Applications of Framework for Optimization, Quantification of Uncertainty, and Surrogates (FOQUS) to Modeling of CO_2 Capture Technologies

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Presentation Outline

- Introduction to $CCSI^2$ and CCSI Computational Toolset
- Overview of Framework for Optimization, Quantification of Uncertainty, and Surrogates (FOQUS) Software
- Applications of FOQUS Software in Carbon Capture Modeling
  - Stochastic Model Development
  - Sequential Design of Experiment (SDoE) for Pilot Testing
  - Techno-Economic Analysis and Optimization
- Summary and Conclusions

CCSI Toolset

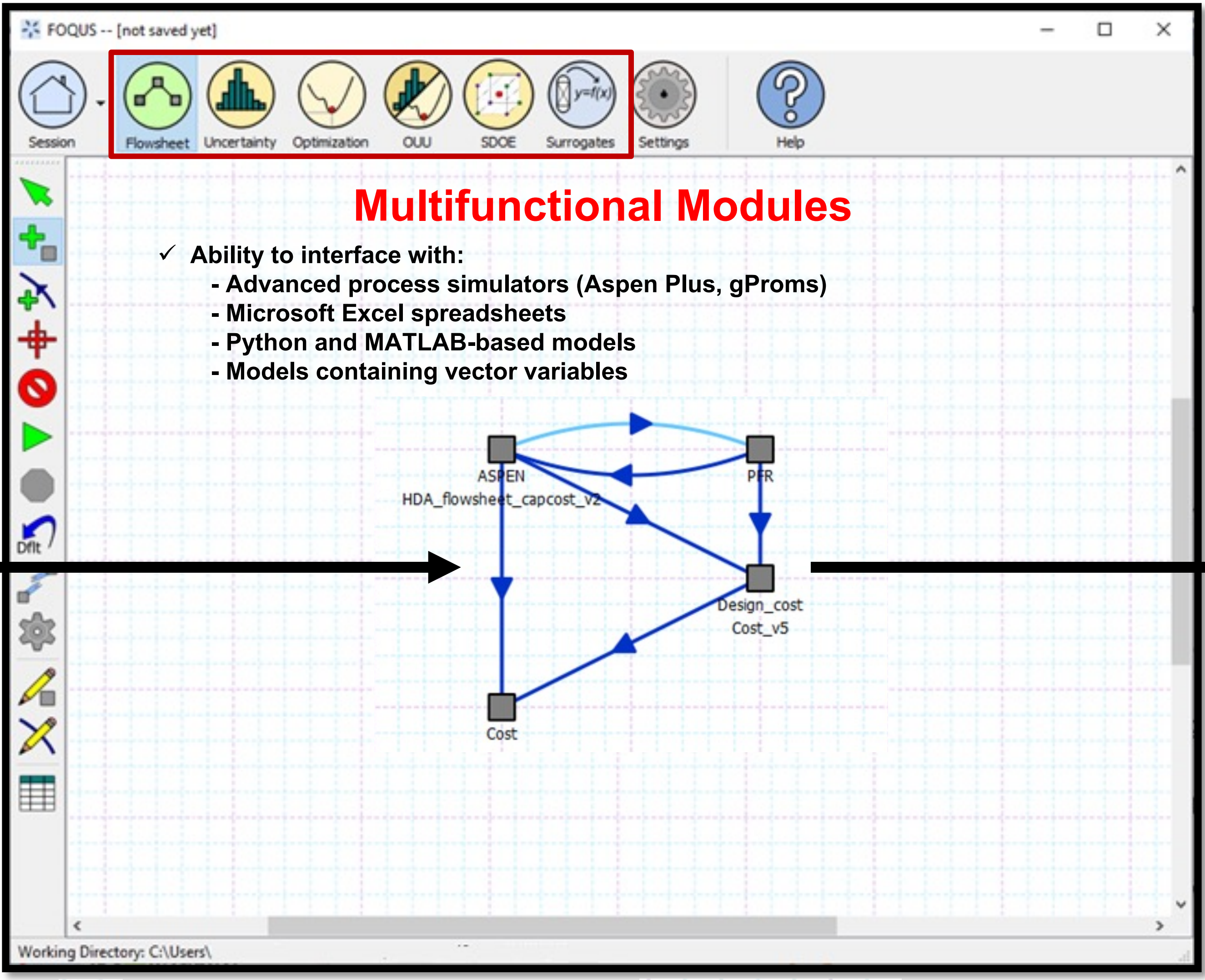
- Open-source suite of computational tools and models designed to maximize learning and reduce risks associated with scaling up carbon capture technologies
- Developed through Carbon Capture Simulation Initiative (CCSI) program (2010–2017)
- Carbon Capture Simulation for Industry Impact ($CCSI^2$) continues to enhance the toolset and apply it to novel CCS technologies in collaborations with national laboratories, industrial organizations, and academia

