CCSI^2 Process Modeling and Optimization Highlights

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2022 Carbon Management Project Review Meeting
Pittsburgh, PA
August 17, 2022

Presentation Outline

- Overview of $CCSI^2$ Program and CCSI Toolset
- Highlights of EY21 Work
  - Modeling and Optimization
    - Integrated NGCC-MEA System with High CO_2 Capture Levels
    - Advanced Flash Stripper Configuration
    - Sorbent Systems – Metal Organic Framework
  - Large Pilot Support
    - RTI Non-Aqueous Solvent
    - MTR Membrane System
    - Hybrid TDA Sorbent / MTR Membrane System
    - Model Development – CESAR1 Blend
- Future Directions in $CCSI^2$
  - Industrial Capture Systems
  - Conceptual Design and Robust Optimization

CCSI^2 – Carbon Capture Simulation for Industry Impact

- **CCSI^2 Mission: Accelerate CO_2 Capture Research and Development**
  - Collaborations among national laboratories, academia, and industry to identify promising novel CCS technologies and reduce scale-up risk through rigorous modeling, optimization, uncertainty quantification, and economic analysis
  - Development of CCS models from multiple classes (solvents, sorbents, membrane technologies)
  - Maintenance and continuing development of CCSI Computational Toolset (2016 R&D 100 winner)
  - Flagship software platform FOQUS enables advanced modeling capabilities for process analysis

2016 R&D 100 WINNER

https://github.com/CCSI-Toolset/foqus

https://github.com/CCSI-Toolset/

Upcoming Presentation:

CCSI^2 FOQUS/Toolset Capabilities
Anuja Deshpande (NETL)
Wednesday, August 17, 2022 (5:05 PM)
Point Source Carbon Capture Session

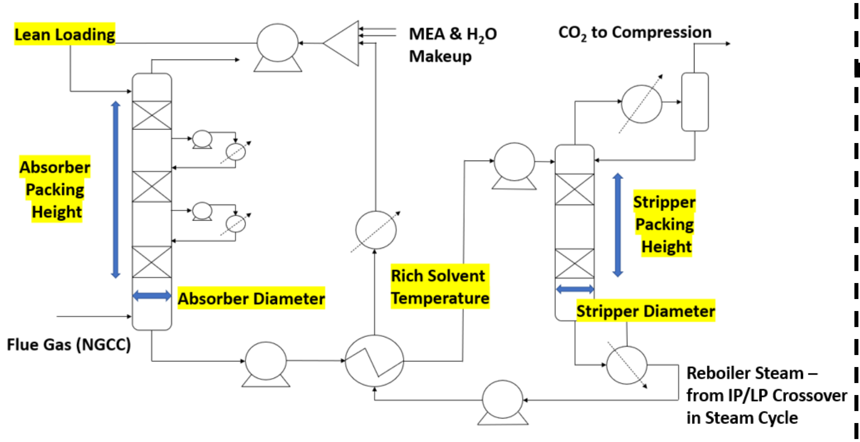
Solvent-Based CO_2 Capture: Techno–Economic Analysis for High Capture Levels

Project Objectives

- Optimize model of NGCC plant with aqueous MEA solvent-based CO_2 capture system for capture levels beyond net-zero emissions
- Understand incremental cost of high capture – compare with direct air capture (DAC) and other net-negative emission technologies
- Understand optimal operation and design of CCS unit to achieve high capture with minimal increase in cost

Problem Formulation in FOQUS

Carbon Capture System Process Model (Aspen Plus®)



Decision Variables for Optimization Problem ($\tilde{x}$)

Variable Transfer

Economic Model (Python)

Calculates levelized cost of electricity (LCOE) for integrated NGCC-MEA system.

Developed from:
- NETL cost and performance baseline [1] for NGCC system
- CSIRO study [2] for capture unit

Optimization Formulation

$\min_{\tilde{x}} f(\tilde{x})$ Minimize LCOE

s.t.

$\tilde{x}^L \le \tilde{x} \le \tilde{x}^U$ Bounded decision variables: design and operation of capture unit

$h(\tilde{x}) = 0$ Fixed level of CO_2 capture & material/energy balances

$g(\tilde{x}) \le 0$ Maximum flooding in columns: 80%

Poster Presentation: Deshpande, A., Morgan, J., Paul, B., Zamarripa, M., Matuszewski, M., Omell, B., **Techno-Economic Analysis and Optimization of Integrated NGCC – MEA System at High CO_2 Capture Levels**.

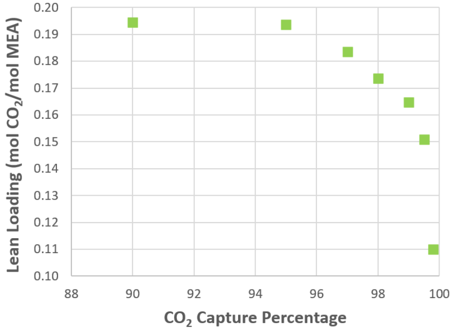
[1] James, R., Zoelle, A., Keairns, D., Turner, M., Woods, M., Kuehn, N., 2019. Cost and performance Baseline for Fossil Energy Plants Volume 1: Bituminous Coal and Natural Gas to Electricity. NETL-PUB-22638

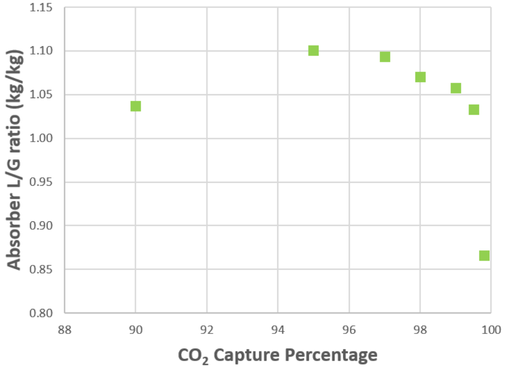
[2] Li, K., Leigh, W., Feron, P., Yu, H., Tade, M., 2016. Systematic study of aqueous monoethanolamine (MEA)-based CO_2 capture process: techno-economic assessment of the MEA process and its improvement. Applied Energy 165: 648-659.

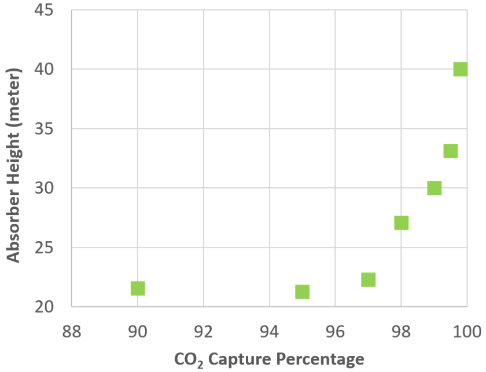
CCSI²
Carbon Capture Simulation for Industry Impact

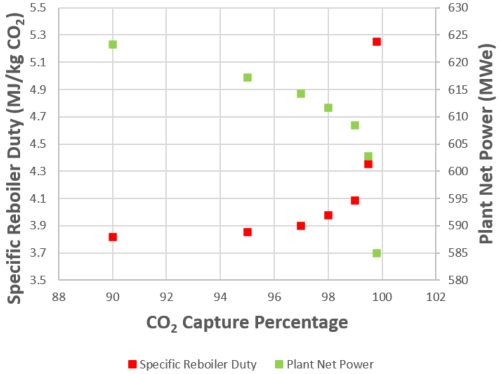
Solvent-Based CO_2 Capture: Techno–Economic Analysis for High Capture Levels

Optimization Results









Optimal lean loading remains flat for 90-95% CO_2 capture, and then decreases with increasing CO_2 capture to alleviate the rapid rise in reboiler duty and steam extraction. As a result, solvent circulation rate drops and absorber height increases.

Cost of Avoided Carbon

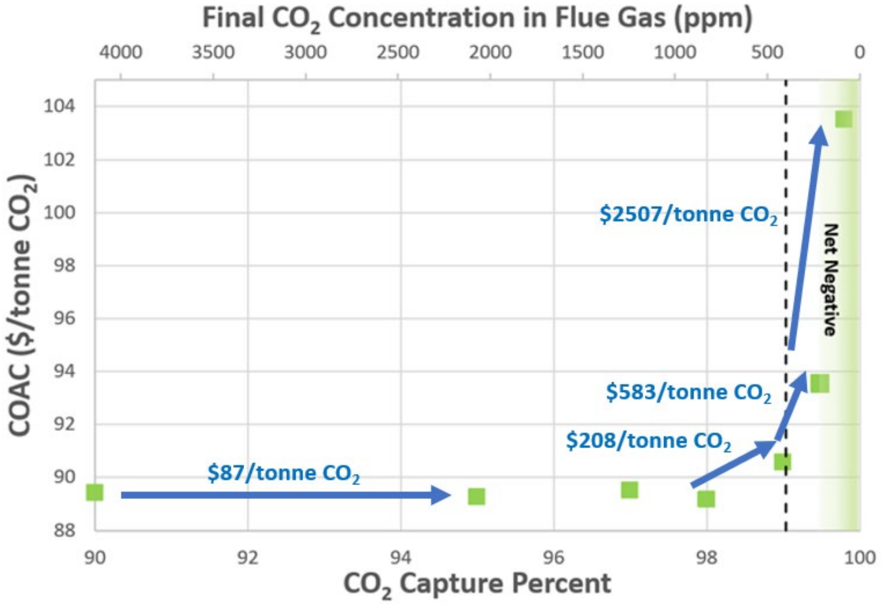
$$COAC[i] = \frac{LCOE[i] - LCOE[0]}{\dfrac{CO_2\ Emissions[0]}{Plant\ Net\ Power[0]} - \dfrac{CO_2\ Emissions\ [i]}{Plant\ Net\ Power[i]}}$$

