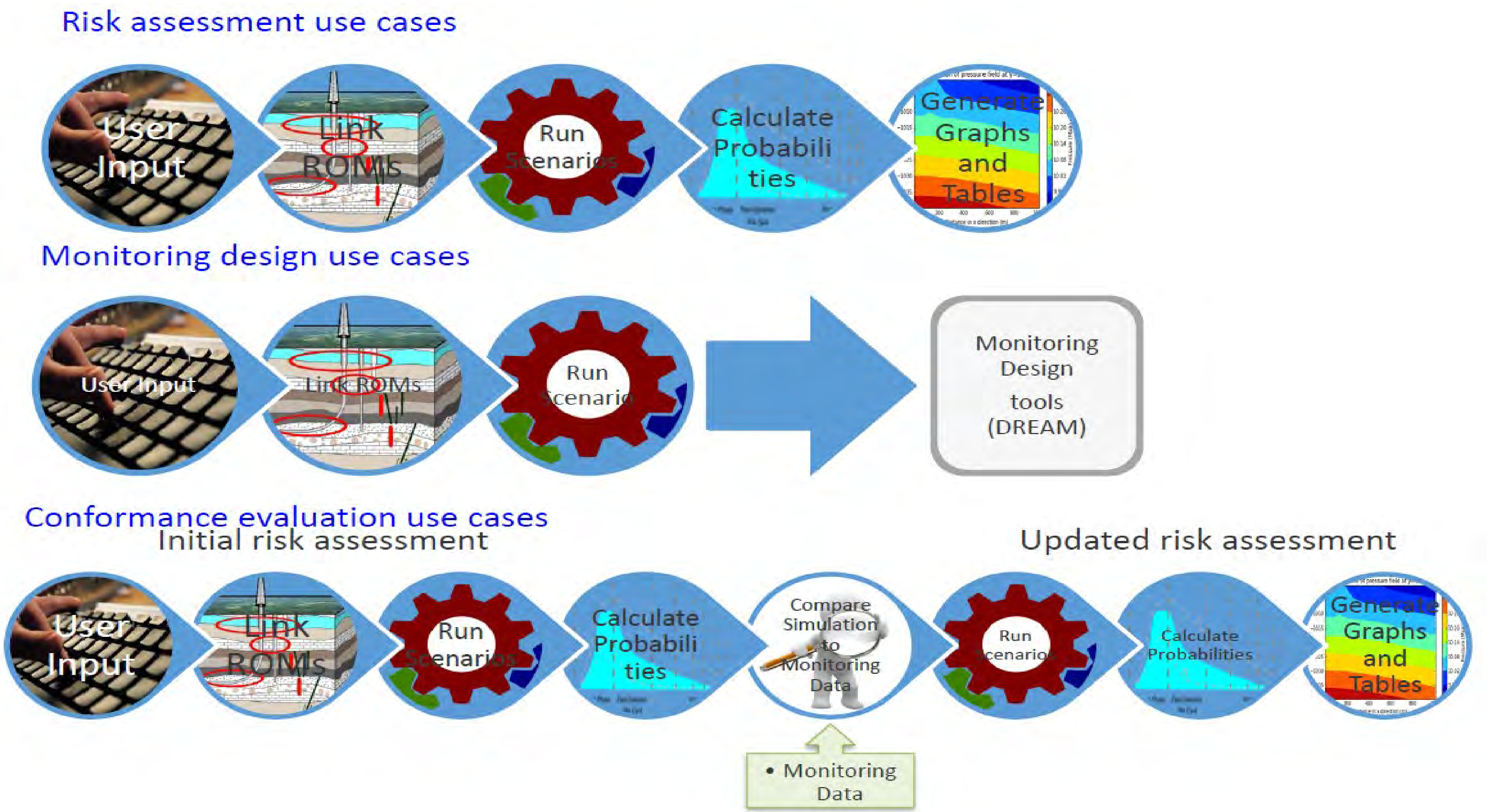
- Monitoring during injection yields a better understanding of reservoir performance and builds confidence in safe, long-term storage.
- Drivers for leakage decrease once injection stops.
- PISC period can be reduced for many storage reservoir systems.



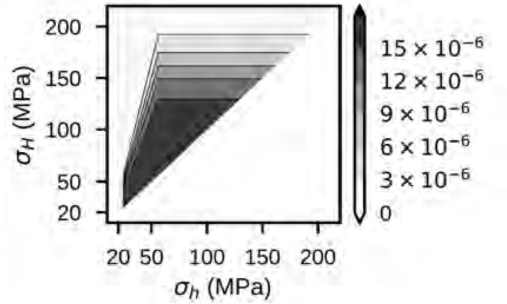
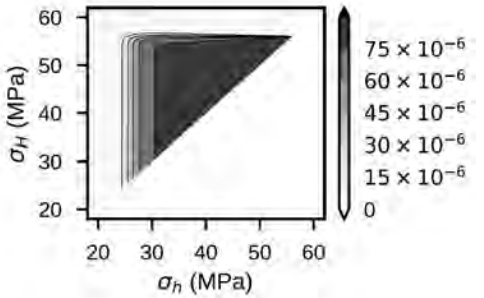
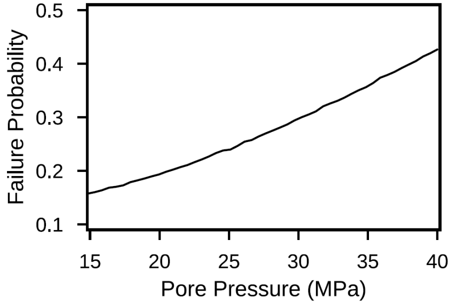
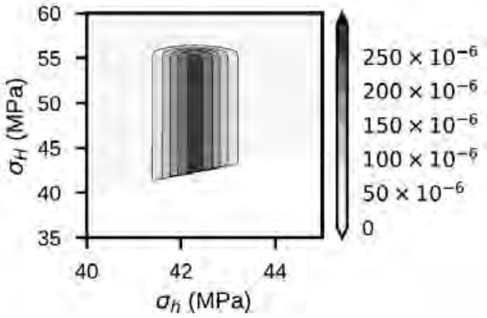
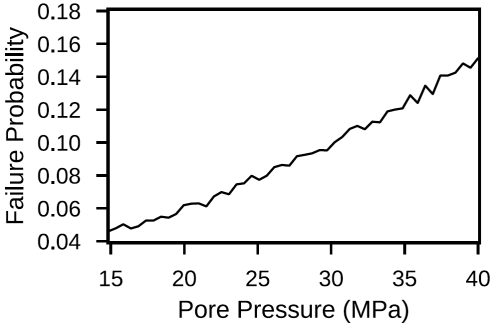
Thanks!

