CCSI^2
Carbon Capture Simulation for Industry Impact

2024 PSE+ Stakeholder Workshop:
Timeline and Scope of CCSI^2 Support for CO$_2$ Capture Technology Pilot Test Campaigns

Michael Matuszewski
CCSI^2 Associate Technical Director

Pittsburgh Marriott City Center
Pittsburgh, PA
9/18/2024

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 · Carnegie Mellon · THE UNIVERSITY OF TEXAS AT AUSTIN · U.S. DEPARTMENT OF ENERGY

Key Points to Consider for Pilots

- **Conventional Design of Experiments at Pilot Scale:**
  - Has unanticipated consequences
  - Can be inefficient

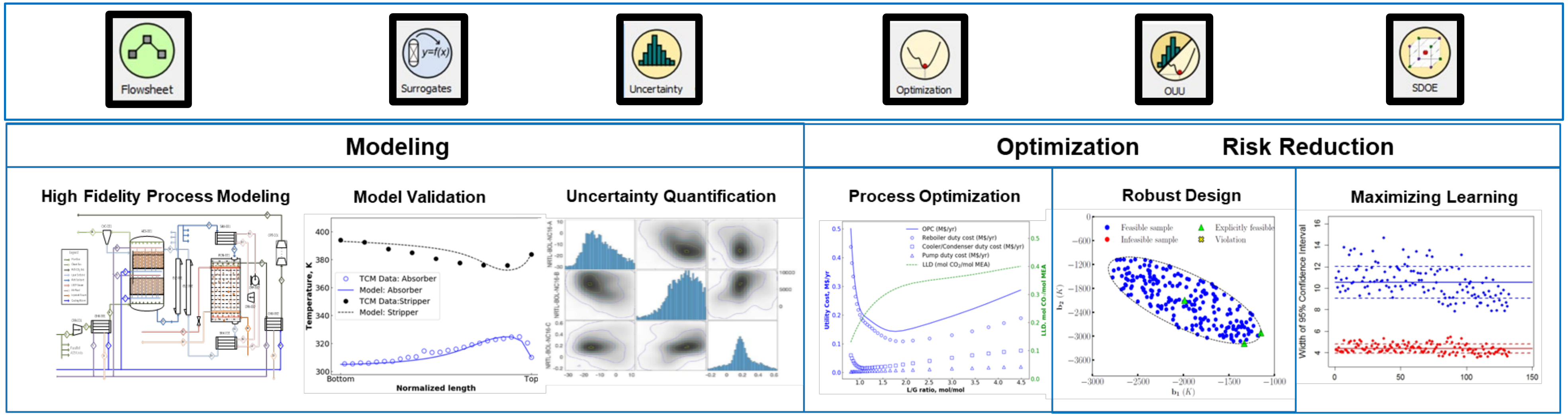
- **Economic Modeling**
  - Supports testing in commercially optimal, relevant scenarios

- **Uncertainty Should be Explicitly Considered**
  - Characterizes most impactful behavior
  - Uncovers process improvement opportunities

- **How to Implement the Right Test Plan**
  - Activities, Data Requirements, Model Requirements, Schedule

Fossil Energy Involvement in Pilot Campaigns

- **Optimizing the Value of Industrial Collaboration**



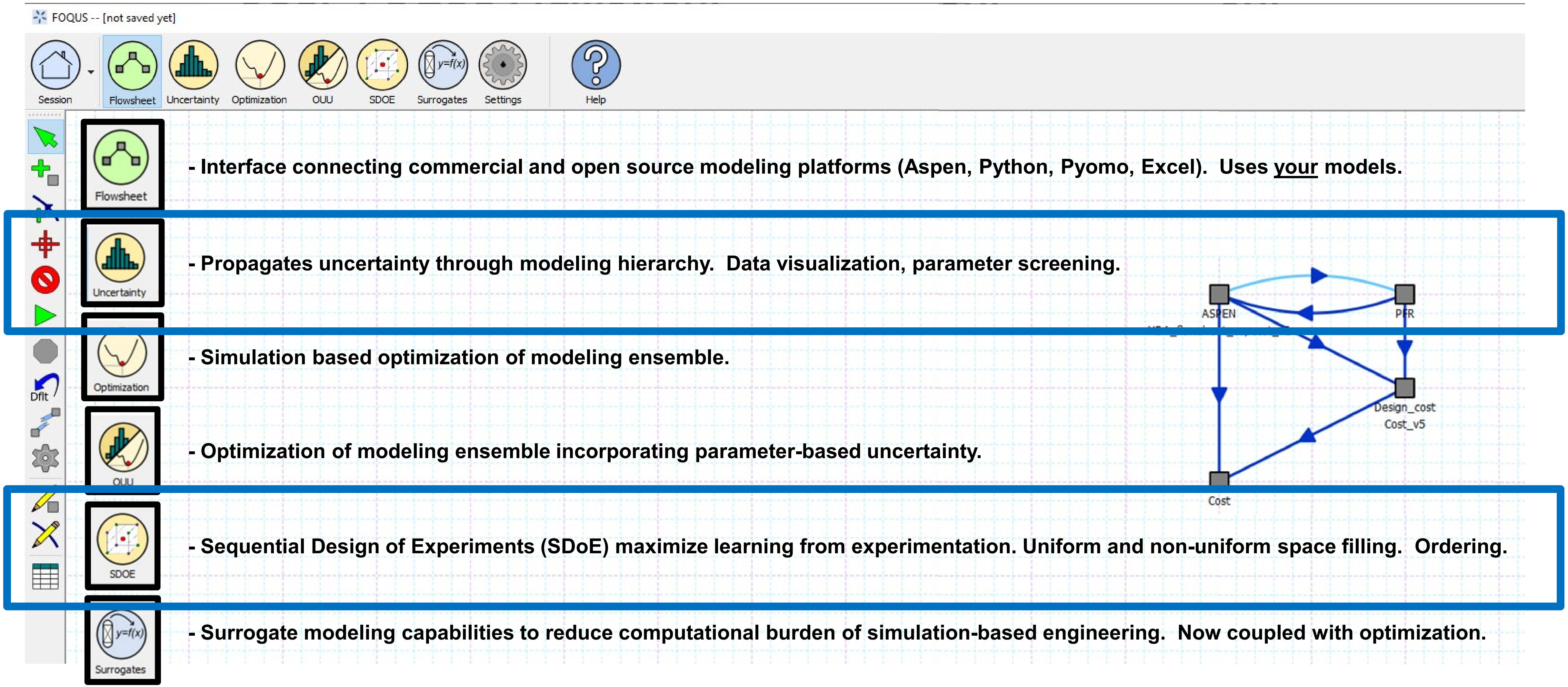
NATIONAL CARBON CAPTURE CENTER

TECHNOLOGY CENTRE MONGSTAD

- Ensures an integrated modeling and testing framework demonstrated to ***eliminate years from scale up***
- Underpins ***Sequential Design of Experiments (SDoE)*** for ***optimizing value of pilot test data***
- ***Can save millions of dollars*** in test costs
- ***Minimizes commercial technology costs*** with rigorous, large-scale optimization
- ***Reducing uncertainty to increase confidence*** in commercialization of carbon capture technologies

$CCSI^2$
Carbon Capture Simulation for Industry Impact

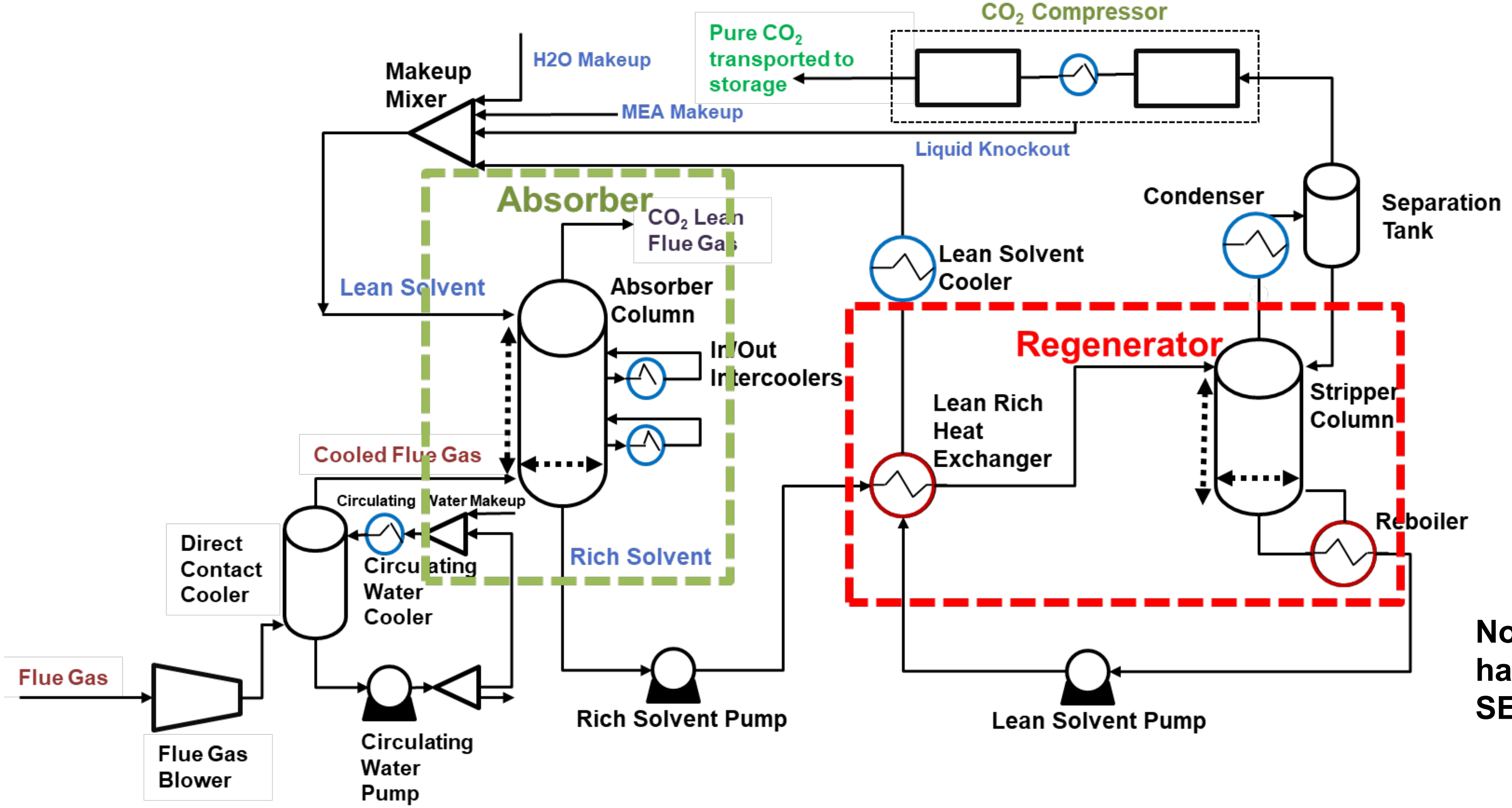
CCSI^2 FOQUS Framework



- Interface connecting commercial and open source modeling platforms (Aspen, Python, Pyomo, Excel). Uses your models.
- Propagates uncertainty through modeling hierarchy. Data visualization, parameter screening.
- Simulation based optimization of modeling ensemble.
- Optimization of modeling ensemble incorporating parameter-based uncertainty.
- Sequential Design of Experiments (SDoE) maximize learning from experimentation. Uniform and non-uniform space filling. Ordering.
- Surrogate modeling capabilities to reduce computational burden of simulation-based engineering. Now coupled with optimization.

Uncertainty Analysis at 97% and 99.5% Capture

Thirteen parameters considered in the thermodynamic and mass transfer models, selected based on Sobol analysis[1,2]

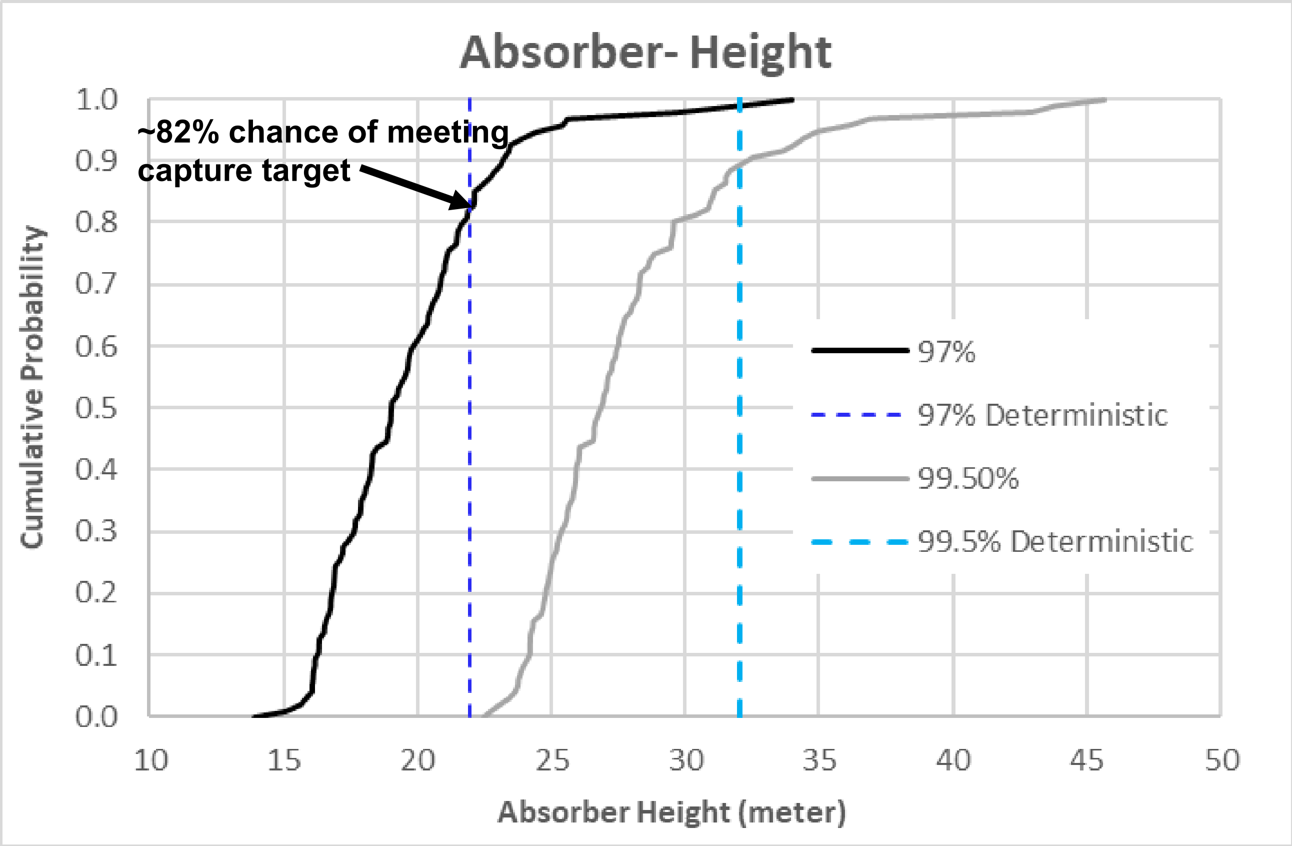


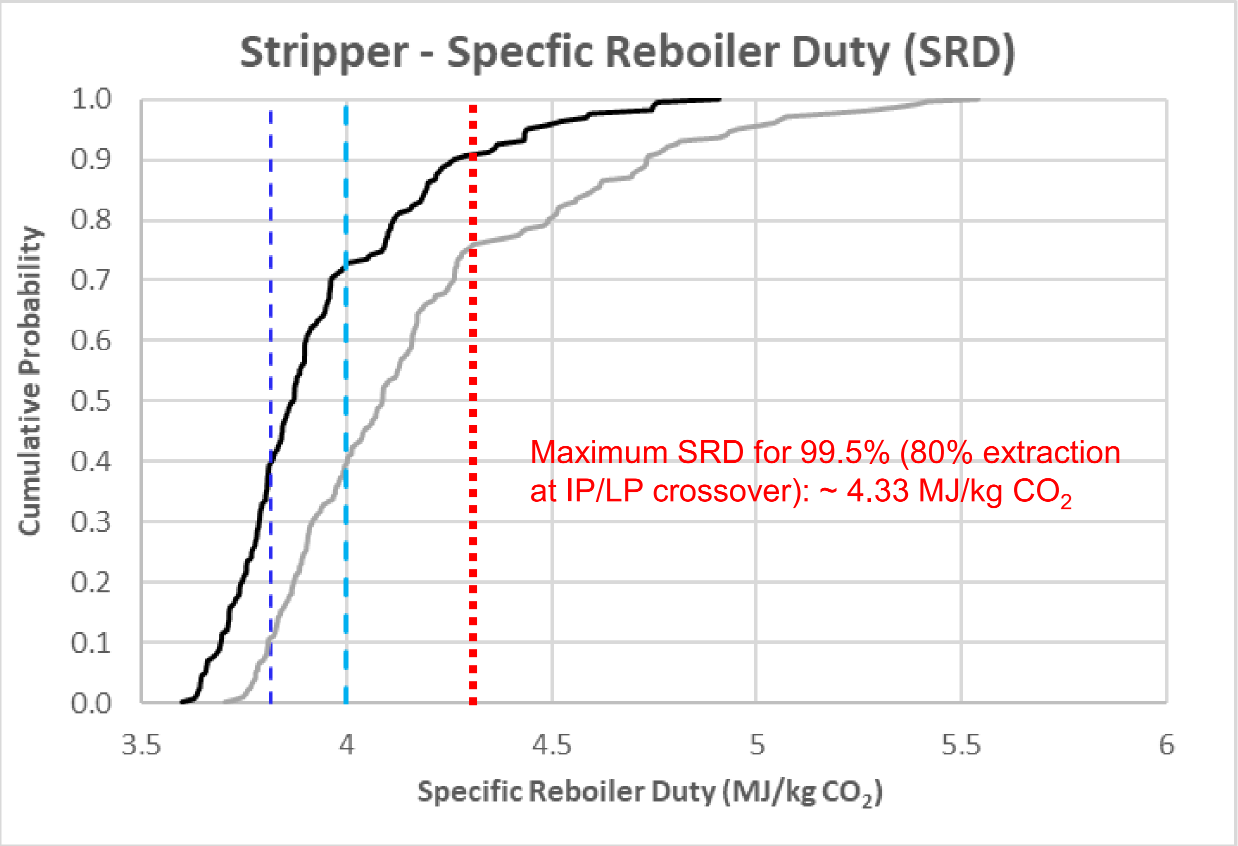
Note: This analysis has been done for the SE case

1. Morgan JC, Chinen AS, Omell B, Bhattacharyya D, Tong C, Miller DC, 2017. Thermodynamic modeling and uncertainty quantification of CO$_2$-loaded aqueous MEA solutions. Chem. Eng. Sci. 168: 309-324.
2. Chinen AS, Morgan JC, Omell B, Bhattacharyya D, Tong C, Miller DC, 2018. Development of a rigorous modeling framework for solvent-based CO$_2$ capture. Part 1: hydraulic and mass transfer models and their uncertainty quantification. Ind. Eng. Chem. Res. 57: 10448-10463.