[0] Plant without CO_2 capture
[i] Plant with given level of CO_2 capture

Incremental Cost of Avoided Carbon

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

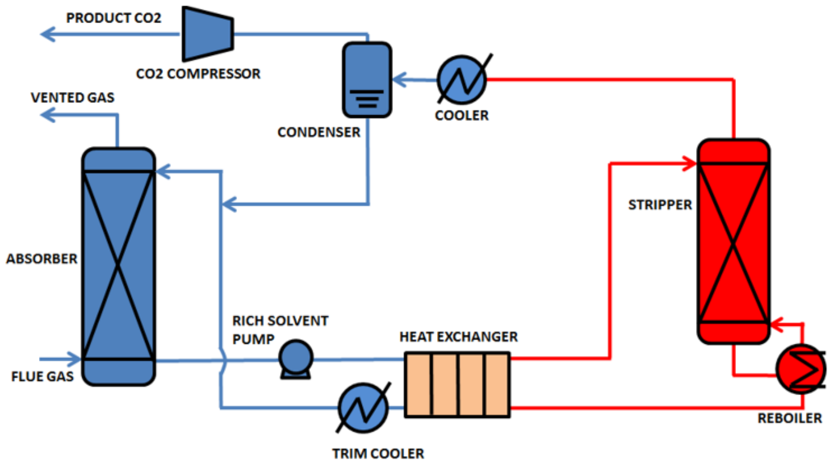
Associated with increase in CO_2 capture level from i to i+Δi



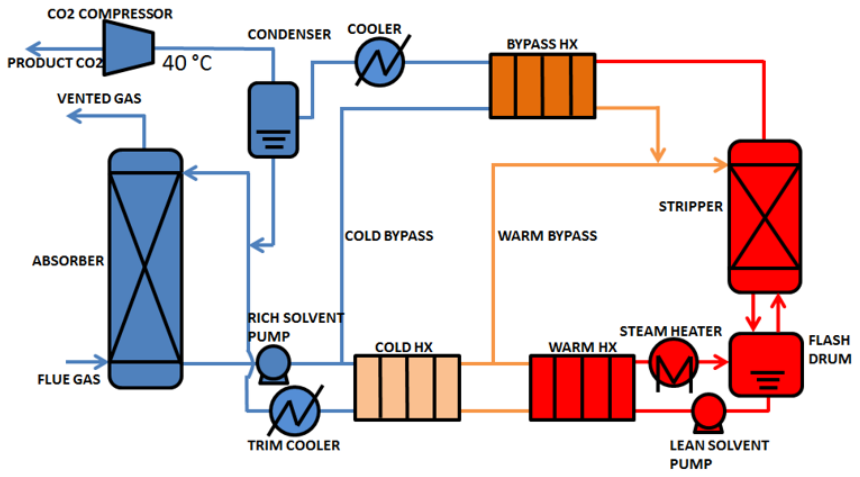
Incremental COAC between capture levels increases exponentially above 98% capture

Advanced Flash Stripper Modeling and Optimization

Simple Stripper



Advanced Flash Stripper



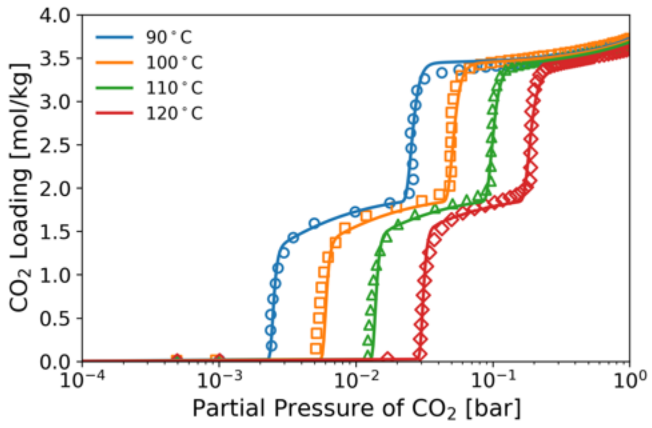
- AFS configuration increases heat recovery from stripper overhead vapor → trade-off in capital costs associated with additional heat exchangers
- Model development and optimization for aqueous solvent systems (MEA and piperazine) and novel water-lean CO_2BOL solvent system (collaboration with PNNL) with simple stripper and advanced flash stripper configurations
- Modeling results predict ~ 2% reduction in COE for aqueous solvent systems (subject to model and economic uncertainty) for AFS process but no improvement for CO_2BOL due to negligible water evaporation
- Future application of work: Conceptual design and superstructure optimization of advanced absorber and stripper configurations

Techno-Economic Analysis for Metal Organic Framework (MOF) – Based CO_2 Capture from NGCC Applications

Project Objectives

- Development of isotherm model for a tetraamine-appended MOF
- Development of fixed bed and moving bed contactor models
- Techno-economic optimization of post-combustion capture processes from NGCC flue gas

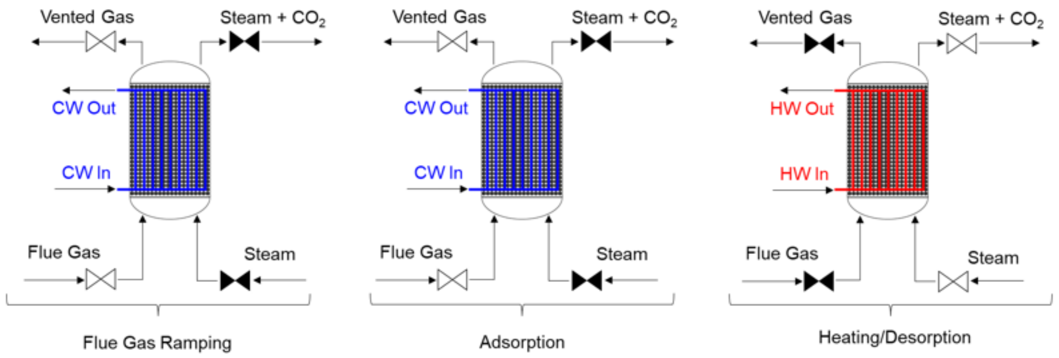
Isotherm Model



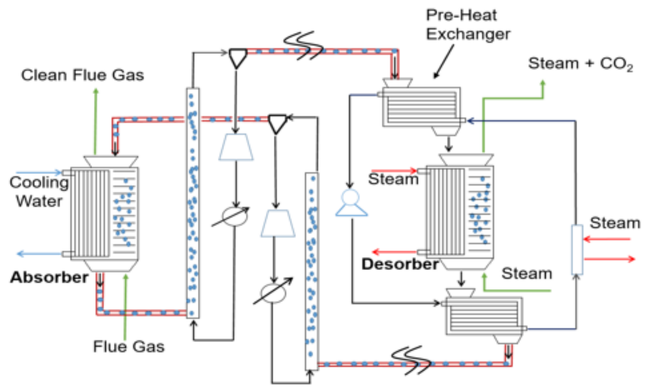
Weighted Langmuir model extended to multiple adsorption steps

Process Models

Fixed Bed TSA Process



Moving Bed TSA Process

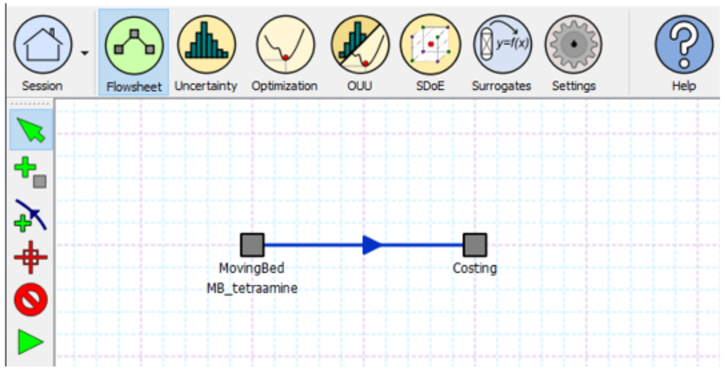


Poster Presentation: Hughes, R., Caballero, D.Y., Zamarripa, M., Bhattacharyya, D., Matuszewski, M., Omell, B., **Techno-Economic Analysis for MOF-based CO_2 Capture from NGCC Applications**.

Techno-Economic Analysis for Metal Organic Framework (MOF) – Based CO_2 Capture from NGCC Applications

Optimization Problem

Process models (fixed and moving bed contactors) integrated with costing module and derivative free optimization algorithms within the FOQUS tool



$\min_x \; f(x)$	Minimize Total Annualized Cost ($MM/y)
$s.t.$	
$x^L \le x \le x^U$	Decision variable bounds
$h(x) = 0$	Modeling eqs. (mass balances, energy balances, etc.)
$g(x) \le 0$	CO_2 capture, velocity constraints, etc.

