Framework for Optimization, Quantification of Uncertainty, and Surrogates (FOQUS) – Demonstration

Katherine Hedrick[a,b]

[a] **National Energy Technology Laboratory**
[b] **NETL Support Contractor**

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Westin Hotel and Conference Center
Tysons Corner, VA
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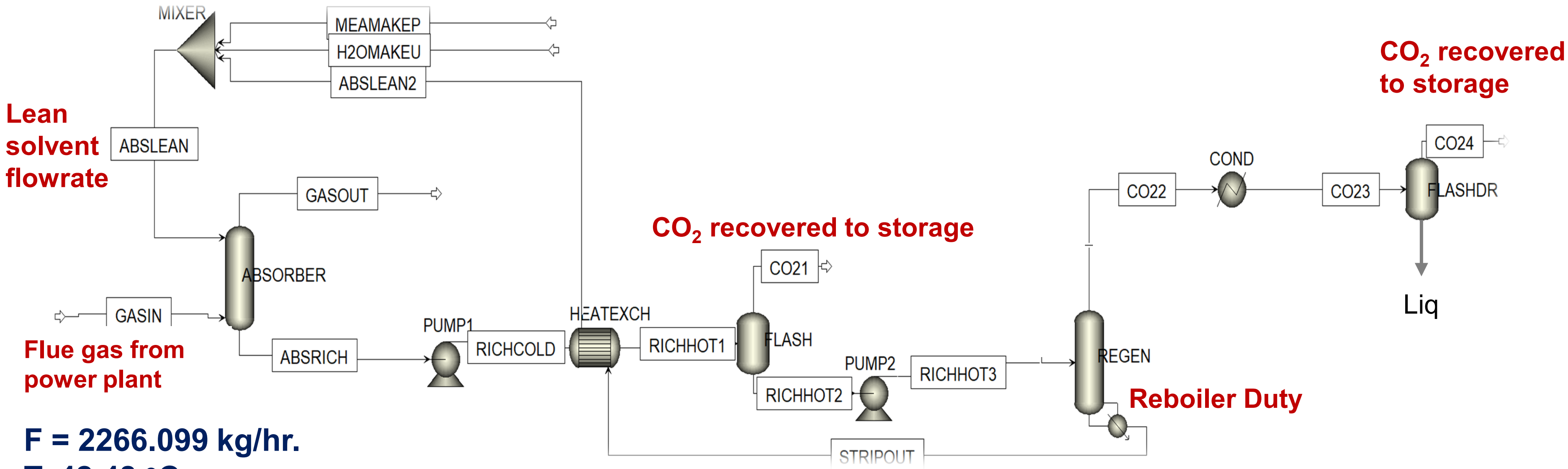
Demonstration Sequence

- Problem Statement: Comprehensive analysis of an monoethanolamine (MEA) solvent-based carbon capture system
- FOQUS Flowsheet setup
- Setup and implementation of the following FOQUS modules:
  - Uncertainty Quantification (UQ)
  - Surrogate Modeling
  - Optimization
- List of available $CCSI^2$ toolset resources

FOQUS – Framework for Optimization, Quantification of Uncertainty, and Surrogates

Problem Statement

Perform a comprehensive analysis of an MEA solvent-based carbon capture system (0.5 MWe)



F = 2266.099 kg/hr.
T: 42.48 °C.
P = 108.82 kPa.

Input variables of interest:

1. CO_2 lean loading
2. Lean solvent flowrate
3. MEA concentration in lean solvent
4. Stripper pressure
5. Flue gas flowrate
6. Flue gas CO_2 concentration

Output variables of interest:

1. CO_2 Capture Rate (%)
2. Reboiler Duty
3. Specific Reboiler Duty (SRD)

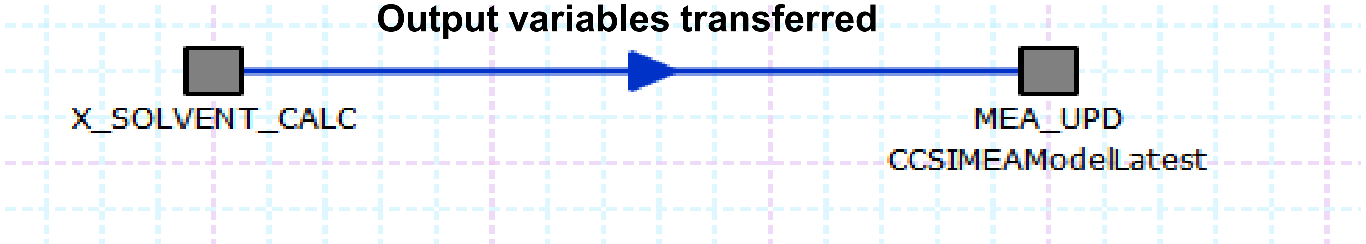
*Aspen Plus v11 model. Process Design and Operating Specifications are based on the **National Carbon Capture Center Pilot System (0.5 MWe)****

$$\mathrm{CO_2\ Lean\ Loading\ (lean\ solvent)} = \frac{mol\ CO_2}{mol\ MEA}$$

$$\mathrm{Specific\ Reboiler\ Duty} = \frac{Reboiler\ Duty}{Total\ rate\ of\ CO_2\ \ Recovered}\ [\mathrm{MJ/kg\ CO_2}]$$

***CCSI-Toolset MEA Steady State Model –** https://github.com/CCSI-Toolset/MEA_ssm/releases/tag/3.2.1

FOQUS Flowsheet Setup



Python-based node:

Input:
- CO_2 Lean Loading
- MEA concentration in lean solvent

Output:
- Mole fractions (CO_2, MEA, H_2O) in lean solvent entering the absorber

Turbine model-based node (MEA Steady-State Aspen Model):

Input:
- Flue gas – flowrate, wt. fraction of components (CO_2, H_2O, N_2, O_2)
- Lean solvent – flowrate, mole fraction of components (CO_2, MEA, H_2O)
- Stripper Pressure

Output:
- CO_2 Capture Rate (%)
- Reboiler Duty
- Specific Reboiler Duty

Process Simulation Inputs (base case)

Process Parameters	Input values
Solvent Flowrate (kg/hr)	6803.7
MEA Concentration (wt fraction, CO_2 free basis)	0.3
CO_2 Lean Loading	0.1
Stripper Pressure (kPa)	183.87
Flue Gas (FG) Flowrate (kg/hr)	2266.099
CO_2 conc. in FG (wt frac)	0.17314

Process Simulation Results

Key output variables	Values
CO_2 Capture Rate (%)	99.98
Amount of CO_2 Recovered (kg/hr)	386.23
Reboiler Duty (W)	800781
SRD (MJ/kg CO_2)	7.464

Uncertainty Quantification (UQ)

Uncertainty

Motivation: Improve our understanding of the process

Sensitivity Study

- Understand the effect of variability/uncertainty of input variables on important output variables of interest
  - Cause-Effect Relationship
  - Extent of the effect
- Supports decision making related to process design, scale-up, optimization, and control

Parameter Screening

- Understand the order of importance for input variables of interest – extent of influence on output variables
- Supports decision making related to process optimization & extensive uncertainty quantification

Overall Importance

- Thorough characterization and understanding of process behavior in a particular range of operating conditions
- Supports decision making related to process scale-up and optimization