www.edx.netl.doe.gov/nrap
NRAP@netl.doe.gov

Additional Workflows

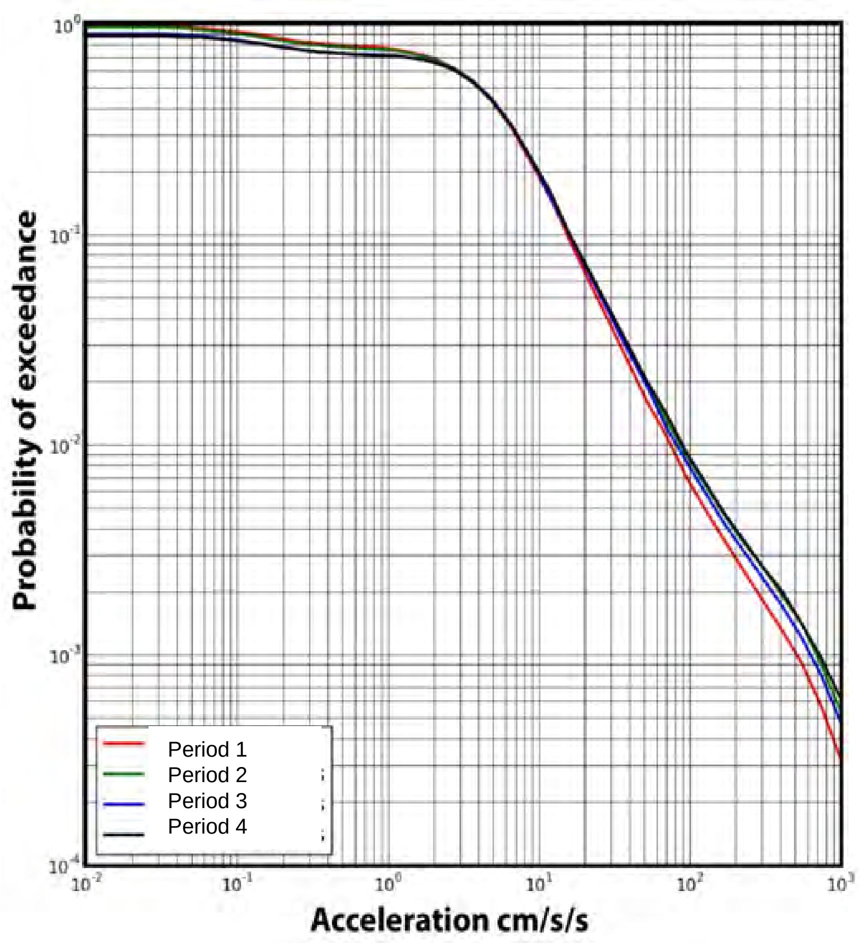


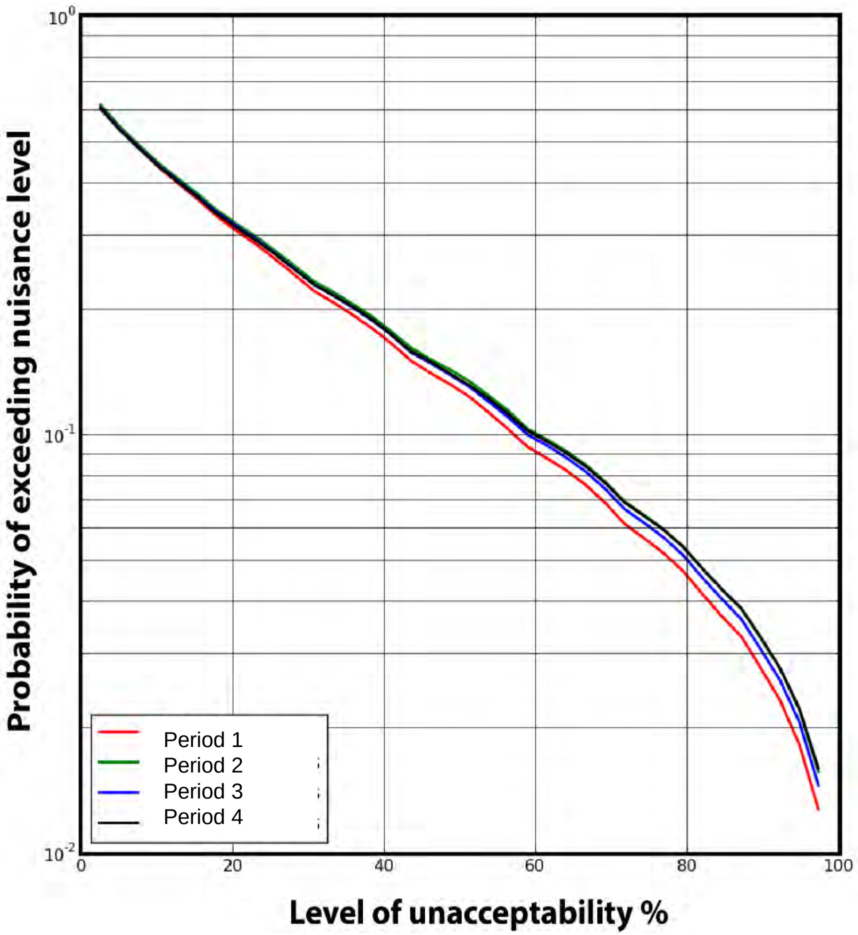
State-of-Stress Assessment Tool (SoSAT)

Input data available	Joint probability for σ_H and σ_h	Probability of activating critically-oriented fault
• Pore pressure • Overburden density		
• Regional stress indicators • Geodetic data		
• Local measurement of σ_h		

Reference: Jeff Burghardt (2018) SOSAT User's Manual.

Probabilistic Seismic Risk Assessment Tool (RiskCat)





Reference: Jean Savy and Bill Foxall (2018) RiskCAT User's Manual.