Decision Variables

Fixed Bed: *L, D, tube pitch, F_{FG}, F_{steam}, step times, lean loading, working capacity*

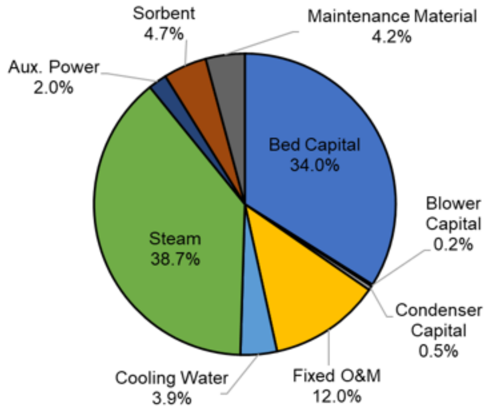
Moving Bed: *L_{ads}, D_{ads}, L_{des}, D_{des}, tube pitch, lean sorbent loading*

Optimization Results

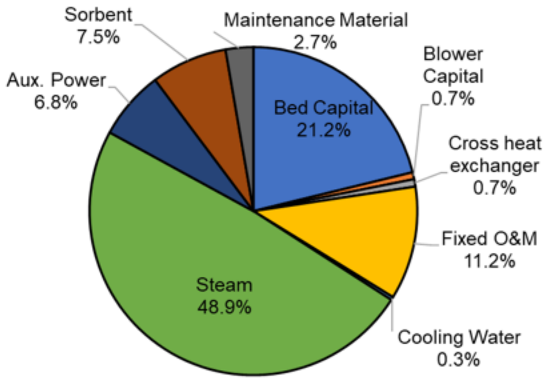
Compared to reference MEA system, the optimal cost of capture:

- Increases 48% for fixed bed process
- Decreases 9% for moving bed process

Fixed Bed Cost Breakdown



Moving Bed Cost Breakdown



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CCSI[2] Carbon Capture Simulation for Industry Impact

Large Pilot Support

Photograph from www.tcmda.com

TECHNOLOGY CENTRE MONGSTAD – catching our future

- Multiple collaborations between CCSI[2] and industrial organizations focused on demonstration of novel CO_2 capture technologies at Norway's Technology Centre Mongstad (TCM) - one of the world's largest venues for testing capture technologies (~ 12 MWe)
- CCSI[2] contributed expertise in process modeling and sequential design of experiments (SDoE)
  - SDoE ensures efficient allocation of resources for expensive test campaigns → extract maximum information with a fixed budget
  - **Forthcoming Presentation: SDoE Capabilities, Progress, and Applications (Abby Nachtsheim – Los Alamos National Laboratory)**

RTI INTERNATIONAL

Research Triangle Institute: Non-Aqueous Solvent (NAS)

MTR

Membrane Technology & Research: Novel Membrane System

TDA

TDA Research: Sorbent System

Large Pilot Support: RTI Non-Aqueous Solvent

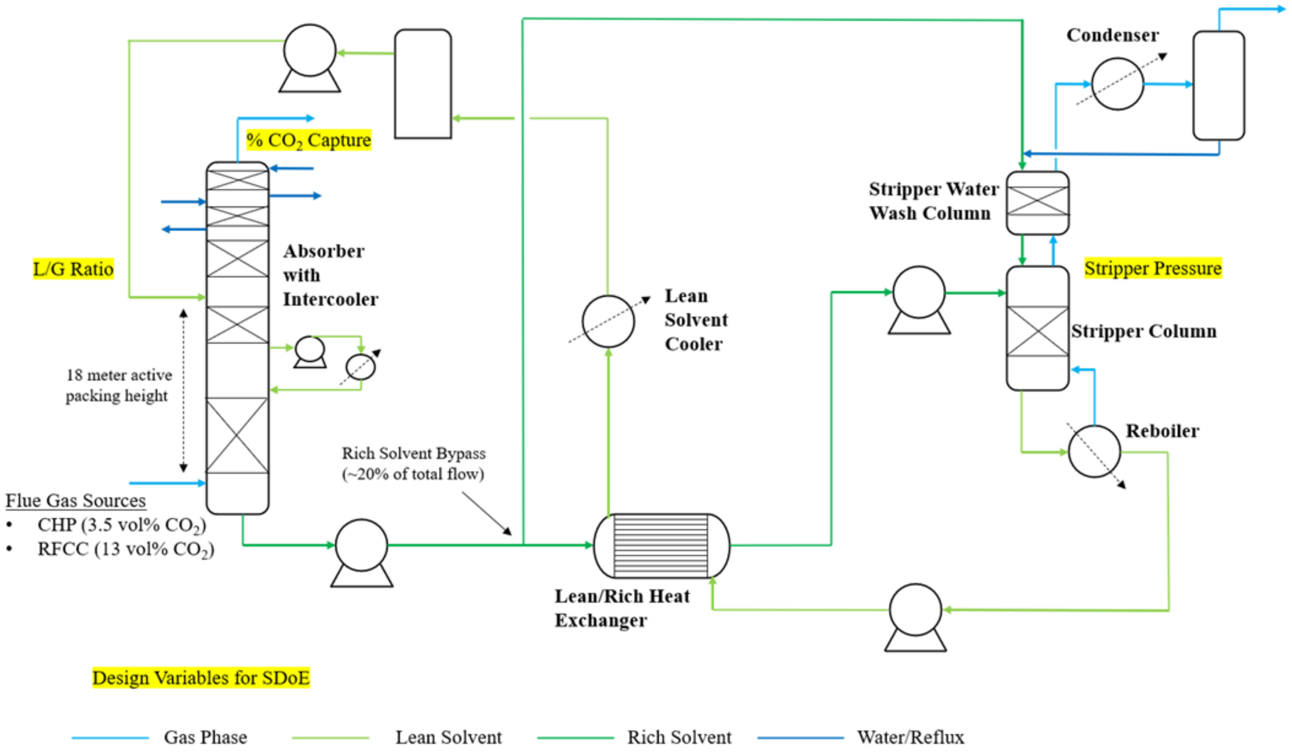
Project Objectives

- Collaboration between RTI and CCSI[2] on multi-scale modeling of non-aqueous solvent system (NAS)
- Leverage 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

TCM Test Campaign

- 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

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



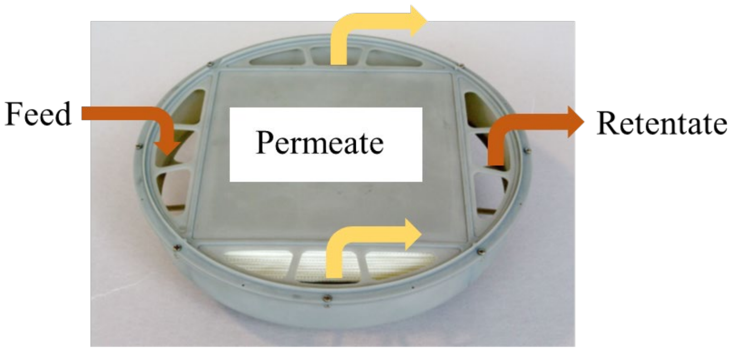
- Ongoing work for development of thermodynamics and other sub-models of NAS solvent system, followed by validation of process models for TCM (12 MWe) and Tiller (60 kWe) pilot plant facilities.
- **Work expected to wrap up at the end of 2022**

Large Pilot Support: Membrane Technology Research

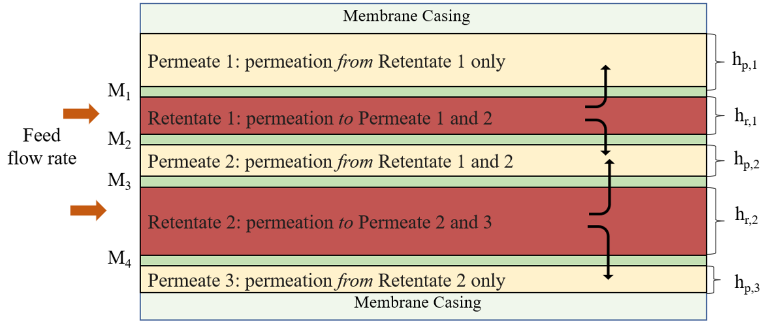
Project Highlights

- 1D model developed for MTR flat sheet membrane with non-uniform channel heights
- SDoE performed with commercial nitrogen membrane model to demonstrate the potential for stochastic parameter estimation