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

2016 R&D 100 WINNER

FOQUS at a Glance

Advanced Process Simulators and Modeling Environments



Comprehensive Analysis of Process Systems

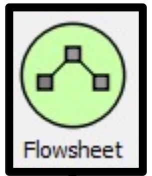
- Uncertainty Quantification
- Simulation-Based and Mathematical Optimization
- Surrogate Modeling
- Sequential Design of Experiments
- Optimization Under Uncertainty

Nodes: Contain Individual Models

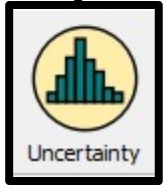
Edges: Transfer variables between nodes

CCSI[2]
Carbon Capture Simulation for Industry Impact

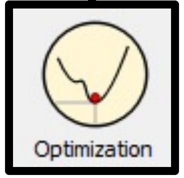
Overview of FOQUS Capabilities



Flowsheet
An interface to set up and integrate various models
- Python
- Pyomo
- Aspen Plus
- MATLAB
- Microsoft Excel

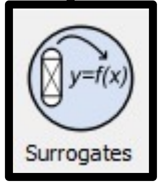


Uncertainty Analysis
- Data Visualization
- Parameter Screening
- Sensitivity Analysis
- Stochastic Parameter Estimation through Bayesian Inference
- Response Surface Construction and Validation

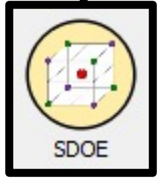


Optimization
- Includes multiple derivative-free optimization solvers
- Flowsheet variables may be incorporated as decision variables and into expressions for objective function and constraints

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

Overview of FOQUS Capabilities

Capabilities to be discussed further in forthcoming case studies

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Comprehensive Analysis of Process Systems