Uncertainty Analysis of Column Height and SRD

Thirteen parameters considered in the thermodynamic and mass transfer models, selected based on Sobol analysis[1,2]





- Driven by mass transfer uncertainty
- Low risk of not meeting performance target

- Driven by thermodynamic uncertainty
- Higher risk of not meeting expected performance (similar in both cases as both use lower lean loadings)
- Steam extraction constraints provide less recourse

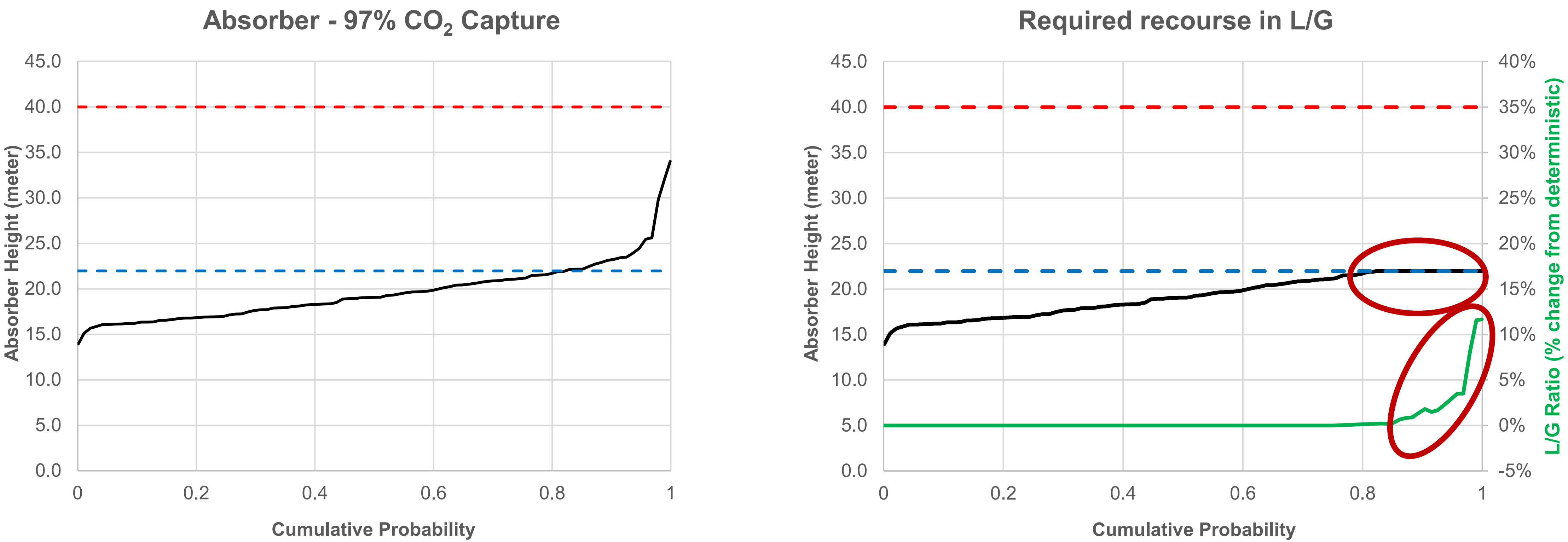
---

[1] Morgan JC, Chinen AS, Omell B, Bhattacharyya D, Tong C, Miller DC, 2017. Thermodynamic modeling and uncertainty quantification of CO_2-loaded aqueous MEA solutions. Chem. Eng. Sci. 168: 309-324.

[2] Chinen AS, Morgan JC, Omell B, Bhattacharyya D, Tong C, Miller DC, 2018. Development of a rigorous modeling framework for solvent-based CO_2 capture. Part 1: hydraulic and mass transfer models and their uncertainty quantification. Ind. Eng. Chem. Res. 57: 10448-10463.

CCSI²
Carbon Capture Simulation for Industry Impact

Additional Recourse for 97% CO_2 Capture Case



Blue dash – actual installed column height
Red dash – technical feasible height

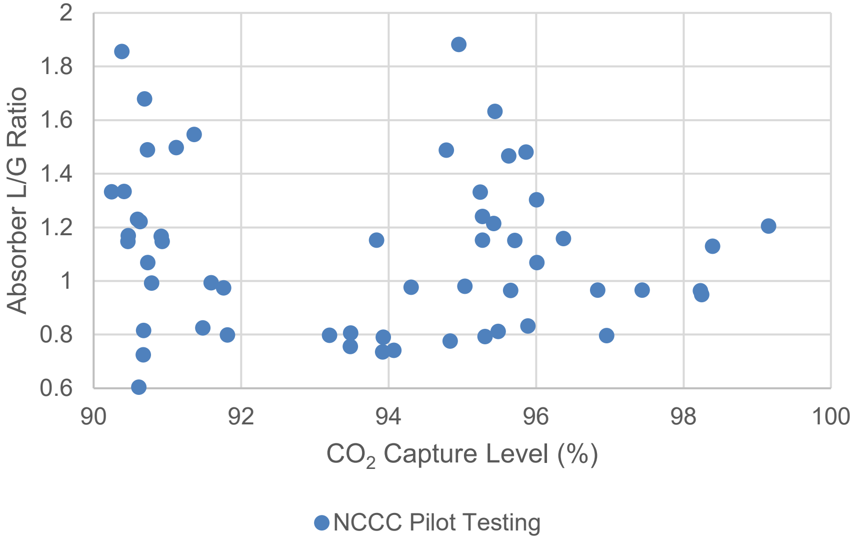
- Deterministic design can achieve capture targets amidst uncertainty with a small increase in liquid flowrates (~2%-12%).
- Increase in L/G may have other impacts

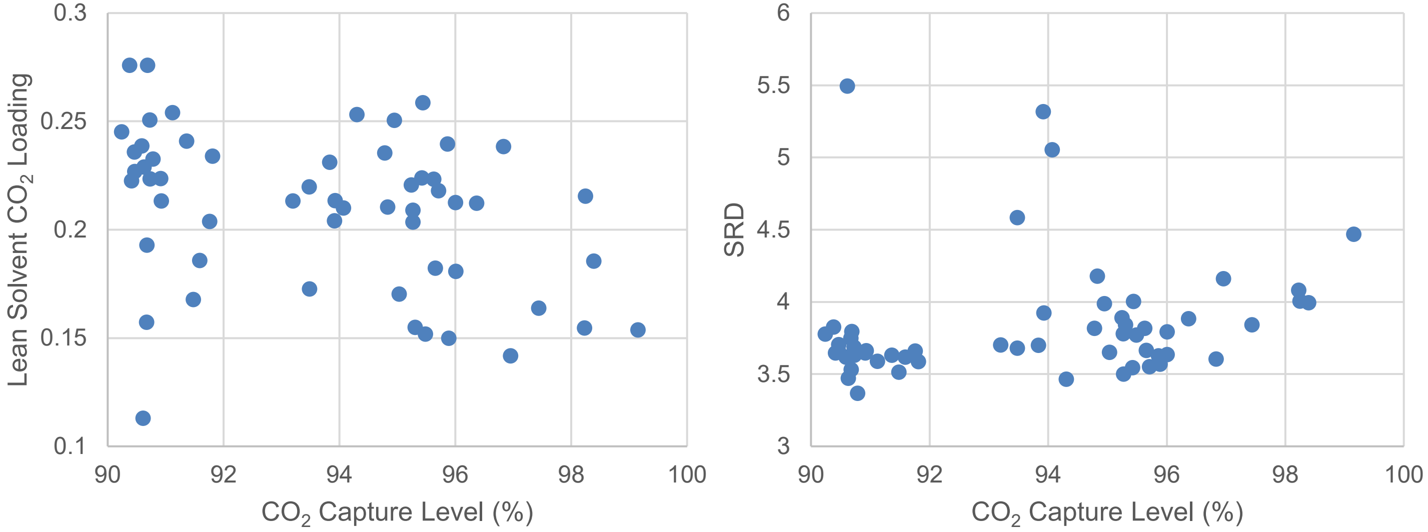
CCSI²
Carbon Capture Simulation for Industry Impact

13 parameters considered in the thermodynamic and mass transfer models, selected based on Sobol analysis

High Capture Example: Considerations for Model Validations

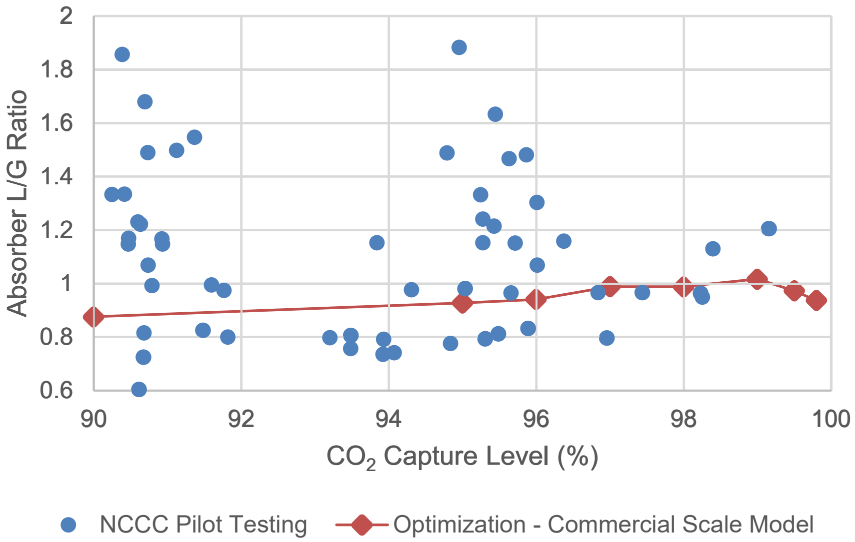
- 2022 NCCC Campaign that targeted high capture
  - 88 runs with NGCC conditions
  - Far more parametric runs than a normal campaign





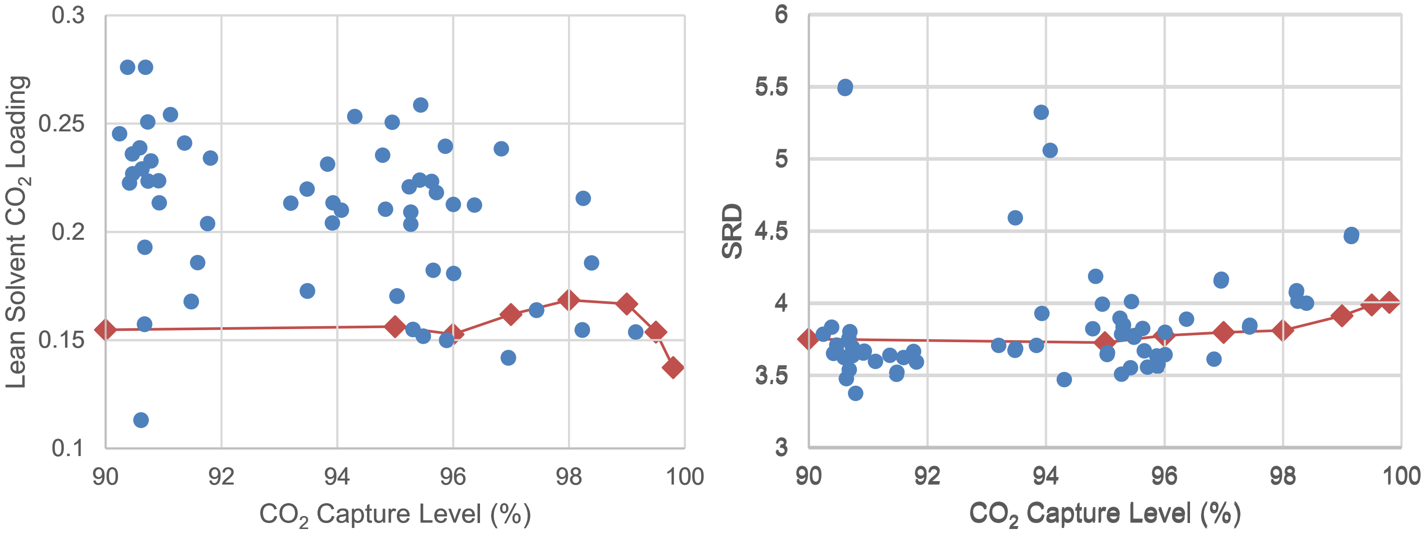
High Capture Example: Considerations for Model Validations

- 2022 NCCC Campaign that targeted high capture
  - 88 runs with NGCC conditions
  - Far more parametric runs than a normal campaign
  - Of those, 12 are close to optimal trend
  - **Of those, 8 are 95% capture or above (<10%)**
  - Only 99%+ case (past the reflection point) off the trend



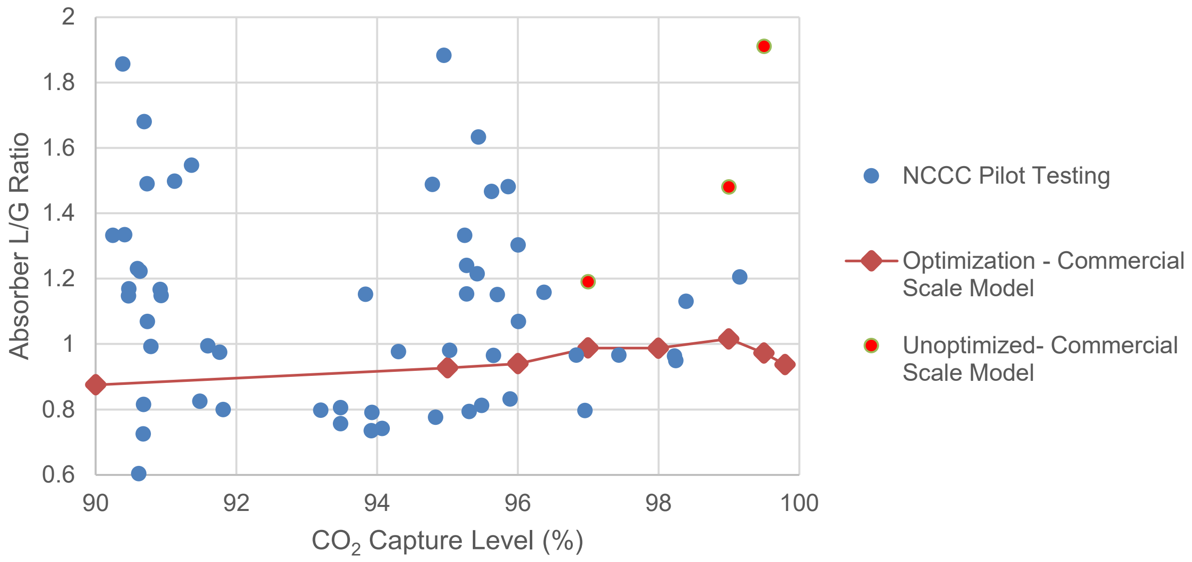
- **High capture rates** not guaranteed to be well represented