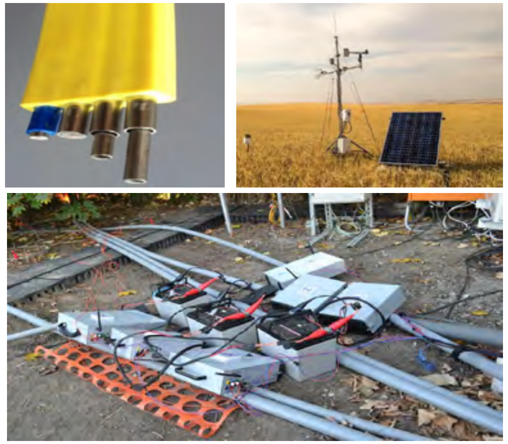
Carbon Storage Program

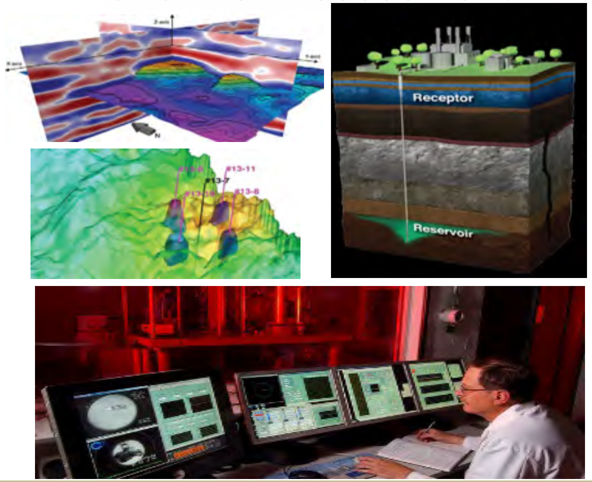
MISSION

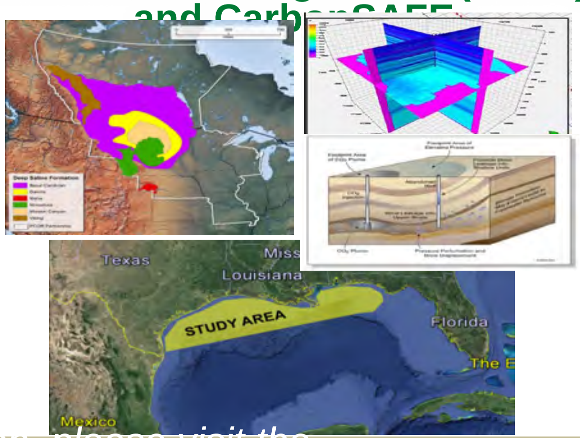
Ensure Permanence – Protect Environment – Facilitate Awareness – Improve Storage Efficiency – Commercial-Readiness by 2030

Program Approach & Technical Accomplishments

ADVANCED STORAGE		STORAGE INFRASTRUCTURE	
Monitoring, Verification, and Accounting	Geologic Storage, Simulation, and Risk Assessment	Regional Carbon Sequestration Partnership Initiative	Onshore and Offshore Characterization, Brine Extraction Storage Tests (BEST), and CarbonSAFE







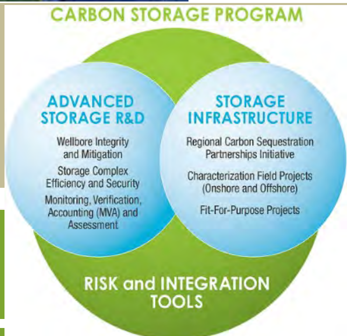
Risk and Integration Tools

CO2 SCREEN

EDX Energy Data eXchange

NRAP National Risk Assessment Partnership

For more information, please visit the Carbon Storage Program web page at: https://www.netl.doe.gov/coal/carbon-storage

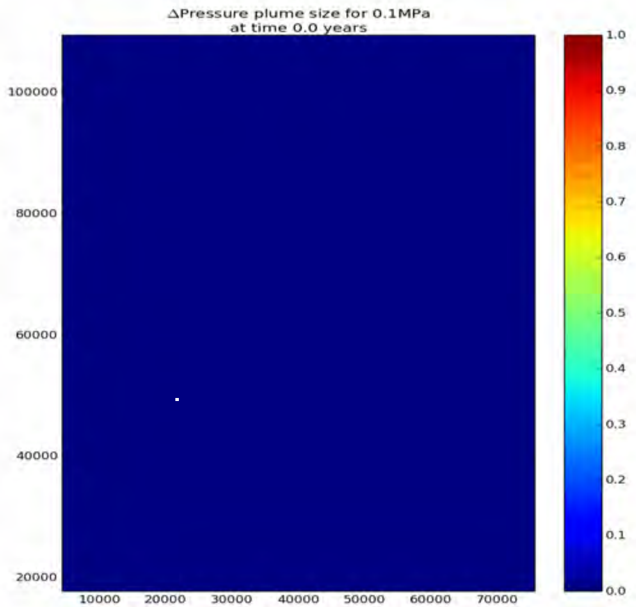


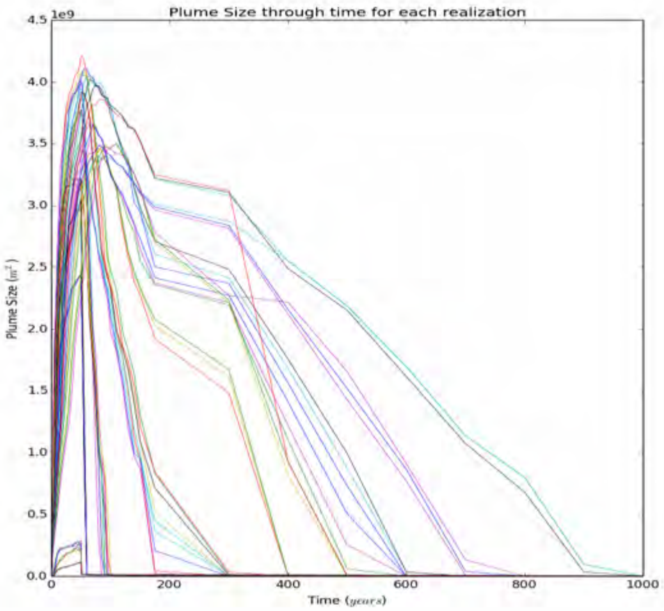
U.S. DEPARTMENT OF ENERGY

– NETL – Industry – Universities – National Labs –

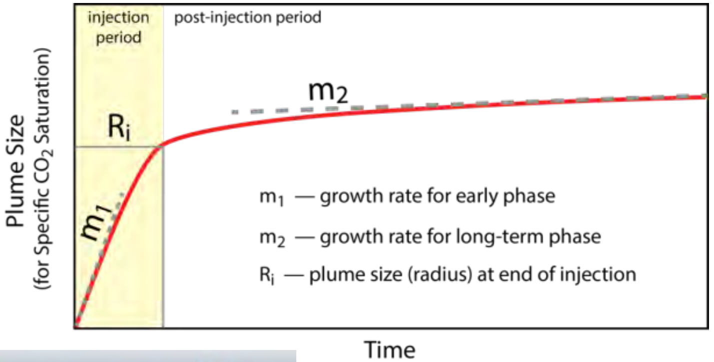
Using Science-Based Prediction to Probe Reservoir Behavior and the Reservoir Evaluation and Visualization (REV) tool