CCSI Model of Aqueous MEA System Implemented in Aspen Plus

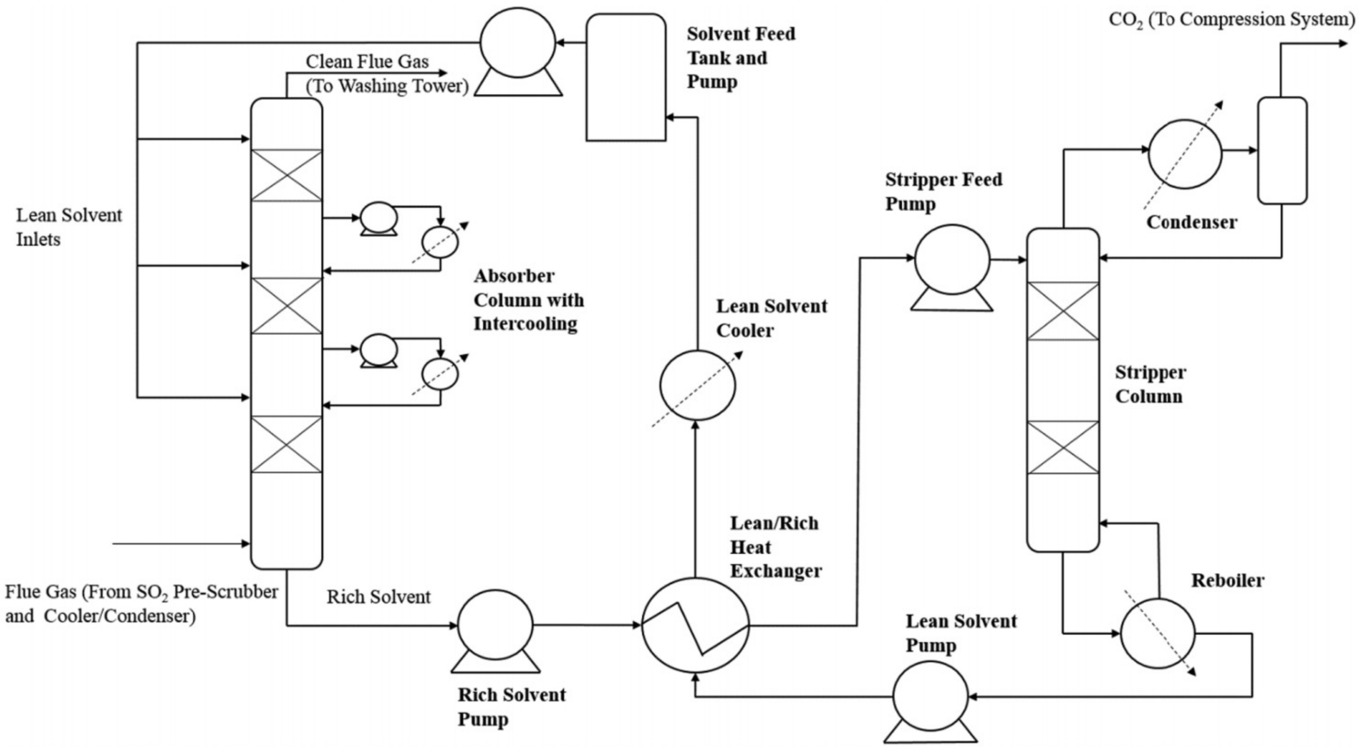


Figure adapted from Morgan et al., Appl. Energy, 2020, 262, 114533

Model Features

Model Scale: ~ 0.5 MWe, baseline CO_2 capture of ~ 10 tpd

Property Method: ELECNRTL

Absorber and stripper modeled as rate-based columns with liquid-phase reactions with equilibrium chemistry:

$$2MEA + CO_2 \leftrightarrow MEAH^+ + MEACOO^-$$

$$MEA + CO_2 + H_2O \leftrightarrow MEAH^+ + HCO_3^-$$

Fortran User Subroutines:
- Liquid Properties (Viscosity, Molar Volume, Surface Tension, Diffusivity)
- Reaction Kinetics
- Mass Transfer
- Interfacial Area
- Liquid Holdup

Parameters Represented by Distributions:
- Property Models – Viscosity, Density, Surface Tension
- Thermodynamic Framework
- Mass Transfer and Interfacial Area

Bayesian Inference

- **Bayesian inference** provides a framework for updating beliefs of model parameters characterized by *epistemic uncertainty* in light of collection of new data

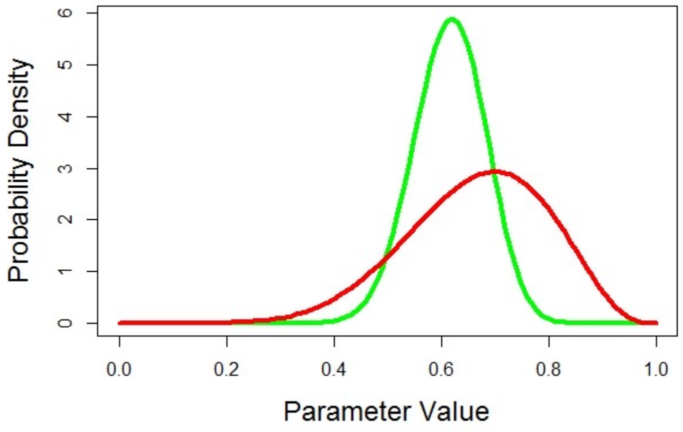
$$\pi(\theta|Z) \propto P(\theta) * L(Z|\theta)$$

Posterior Prior Likelihood

Typical Likelihood Function:

$$L(Z|\theta) = exp\left(-0.5\sum_{i=1}^{M}\frac{\left[F^{*}(x_{i,}\theta) - Z(x_i)\right]^2}{M\sigma_i{}^2}\right)$$

Representation of Prior and Posterior Distributions (reduction in uncertainty through data collection):



PSUADE

Problem Solving Environment for Uncertainty Analysis and Design Exploration

- Software package, developed and maintained by PNNL, integrated into Uncertainty module in FOQUS

Objectives for Pilot Testing

- Develop systematic approach to conducting pilot plant testing regardless of scale, process configuration, technology type, etc.
- Ensure right data are collected
- Maximize value of data collected
- **Design of Experiments (DoE)** is a powerful tool to accelerate learning by targeting optimally useful input combinations to match experiment goals
- **Sequential DoE (SDoE)** allows for incorporation of information from an experiment as it is being conducted by updating input selection criteria based on new information

Sequential Design of Experiments (SDoE)

- SDoE, coupled with detailed process models, can maximize knowledge gained from budget- and schedule-limited pilot testing by optimizing resource allocation
- Reduction of model uncertainty leads to refined understanding of processes and, ultimately, reduction of technical risk associated with scale-up