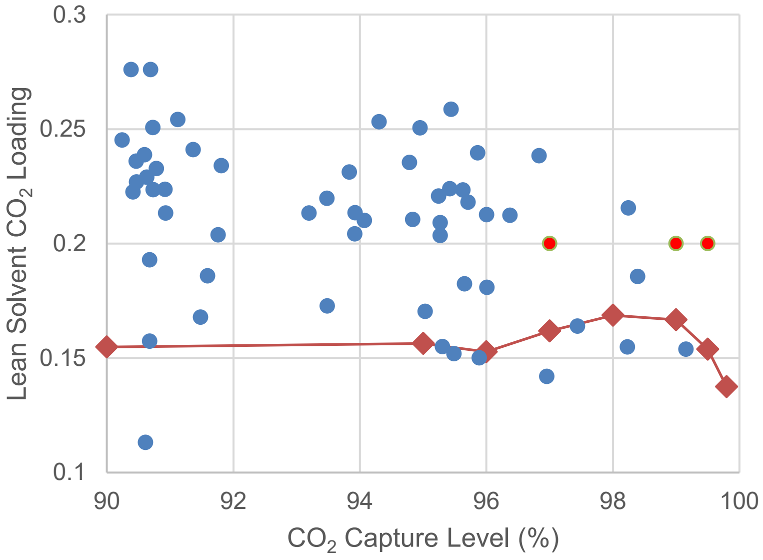
- **Optimal operation** not guarantee to be well represented

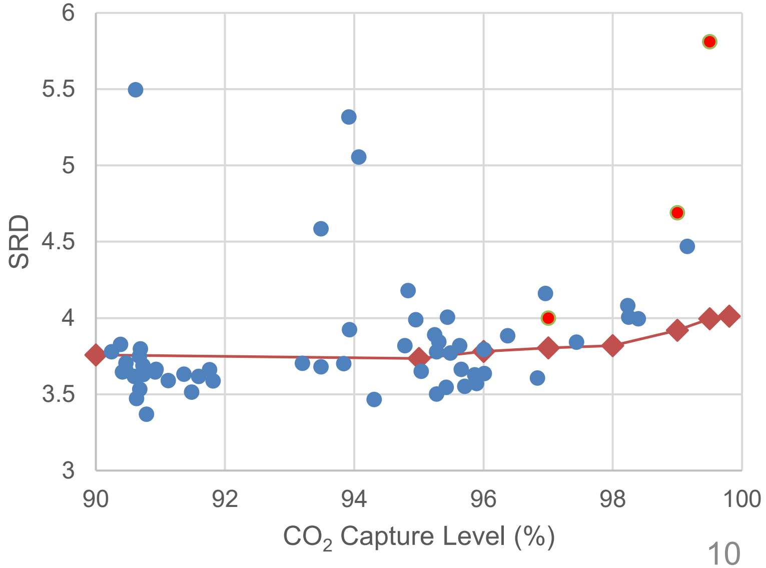


Economic Feasibility of Unoptimized Cases

Unoptimized Case Comparison (lean loading set at 0.2)			
% CO_2 Capture	97	99	99.5
L/G (kg/kg)	1.19	1.48	1.91
SRD (MJ/kg CO_2)	4.00	4.69	5.81
LCOE (\$/MW-hr)	73.37	76.18	80.16
COAC (\$/tonne CO_2)	90.50	96.63	107.77
Incremental COAC (\$/tonne CO_2)		**341.45**	**1937.15**
Optimized Incremental COAC (\$/tonne CO_2)			

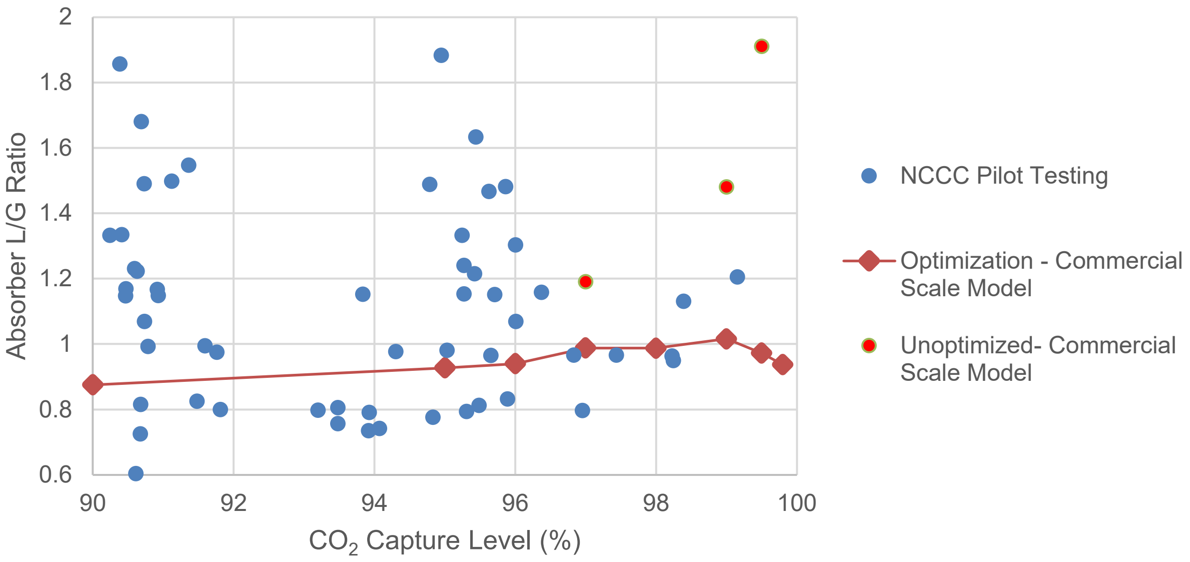




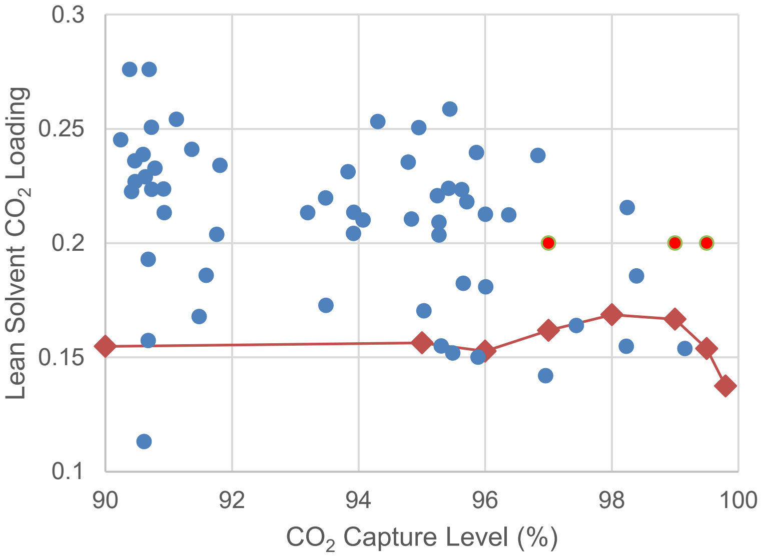


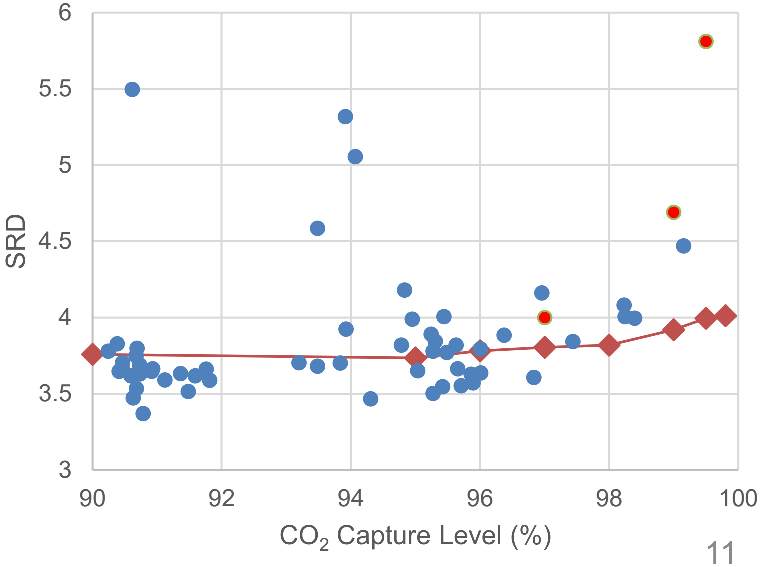
Economic Feasibility of Unoptimized Cases

Unoptimized Case Comparison (lean loading set at 0.2)			
% CO_2 Capture	97	99	99.5
L/G (kg/kg)	1.19	1.48	1.91
SRD (MJ/kg CO_2)	4.00	4.69	5.81
LCOE ($/MW-hr)	73.37	76.18	80.16
COAC ($/tonne CO_2)	90.50	96.63	107.77
Incremental COAC ($/tonne CO_2)		341.45	1937.15
Optimized Incremental COAC ($/tonne CO_2)	1.27x	269.40	4.8x 406.07



Models are important to determine test cases!



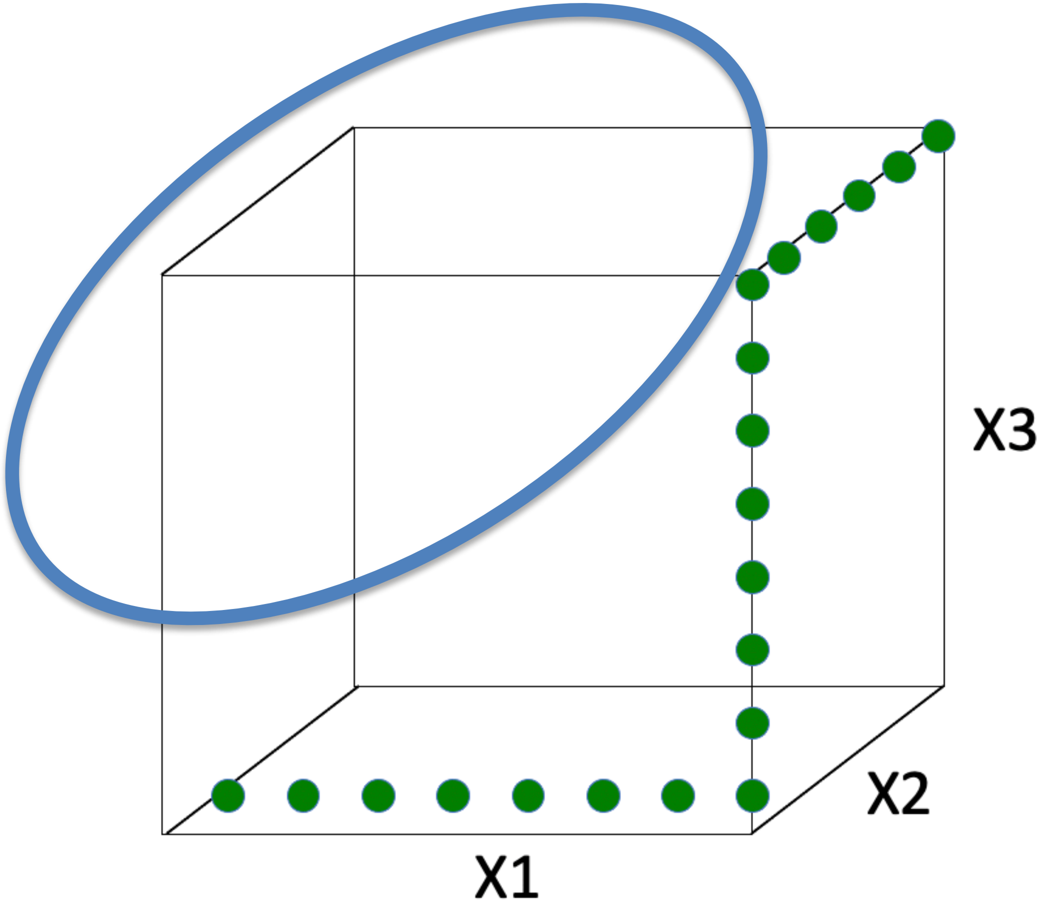


What is Design of Experiments (DoE)?

- **Mathematical strategy for selecting input combinations**
  - Compute output (computer experiment)
  - Operate system (physical experiment)
- **Series of these experimental runs/tests forms experiment**
  - **Purposeful changes** to inputs of process or system
  - **Identify the reasons** for any changes in output
- **A well-designed experiment is critical**
  - Results and conclusions depend on how the data is collected

Design of Experiments not the same as One-Factor-at-a-Time

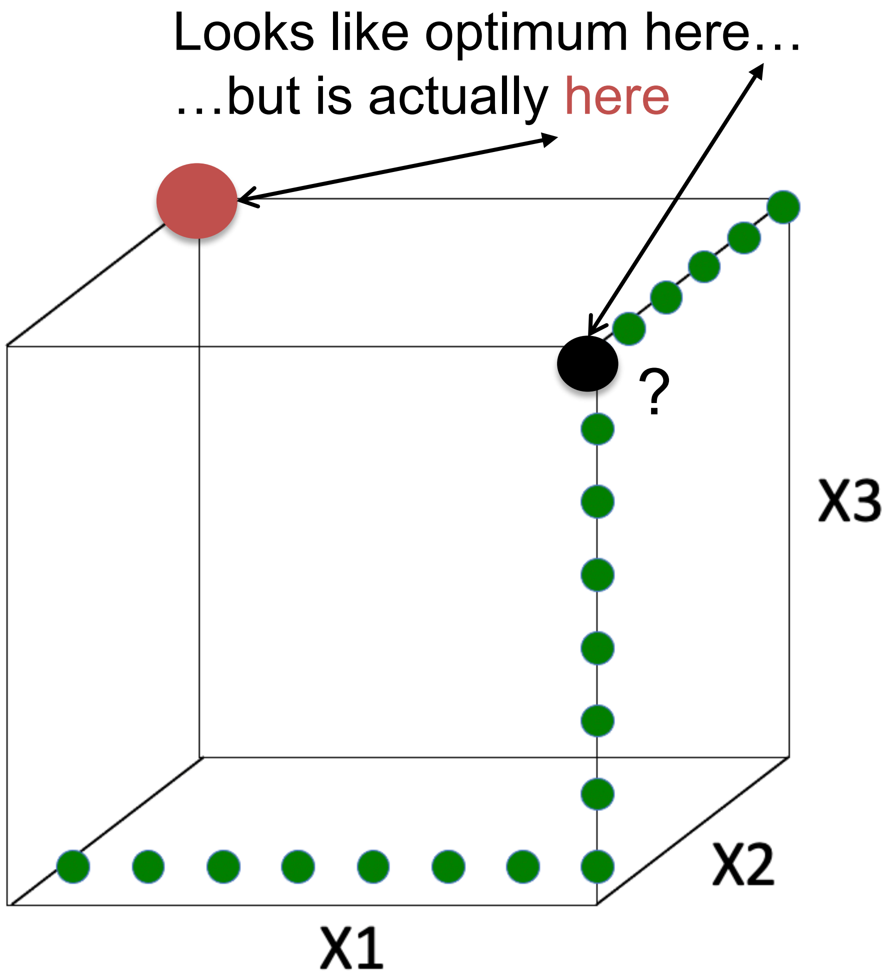
- **OFAAT strategy:**
  - Change only one input (factor) at a time
  - Hold all others constant
- **Inefficient use of budget**
- **Cannot identify interactions**
  - Effect of one factor changes when another factor changes
  - Finding optimal operating conditions is unlikely



CCSI²
Carbon Capture Simulation for Industry Impact

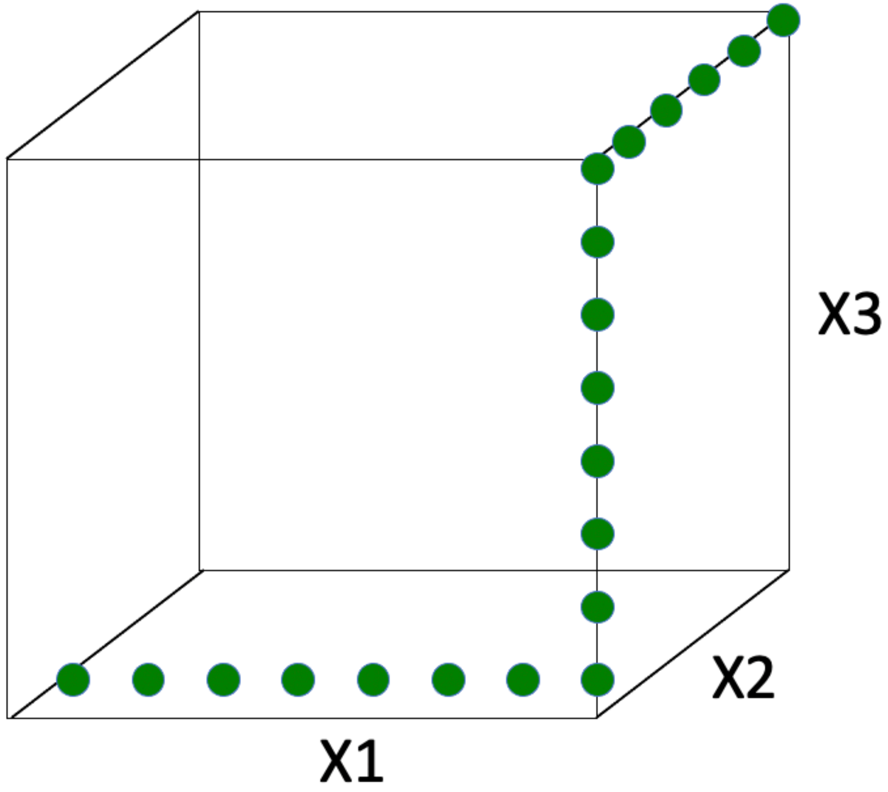
Design of Experiments not the same as One-Factor-at-a-Time

- **OFAAT strategy:**
  - Change only one input (factor) at a time
  - Hold all others constant
- **Inefficient use of budget**
- **Cannot identify interactions**
  - Effect of one factor changes when another factor changes
  - Finding optimal operating conditions is unlikely