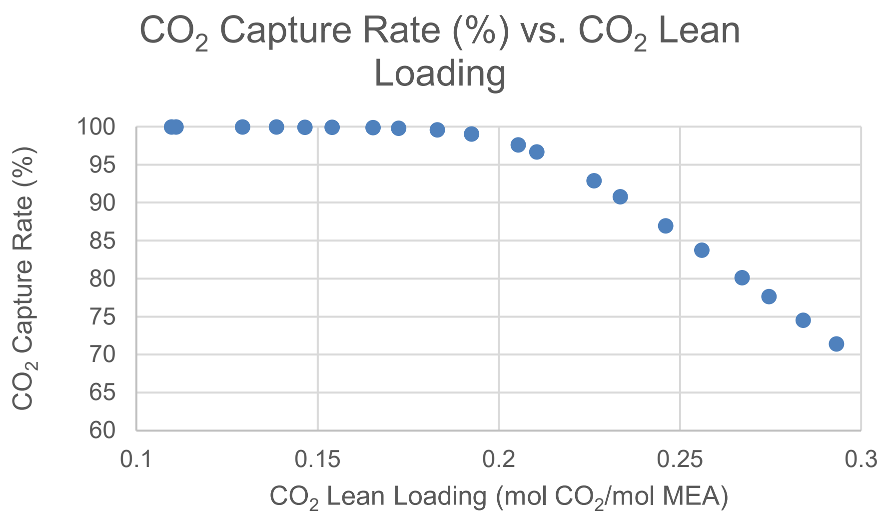
Uncertainty Quantification

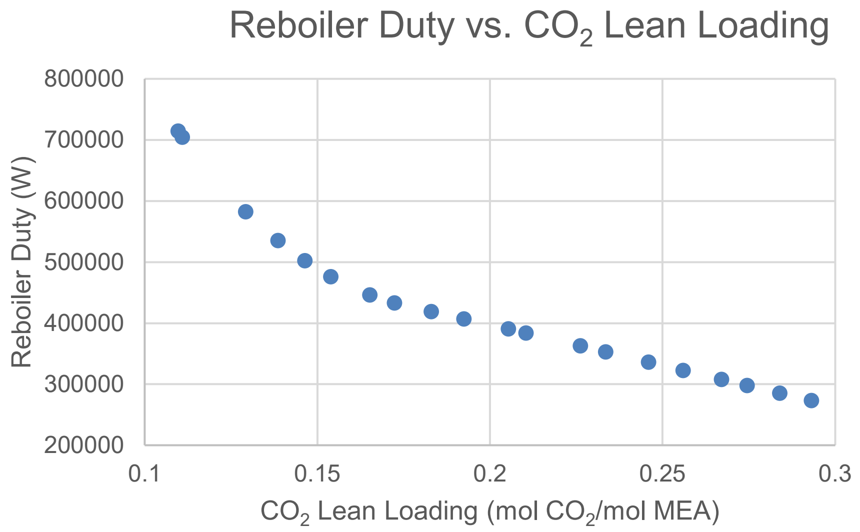
Single Variable Sensitivity Study

Run Simulation Ensemble – 1 process parameter changed at a time

Process Parameter	Range of Variation	Sampling	No of Points
CO_2 Lean Loading	0.1-0.3	LHS	20

Other input parameter values are the same as base case





Cause for the trend – Reduction in CO_2 absorption capacity by the lean solvent in the absorber with higher CO_2 lean loading

Cause for the trend – With increased CO_2 lean loading, there is a decrease in the amount of CO_2 that needs to be stripped from the rich solvent entering the stripper, hence the lower requirement for reboiler duty

Uncertainty Quantification

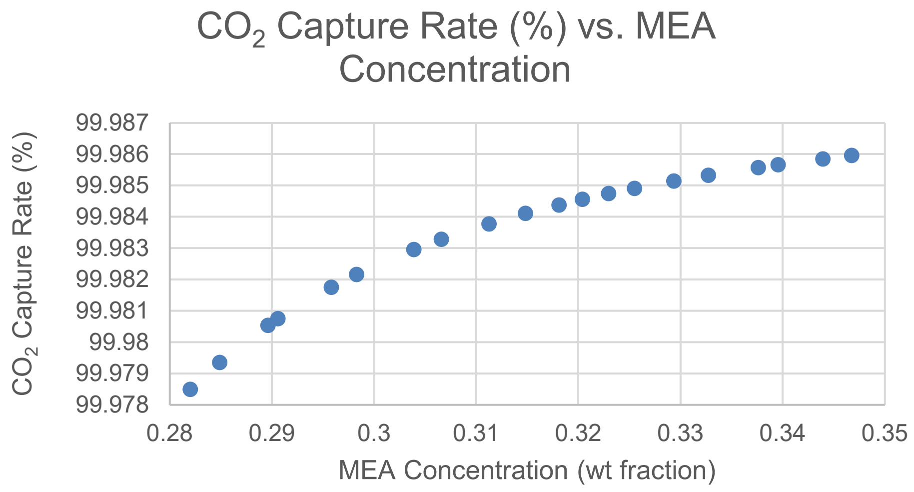
Uncertainty

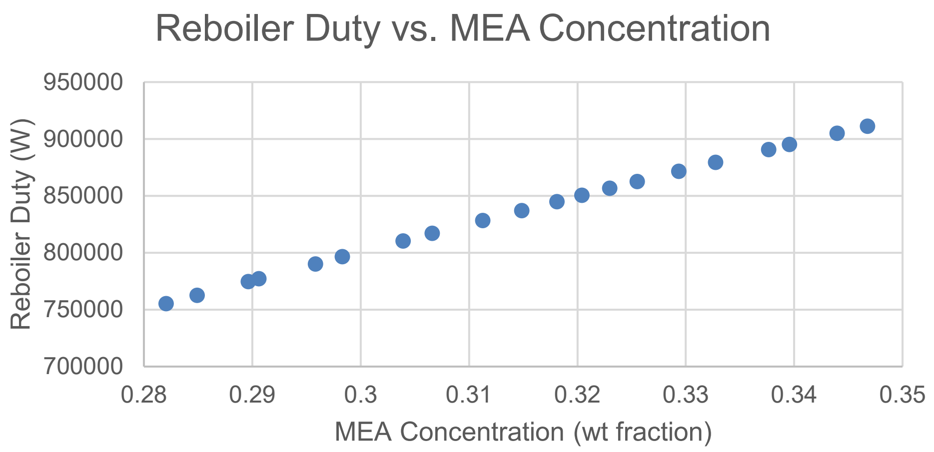
Single Variable Sensitivity Study

Run Simulation Ensemble – 1 process parameter changed at a time

Process Parameter	Range of Variation	Sampling	No of Points
MEA Concentration	0.28-0.35	LHS	20

Other input parameter values same as default





Cause for the trend – Increase in rate of absorption of CO_2 by the lean solvent in the absorber with higher MEA concentration

Cause for the trend – System thermodynamics dictate that higher reboiler duty is required for stripping CO_2 when the MEA concentration is higher