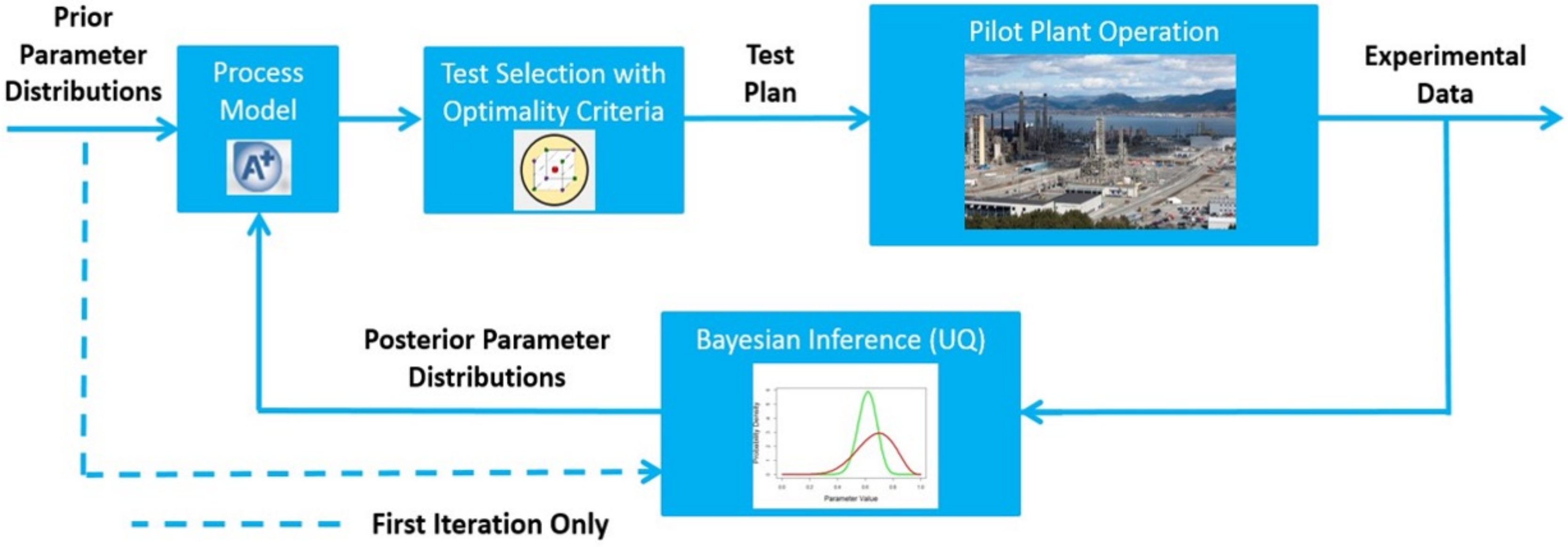


Figure adapted from Morgan et al., GHGT-15 Proceedings, 2021, https://ssrn.com/abstract=3811695

Utility Functions for SDoE

- Space-filling designs
  - **Minimax**: Ensure all points in the candidate set are in close proximity to a point in the design
  - **Maximin**: Ensure all points in the chosen design are not too close together
- Various classes of uncertainty-based designs
  - Minimize variance of parameter estimations
  - Minimize variance of model predictions
    - **G-optimality**: Minimizing the maximum output predicted variance in the design space

Applications of SDoE to Pilot-Scale Testing

National Carbon Capture Center (NCCC)

0.5 MWe test facility
Wilsonville, Alabama

Collaborated with CCSI^2 on aqueous MEA test campaigns in 2014 and 2017

Technology Centre Mongstad (TCM)

12 MWe test facility
Mongstad, Norway

Collaborated with CCSI^2 on aqueous MEA test campaign in 2018

Upcoming test campaigns for novel CO_2 capture technologies in collaboration with commercial developers

Both test campaigns used CCSI aqueous MEA model:

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

Phases of Test Campaign at TCM

Phase 1
Use space-filling design for evaluating quality of prediction of existing model

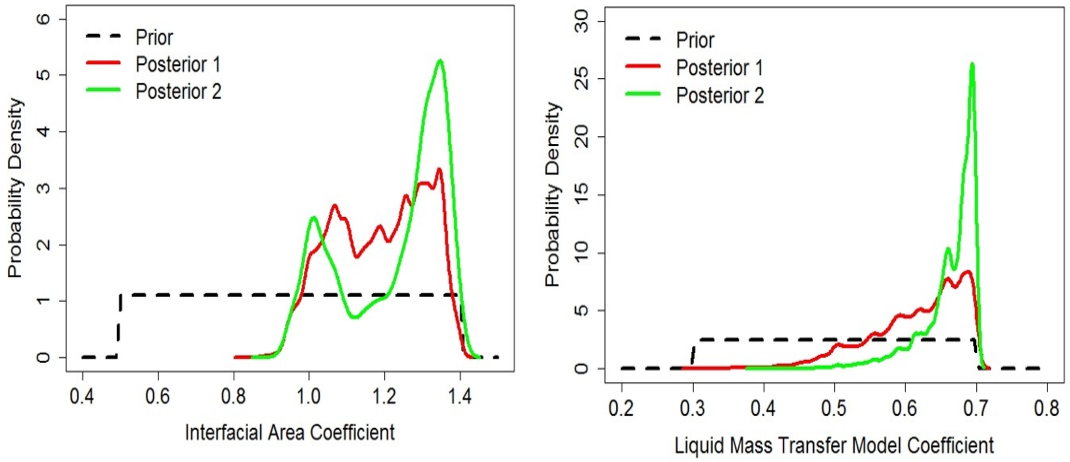
Phase 2
Determine input combinations for testing based on economic objective function