- **Size of CO_2 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

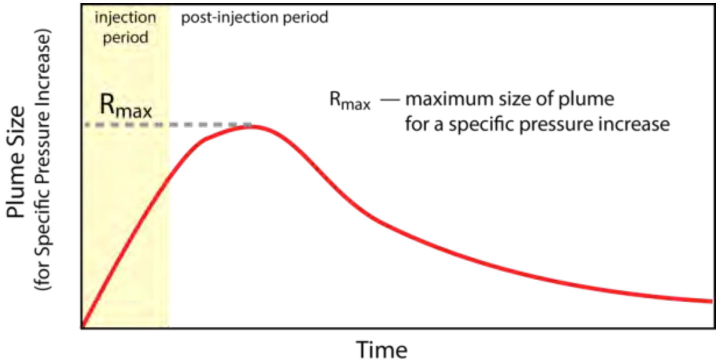




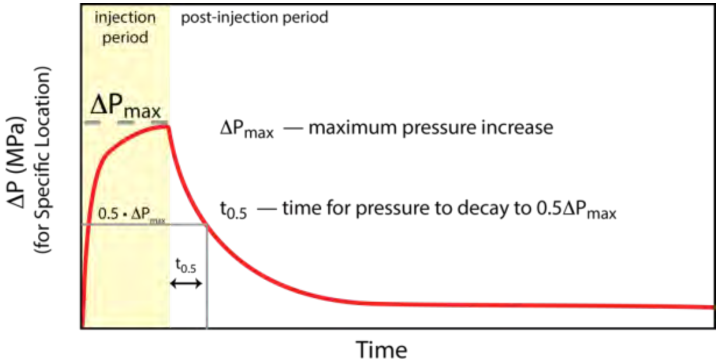
Size of CO_2 Plume



Size of Pressure Plume



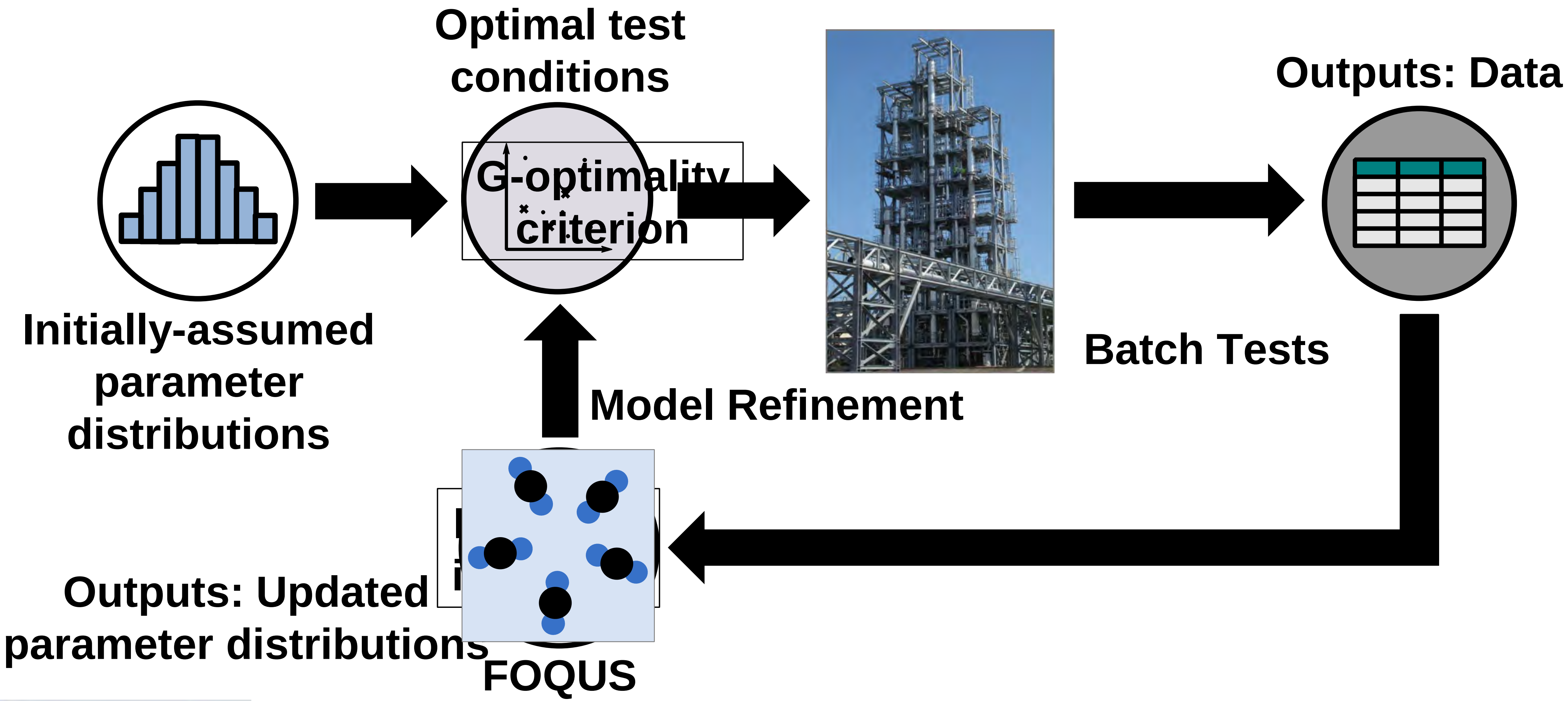
Pressure at a Location



GCS Site Closure Products

- Demirkanli, Bacon, White, Risk-based Area of Review (AoR) Determination for a Deep-Saline Carbon Storage Site Using National Risk Assessment Partnership's Open-Source Integrated Assessment Model (NRAP-IAM-CS v2)." submitted to IJGGC
- 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 CO_2 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 CO_2 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 CO_2 storage sites. submitted to IJGGC
- Harp, D., Ohishi, T., Chu, S., Chen, S., Pawar, R. Development of quantitative metrics of plume migration at geologic CO_2 storage sites. submitted to Greenhouse Gas Science
- Chen, B., Harb, D., Lu, Z., Pawar, R. On Reducing Uncertainty in Geologic CO_2 Sequestration Risk Assessment by Assimilating Monitoring Data in preparation to be submitted to IJGGC
- Lackey, G.; Vasylkivska. V.; Huerta, N.; King, S.; Dilmore, R. Managing Well Leakage Risks at a Geologic Carbon Storage Site with Many Wells, submitted to IJGGC
- Doughty, C. and Oldenburg, C.M. CO_2 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