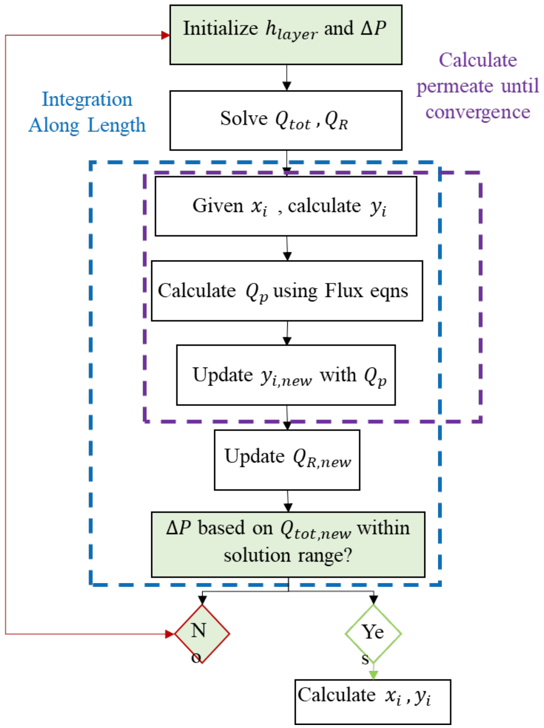
Flat Sheet Membrane Model



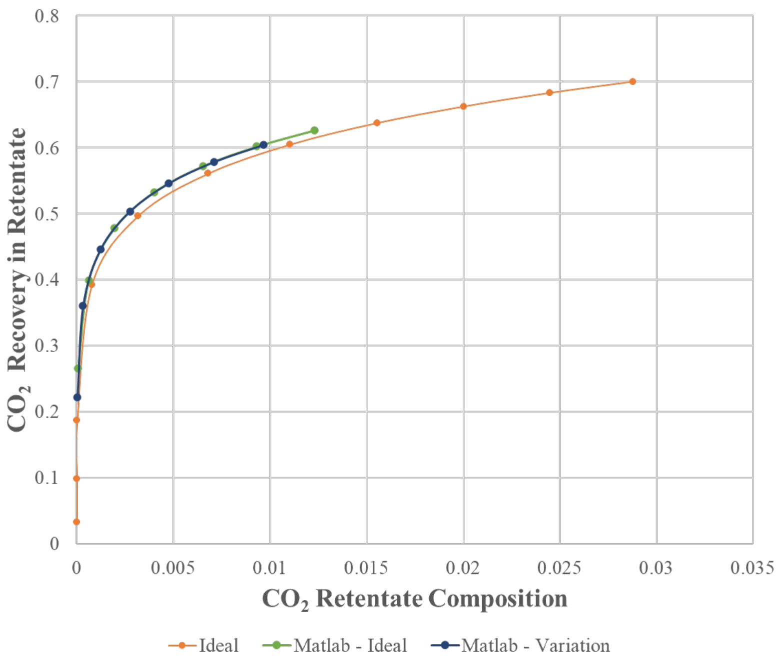
Example of MTR's 100 m^2 plate-and-frame module.



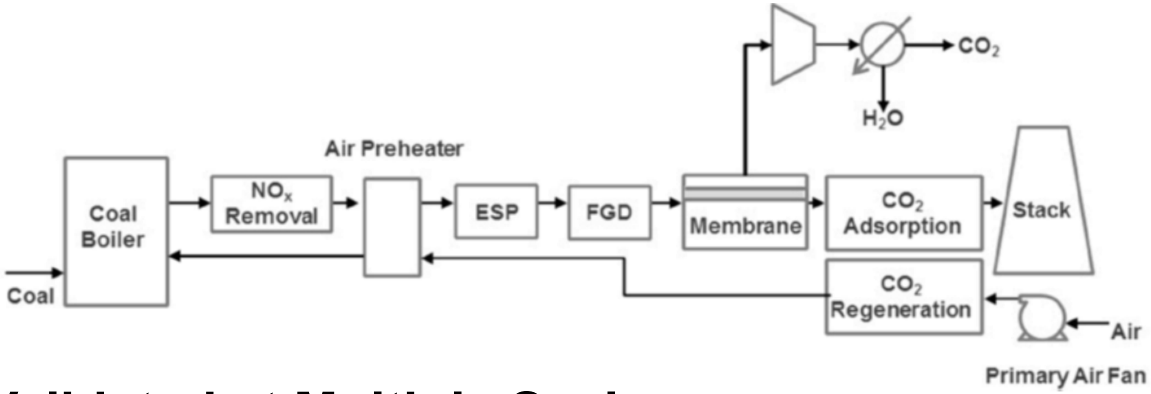
Iterative Solution Methodology



Membrane Performance Compared to Ideal Module



Large Pilot Support: TDA-MTR Technology



Model Developed and Validated at Multiple Scales

SBIR Phase II B: Hybrid Membrane/Sorbent System for Capture 1 ton/day CO_2

50 kWe system

- **More instrumentation than SBIR Phase II B System**
- **Adsorption-desorption cycle data available**

TCM (1 MWe system)

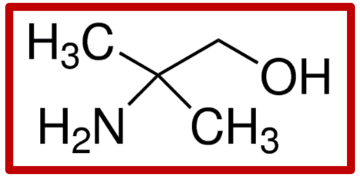
- **Highly instrumented**
- **Can blank off 50% of the bed to avoid channeling at low flow**
- **Design of experiments developed for test runs to be conducted in Dec 2022 – Jan 2023**

Future work will focus on validation with additional data from TCM, process optimization, and uncertainty quantification

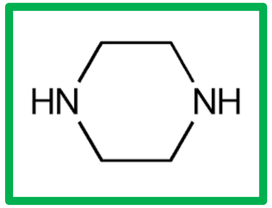
CCSI[2]
Carbon Capture Simulation for Industry Impact

Model Development and Validation – CESAR1

- CESAR (CO_2 Enhanced Separation and Recovery) project funded by EU (2008-2011)
- CESAR1: Aqueous blend of 2-amino-2-methyl-1-propanol (AMP) and piperazine (PZ)



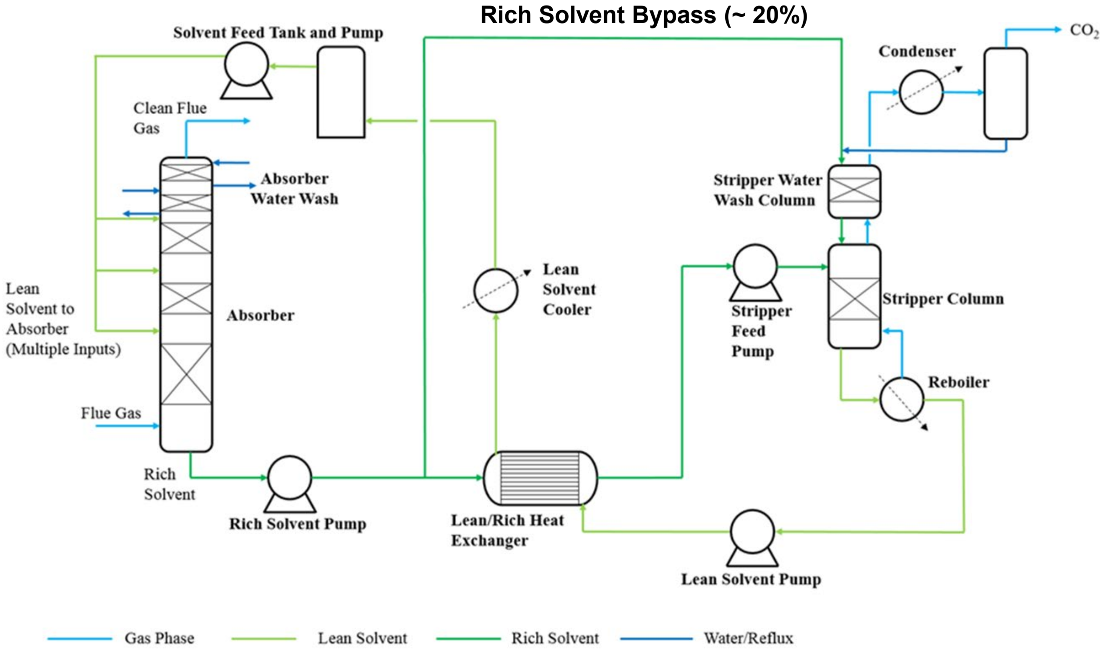
5.0 m AMP



2.5 m PZ

- Blended system combines advantages associated with PZ (high reactivity) and AMP (relatively low heat requirement for solvent regeneration)

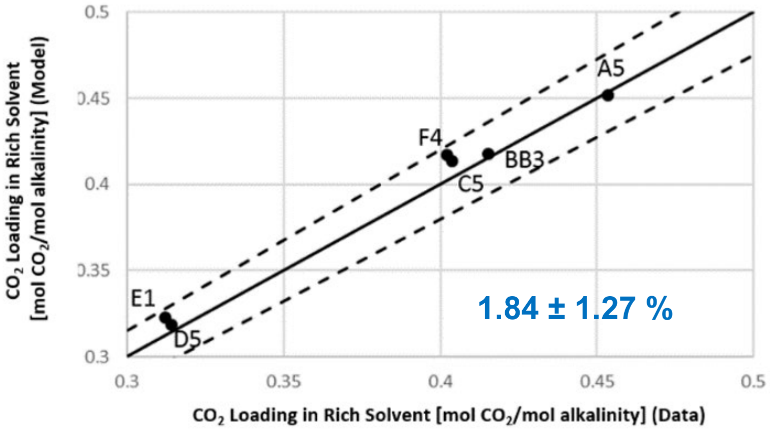
- Process model developed and validated with seven steady-state data sets collected from ALIGN-CCUS campaign at TCM (12 MWe) using natural gas-based combined cycle turbine flue gas