Uncertainty Quantification

Uncertainty

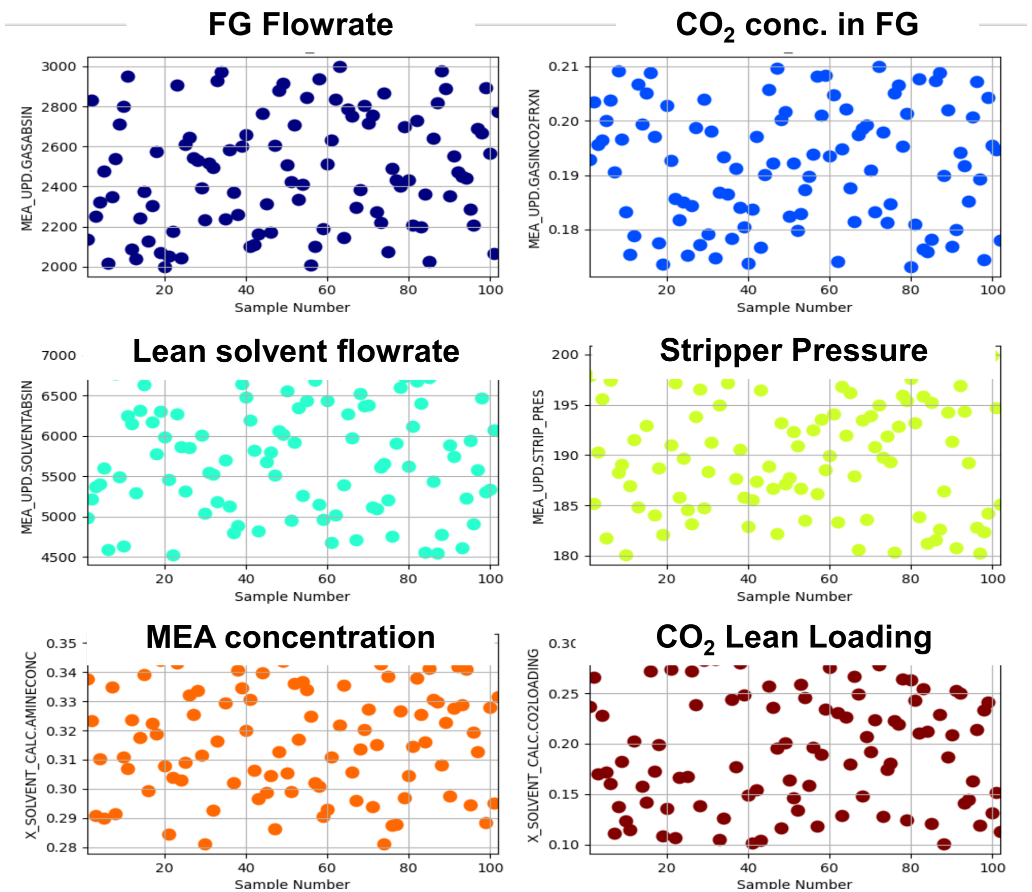
Multi-variable Analysis

Run Simulation Ensemble – 6 process parameters changed at a time

Process Parameter	Range of Variation
Solvent Flowrate (kg/hr)	4500–7000
MEA Concentration	0.28–0.35
CO_2 Lean Loading	0.1–0.3
Stripper pressure (kPa)	180–200
Flue gas flowrate (kg/hr)	2000–3000
FG CO_2 concentration	0.17314–0.21

- Latin Hypercube Sampling
- Number of points:102

Data Visualization – 1 variable scatter plots



Uncertainty Quantification

Uncertainty

Multi-variable Analysis

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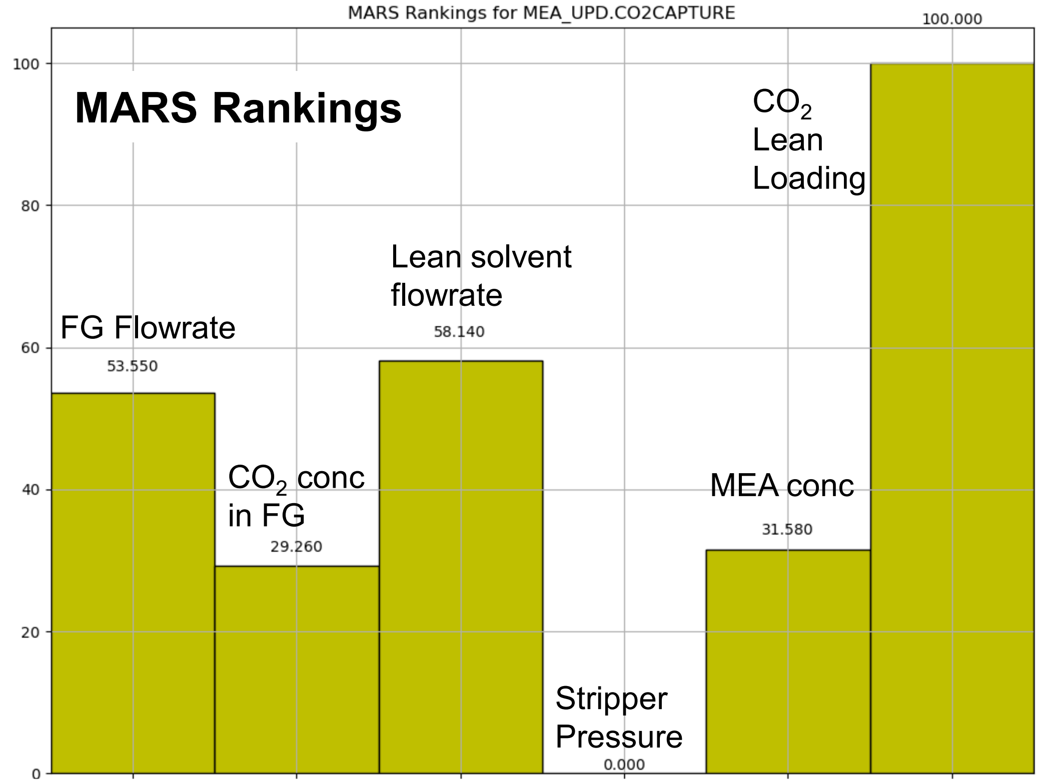

Parameter Screening for CO_2 Capture %

Uncertainty Quantification

Multi-variable Analysis

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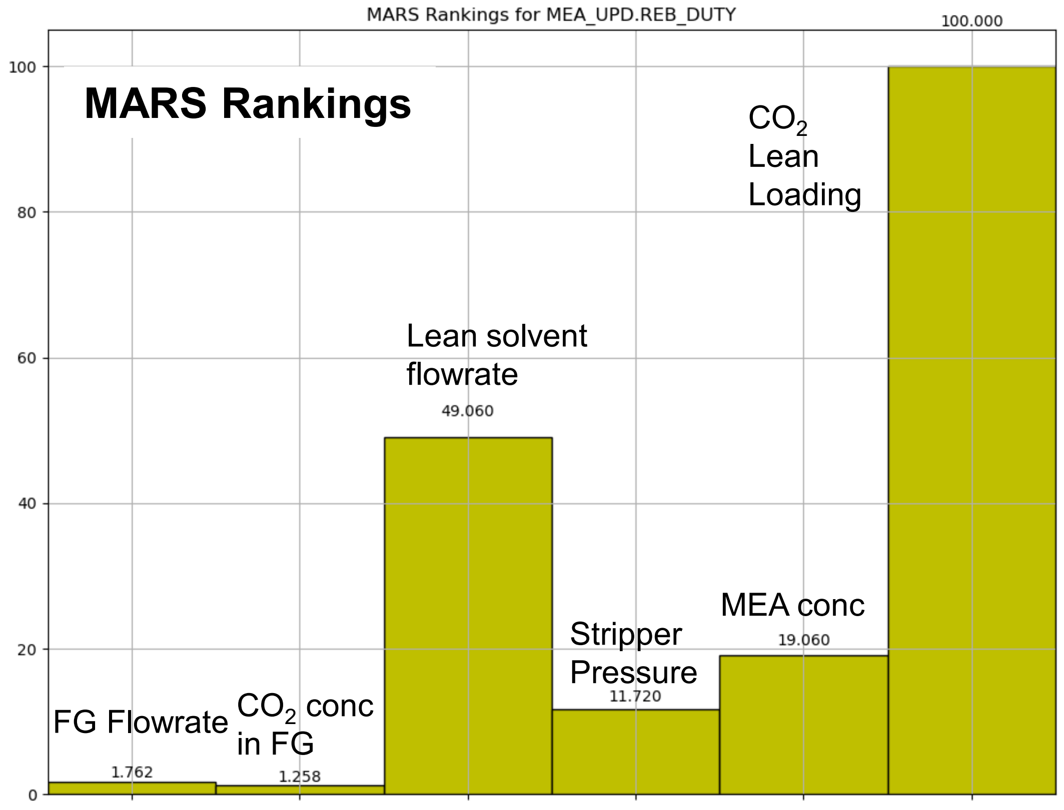


Parameter Screening for Reboiler Duty

Surrogate Modeling

Surrogates

Motivation

- Simple algebraic model-based representation of a complex simulator model without compromising accuracy
- Saves time for simulation, uncertainty quantification, and optimization
- Enables connection with other equation-oriented models and perform analysis on the combined model

Surrogate Modeling

Surrogates

(Based on 102 pt. dataset from UQ Simulation Ensemble)

Surrogate Input Variables
Lean solvent flowrate (kg/hr)
MEA Concentration (wt frac)
CO_2 Lean Loading
Stripper Pressure (kPa)
Flue Gas (FG) Flowrate (kg/hr)
CO_2 conc in FG (wt frac)