Looks like optimum here…
…but is actually here

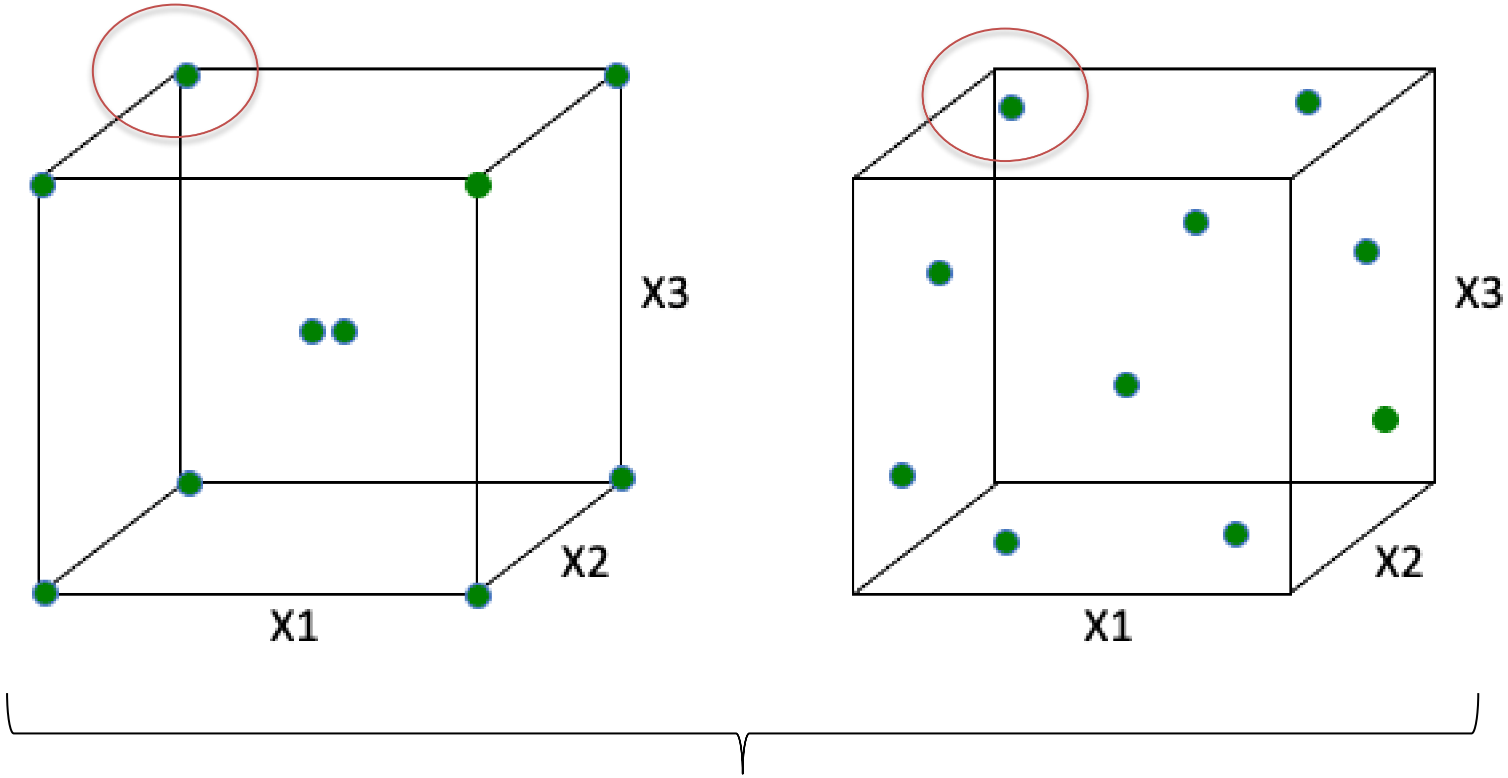
Design of Experiments not the Same as One-Factor-at-a-Time

- **OFAAT strategy:**
  - Change only one input (factor) at a time
  - Hold all others constant
- **Inefficient use of budget**
- **Cannot identify interactions**
- **Not randomized**
  - Changing conditions can negatively affect the results

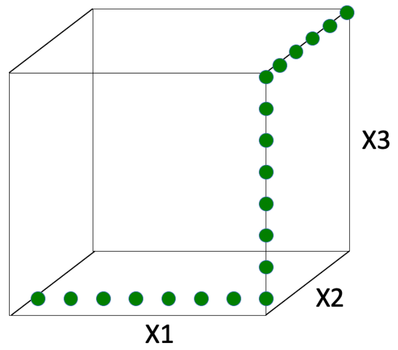


CCSI²
Carbon Capture Simulation for Industry Impact

DoE Avoids These Drawbacks – Is Always More Efficient



Two Different SDoE Approaches
Each uses **10 runs**



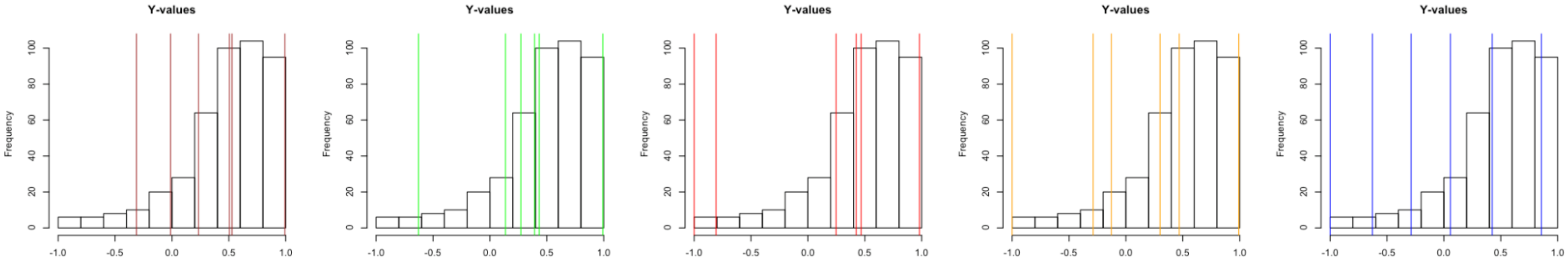
Uses **20 runs**

Balancing Input vs. Output Space

$$\boxed{d(v_1, v_2|w) = \overset{\text{Tuning parameter}}{w}\, d\overbrace{(x_1, x_2)}^{\text{inputs}} + (1-w)\, d\overbrace{(y_1, y_2)}^{\text{outputs}}}$$

$$d(x_1, x_2) = \sqrt{\sum (x_{1j} - x_{2j})^2} \quad d(y_1, y_2) = |y_{1j} - y_{2j}|$$

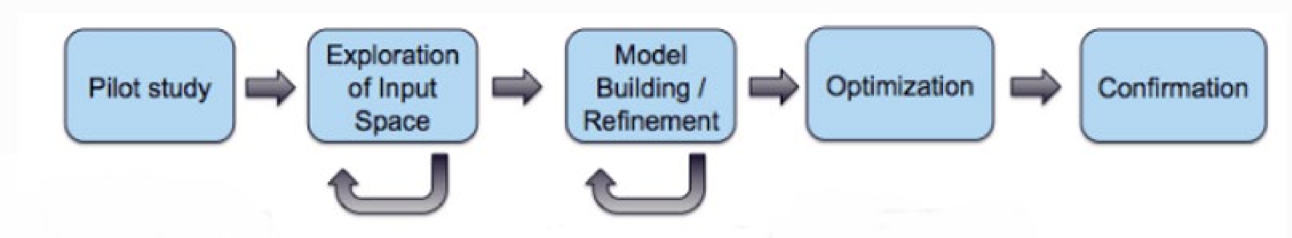
Increase Range of Model Predictions

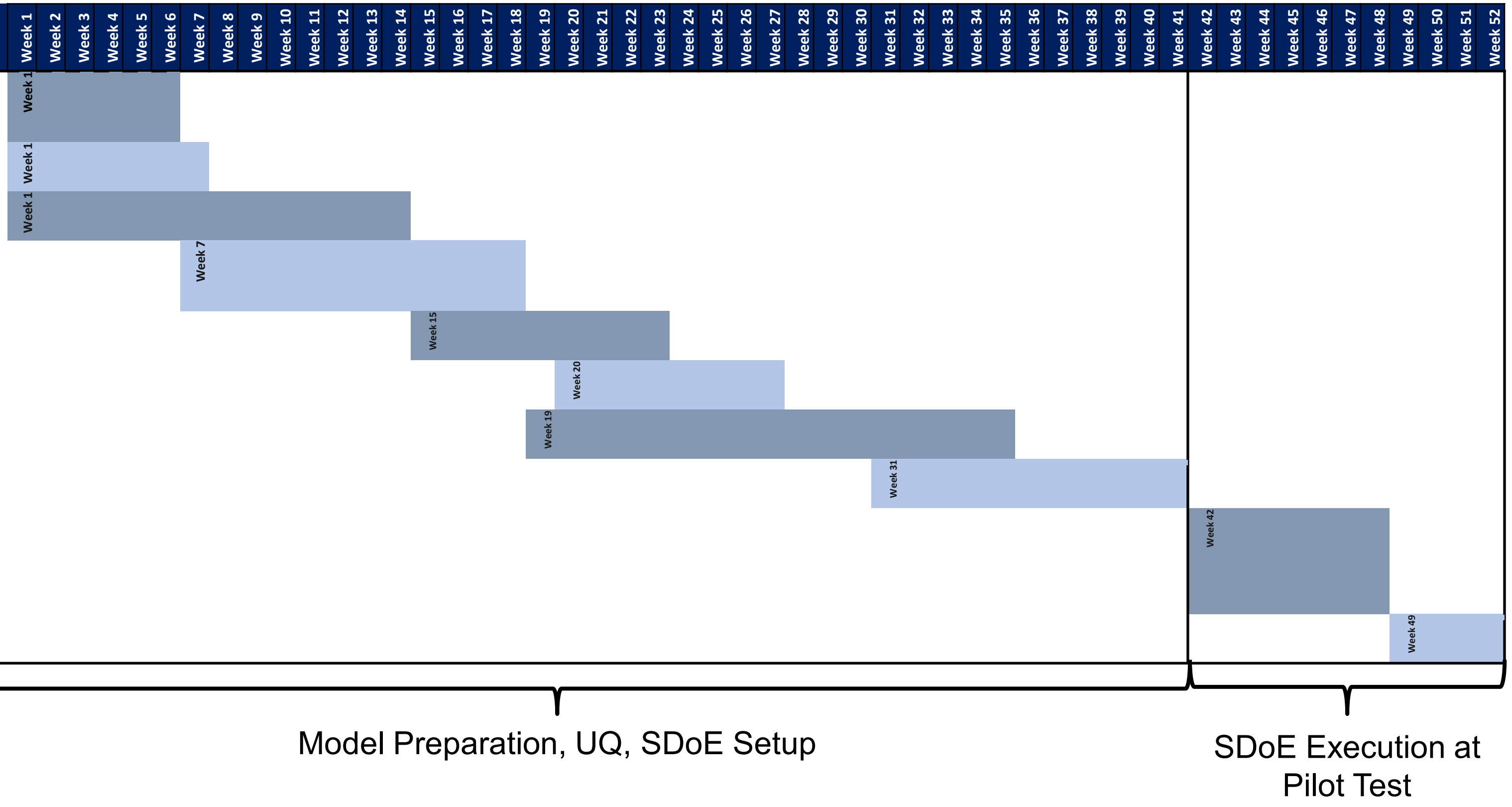


Output space spread increasing

CCSI²
Carbon Capture Simulation for Industry Impact

Notional Gantt Chart for Designing Pilot Tests





Step/Action	Total Weeks
Determine the total time available for the experiment and the expected time required for a single experimental run	6
Define the goals of the experiment	7
Assess performance and maturity of system process models	14
Identify and classify the dependent, independent intermediate, and nuisance variables	12
Identify restrictions on the experiment	9
Identify region of interest for experiment	8
Determine appropriate sequential plan for SDoE	17
Construct design(s) to be used in initial phase of the SDoE	11
Execute SDoE: collect data from current phase, assess results, construct design(s) for next phase. Repeat to align with overall goals of experiment	7
Collect results of SDoE, summarize key takeaways	4

Model Preparation, UQ, SDoE Setup

SDoE Execution at Pilot Test

TCM CO_2 Capture Pilot Support

Open-Source CESAR-1 Baseline Campaign Guidance and Methods Standardization

Objective

Maximize value of pilot testing by ensuring the right data is collected to aid in reduction of technical risk associated with process scale-up

Rationale

This task will provide quality data for refining existing open gen2 solvent process models and incorporating uncertainty quantification (UQ) as appropriate. The refined models will be scaled up to enable work in techno-economic analysis and optimization for plant-level processes of interest, targeting high capture. This will enable establishment of CESAR1 as a baseline for comparison for novel CO_2 capture technologies – particularly with respect to deep decarbonization applications.

Approach

- Refine process models of CESAR1 solvent system with goal of supporting future test campaign focused on amine emissions characterization and reduction

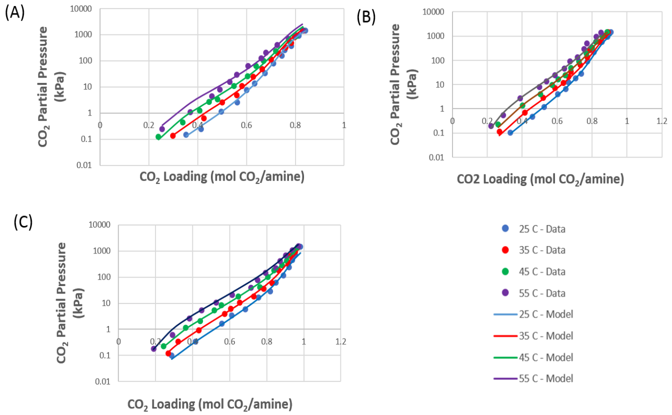
Outcome

- Development of rigorous and predictive process models with uncertainties quantified for key process indicators – reduce risk associated with process scale-up
- Sequential design of experiments (SDoE) maximizes the value of data collected – flexible for various test campaign goals and classes of technologies

Deliverables

- Refinement of CESAR1 process models for the TCM pilot plant,
- Identify goals for the test campaign and developing a strategy to incorporate SDoE into a pilot campaign.

CESAR-1 VLE Model



EPRI/PNNL EEMPA CO_2 Solvent Pilot Support

Model Development, Optimization, SDoE

Objective

Maximize value of pilot testing by ensuring the right data is collected to aid in reduction of technical risk associated with process scale-up of EEMPA being tested at NCCC in collaboration with EPRI

Rationale

Provide computational support and development of tools, methods, benchmarks, and guidelines to aid in the capture pilot and demonstration projects through process modeling, quantification of uncertainty, and development of optimal test plans to maximize the value of data generated

Approach

- PNNL/EPRI Pilot Support
- Support test campaign for novel solvent at National Carbon Capture Center
  - focus on controlling water balance and achieving high levels of CO2 capture

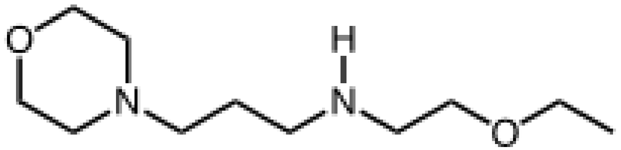
Outcome

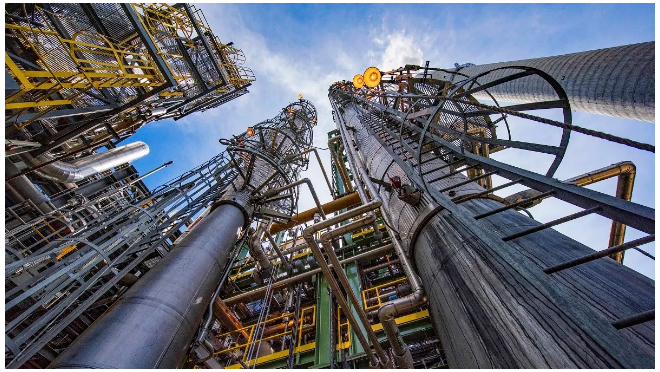
- Development of rigorous and predictive process models with uncertainties quantified for key process indicators – reduce risk associated with process scale-up
- Sequential design of experiments (SDoE) maximizes the value of data collected – flexible for various test campaign goals and classes of technologies

Deliverables

- SDoE test strategy for EEMPA at NCCC
- Complete integration of the fundamental knowledge on solvent-packing interactions into the multiscale framework for column scale design and optimization.

EEMPA





UKy/Nucor CO_2 Capture Pilot Support

Technology Development Support – UKy/Nucor Steel Plant Pilot Support

Objective

Provide process and economic modeling support, optimization, and UQ to help guide testing of the University of Kentucky solvent based process at the Nucor facility.