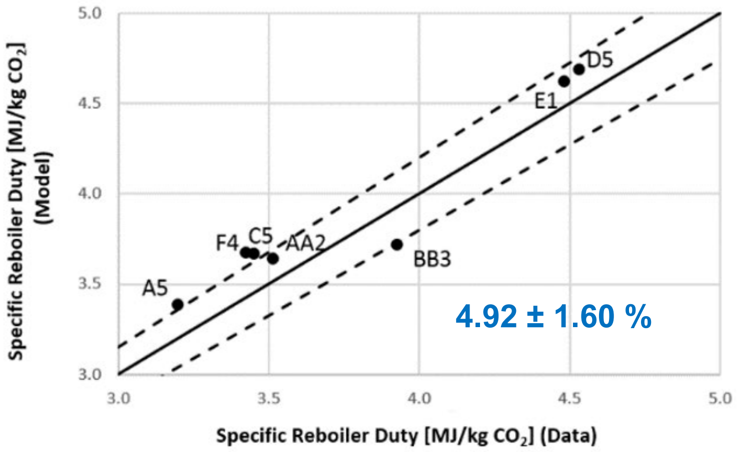


Model Development and Validation – CESAR1

Model Validation Data

	C5	D5	E1	F4	AA2	BB3	A5
Absorber Packing Height (m)	18	18	12	18	24	24	24
Flue Gas Flowrate (kg/hr)	59853	59803	59821	70675	60101	60086	60451
Absorber L:G Mass Ratio	0.66	0.92	1.09	0.57	0.74	0.58	0.66
Lean CO_2 Loading (mol CO_2/mol alkalinity)	0.135	0.109	0.147	0.087	0.135	0.049	0.176
Rich CO_2 Loading (mol CO_2/mol alkalinity)	0.404	0.314	0.312	0.402	NA	0.415	0.454
Lean Solvent Molality (AMP/PZ)	5.206/ 2.616	5.077/ 2.669	4.907/ 2.574	5.022/ 2.470	5.460/ 2.482	5.541/ 2.492	4.490/ 2.314
Flue Gas Temperature (°C)	40.00	40.12	40.15	40.20	40.13	40.17	30.43
Stripper Pressure (kPa)	191.9	191.9	191.8	221.4	192.0	192.1	191.4





Average percent error

- Future work will focus on uncertainty quantification in process submodels (e.g., thermodynamics, mass transfer/interfacial area, reaction kinetics, hydraulics)
- Model will be released to open-source CCSI Toolset and applied to process modeling efforts in the Sustainable OPeration of post-combustion Capture plants (SCOPE) program → focus on characterization of amine emissions

CCSI^2 Process Modeling: Future Directions (EY22 and Beyond)

- Pilot Support
  - Wrap-up of TCM SDoE projects (RTI, MTR, TDA)
  - Initiate work on small-pilot support for natural gas-based point sources

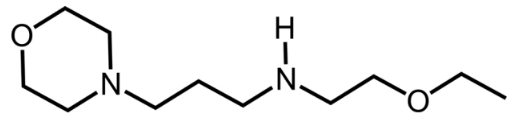
Solid Sorbent Technology
Initial work will focus on development of rotary packed bed contactor model

Develop generic capabilities for sorbent properties and kinetic modeling

Implement newly-developed capabilities in science-based design of experiments (SBDoE) for testing technology at pilot scale

EEMPA Solvent System
Low-aqueous diamine solvent system developed by PNNL to be tested at National Carbon Capture Center (~ 0.5 MWe)

Initial work will focus on model development and improvement through bench-scale experimentation and uncertainty quantification



NATIONAL CARBON CAPTURE CENTER

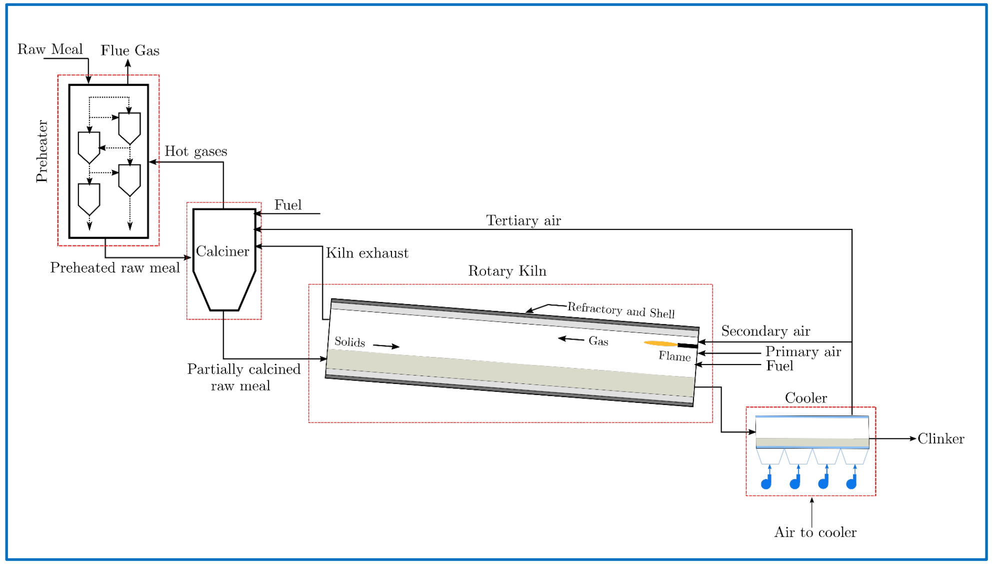
Pacific Northwest NATIONAL LABORATORY

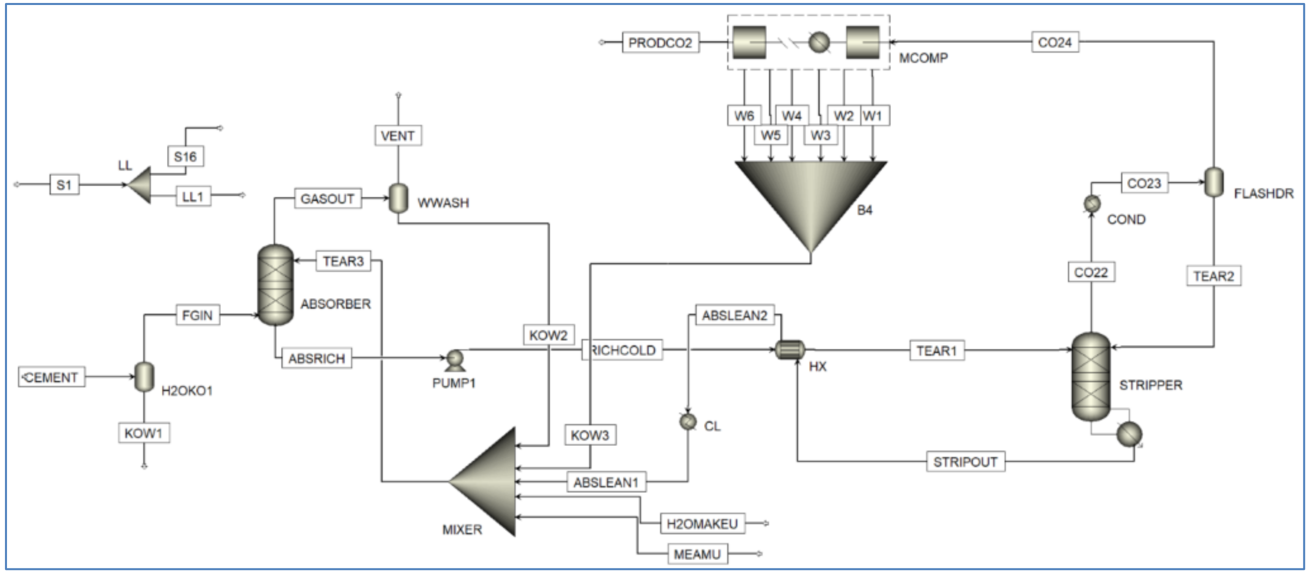
- Industrial Capture Modeling
- Conceptual Design and Robust Optimization
- Development of Rigorous Cost Analysis Methods for CCS Equipment

Industrial Capture Modeling & Pilot Support

Preliminary Analysis

- Integrated cement kiln model (MATLAB) with MEA-based carbon capture model (Aspen Plus) in FOQUS





Future Directions

- Rigorous modeling of steel production process with focus on understanding key sources of emissions and energy consumption and integration with CCS systems
- Initiate work on characterization of cryogenic CO_2 separation – with focus on modeling thermodynamic processes and heat integration
- Expected to provide support to pilot projects for CCS from industrial sources

Conceptual Design and Robust Optimization

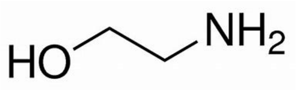
Motivation

- Achieving net-zero CO_2 emissions in CCS applications in an economically efficient manner requires consideration of various classes (solvents, sorbents, membranes, etc.) and configurations of technologies → need for rigorous process modeling and optimization
- Complexity of modeling effort compounded by economic and epistemic uncertainties in process sub-models and variability in feedstock quality

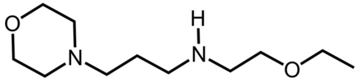
Example: Decision Points for Solvent-Based CO_2 Systems

<u>Solvent Classes</u>

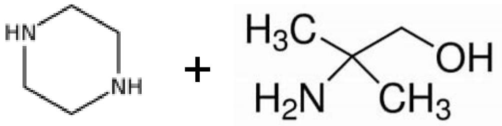
Traditional Aqueous Amines



Low-Aqueous Systems

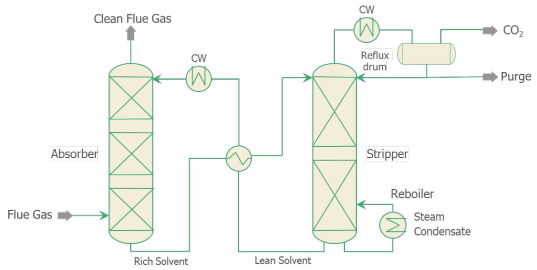


Solvent Blends

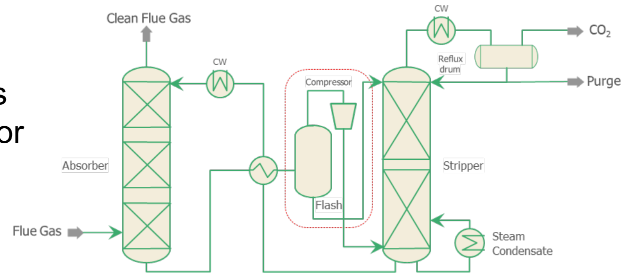


<u>Process Configurations</u>

Typical Configuration



Advanced Configurations (e.g., rich vapor compression)