Surrogate Output Variables
CO_2 Capture Rate (%)
Reboiler Duty (W)

ALAMO Settings

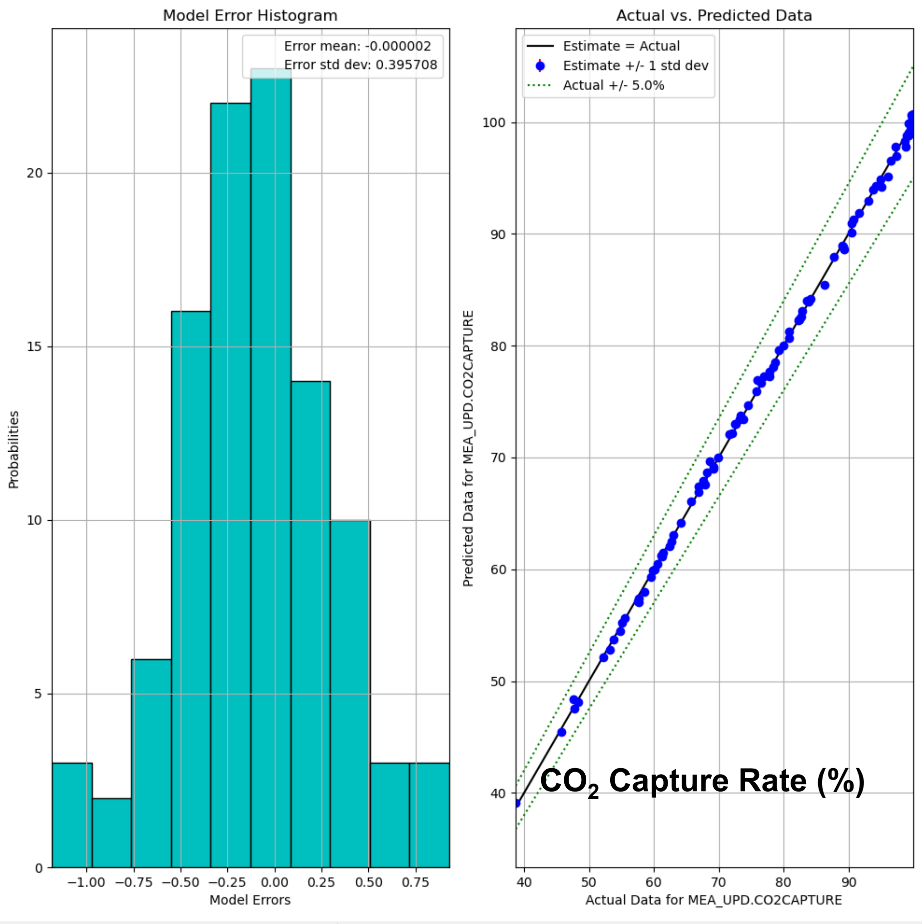
MAXTIME	2000
MINPOINTS	0
NSAMPLE	0
MAXSIM	5
SAMPLER	"None"
MAXITER	1
PRESET	-111111
MONOMIALPOWER	[1, 2, 3]
MULTI2POWER	[1, 2, 3]
MULTI3POWER	[1, 2, 3]
RATIOPOWER	[1, 2, 3]
EXPFCNS	☑
LOGFCNS	☑

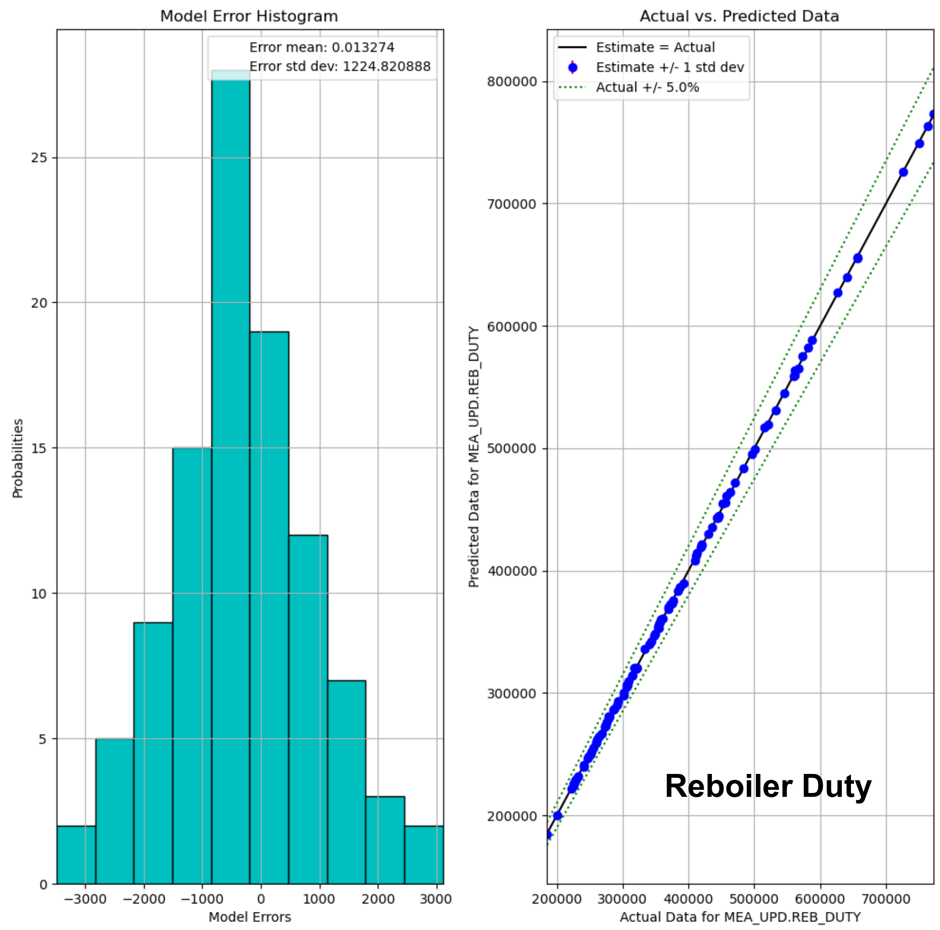
	Setting Name	Value
21	MODELER	"BIC"
22	CONVPEN	10.0
23	SCREENER	"No Screening"
24	SCALEZ	☑
25	GAMS	"gams"
26	GAMSSOLVER	"BARON"
27	SOLVEMIP	☑
28	FUNFORM	"Fortran"
29	MIPOPTCA	0.05
30	MIPOPTCR	0.0001
31	LINEARERROR	☐
32	CONREG	☐
33	CRNCUSTOM	☐
34	CRNINITIAL	0
35	CRNMAXITER	10
36	CRNVIOL	100
37	CRNTRIALS	100
38	CRTOL	0.001
39	Input File	"alamo.alm"
40	FOQUS Model (for UQ)	"alamo_surrogate_uq.py"
41	FOQUS Model (for Flowsheet)	"alamo_surrogate_fs.py"

Surrogate Modeling

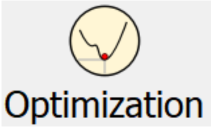
(Based on 102 pt. dataset from UQ Simulation Ensemble)

Parity Plots





Process Optimization



Motivation

- Improve the process in terms of maximizing product purity or minimizing waste generation and energy requirement
- Improves economic feasibility of the process

Optimization

Optimization Problem

$$\min_{x} \mathrm{f}(x)$$ → **Objective Function**; x → **Decision Variables**

St: $h(x) = 0$, $g(x) \leq 0$ → **Constraints**

h(x) represents Process Model:

- Mass, energy balances
- Stream connections
- Design specification
(CO_2 Capture Rate = 90 %)

Objective Function f(x): SRD
Decision Variables (x): CO_2 Lean Loading

Other Process Parameters – fixed at default values

DFO Solver: NLopt (default settings)

Result:

Objective Function (SRD)* = 3.465

Process Parameter	Type	Range of Variation	Initialization (default values)	Optimum Value
CO_2 Lean Loading	Decision	0.15–0.25	0.15	0.17036