Phase 3
Determine input combinations in order to minimize the maximum model prediction variance in the design space

Phases 4–5
Minimize solvent regeneration energy requirement
(Note: absorber packing height reduced and rich solvent bypass configuration used for this part of the test campaign)

SDoE Results (TCM Campaign)

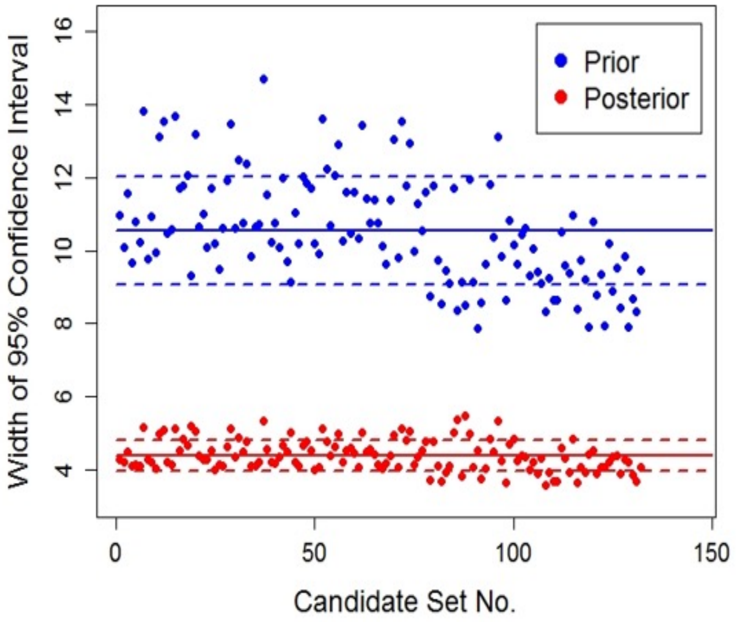
Effect of two iterations of SDoE process on distributions of interfacial area and mass transfer parameters



Through data collection, feasible ranges of mass transfer and interfacial parameters are reduced by refining their distributions

Figures adapted from Morgan et al., GHGT-15 Proceedings, 2021, https://ssrn.com/abstract=3811695

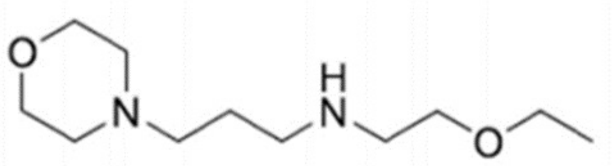
Effect of Bayesian inference on capture prediction confidence interval for individual combinations in candidate sets (candidate set includes variation in flue gas flowrate, CO_2 capture percentage, lean solvent CO_2 loading, and flue gas CO_2 concentration)



Average reduction of ~ 58% in the uncertainty of CO_2 capture percentage predicted by the model due to refinement of mass transfer and interfacial area parameters