<u>Process Design and Operation</u>

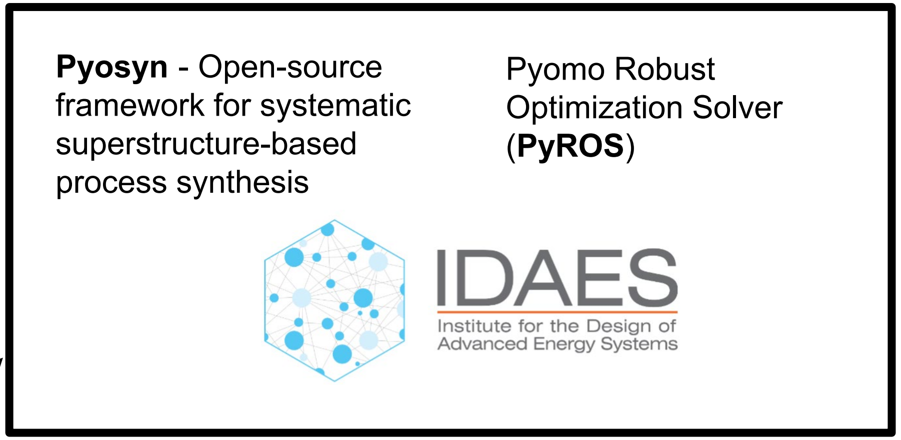
- L/G Ratio
- Steam Input (Reboiler Duty)
- Absorption Temperature
- Stripper Pressure
- Equipment Design (e.g., sizes, choice of internals for absorber/stripper columns)
- Number of parallel trains for CCS unit and/or individual equipment

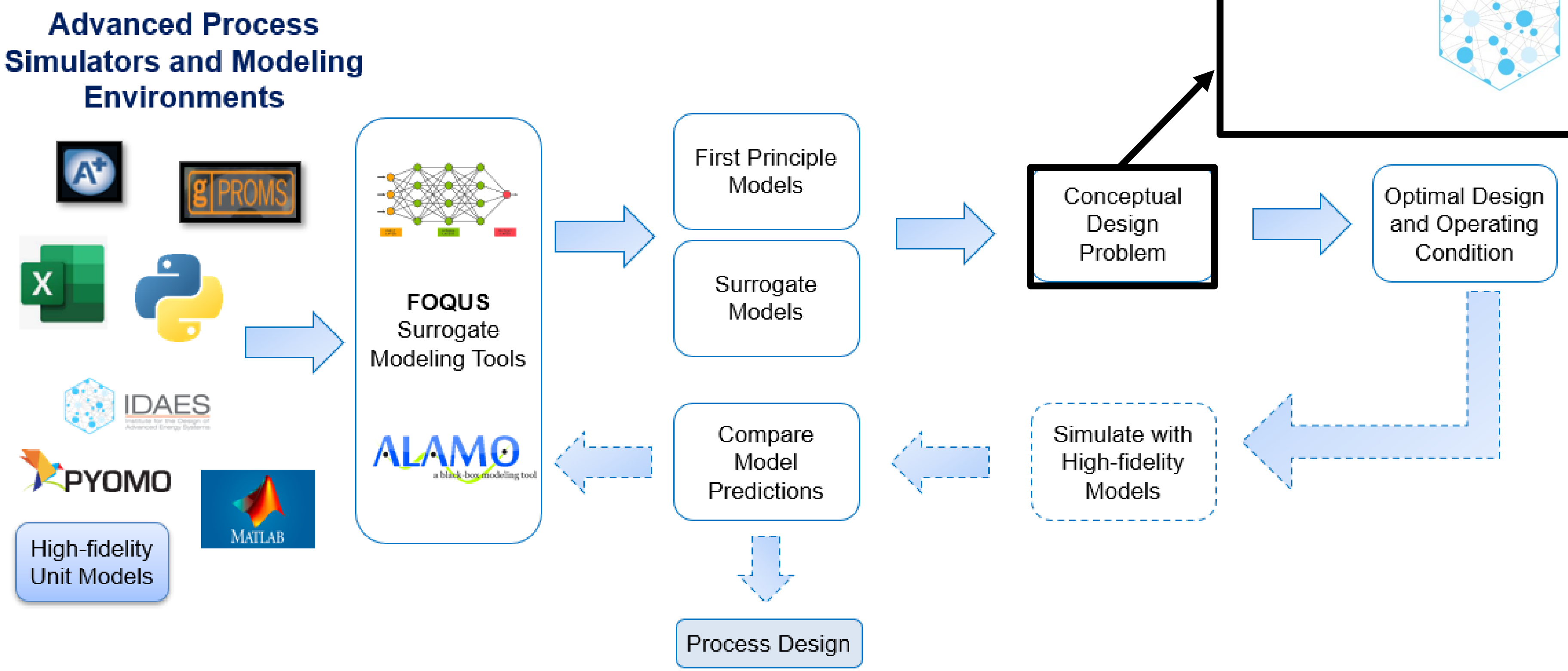
<u>Process and Model Uncertainty</u>

- Process thermodynamics and kinetics
- Equipment variables – mass transfer, interfacial area, hydraulics for packing
- Feedstock variability
- Economics

Reducible through targeted data collection

Conceptual Design and Robust Optimization





Open – source toolsets developed and evaluated in other process systems engineering applications will be leveraged for rigorous design and optimization of CCS systems while accounting for predictions of model uncertainties, which are highly dependent upon process variables

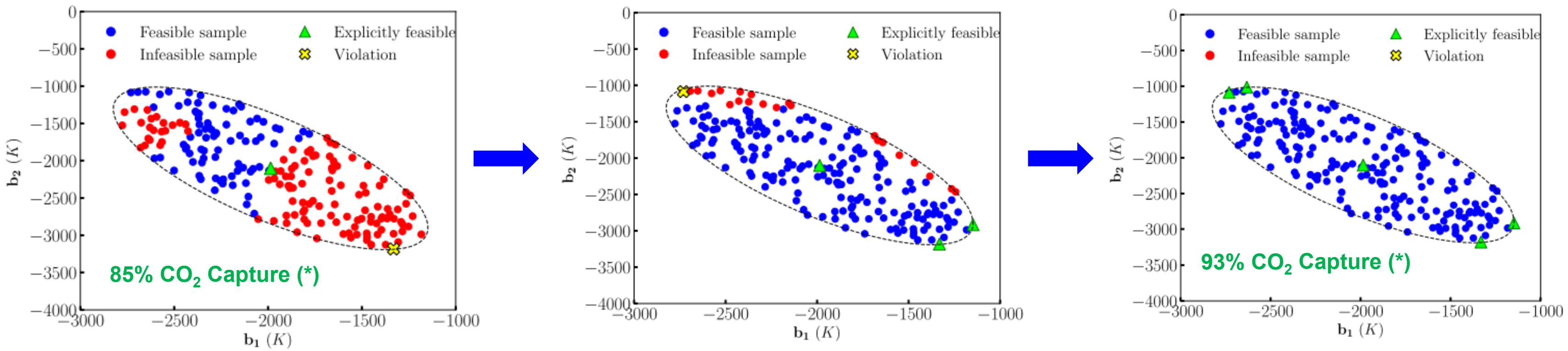
Application areas include superstructure-based optimization under uncertainty for advanced configurations of solvent-based CO_2 capture systems

Robust Optimization – PyROS Capability in IDAES

MEA Solvent System Example

- Optimization Problem: Minimize equivalent annual cost of CO_2 capture unit subject to minimum capture of 85%
- Decision variables: Absorber and stripper sizes, lean-rich heat exchanger area
- Control variables: Reboiler and condenser duties

(*) Deterministic Value



Nominal Design (k = 0) **Intermediate Design (k = 2)** **Final GRCS Design (k = 4)**

$$2\,MEA + CO_2 \overset{K_{eq-1}}{\Longleftrightarrow} MEA^+ + MEACOO^-$$

$$MEA + CO_2 + H_2O \overset{K_{eq-2}}{\Longleftrightarrow} MEA^+ + HCO_3^-$$

$$K_{eq-1} = a_1 + \boldsymbol{b_1}\ln(T) + \frac{c_1}{T}$$

$$K_{eq-2} = a_2 + \boldsymbol{b_2}\ln(T) + \frac{c_2}{T}$$

Uncertain Parameters

- Generalized Robust Cutting Set (GRCS) algorithm yields optimal robust solution in four iterations – constraints satisfied for full parametric uncertainty set
- Capability can be leveraged in future CCSI[2] work to ensure process designs for systems with high levels of CO_2 capture are robust in light of epistemic uncertainty associated with property and process sub-models

Example adapted from:
Isenberg NM, Akula P, Eslick JC, Bhattacharyya D, Miller DC, Gounaris CE, 2020. A generalized cutting-set approach for nonlinear robust optimization in process systems engineering. *AIChE J*. 2021;67:e17175 https://doi.org/10.1002/aic.17175