Advanced FOQUS Capabilities and Updates

- AWS FOQUS Cloud
  - Can be used instead of TurbineLite to run Aspen simulations
  - Users don’t have to install Aspen on their local machine
  - Simulations can be run in parallel to reduce computational time and reduce resources on a user's local machine
  - Latest Updates:
    - Improvements to multi-user support and resource isolation
    - Enhancements to SDOE function parallelism on AWS Lambda to enable testing of 1000s of executions
    - Additional Cloud Metrics and Jupyter Notebook support for monitoring and insight

- Major Updates to SimSinter
  - Behind the scenes rehaul to improve maintainability
  - Support for current versions of Windows and Aspen
  - Security updates
  - Latest release: https://github.com/CCSI-Toolset/SimSinter/releases/tag/3.0.0

Summary

- FOQUS – useful tool for realistic application-based modeling & analysis
  - Covers wide range of system types & scales
  - Solvent, sorbent, membrane carbon capture systems
  - Bench, pilot, commercial scale
  - Combined system models - Power plant with CO_2 capture

- FOQUS capabilities are interconnected – flexible to use

- Each capability provides valuable information – enables decision making for the path forward

CCSI^2 Toolset Resources

CCSI^2 Additional Information

https://www.acceleratecarboncapture.org/

CCSI^2 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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Carbon Capture Simulation for Industry Impact

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Carbon Capture Simulation for Industry Impact

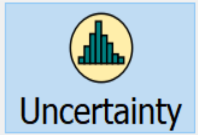
For more information

https://www.acceleratecarboncapture.org/

Katherine.Hedrick@netl.doe.gov

2023 Joint CCSI2/IDAES Technical Team Meeting, Lawrence Berkeley National Lab

Uncertainty Quantification

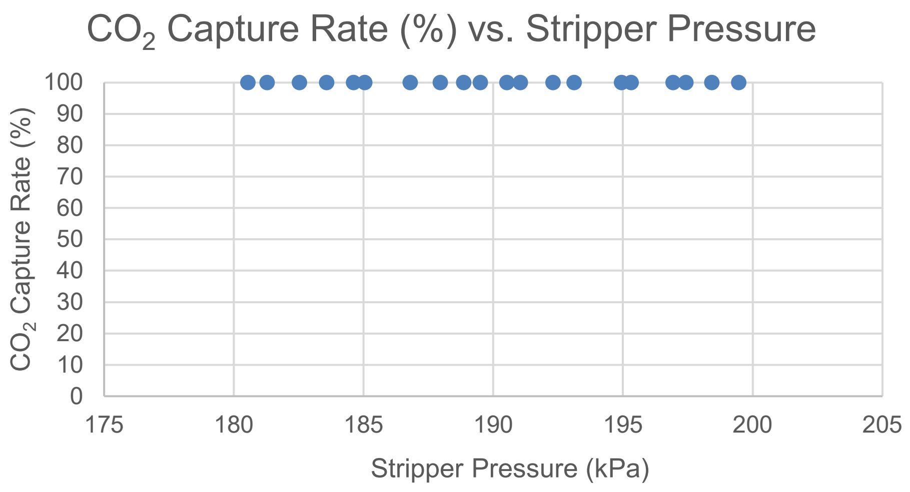


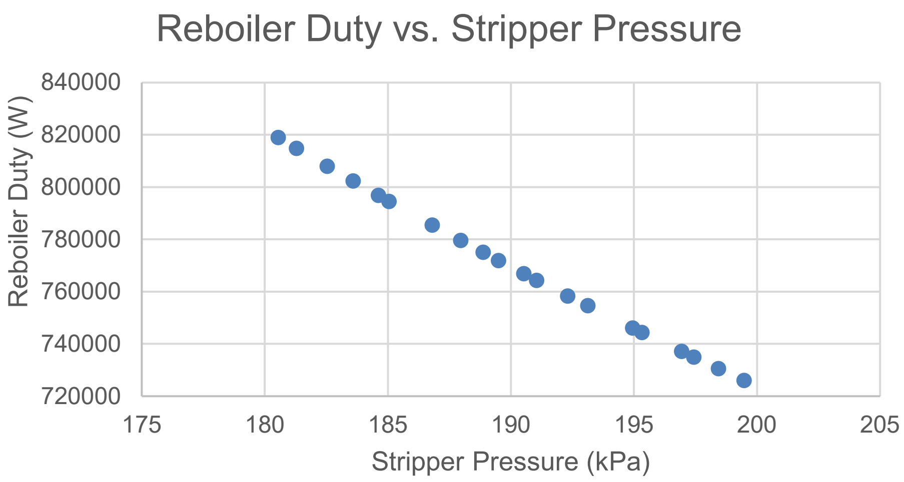
Single Variable Sensitivity Study

Run Simulation Ensemble – 1 process parameter changed at a time

Process Parameter	Range of Variation	Sampling	No of Points
Stripper pressure	180-200	LHS	20

Other input parameter values same as defaul





Cause for the trend – Model is set up such that absorber is not affected by the stripper pressure, hence there is no effect on the CO_2 Capture Rate

Cause for the trend – Higher stripper pressure implies higher rich solvent temperature entering the reboiler, hence the reboiler duty decreases to maintain the same CO_2 lean loading

Uncertainty Quantification

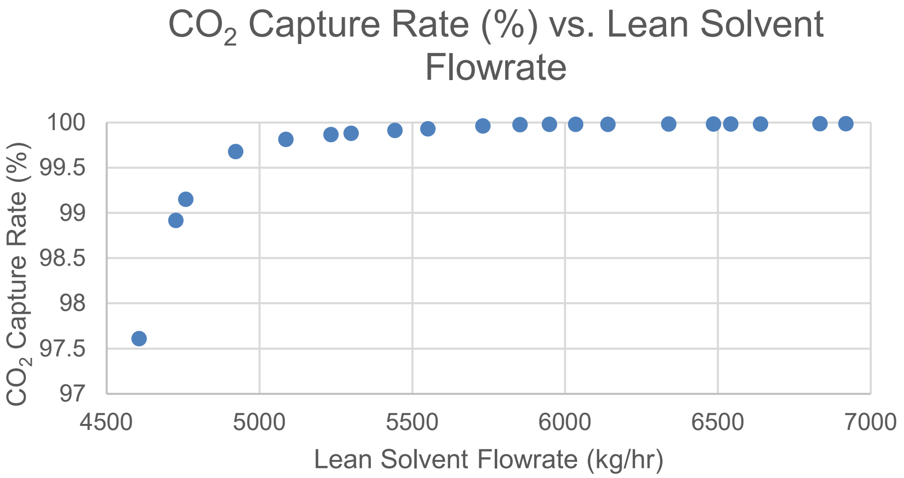
Uncertainty

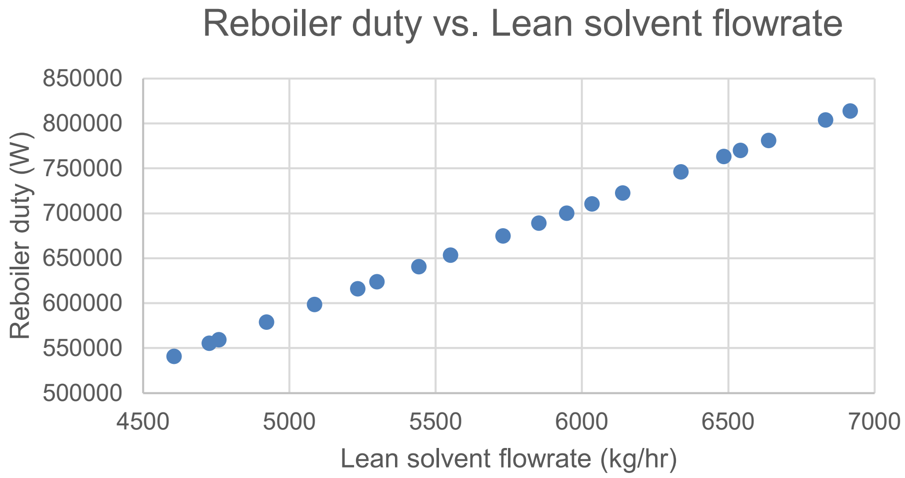
Single Variable Sensitivity Study

Run Simulation Ensemble – 1 process parameter changed at a time

Process Parameter	Range of Variation	Sampling	No of Points
Solvent Flowrate (kg/hr)	4500-7000	LHS	20