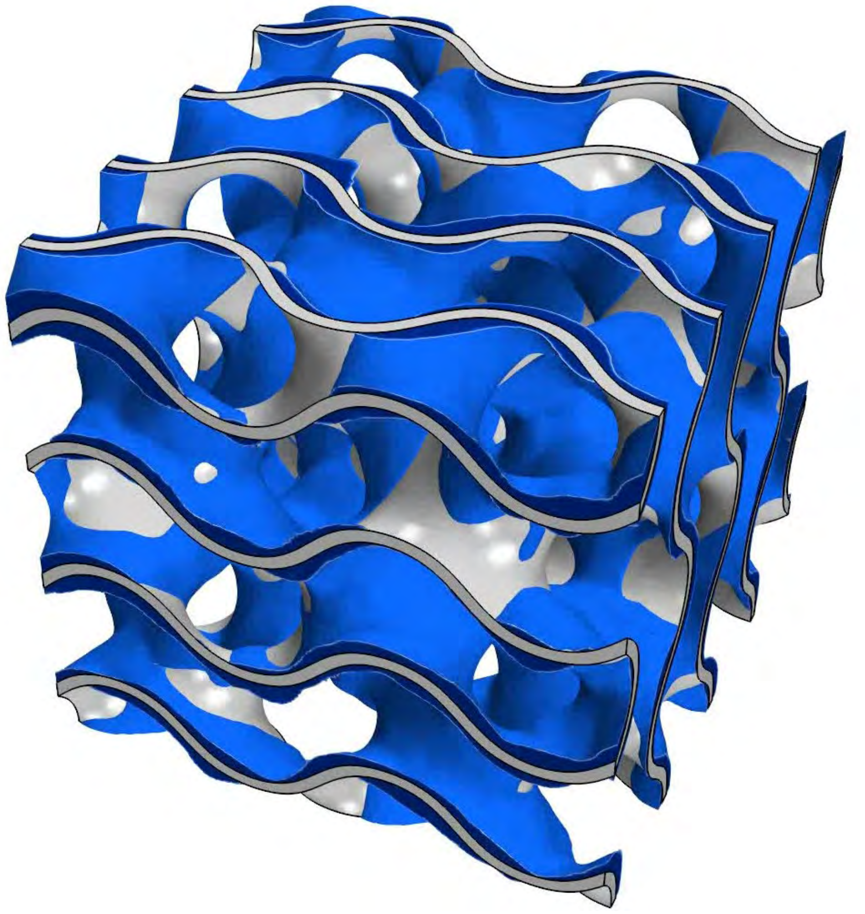


Conclusions: LLNL Reactor Geometry

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

Future Work

- Geometry design to optimize countercurrent gas/solvent flow and heat transfer for MEA
- Apply framework to CO_2BOL
- Characterize performance as a function of geometry and solvent characteristics



Rivulet Flow Example

Task 2.2: CFD Validation Effort

Packed column

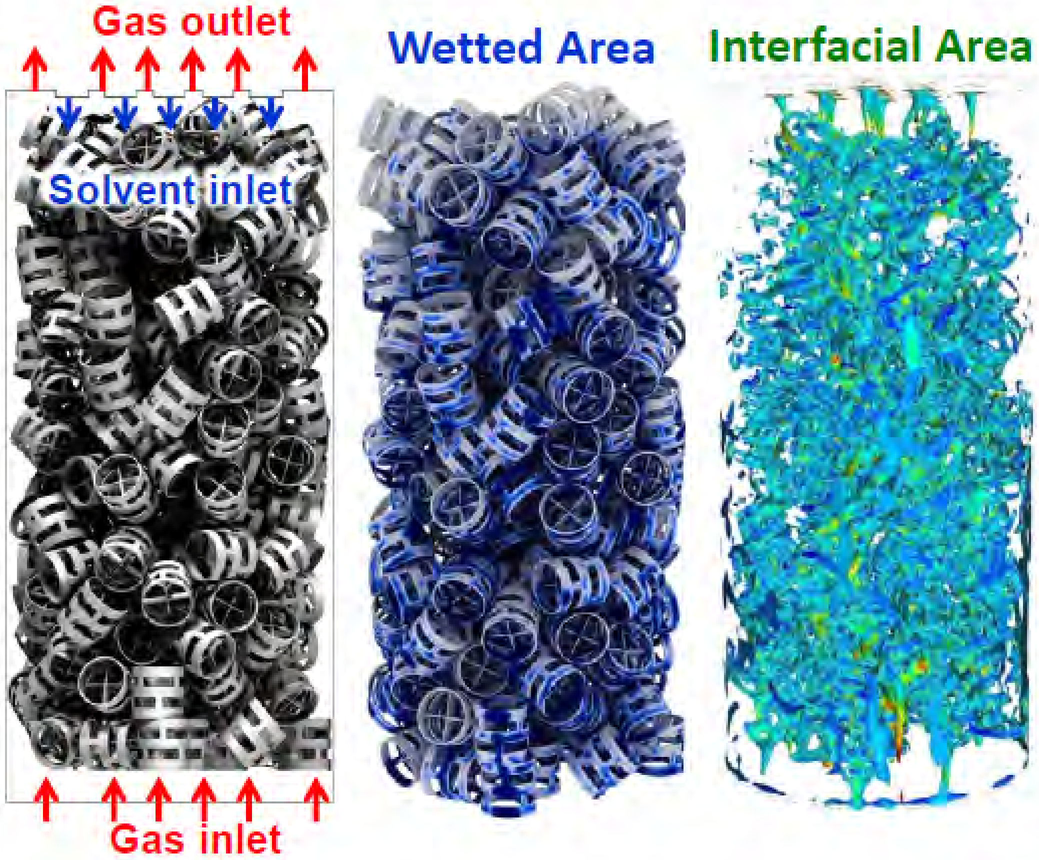
- Column diameter: 100 mm
- Column height: 200 mm
- Number of rings: 160