Rationale

Provide computational support and development of tools, methods, benchmarks, and guidelines to aid FECM and DOE funded point source capture pilot and demonstration projects through process modeling, quantification of uncertainty, and development of optimal test plans to maximize the value of data generated

Approach

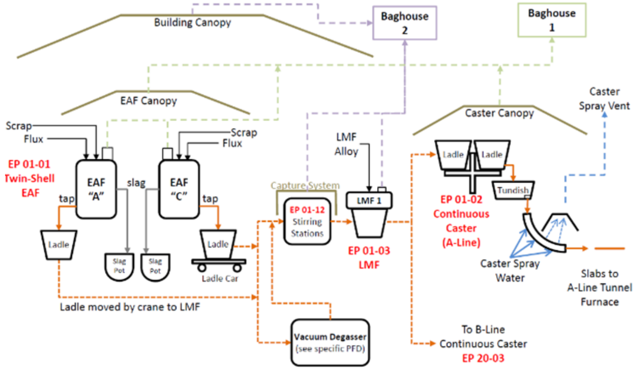
- Process analysis for solvent-based CO_2 capture system implemented at Nucor Steel Gallatin (e.g., understand impact of low L/G on packing performance, determine optimal process set points)
- Apply CCSI Toolset optimization techniques to determine optimal set points of the process.

Outcome

- Understand wettability of the packing with lower L/G ratios, using predictive CFD models with measured physical properties of the solvent such as viscosity, surface tension, and contact angle.
- Sequential design of experiments (SDoE) maximizes the value of data collected – flexible for various test campaign goals and classes of technologies

Deliverables

- Report out on optimal operating conditions for various disturbances and arc furnace steady-states
- Report out on impacts of wettability with low L/G ratios



CO_2 Capture from Nucor Steel Electric Arc Furnace

US Steel Membrane CO_2 Capture Pilot

Model Development, SDoE

Objective

Maximize value of pilot testing by ensuring the right data is collected to aid in reduction of technical risk associated with process scale-up of a polymeric membrane developed by NETL at US Steel test facility

Rationale

Ensure optimal test plans to inform developed membrane and integrated process models with refined parametric uncertainty, maximizing the value of data generated

Approach

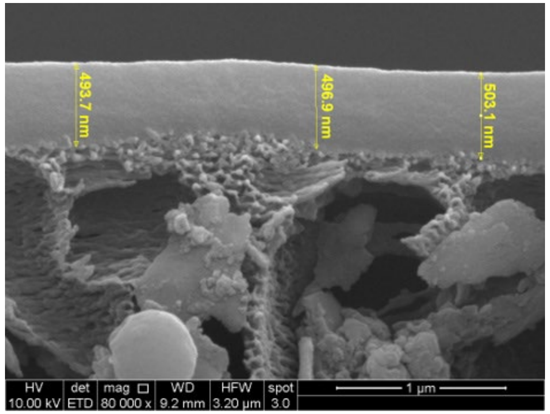
- Development of rigorous and predictive process models with uncertainties quantified for key process indicators – reduce risk associated with process scale-up
- Sequential design of experiments (SDoE) maximizes the value of data collected – flexible for various test campaign goals and classes of technologies

Outcome

- Quantification and estimation key performance indicators over a wide range of conditions
- Reduced uncertainty in performance, improving predictions at larger scales and alternate configurations.

Deliverables

- Membrane module model that captures impacts of varying temperature, flow maldistribution and real gas behavior.
- Process flow diagram for integration with US Steel process
- Execute test campaign informed by SDoE



NETL Membrane Development

Honeywell UOP CO_2 Solvent Pilot Support

Technology Development Support – Honeywell Piperazine Pilot Support

Objective

Estimate performance of piperazine under varying conditions, including estimation of performance for emission control systems (that could be potentially applied to other technologies).

Rationale

Provide methodologies to approximate waterwash performance utilizing extensive data collected at NCCC and other pilots and provide modeling and process optimization using detailed costing data.

Approach

- Utilize available data for water wash and prescubber performance at NCCC, TCM, and other pilots to develop and validate an approximate water wash model
- A cost model based on the FEED results will be coded in gPROMS and linked to an equation-based optimization tool to optimize designs for representative applications
- Refinement of Piperazine model in gPROMS

Outcome

- Development of rigorous and predictive process models with uncertainties quantified for key process indicators – reduce risk associated with process scale-up
- Sequential design of experiments (SDoE) maximizes the value of data collected – flexible for various test campaign goals and classes of technologies

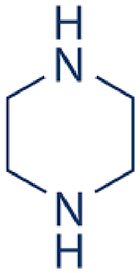
Deliverables

- gPROMS equation-based model of piperazine
- Approximated model of waterwash based on gas film coefficients

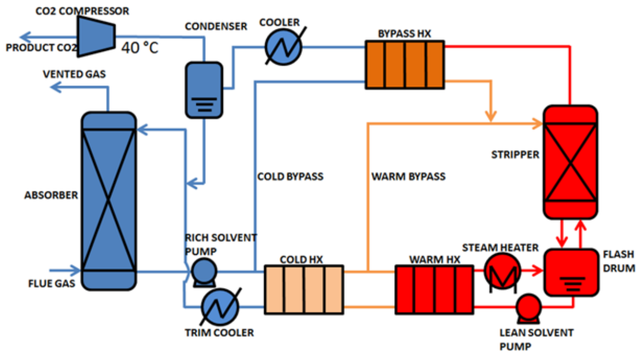
Honeywell uop

TEXAS
The University of Texas at Austin

Piperazine



PZAS Process



OSU Membrane CO_2 Capture Pilot Support

Technology Development Support – OSU Facilitated Transport Membrane Pilot Support

Objective

Support OSU's Facilitated Transport Membrane pilot testing at Holcim US's cement plant in Holly Hill, South Carolina and the NGCC power plant located at the Wyoming Integrated Test Center in Gillette, Wyoming

Rationale

Provide computational support and development of tools, methods, benchmarks, and guidelines to aid OSU facilitated transport membranes pilots at a cement plant and the Wyoming Integrate Test Center.

Approach

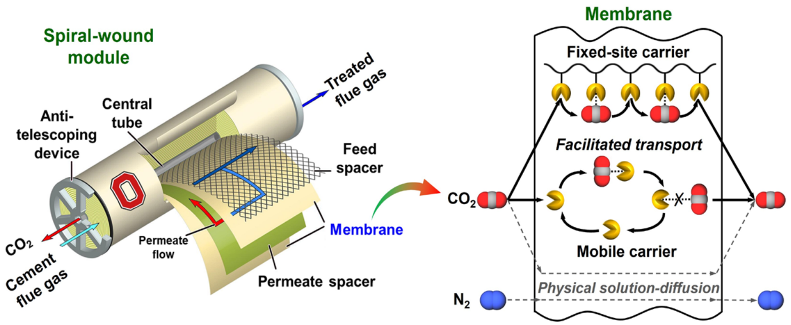
- Develop a membrane module performance model for facilitated transport membranes that also captures the effects of varying temperature, flow maldistribution, and real gas behavior.
- Execute an experimental test campaign informed by the CCSI2-developed SDoE framework.
- Refine parametric uncertainty in the modeling framework using data gathered in ongoing pilot demonstrations.

Outcome

- Development of rigorous and predictive process models with uncertainties quantified for key process indicators reducing risk associated with process scale-up
- Sequential design of experiments (SDoE) maximizes the value of data collected – flexible for various test campaign goals and classes of technologies

Deliverables

- Develop facilitated transport membrane module performance model into Aspen



CCSI^2

Carbon Capture Simulation for Industry Impact

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

Michael.matuszewski@netl.doe.gov

Disclaimer

ACT – Sustainable OPEration of post-combustion Capture plants (EY23)

Solvent Emission Prediction Modeling Tools

Objective

Rationale

- The SCOPE project is a multi-national, multi-disciplinary, and multi-hierarchical project which aims to understand the nature of solvent emission losses and mechanisms to mitigate.
- Modeling work needed to support design and operational strategies to minimize the cost to mitigate solvent emissions

Approach

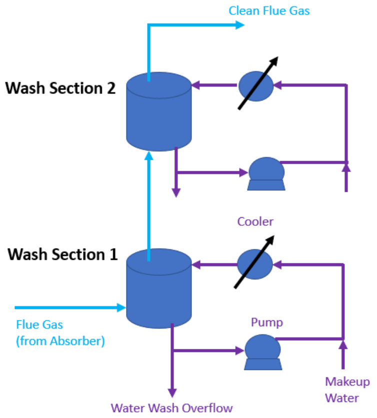
- Refine solvent vapor-liquid equilibrium predictions based upon data collected from Heriot Watt University (HWU)
- The project team will integrate solvent models to be refined with test data with OGT equipment models and CCSI2 process models to properly represent MEA and CESAR-1 solvent based capture system performance
- Emission control technologies will be modelled and then validated against plant data from project partners (TCM)

Outcome

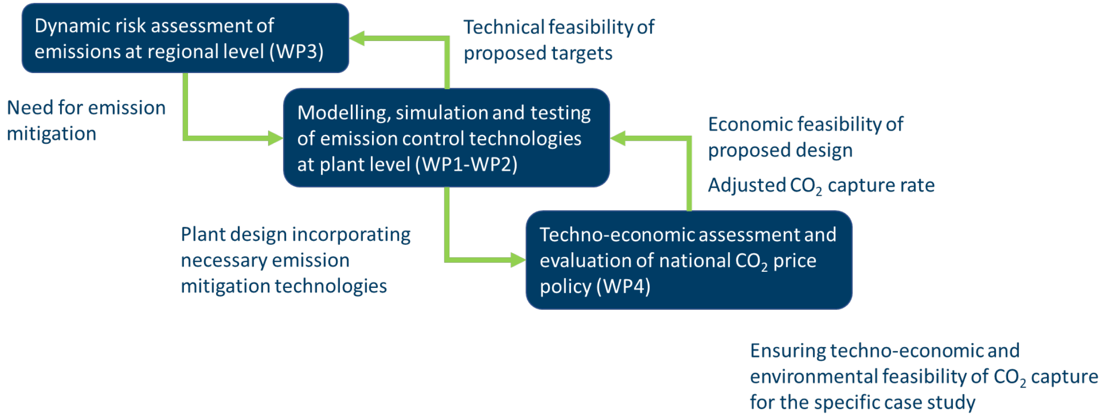
- New set of modeling capability for predicting volatile and aerosol-based emissions, both for MEA and CESAR1 solvents
- A process level understanding of emissions mitigation requirements

Deliverables

SCOPE



Case studies in SCOPE : multi-level approach



Dynamic risk assessment of emissions at regional level (WP3)

Technical feasibility of proposed targets

Need for emission mitigation

Modelling, simulation and testing of emission control technologies at plant level (WP1-WP2)

Economic feasibility of proposed design

Adjusted CO_2 capture rate

Plant design incorporating necessary emission mitigation technologies

Techno-economic assessment and evaluation of national CO_2 price policy (WP4)

Ensuring techno-economic and environmental feasibility of CO_2 capture for the specific case study

Validation of Models

- **First principle process models** are a key component in demonstrating **risk reduction** for process scale-up
- **Model demonstration and validation** at pilot scale is understood to be an **important component** of the FOA
- **All pilots** in 2614 Round 3 expected to **develop and validate process models** of their technology
  - Models **do not** have to be provided to NETL/FECM, however details of models and submodels, data sets, and validations will be examined
- **CCSI^2 can provide support** for model development, optimal DoE, uncertainty quantification and validation

What Is DoE Used For?

Development

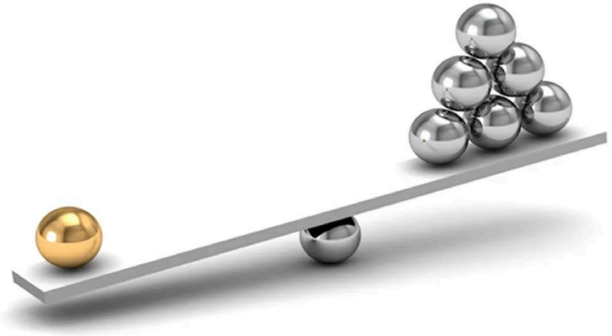
- Evaluate and compare product configurations
- Evaluate material alternatives
- Determine parameters settings to work well under variable field conditions
- Determination parameters that impact product performance

Improvement

- Reduce variability
- Obtain closer conformance to target requirements
- Reduce development time
- **Reduce overall costs**

Why Use Statistically Designed Experiments?

- **Extract maximum information with a fixed budget**
  - Produces exceptionally high-quality data
- **Can save years off pilot test schedule**
- **Proven track record from past applications**
  - Over 25% reduction in model uncertainty
  - CO_2 Capture percentage within 3-6% with 95% confidence



Plan for CCSI² Contributions to Support of EPRI/ EEMPA Campaign

Initial Phase

- Plant start-up
- Achieve steady-state water loading

Phase 1

- Demonstrate 90% CO_2 capture for coal, natural gas flue gases
- Use designed experiments to strategically manipulate chosen variables (e.g., solvent circulation, stripper temperature)

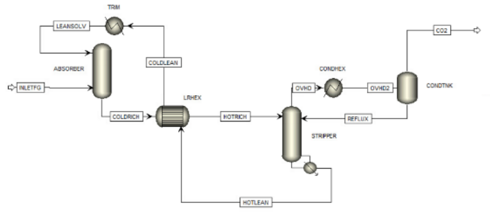
Additional Phases

- Target high capture
- Minimize solvent regeneration energy
- Evaluate effect of solvent water content on CO_2 capture
- Investigate effect of flue gas flowrate and temperature
- Analysis of metal vs. plastic packing

Process Model Refinement

Process Inputs

Solvent Circulation
Solvent Capacity
CO_2 Capture Target
Operating T, P



Process Outputs

CO_2 Capture
Specific Reboiler Duty

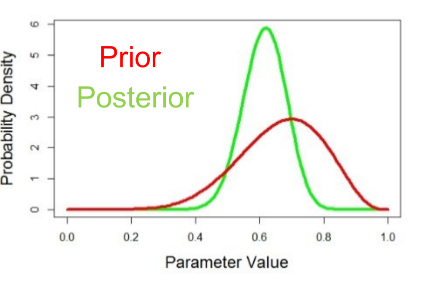
Model Parameters

Thermodynamics
Mass Transfer
Interfacial Area
Kinetics

Sequential design of experiments (SDoE) enables direct incorporation of knowledge learned in previous stages for strategic data collection

Stochastic Model

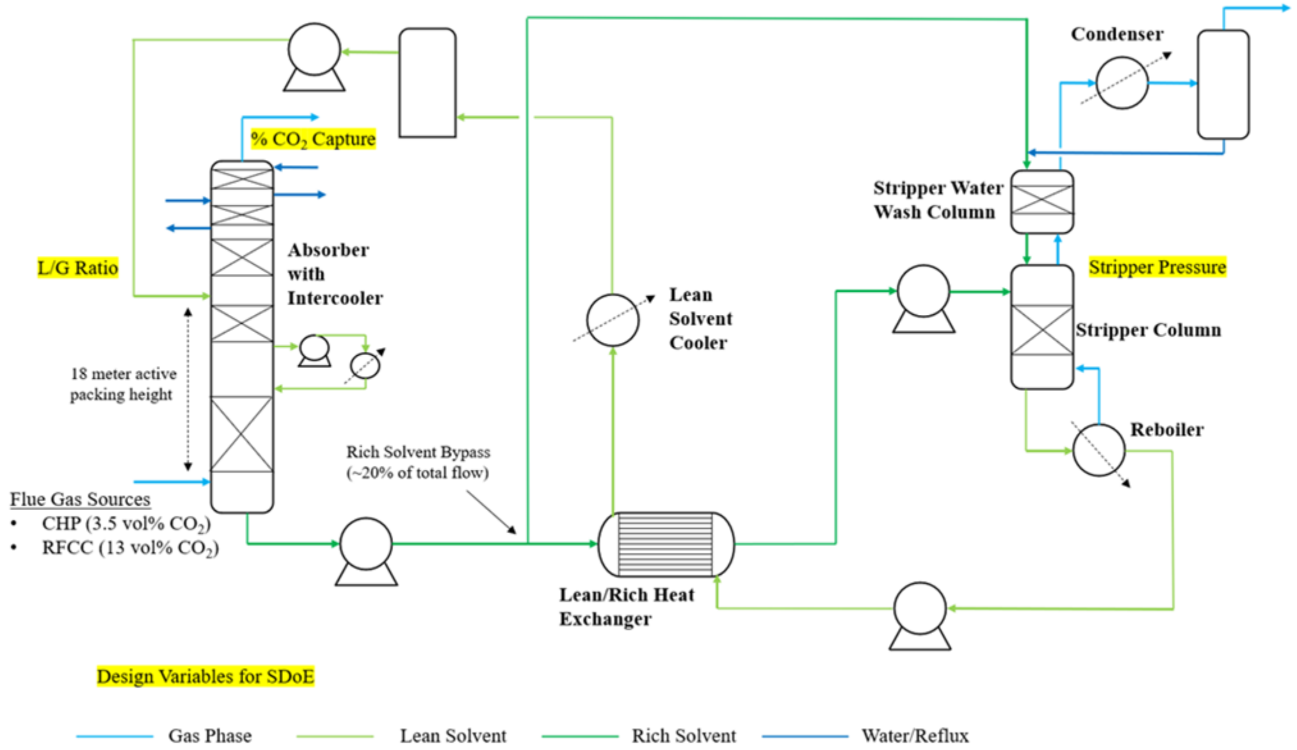
- Reduce risk associated with process scale-up