Other input parameter values same as default

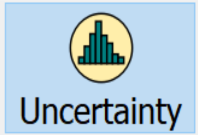




Cause for the trend – Increase in rate of absorption of CO_2 by increase in lean solvent flowrate in the absorber

Cause for the trend – Increase in sensible heat requirement in the reboiler for solvent regeneration

Uncertainty Quantification

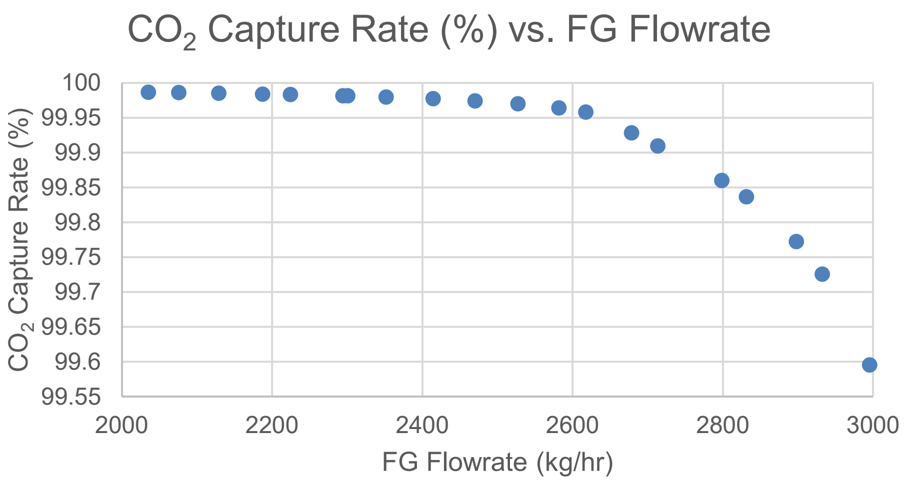


Single Variable Sensitivity Study

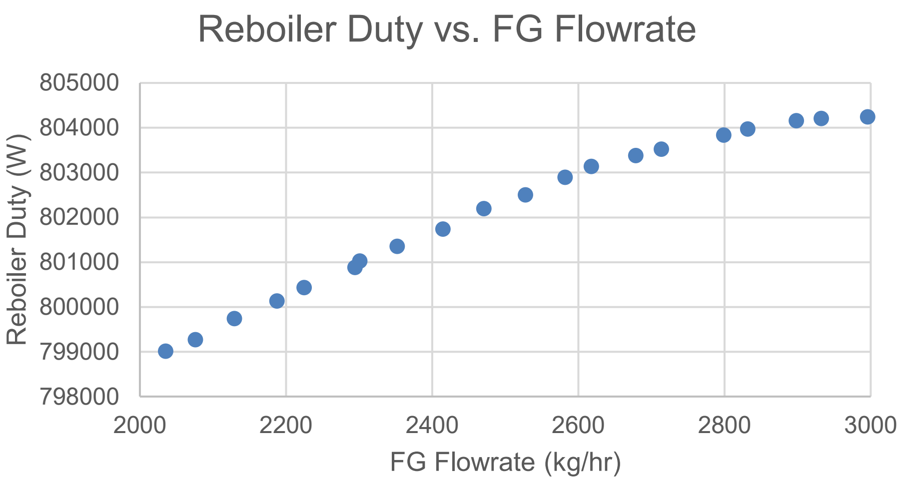
Run Simulation Ensemble – 1 process parameter changed at a time

Process Parameter	Range of Variation	Sampling	No of Points
Flue gas flowrate	2000-3000	LHS	20

Other input parameter values same as default



Cause for the trend – Increase in CO_2 flowrate in the flue gas, which causes a decrease in capture rate with the same lean solvent flowrate and composition entering the absorber



Cause for the trend – Increase in flue gas flowrate leads to a slight increase in the amount of CO_2 captured, hence reboiler duty increases to maintain the same CO_2 lean loading

Uncertainty Quantification

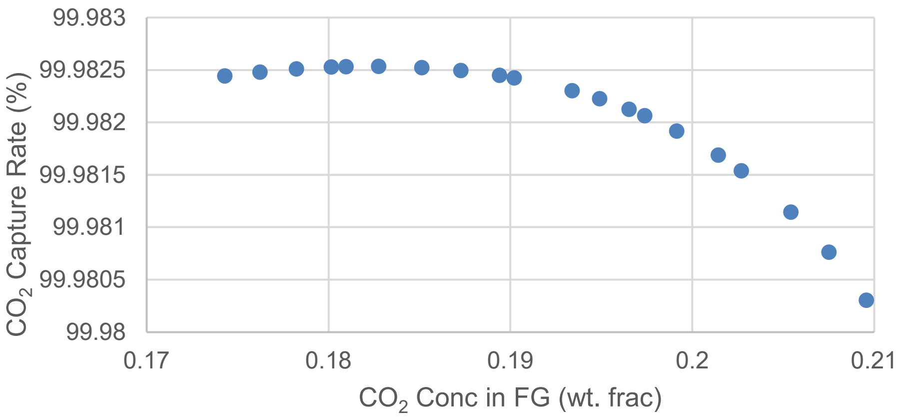
Single Variable Sensitivity Study

Run Simulation Ensemble – 1 process parameter changed at a time

Process Parameter	Range of Variation	Sampling	No of Points
FG CO_2 concentration	0.17314-0.21	LHS	20

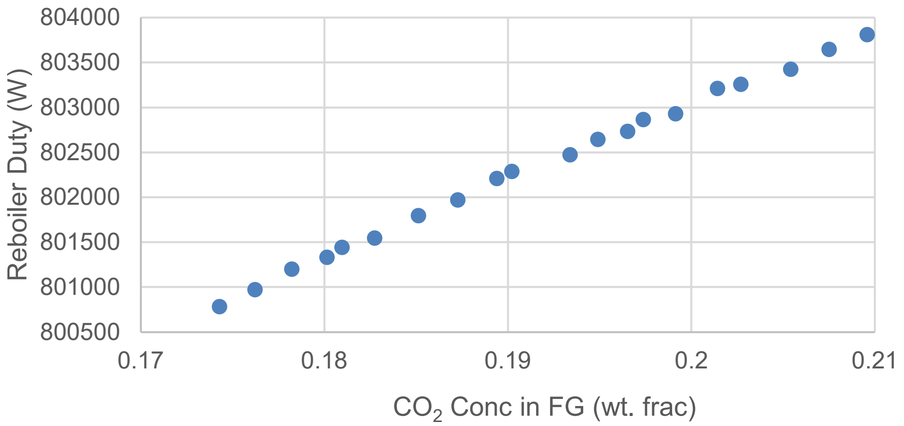
Other input parameter values same as default

CO_2 Capture Rate (%) vs. CO_2 conc. in FG



Cause for the trend – Increase in CO_2 flowrate in the flue gas, which causes a decrease in the capture rate with the same lean solvent flowrate and composition entering the absorber

Reboiler Duty vs. CO_2 conc. in FG



Cause for the trend – Increase in flue gas CO_2 concentration leads to a slight increase in the amount of CO_2 captured, hence reboiler duty increases to maintain the same CO_2 lean loading