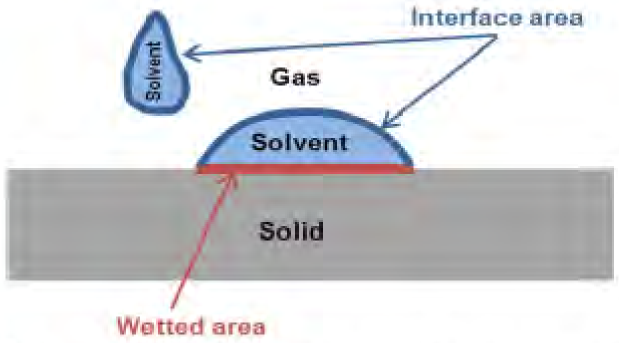
Design of pall ring

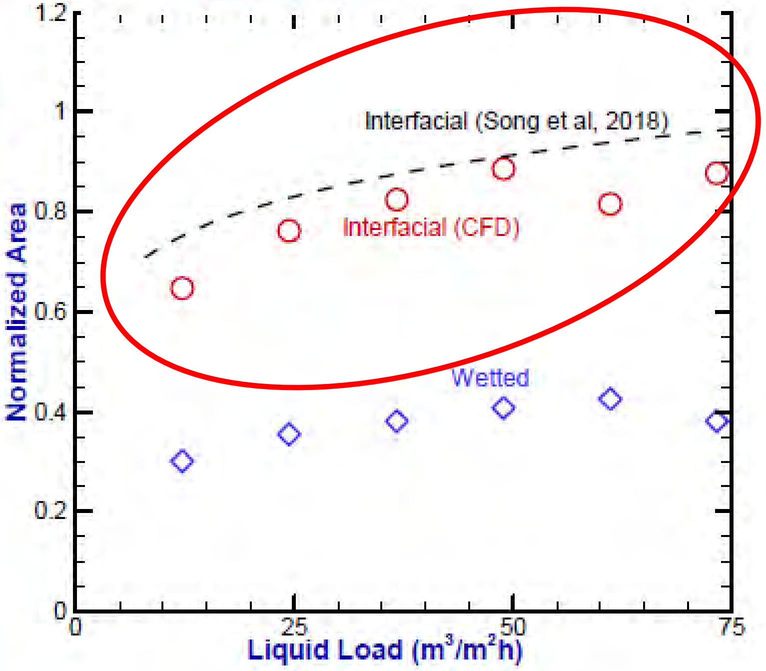
- Diameter: 16 mm
- Height: 16 mm
- Thickness: 0.5 mm
- Specific Area: 282 m^2/m^3

Solvent Properties (30% MEA)

Physical Properties	
Density ρ (kg/m^3)	1000
Viscosity μ (cP)	2.46
$D_{CO_2}[l]$ (m^2/s)	1.0×10^{-9}
$D_{CO_2}[g]$ (m^2/s)	1.0×10^{-5}
Reaction Rate	5.96
Henry's constant (Dimensionless)	1.228
Surface Tension (N/m)	0.065
Contact angle (°)	40







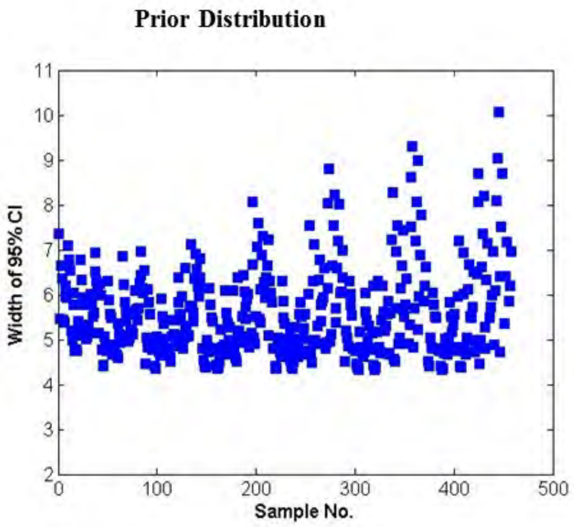
Validation

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

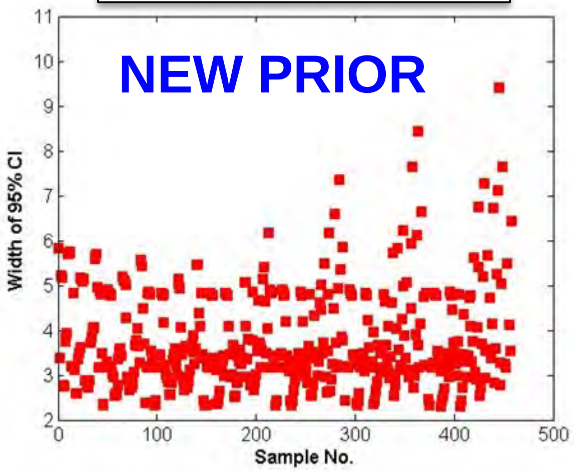
Song et al. (Ind. Eng. Chem. Res. 2018, 57, 718–729)

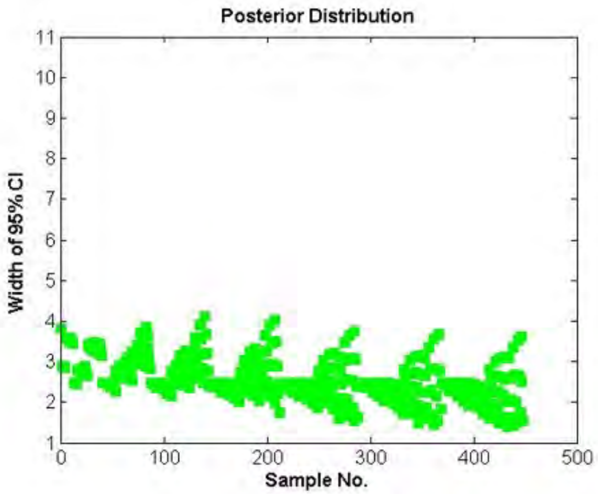
Optimal Design of Experiments: NCCC Trial