Summary and Conclusions

- Multi-year collaborations with industrial partners testing novel CCS systems at TCM have resulted in successful test campaigns and improved understanding of technologies
  - Established statistical approaches to experimental design as best practice for pilot testing
  - Pilot support will remain foundational in $CCSI^2$ work in EY22 and beyond

- Process modeling efforts are shifting away from CCS system operation at baseline levels (e.g., 90%) to focus on higher capture levels - up to net-zero emissions for natural gas source systems
  - Necessitates enhanced focus on risk assessment through economic analysis, UQ, robust optimization, and conceptual design → **synergistic application of these tools across projects will be a major EY22 priority**

- New $CCSI^2$ projects initiated in EY22 will focus on expanding capabilities to industrial source CCS applications

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CCSI²

Carbon Capture Simulation for Industry Impact

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

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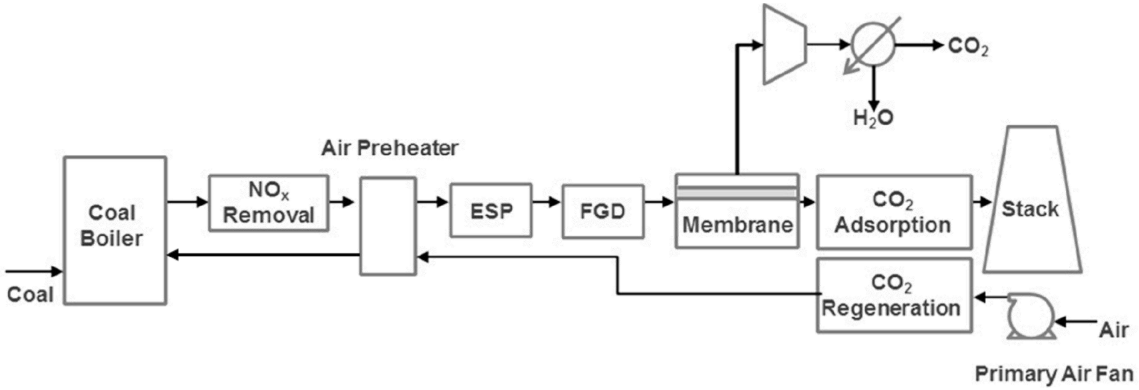
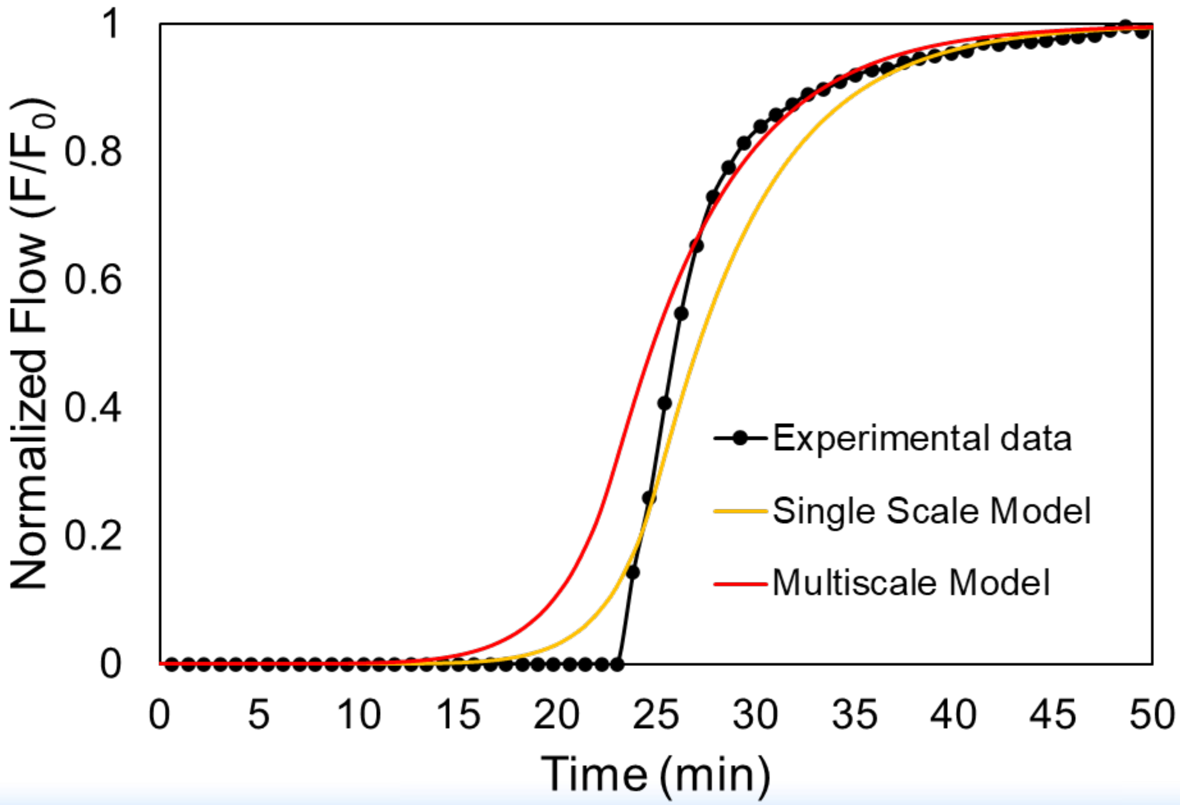
Backup Slides

TDA-MTR Technology*

- Membrane captures about 50% of CO_2 while the remaining desired amount of CO_2 is removed by TDA sorbent
- Boiled feed air is used as sweep gas for sorbent regeneration
- Solid sorbent is a mesoporous carbon with a surface functional group capturing CO_2 by physisorption
- Multi-scale radial-flow bed model developed by modeling both the bulk scale and particle scale and by incorporating inter-particle and intra-particle mass and heat transfer resistances.
- Particle scale model is validated using data available for functionalized MOF
- Model developed and validated for 3 scales





*https://www.netl.doe.gov/node/6161

Three Different Systems Modeled

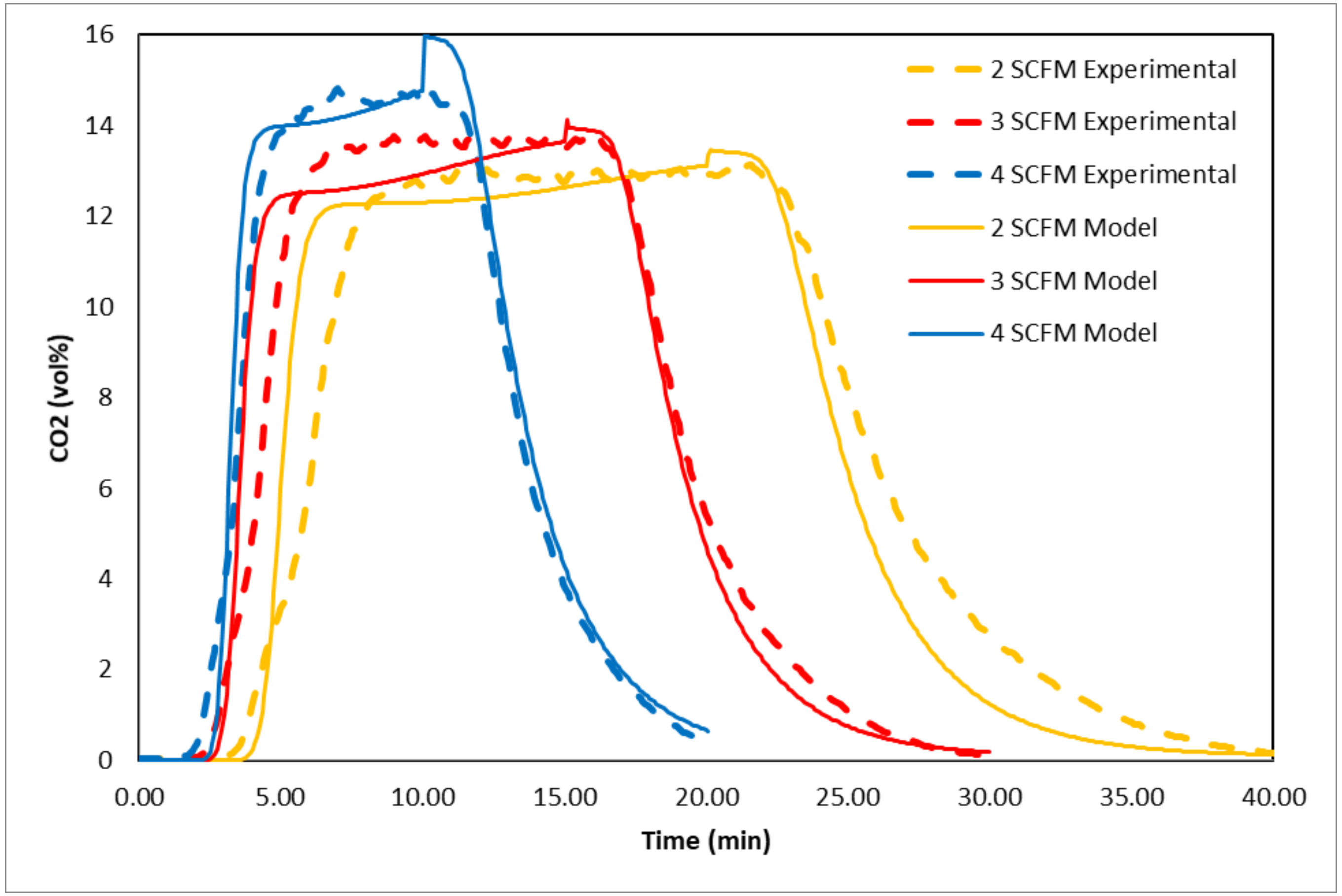
- SBIR Phase II B: Hybrid membrane sorbent system for capturing 1 ton CO_2 per day
- Lack of measurements