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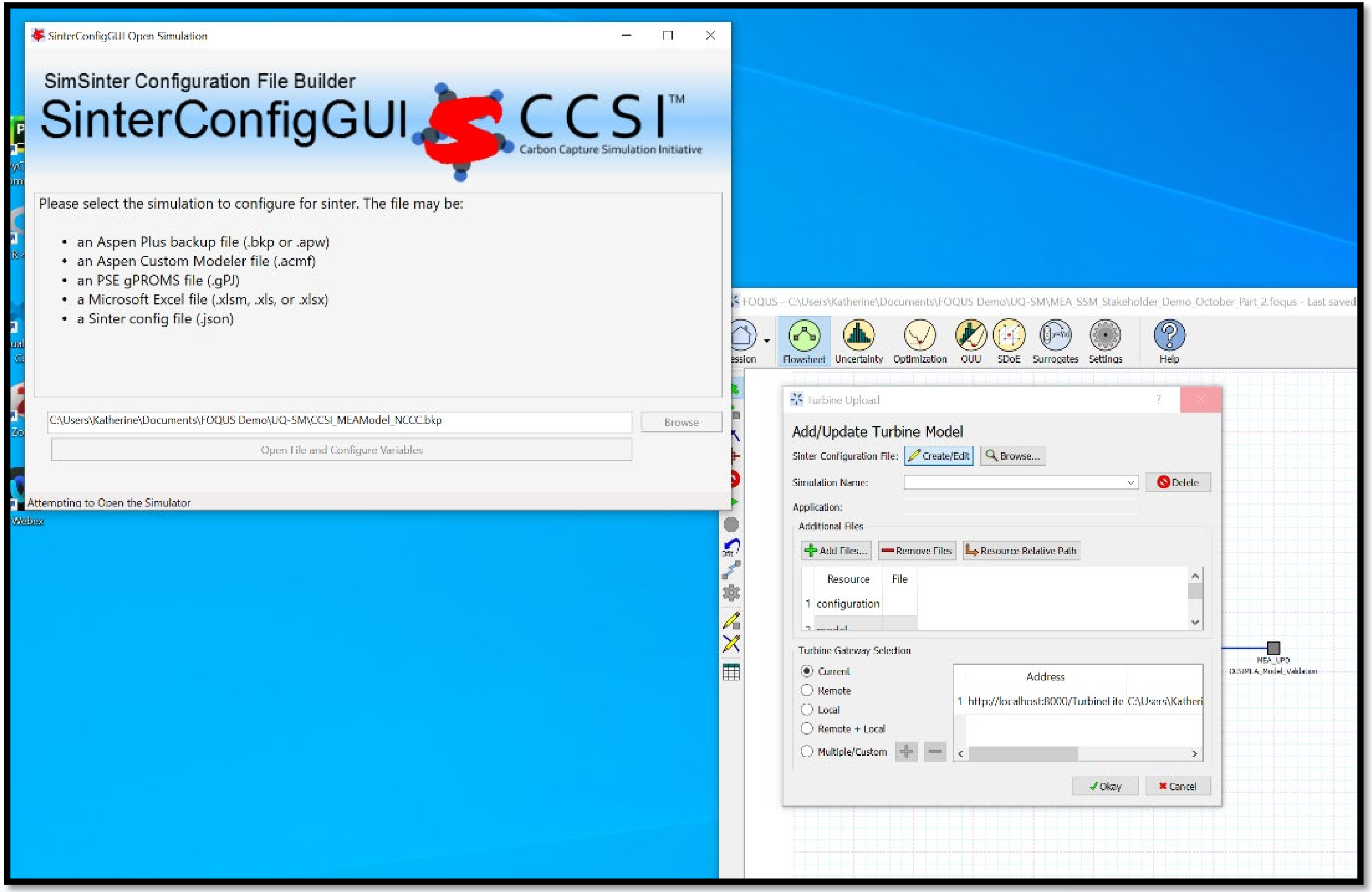
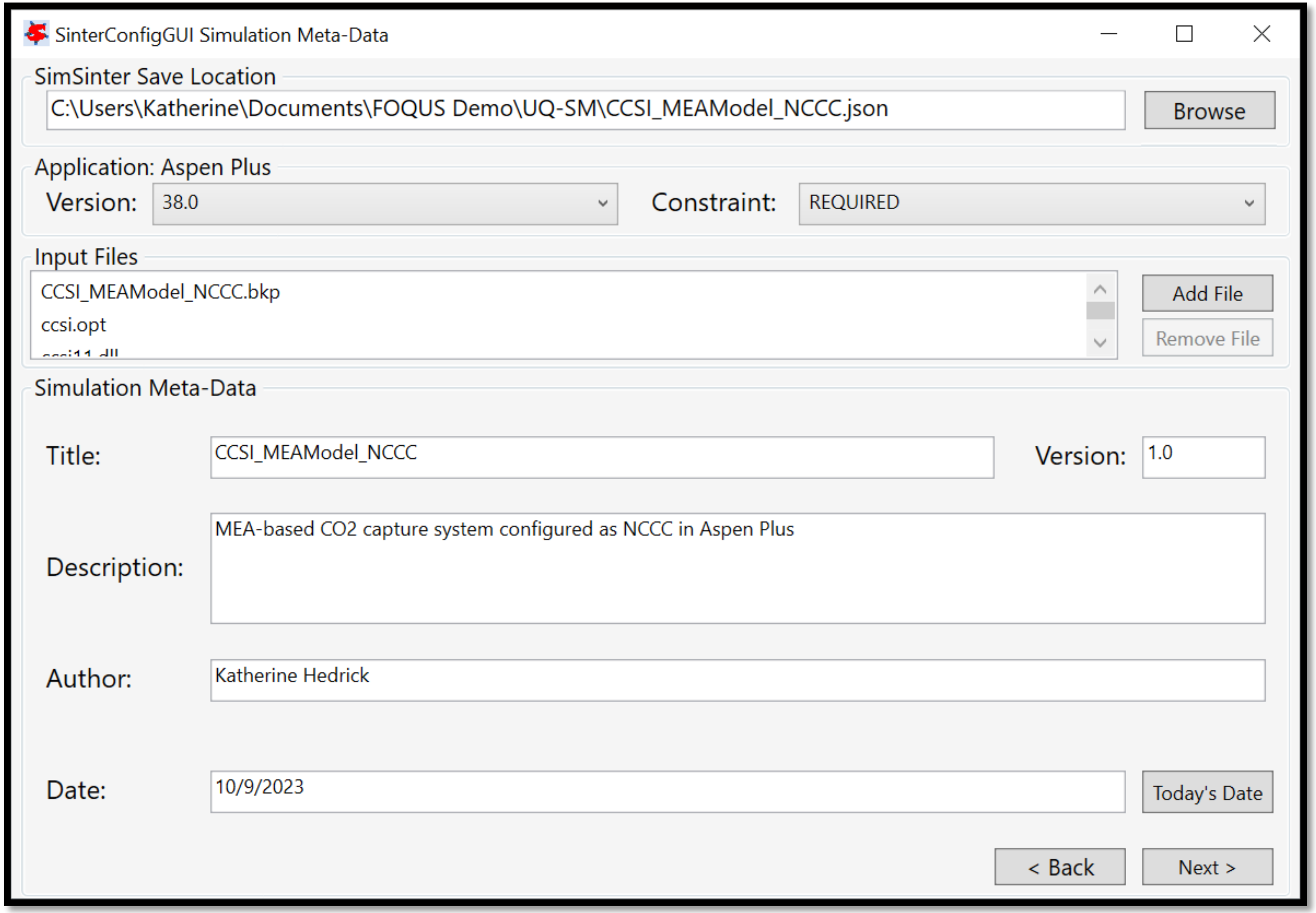
Turbine Setup