Candidate Points

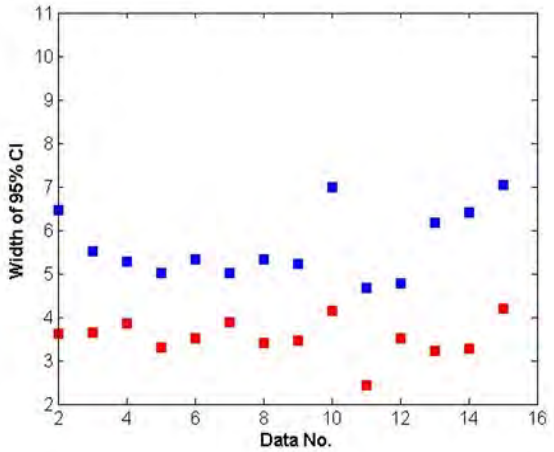


Next iteration

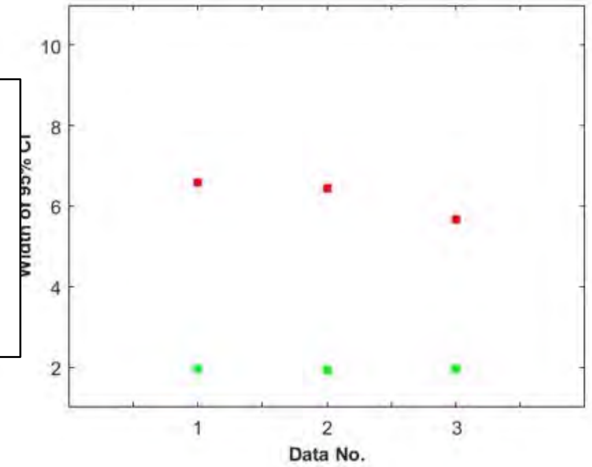




Points with Experimental Data



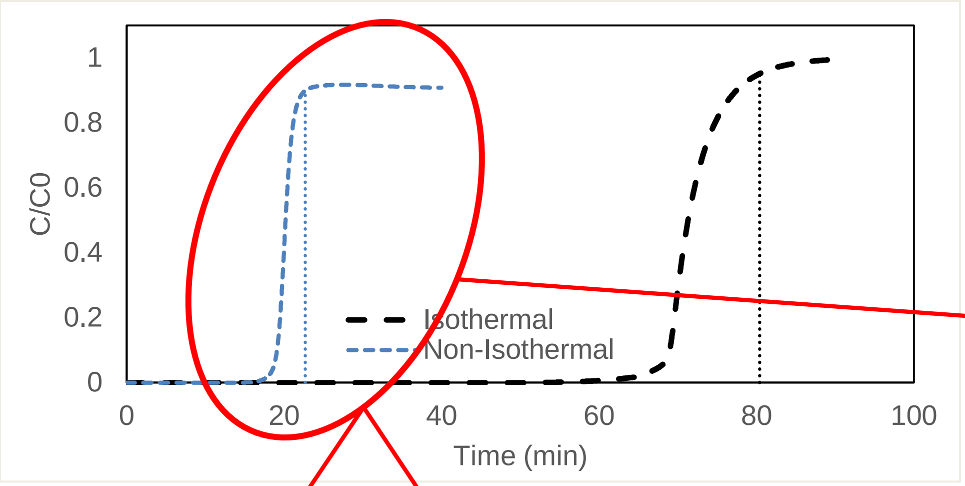
50-70% Reduction in CO_2 Capture Prediction Uncertainty
(18 total runs)



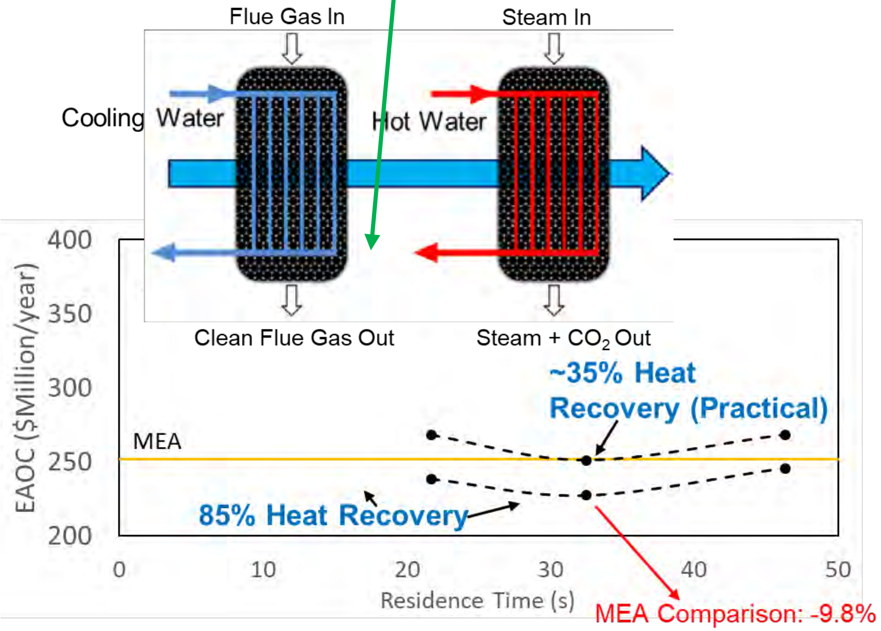
CCSI[2] Carbon Capture Simulation for Industry Impact · National Energy Technology Laboratory · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Pacific Northwest National Laboratory · West Virginia University · The University of Texas at Austin · U.S. Department of Energy

Task 2.1: Fixed Bed Results

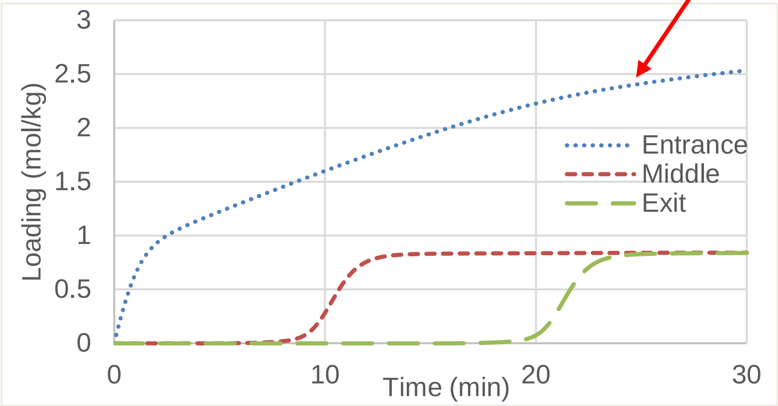
Operating Conditions	
Pressure (bar)	1.1
Temperature (°C)	25
Flow rate (mol/s)	120
y_{CO2}	0.132
y_{H2O}	0.055
y_{N2}	0.813
Bed Length (m)	10
Bed Diameter (m)	3

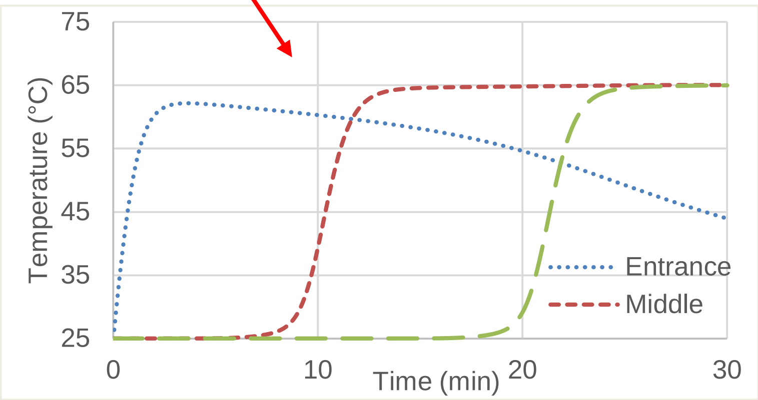


- Large temperature spikes due to high heat of adsorption and poor heat removal from the system
  - Thermal management can considerably increase performance
    - $t_{b, non-intensified}$ = 22.7 min
    - $t_{b, intensified}$ = 80.4 min