Modeling of Second-Generation Solvent System

- EEMPA Solvent System

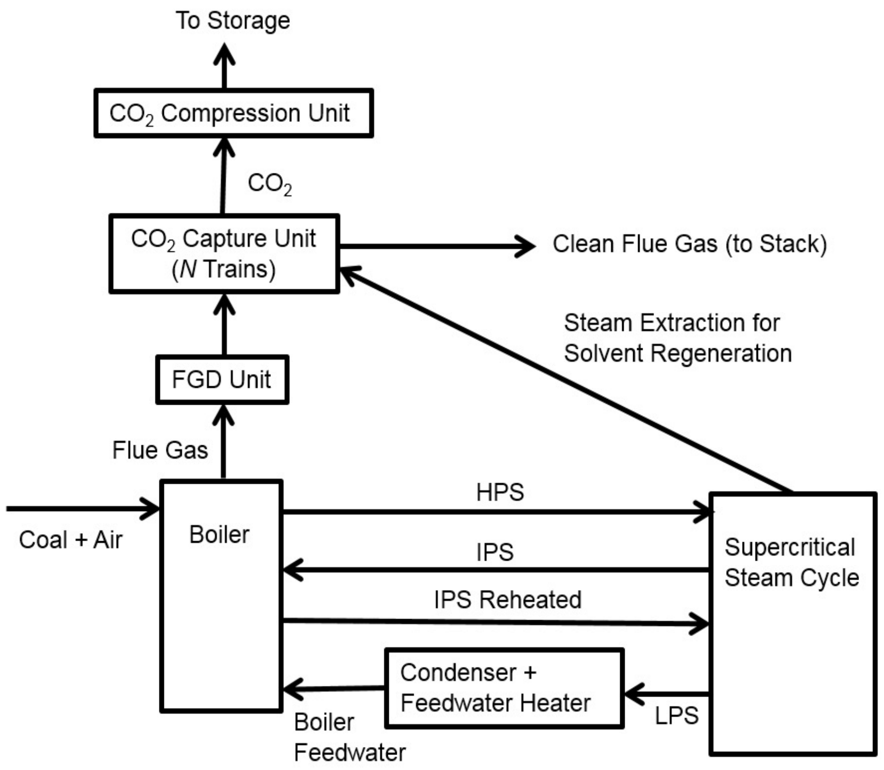


  - Latest in low-aqueous CO_2-binding organic liquid (CO_2BOL) class of solvents developed at Pacific Northwest National Laboratory
  - Reduction in regeneration energy (~40% in comparison to aqueous MEA) and temperature
- CCSI^2 has developed a methodology in FOQUS for economic-based optimization of supercritical PC power plant with CO_2 capture (scale: 650 MWe)
  - EEMPA chosen as solvent system for initial implementation of methodology
  - Ongoing work to extend methodology to a natural gas combined cycle plant

For further reading on EEMPA solvent system:

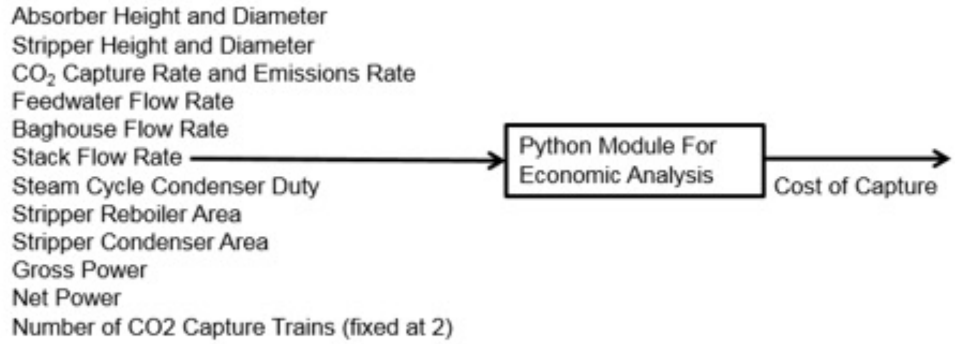
Jiang et al., IJGCC, 2021, 106, 103279

Modeling of Supercritical PC Plant



Aspen Model Node

Variable Transfer



Economic calculations based on:

- Li et al. (2016) [1] paper for capital cost of CO_2 capture unit
- NETL baseline report [2] for all other capital and operating costs (Case B12B)

Python Node

References:

[1] Li et al. (2016), Applied Energy, 165: 648-659

[2] Cost and Performance Baseline for Fossil Energy Plants Volume 1a: Bituminous Coal (PC) and Natural Gas to Electricity Revision 3, DOE/NETL-2015/1723

Optimization Problem Implementation

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

s.t.

$$\tilde{x}^L \leq \tilde{x} \leq \tilde{x}^U$$
$$h(\tilde{x}) = 0$$
$$g(\tilde{x}) \leq 0$$

Variables included in $\tilde{x}$

Variable	Initial Value	Minimum	Maximum
Absorber Packing Height (ft)	71.0	40.0	80.0
Absorber Diameter (ft)	48.0	30.0	50.0
Stripper Packing Height (ft)	40.0	30.0	60.0
Stripper Diameter (ft)	23.0	10.0	40.0
Lean Solvent Loading (mol CO_2/mol DIAM)	0.045	0	1
Rich Solvent Temperature – Exiting Lean Rich Exchanger (°F)	194.0	100.0	200.0