CCSI²
Carbon Capture Simulation for Industry Impact

TCM Test Campaign for RTI NAS Solvent

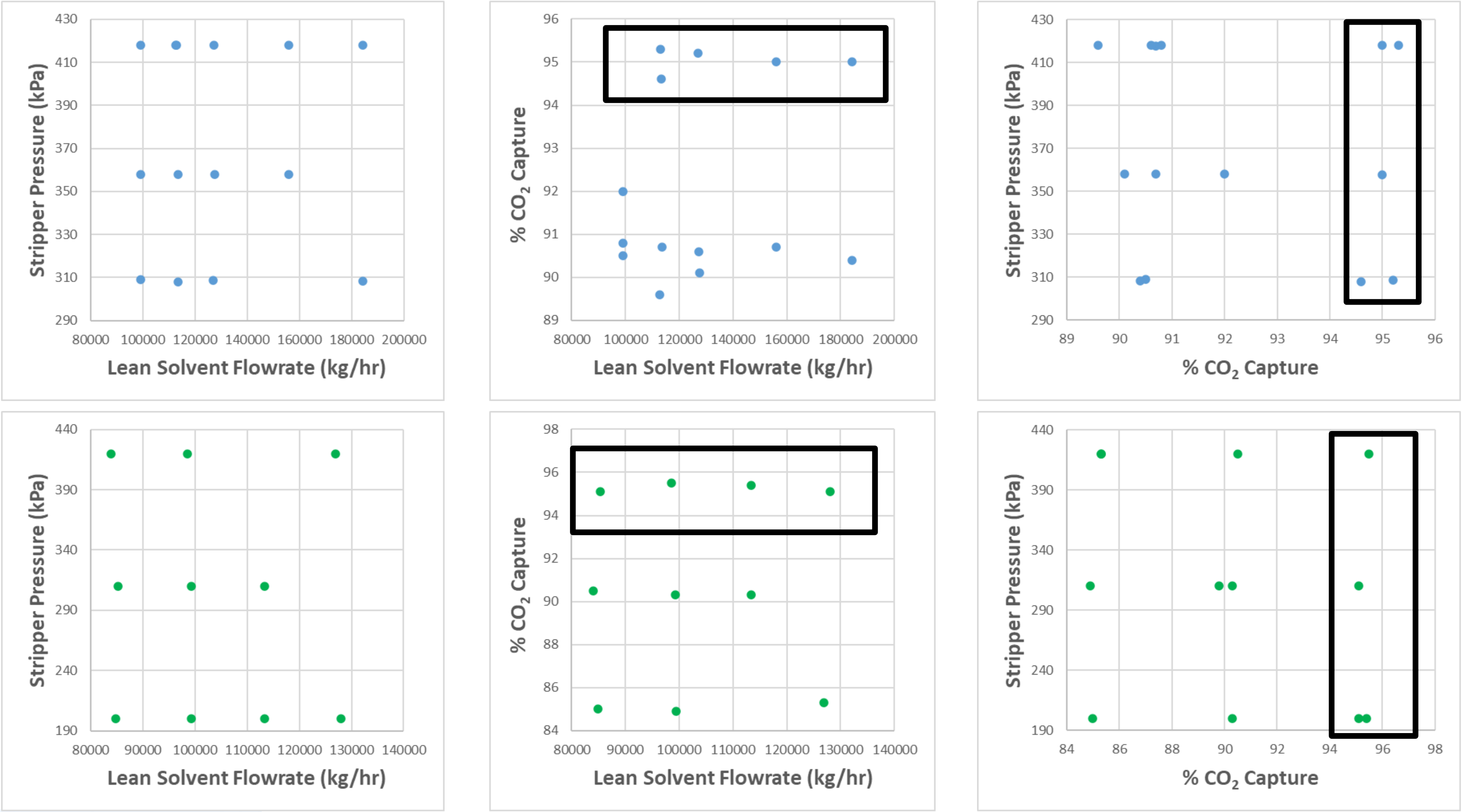
- Leveraged SDoE to guide NAS test campaign at TCM → focused on demonstrating high levels of CO_2 capture with low solvent emissions and regeneration energy requirement
- CCSI^2 team contributed separate designed experiments for gas-fired combined heat and power (CHP) [3.7 vol% CO_2] and residual fluidized catalytic cracker (RFCC) [13.5 vol% CO_2] flue gas sources
- Each designed experiment includes a series of test matrices with 12-22 proposed operating conditions for flexibility in design size



<u>Design factors</u>:
CO_2 Capture: 85 – 95%
Absorber L/G Ratio: 2.5 – 6.5 kg/kg
Stripper Pressure: 0.9 – 3.2 barg

SDoE Results – Data Collection at TCM

Data sets generated for SDoE demonstrate good coverage of operation space:



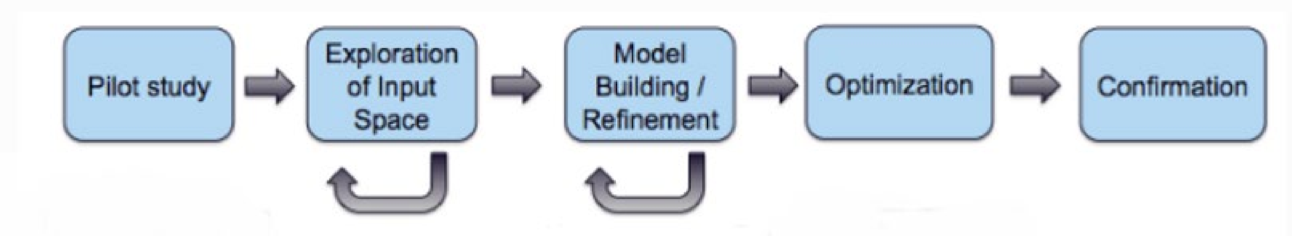
Characterization of parameter interactions through DoE → demonstrates multiple pathways to high capture levels based on the trade-off between solvent circulation and CO$_2$ capacity

● **Coal-based flue gas**

● **NGCC flue gas**

Sequential Design of Experiments (SDoE)

- **Design of experiments (DOE)** is a powerful tool for accelerating learning by targeting maximally useful input combinations to match experiment goals
- **Sequential design of experiments (SDoE)** allows for incorporation of information from an experiment as it is being run, by updating selection criteria based on new information
- Specific algorithms can be tailored to match experimental goals. Options available in the CCSI Toolset include:
  - Uniform Space Filling (USF)
  - Non-Uniform Space Filling (NUSF)
  - Input-Response Space Filling (IRSF)
  - Robust Optimality-Based Design of Experiments (ODoE)
- Recommended to run experiments in phases to take advantage of SDoE capabilities and customize test designs to meet expected project outcomes

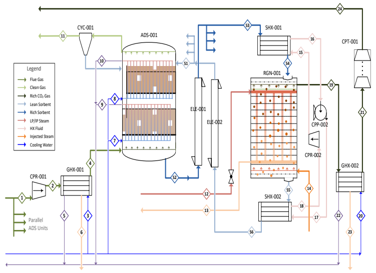


Detailed discussion on SDoE:

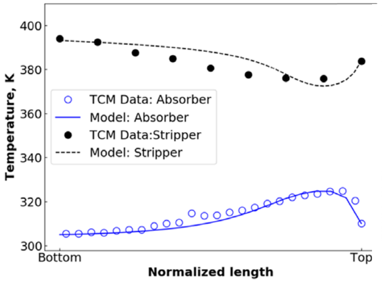
Technical Risk Reduction: Sequential Design of Experiments and Uncertainty Quantification (Abby Nachtsheim – LANL)
Thursday (8/31/2023) @ 9:30 AM during Point Source Carbon Capture Breakout Session

Stochastic Equation-Oriented Modeling and/or "Black Box" Simulations

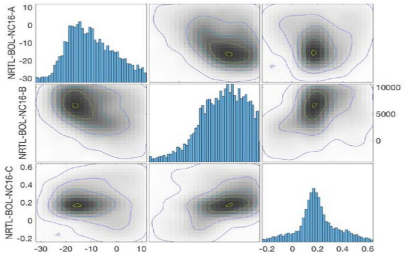
High Fidelity Process Modeling



Model Validation

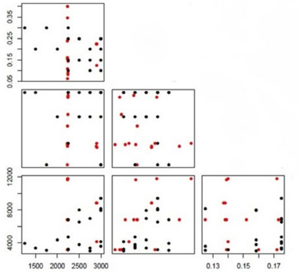


Uncertainty Quantification

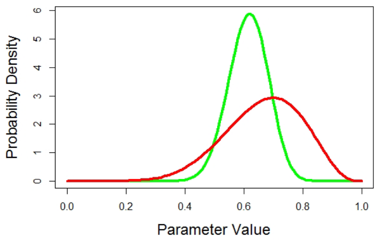


UQ Guides SDoE to Optimize Data Value, Maximize Learning

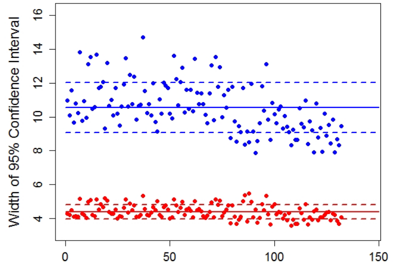
Optimize Experimental Design



Refine Model Parameters

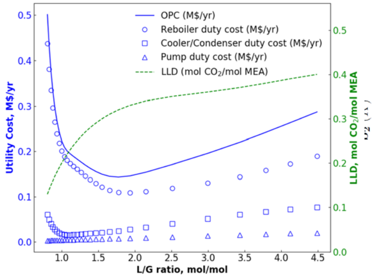


Maximizing Learning

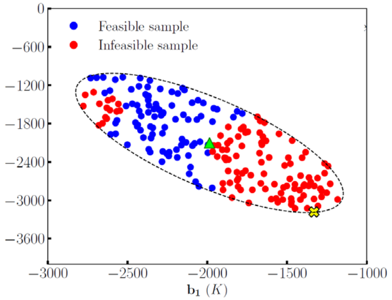


Framework for Robust-Optimal Design and Operation

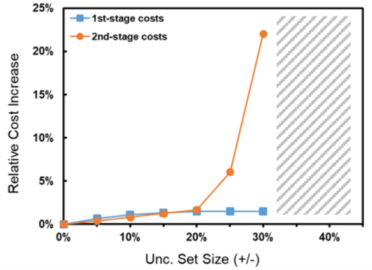
Process Optimization



More Robust Optimal Designs



Quantify Price of Robustness



- **Uncertainty Quantification (UQ)** provides a modeling framework for characterizing epistemic uncertainty - essential for understanding scale-up risk
- **Sequential Design of Experiments (SDoE)** techniques enable reduction of uncertainty through strategic collection of process data to maximize learning from pilot test campaigns
- **Robust Optimization (RO)** framework quantifies cost of accommodating uncertainty in designs ensured to meet performance targets (with a chosen confidence level)

CCSI²
Carbon Capture Simulation for Industry Impact

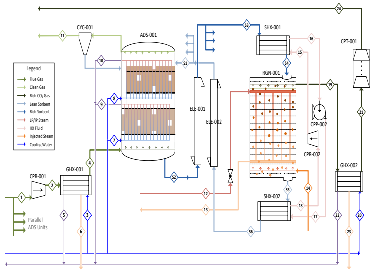
CCSI² – Modeling, Optimization and Technical Risk Reduction

CCSI²
Carbon Capture Simulation for Industry Impact

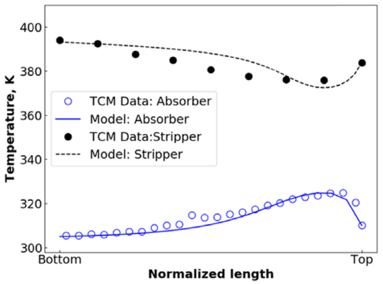
Multi-lab modeling initiative to support carbon capture technology development

NATIONAL ENERGY TECHNOLOGY LABORATORY
BERKELEY LAB
Lawrence Livermore National Laboratory
Los Alamos NATIONAL LABORATORY EST.1943
Pacific Northwest NATIONAL LABORATORY
OAK RIDGE National Laboratory
Carnegie Mellon
WestVirginiaUniversity.
UNIVERSITY OF NOTRE DAME
THE UNIVERSITY OF TEXAS AT AUSTIN
UT
UNIVERSITY OF PITTSBURGH

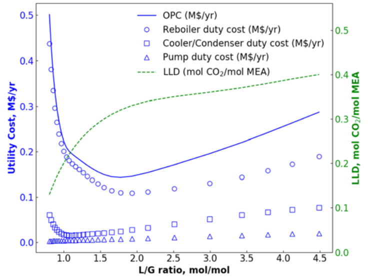
High Fidelity Process Modeling



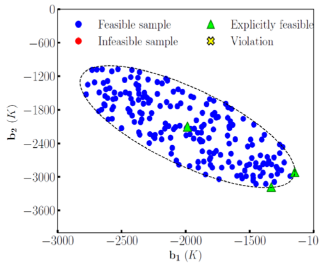
Model Validation



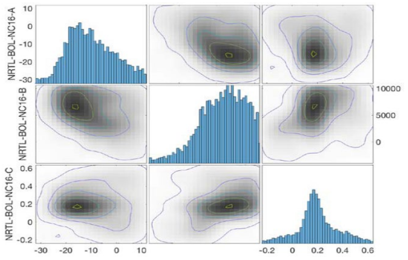
Process Optimization



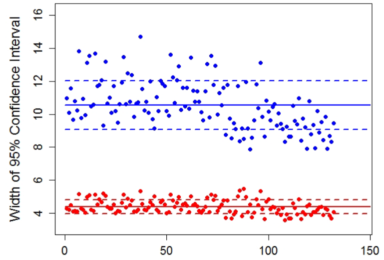
Robust Design

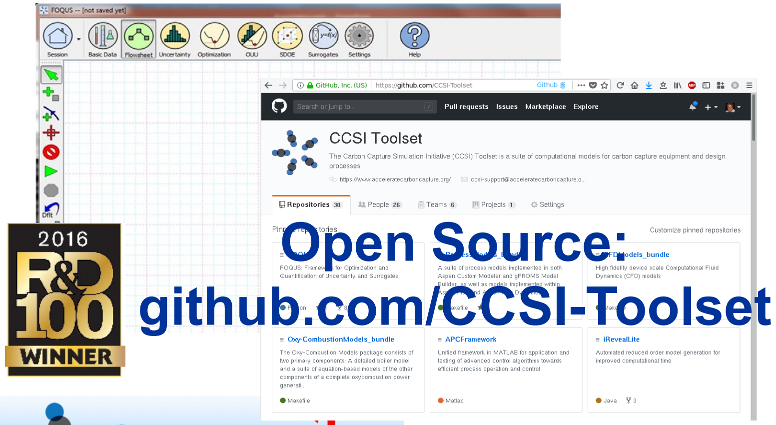


Uncertainty Quantification



Maximizing Learning





CCSI Toolset

The Carbon Capture Simulation Initiative (CCSI) Toolset is a suite of computational models for carbon capture equipment and design processes.

https://www.acceleratecarboncapture.org/
ccsi-support@acceleratecarboncapture.o...

FOQUS: Framework for Optimization and Quantification of Uncertainty and Surrogates

A suite of process models implemented in both Aspen Custom Modeler and gPROMS Model Builder, as well as models implemented within

CFDModels_bundle
High fidelity device scale Computational Fluid Dynamics (CFD) models

Oxy-CombustionModels_bundle
The Oxy-Combustion Models package consists of two primary components: A detailed boiler model and a suite of equation-based models of the other components of a complete oxycombustion power generati...
Makefile

APCFramework
Unified framework in MATLAB for application and testing of advanced control algorithms towards efficient process operation and control
Matlab

iRevealLite
Automated reduced order model generation for improved computational time
Java 3

Open Source:
github.com/CCSI-Toolset

2016 R&D 100 WINNER

CCSI²
Carbon Capture Simulation for Industry Impact

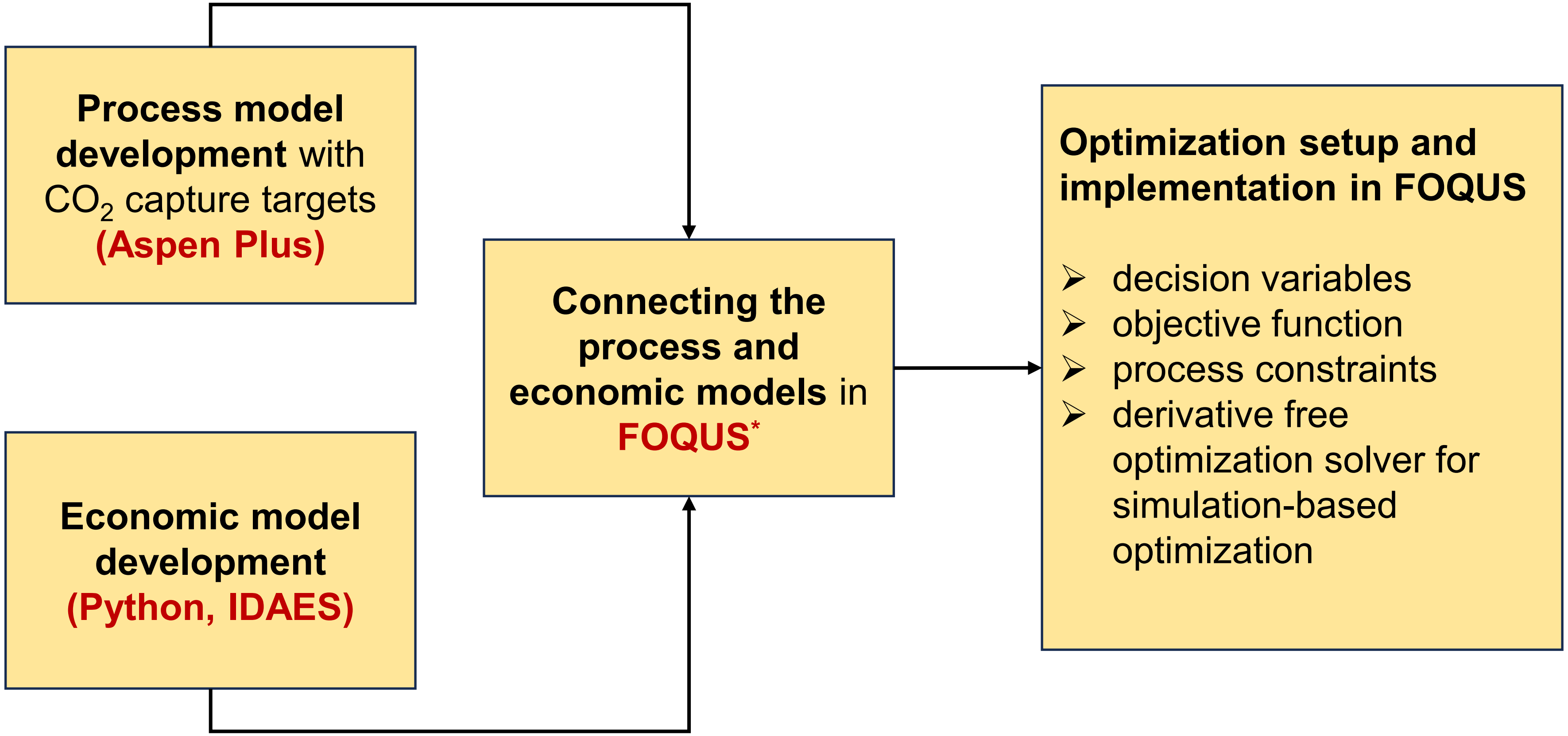
IDAES
Institute for the Design of Advanced Energy Systems