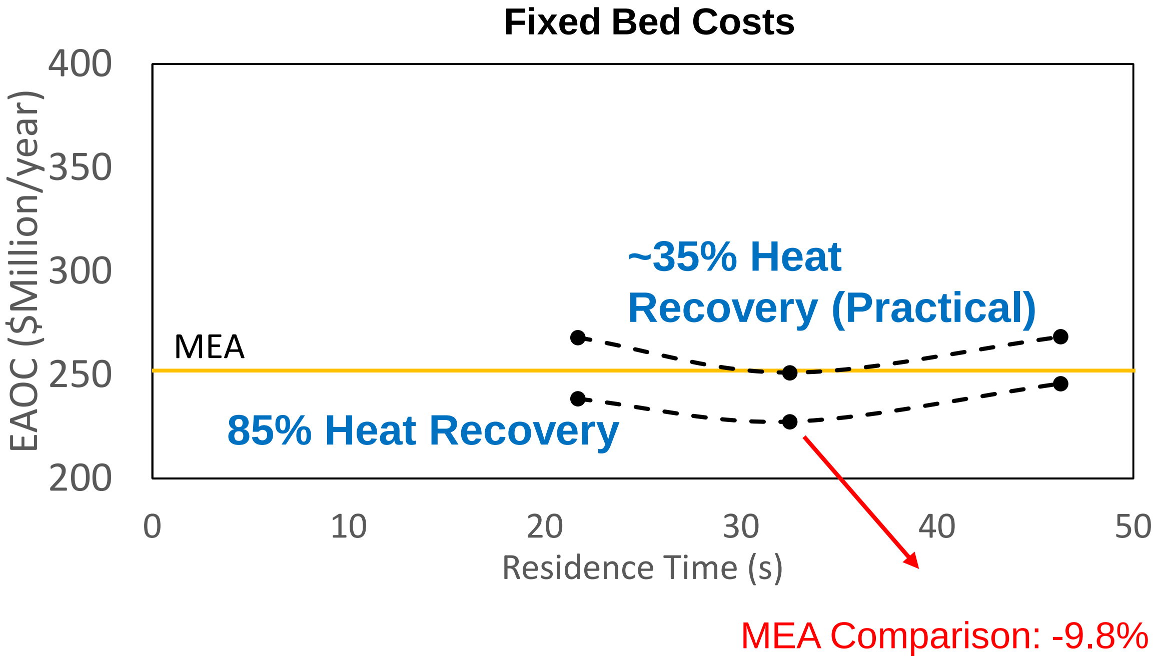
High temperature = poor use of potential working capacity

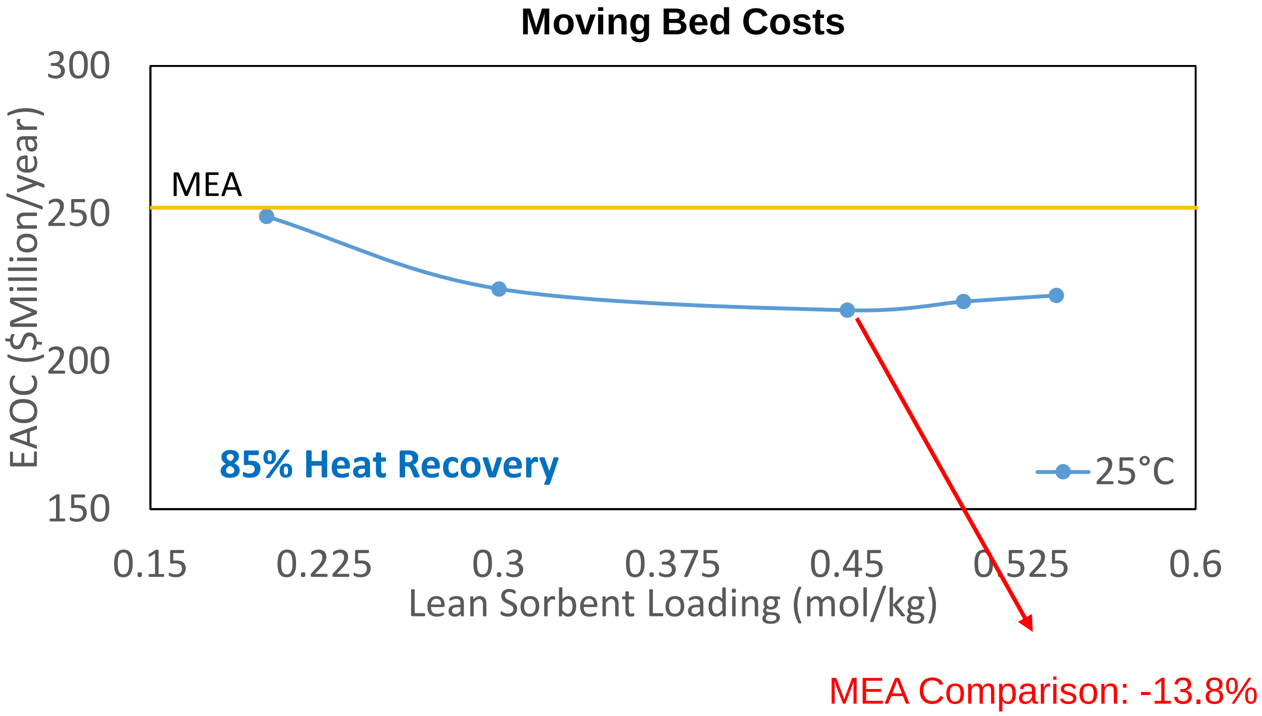




Task 2.1: Moving Bed Results

- **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





Task 2.2: PNNL CO_2BOL Low Aqueous Solvent

- **Technology**
  - Low Aqueous Solvent
  - Polarity swing-assisted regeneration
  - Anti-solvent
- **Multi-scale modeling**
  - CO_2BOL Solvent
  - Equipment
  - System
- **Objective**
  - Elucidate solvent/packing interactions
  - Proper absorber optimization