$f(\tilde{x})$ is Cost of CO_2 Capture (COC) in \$/tonne CO_2

$h(\tilde{x})$ denotes constraints directly included in Aspen model

$g(\tilde{x})$ is used to constrain maximum column flooding to 80%

Optimization Results

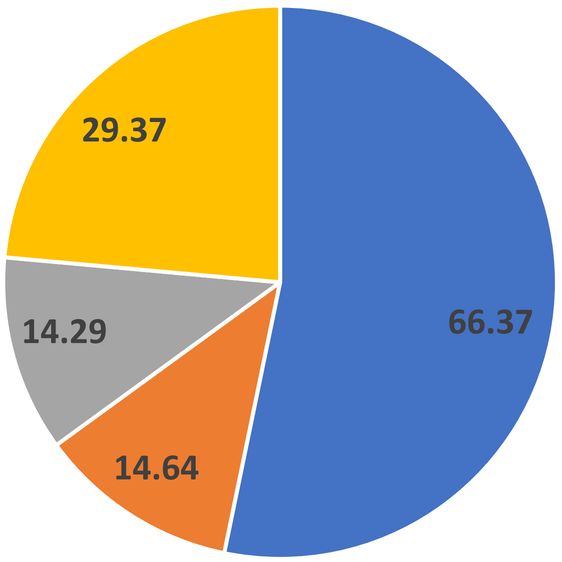
	Range	Optimal Value
Absorber Packing Height (ft)	[40-80]	40.0
Absorber Diameter (ft)	[30-50]	48.2
Stripper Packing Height (ft)	[30-60]	30.1
Stripper Diameter (ft)	[10-40]	23.0
Lean Solvent Loading (mol CO_2/ mol DIAM)	[0-1]	0.069
Rich Solvent Temperature – Exiting Lean Rich Exchanger (°F)	[100-200]	183.1
CO_2 Capture Cost ($/tonne CO_2)		**51.3**

Cost for supercritical PC plant with CANSOLV capture unit (NETL baseline case B12B): $58.2/tonne CO_2

Economic Analysis – Cost of Electricity Comparison

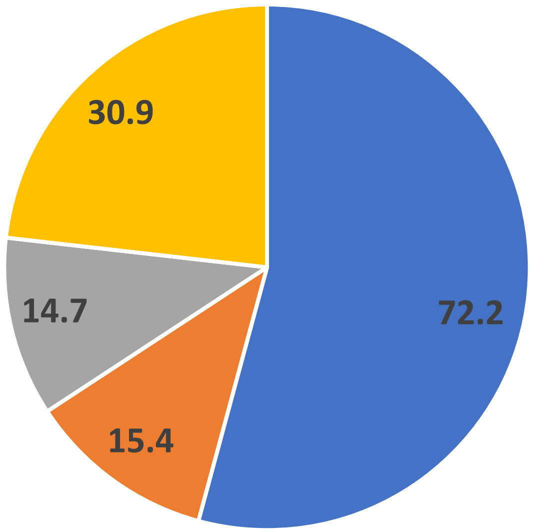
$$Cost\ of\ Capture = \frac{COE - COE_{without\ CO_2\ capture}}{mass\ of\ CO_2\ captured}$$

Cost of Electricity - EEMPA



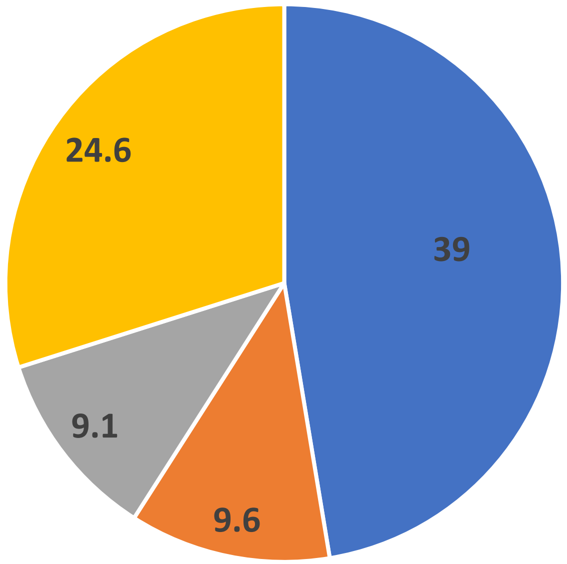
Total = $124.66/MW-hr

Cost of Electricity - CANSOLV (B12B)



Total = $133.2/MW-hr

Cost of Electricity - No Capture (B12A)