Open Source:
github.com/IDAES/idaes-pse

Objective

- Understand high capture process variables important for optimization
- Characterize optimal capture costs and their rate of increase as capture demands rise
- Assess usefulness of pilot data for model validation
- Quantify effects of model uncertainty
- Explore means to accommodate uncertainty

CCSI^2 Techno-Economic Optimization Framework



Process model development with CO_2 capture targets **(Aspen Plus)**

Economic model development (Python, IDAES)

Connecting the process and economic models in **FOQUS***

Optimization setup and implementation in FOQUS

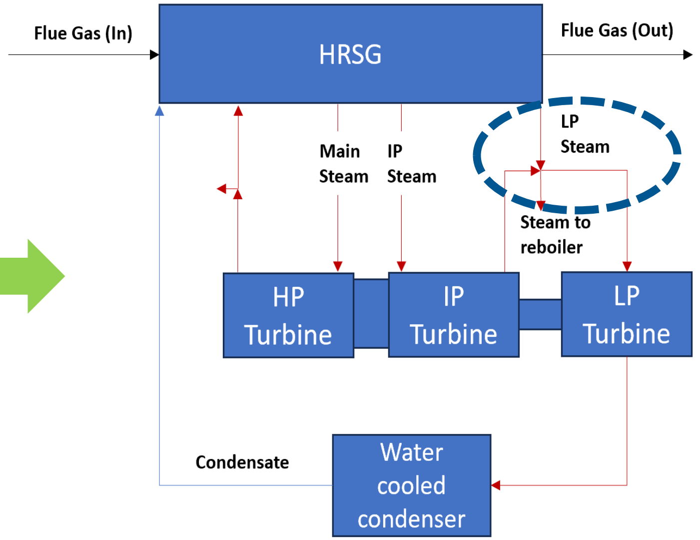
- decision variables
- objective function
- process constraints
- derivative free optimization solver for simulation-based optimization

*** Framework for Optimization and Quantification of Uncertainty and Surrogates**
Open Source: github.com/CCSI-Toolset/FOQUS

Optimization Cases

Case Name	CO_2 Capture Solvent	Steam Source for solvent regeneration	CO_2 Capture Levels (%)
SE	MEA	Steam extraction from NGCC steam cycle	Discrete levels between 90% – 99.8%
AB		Natural gas fired auxiliary boiler	

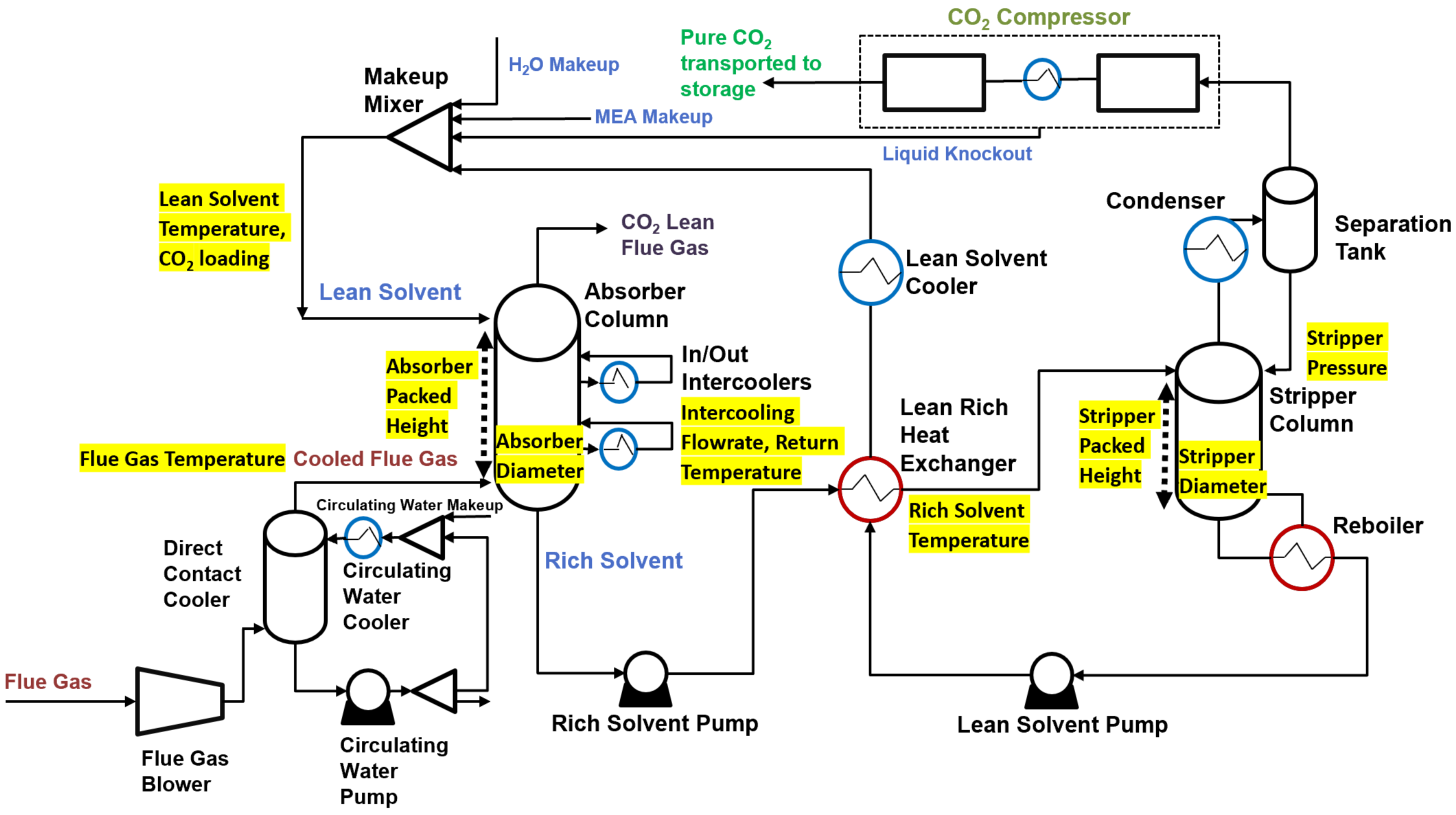
Steam extracted from the IP/LP steam turbine crossover



Auxiliary boiler: No steam extraction from the NGCC steam cycle

SE: MEA with steam extraction
AB: MEA with auxiliary boiler

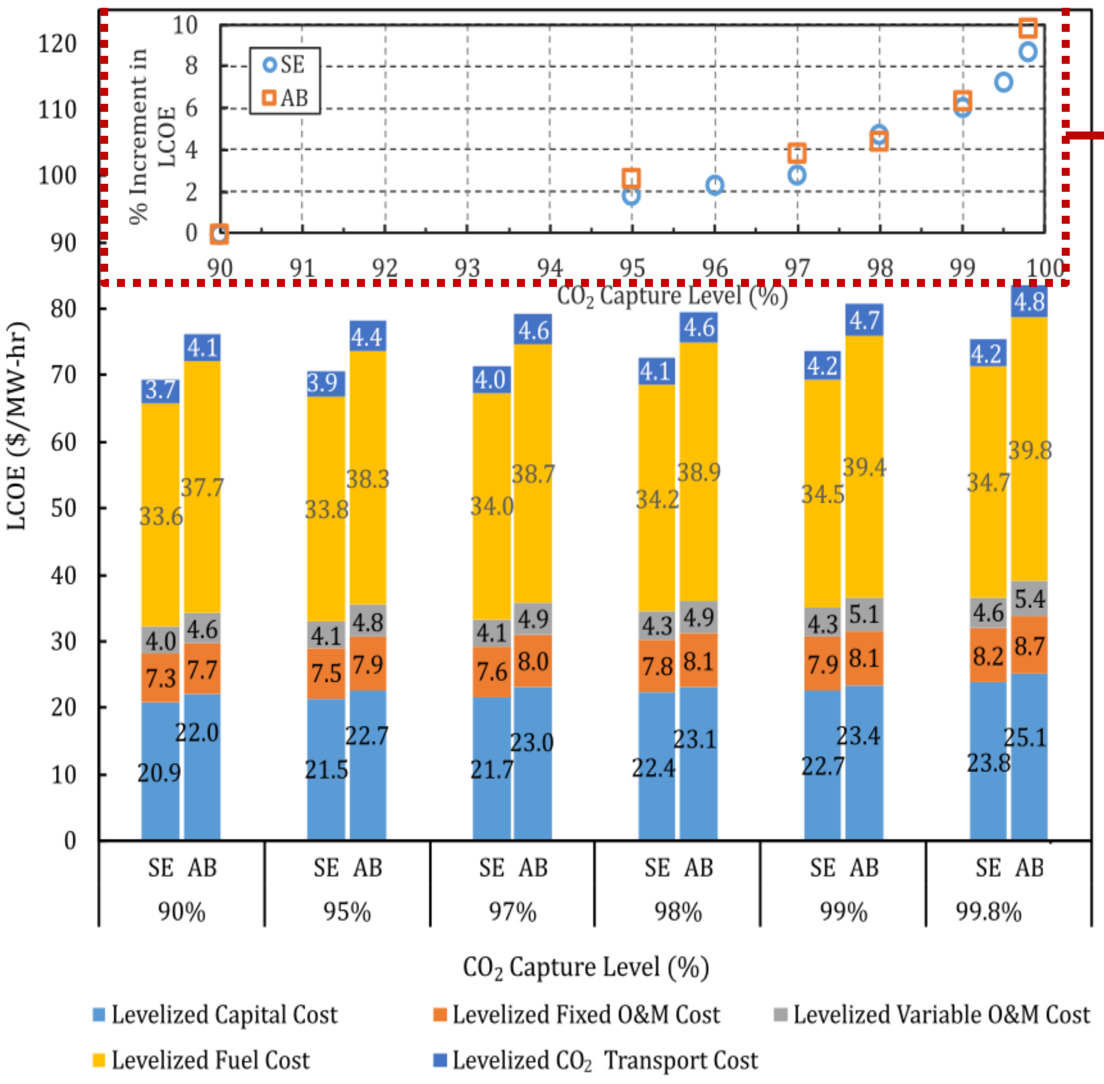
Optimization Decision Variables

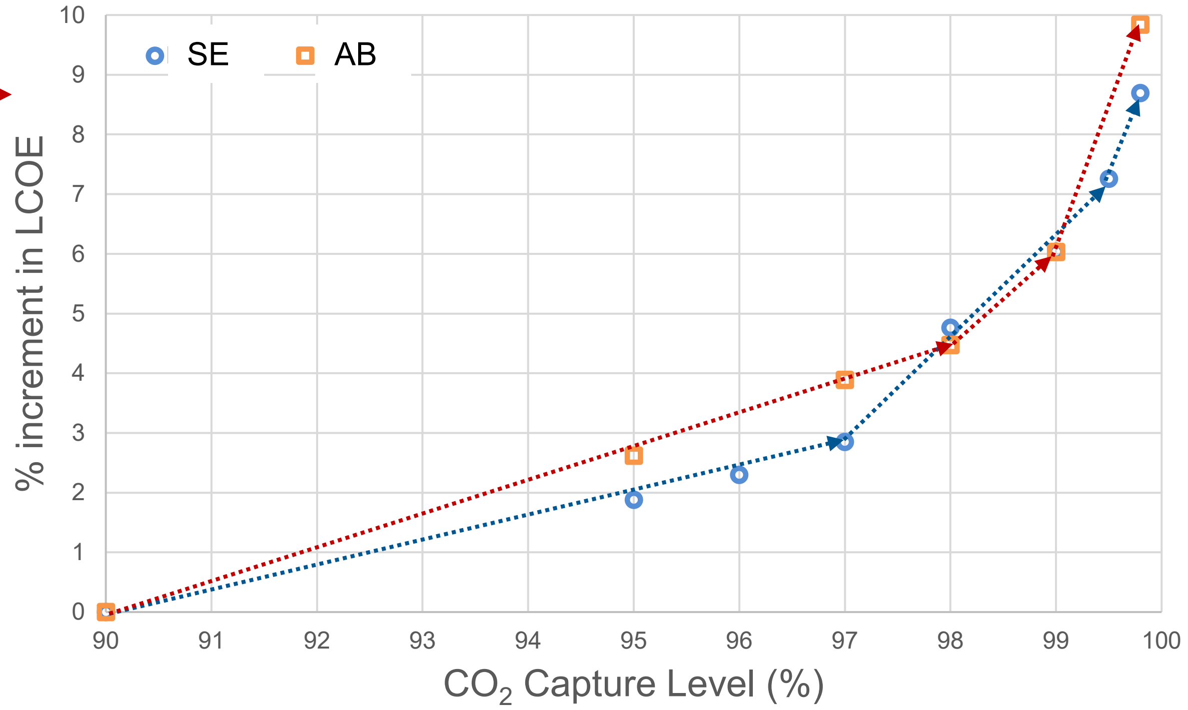


Decision Variables for Optimization Problem

Variable	Unit	Range
Absorber Diameter	meter	12 - 20
Absorber Height	meter	20 - 45
Lean CO$_2$ Loading	$\frac{\text{mol CO}_2}{\text{mol MEA}}$	0.1 - 0.25
Intercooler #1 Temperature	°C	25 - 45
Intercooler #2 Temperature	°C	25 - 45
Intercooler # 1 flow fraction	$\frac{\text{mass flow IC\#1}}{\text{mass flow lean solvent}}$	1e-5 - 1
Intercooler # 2 flow fraction	$\frac{\text{mass flow IC\#2}}{\text{mass flow lean solvent}}$	1e-5 - 1
Lean Solvent Temperature	°C	25 - 45
Rich Solvent Temperature (Lean/Rich HEX Exit)	°C	90 - 115
Stripper Height	meter	4 - 15
Stripper Diameter	meter	3 - 10
Stripper Pressure	kPa	170 - 230
FG Temperature	°C	25 - 45

LCOE Optimization Results

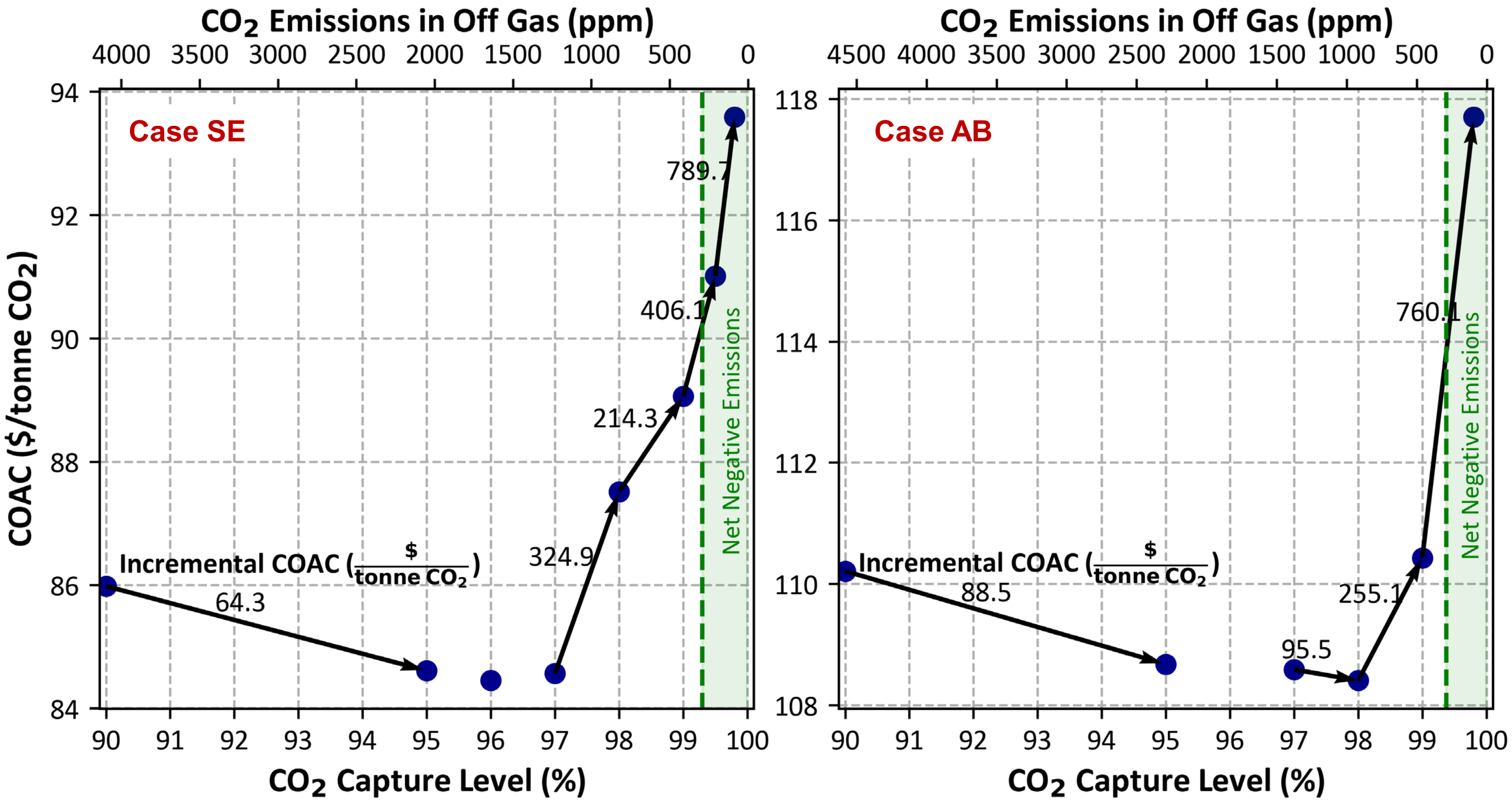




- A sharp increase is observed beyond 97% capture for the SE case and 98% capture for the AB case.
- Across the capture levels and between the steam sources, the cost contribution of the LCOE components does not vary significantly.