Turbine Setup



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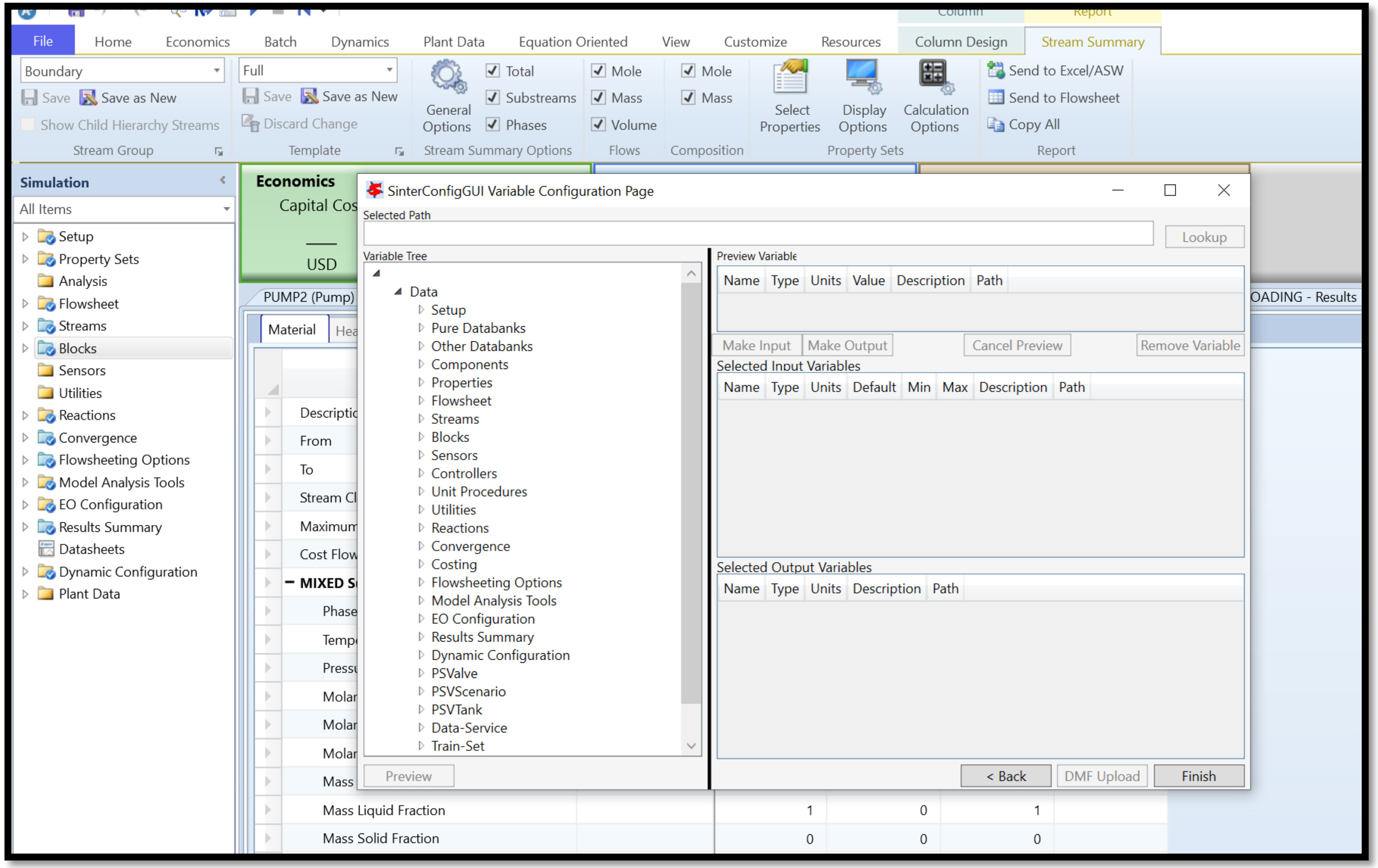

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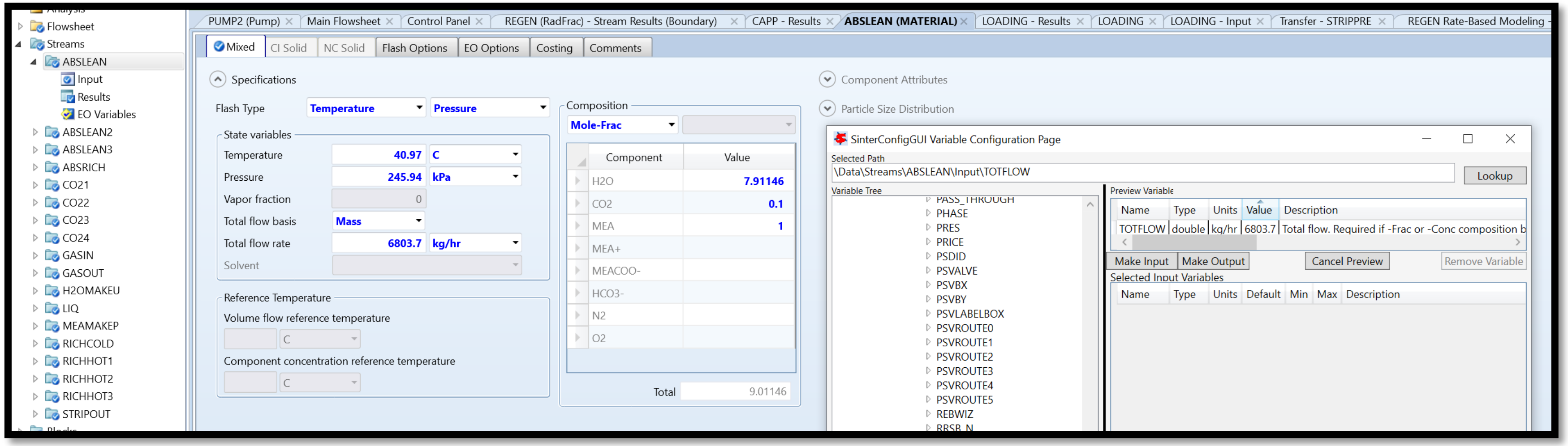

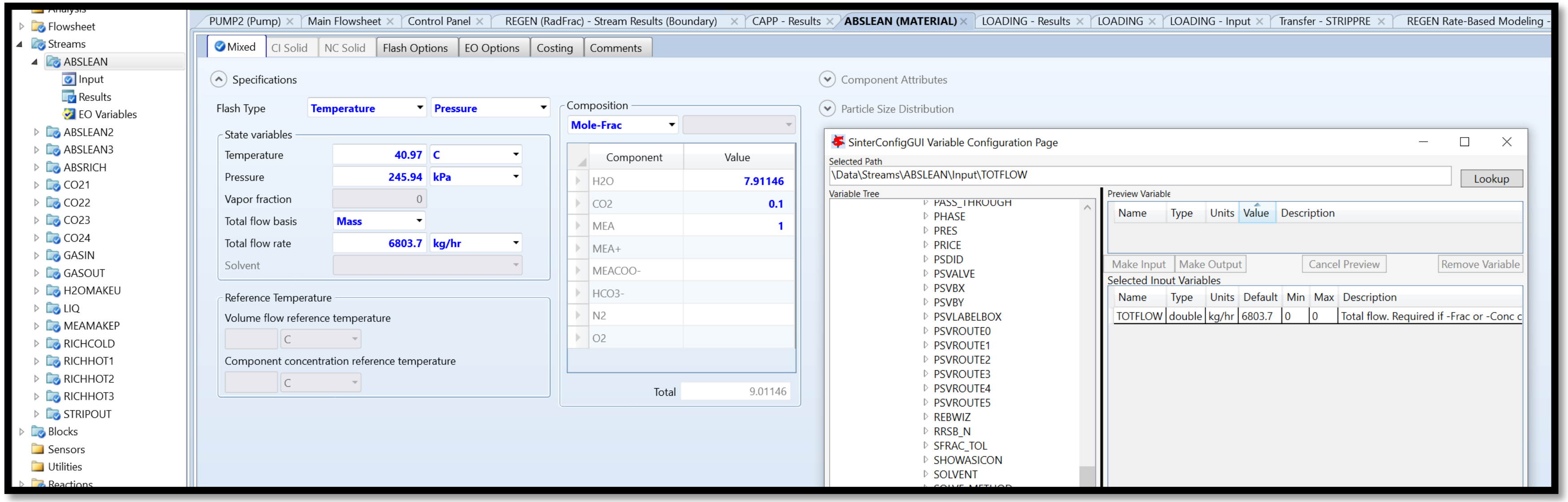

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Turbine Setup