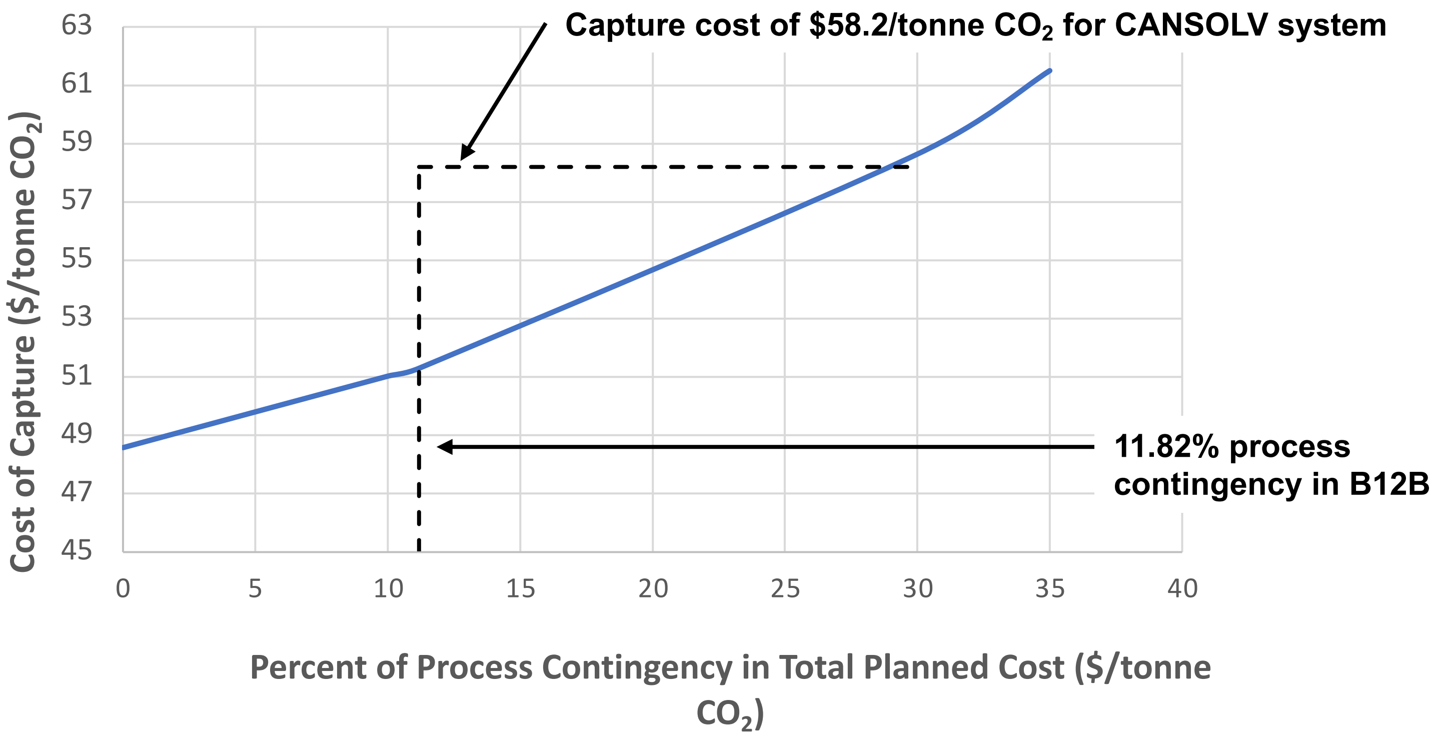
Total = $82.3/MW-hr

■ Captial ■ Fixed ■ Variable ■ Fuel

Sensitivity Study – Effect of Contingency Costs for CO_2 Removal Unit

Process Contingency: Accounts for uncertainty in capital cost estimates due to process performance uncertainty; generally dependent on development status of technology

Project Contingency: Assumed to be ~18% of the sum of bare-erected cost + EPC fees + process contingency [Consistent with Case B12B in baseline report]



- Due to relatively low maturity of EEMPA system technology, it is reasonable to assume higher percentage of process contingency in total planned cost for capture unit
- COC exceeds that of baseline B12B if percent of process contingency for EEMPA system is assumed to be higher than 30%

CCSI²
Carbon Capture Simulation for Industry Impact

Summary and Conclusions

- CCSI² program aims to accelerate the scale-up and commercial deployment of carbon capture technologies through efficient implementation of available computational tools and models
- FOQUS tool facilitates connection between process models of various platforms (e.g., Aspen Plus) and enables advanced modeling capabilities for applications in and beyond carbon capture and storage
- SDoE capability has been demonstrated to be effective in refining, through uncertainty reduction, stochastic models through collection of pilot plant data
  - Reduction of ~60% in prediction of CO_2 capture percentage demonstrated for aqueous MEA in test campaigns at NCCC and TCM
- Optimization capability implemented at plant-scale for second-generation CO_2 capture solvent system for economic comparison with established baseline

Further Information

CCSI² Additional Information

https://www.acceleratecarboncapture.org/

CCSI² Toolset (FOQUS framework + individual models) Downloads

https://github.com/CCSI-Toolset

FOQUS Installation Instructions and Reference Manual

https://foqus.readthedocs.io/en/latest/

FOQUS Video Tutorials

https://www.youtube.com/channel/UCBVjFnxrsWpNlcnDvh0_GzQ?app=desktop

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

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