- 'Small Scale' system: 50 kWe
- Adsorption-desorption cycle data available
- More instrumented than the SBIR Phase II system

- TCM pilot plant: 1 MWe
- Highly instrumented
- Can blank off 50% of the bed to avoid channeling at low flow
- DoE developed for test runs conducted in December,2022-January, 2023

Model Validation and Observation

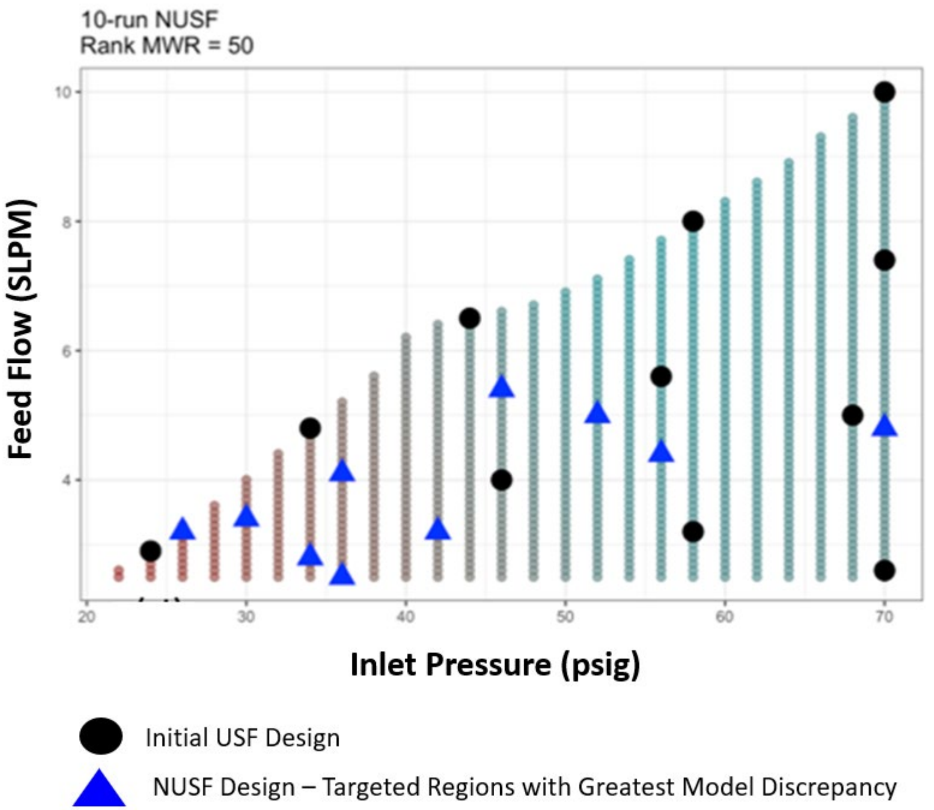
- Under same inlet conditions for adsorption and for same bed height and same solid volume, axial flow and radial flow beds have similar bed average loading and breakthrough time, but the pressure drop through the radial flow beds is about two order of magnitude lower than axial flow beds.
- For regeneration of the bed from similar initial loading to similar end-of-the desorption bed average loading, axial flow beds took about 3-5 times longer time for regeneration.
- Higher entrance loading for radial-flow due to higher surface area that facilitates easier cooling of solids at the entrance
- Future work will focus on validation with additional data from TCM, optimization and uncertainty quantification



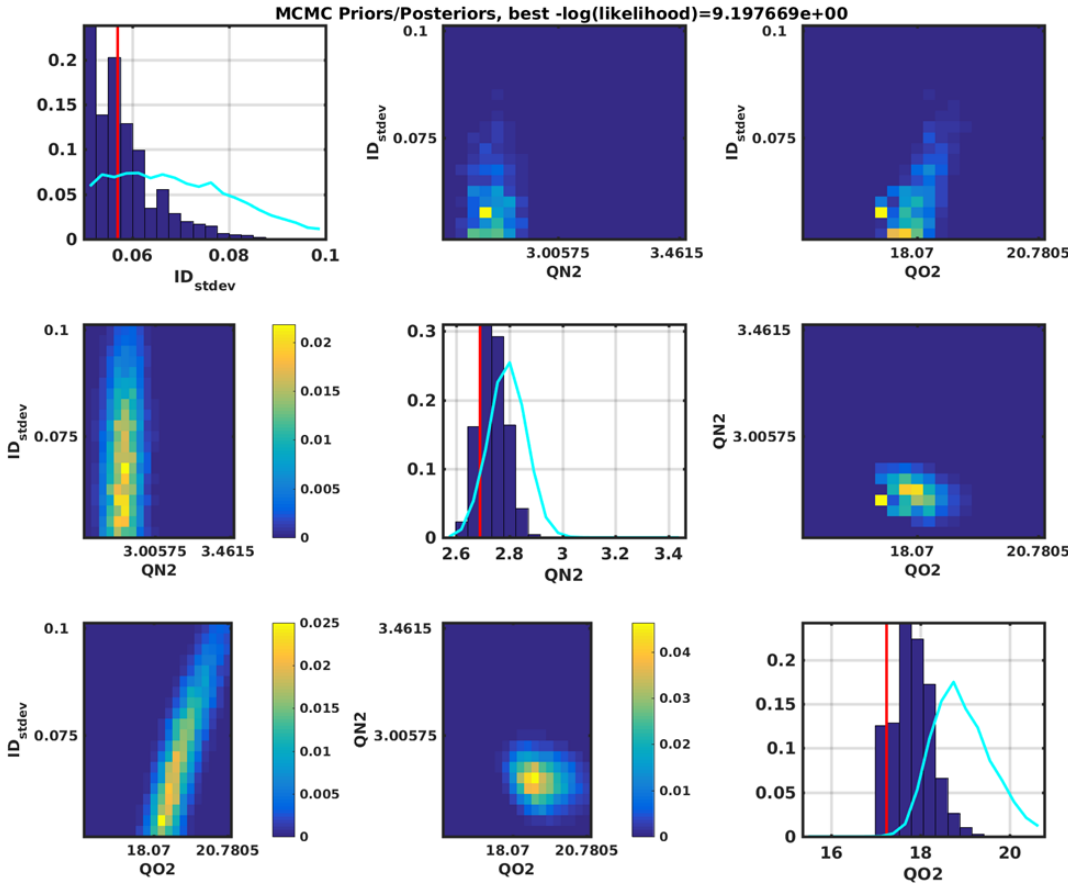
CCSI[2]
Carbon Capture Simulation for Industry Impact

Large Pilot Support: Membrane Technology Research

SDoE Performed for Commercial Nitrogen Module



Stochastic Parameter Estimation



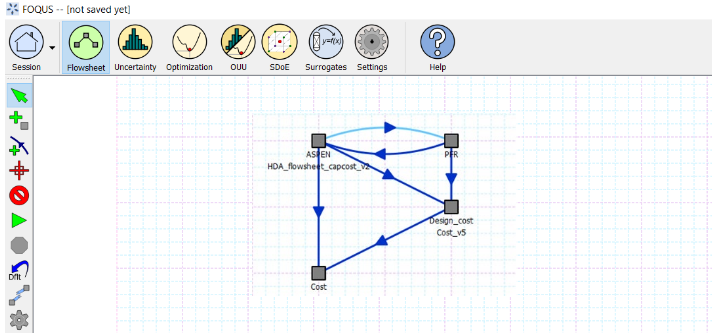
$\mathrm{ID_{stdev}}$ → Variation in fiber internal diameter

$\mathrm{QO2; QN2}$→ Permeance of O_2 and N_2

Framework for Optimization, Quantification of Uncertainty, and Surrogates

Flowsheet – An interface to set up and integrate various models

Flowsheet



Nodes: Contain Individual Models

Edges: Transfer variables between nodes

Uncertainty

Optimization

OUU

Surrogates

SDOE

Uncertainty Analysis
- **Data Visualization**
- **Parameter Screening**
- **Sensitivity Analysis**
- **Stochastic Parameter Estimation through Bayesian Inference**
- **Response Surface Construction and Validation**

Optimization
- **Includes multiple derivative-free optimization solvers**
- **Flowsheet variables may be incorporated as decision variables and into expressions for objective function and constraints**

Optimization under Uncertainty
- **Integrates capabilities of optimization and uncertainty modules to solve stochastic optimization problems with discrete and continuous uncertain parameters**
- **Enables single-stage and two-stage problem formulations**

Surrogates
- **Simplified representation of flowsheet models**
- **Surrogate modeling tools include:**
  - **ALAMO**
  - **ACOSSO**
  - **BSS-ANOVA**

SDOE
- **Sequential design of experiments**
- **Capabilities for space-filling designs:**
  - **Uniform**
  - **Non-uniform**
  - **Input/Response**

Comprehensive Analysis of Process Systems