SE: MEA with steam extraction
AB: MEA with auxiliary boiler

Optimum Cost of Avoided Carbon (COAC)



- COAC has an optimal value near 96% capture.
- Incremental COAC is the change in LCOE wrt the change in CO_2 footprint

$$\Delta\mathrm{COAC}[i+\Delta i] = \frac{\mathrm{LCOE}[i+\Delta i] - \mathrm{LCOE}[i]}{\frac{\mathrm{CO_2\ Emissions}[i]}{\mathrm{Plant\ Net\ Power}[i]} - \frac{\mathrm{CO_2\ Emissions}[i+\Delta i]}{\mathrm{Plant\ Net\ Power}[i+\Delta i]}}$$

- Incremental COAC between capture levels increases exponentially above 97% and 98% CO_2 capture for case SE, and AB respectively

SE: MEA with steam extraction
AB: MEA with auxiliary boiler

Conclusions

- CCSI Toolset provides useful framework for optimizing numerous designs through **coupling of costing models and process models**
- **Inflection point** in cost of capture occurs past 98% for MEA
- **Designs can fail** with expected realizations of uncertain parameters
- **Recourse strategies** can handle much of the uncertainty, but **require insights gained via computational analyses**
- Full techno-economic modeling frameworks support the **test data generation of highest value**

Acknowledgements

Benjamin Omell
David Miller
Tony Burgard
Indra Bhattacharya

Josh Morgan
Brandon Paul (*)
Katie Hedrick (*)
Anca Ostace (*)
Miguel Zamarripa (*)
Daison Yancy Caballero (*)
Sally Homsy
Norma Kuehn (*)
Alex Zoelle (*)
Mike Matuszewski (*)

(*) NETL Support Contractor

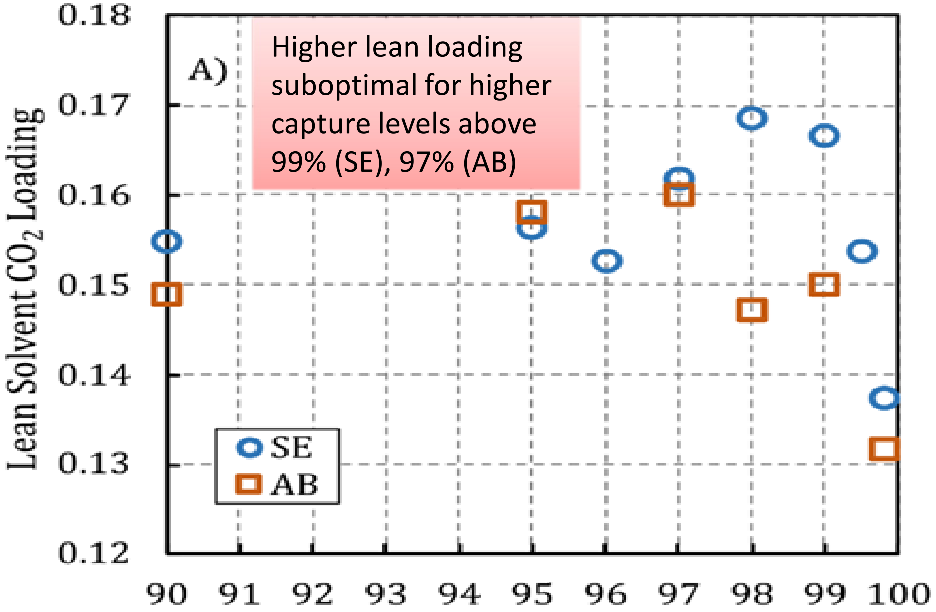
The authors graciously acknowledge funding from the U.S. Department of Energy, Office of Fossil Energy and Carbon Management, through the Carbon Capture Program.

Disclaimer

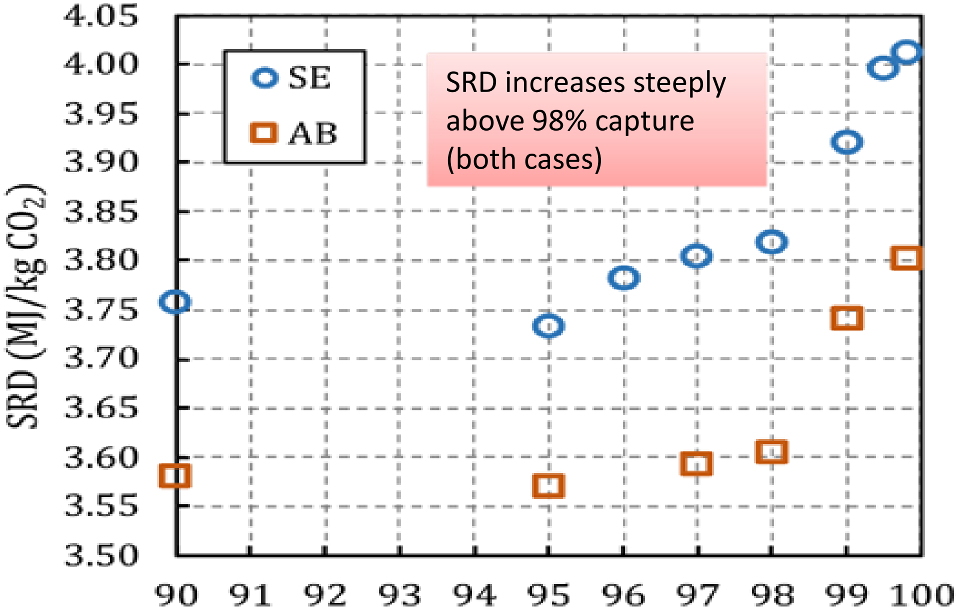
This project was funded by the Department of Energy, National Energy Technology Laboratory an agency of the United States Government, through a support contract. Neither the United States Government nor any agency thereof, nor any of their employees, nor the support contractor, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Optimum Design and Operation of CCS Unit – Case Comparison

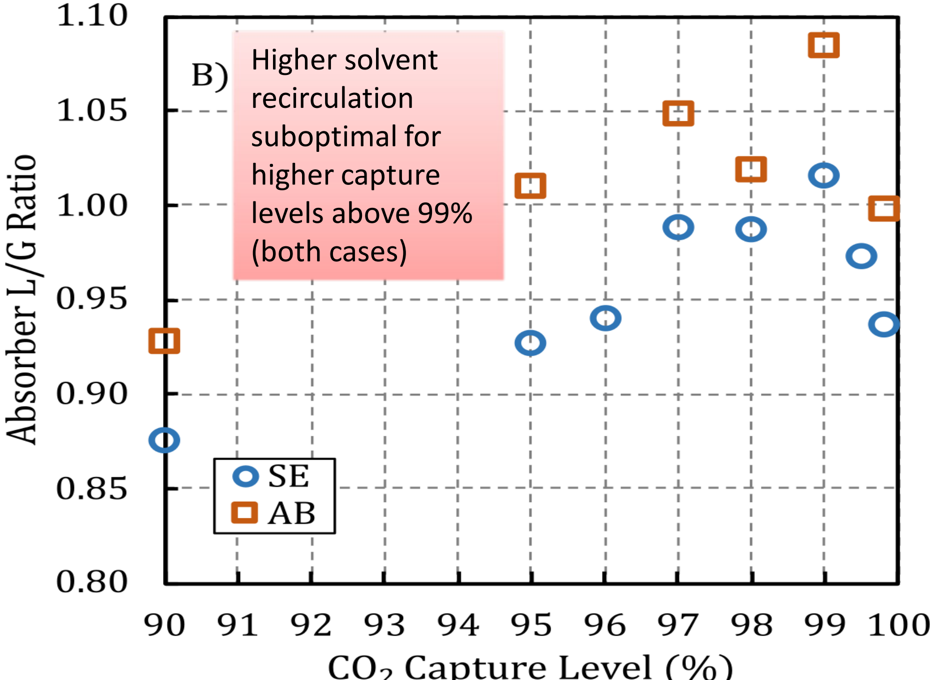
SE: MEA with steam extraction
AB: MEA with auxiliary boiler



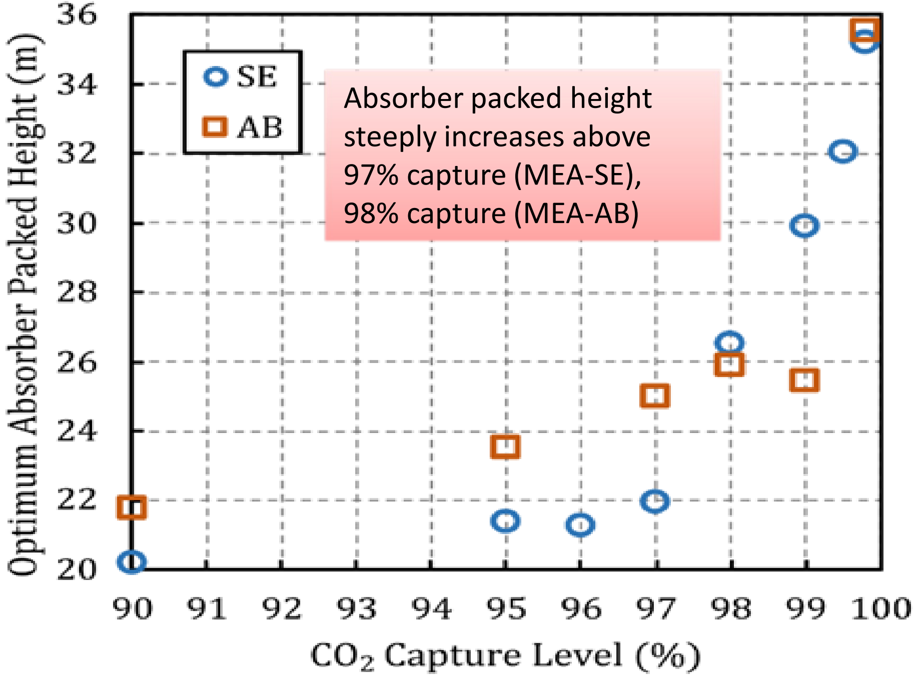
Higher lean loading suboptimal for higher capture levels above 99% (SE), 97% (AB)



SRD increases steeply above 98% capture (both cases)

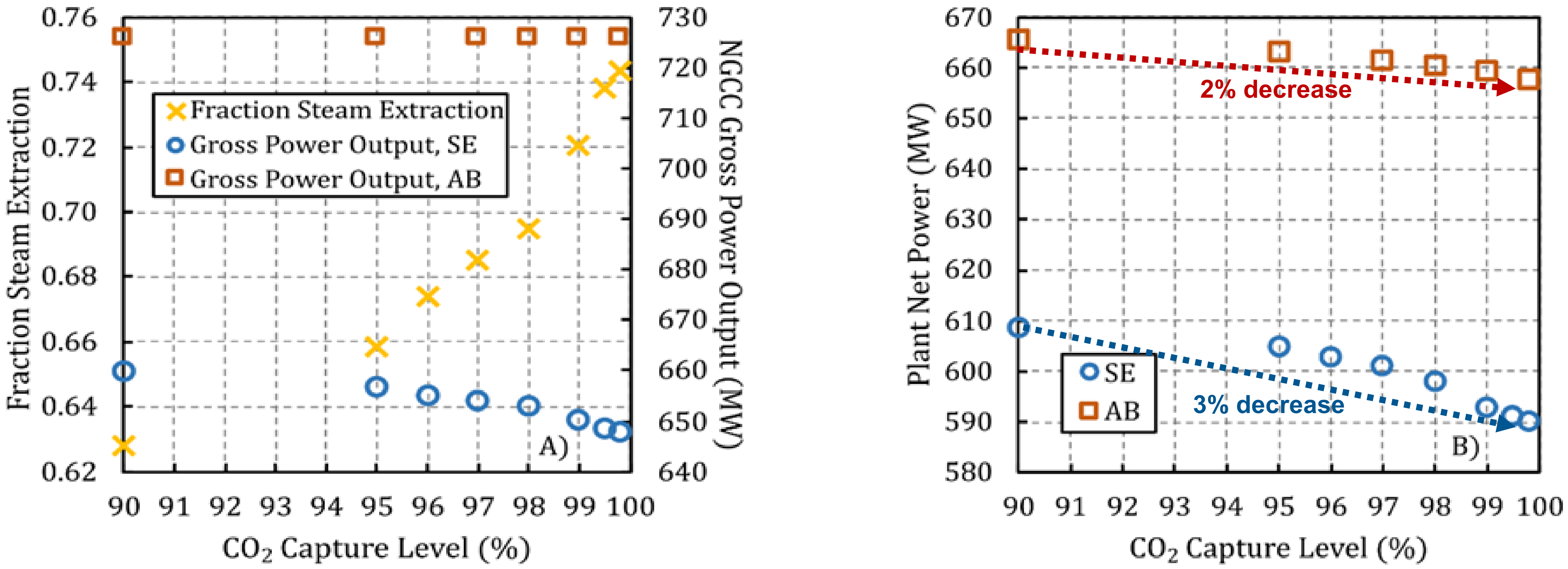


Higher solvent recirculation suboptimal for higher capture levels above 99% (both cases)



Absorber packed height steeply increases above 97% capture (MEA-SE), 98% capture (MEA-AB)

Performance of NGCC at Optimum CCS Conditions



- Optimum steam extraction in the SE case increases by 17% across the capture levels – NGCC Gross Power reduces by 1.8%.
- No steam extraction in the AB case – NGCC Gross Power remains constant—72 MW (on average) higher than SE.
- NGCC Net Power reduces in both cases across capture levels (combined effect of steam extraction and increasing auxiliary load).

SE: MEA with steam extraction
AB: MEA with auxiliary boiler

Economic Model: NGCC Solvent-based CCS System

- Developed in Python using the IDAES Costing Framework[1]
- **Key Inputs:**
  - **Resources and Chemicals:** Natural gas flowrate, solvent initial fill and makeup rate, etc.
  - **Design Conditions:** Absorber and stripper column size, heat exchanger surface area
  - **Operating Conditions:** Flue gas flowrate, solvent circulation rate, CO_2 capture rate
  - **Performance Indicators:** Heat exchanger duties; power requirement for blowers, pumps, and compressors
- **Key Outputs:** Economic Evaluation Metrics
  - **Total Plant Cost (Million $):** NGCC plant, CCS equipment, and full system
  - **Levelized Cost of Electricity ($/MW-hr):** Amount of revenue required per net megawatt-hour during the power plant's operational life to meet all capital and operational costs[2]
  - **Cost of CO_2 Captured ($/tonne CO_2):** Minimum CO_2 plant gate sales price that will incentivize carbon capture relative to a defined reference non-capture plant[2]
  - **Cost of CO_2 Avoided (COAC) ($/tonne CO_2):** Minimum CO_2 emissions price that will incentivize carbon capture relative to a defined reference non-capture plant[2]

[1] IDAES online documentation: https://idaes-pse.readthedocs.io/en/latest/index.html

[2] National Energy Technology Laboratory, "Cost and Performance Baseline for Fossil Energy Plants Volume 1: Bituminous Coal and Natural Gas to Electricity Revision 4a," US DOE, Pittsburgh, PA, 2022.