

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

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**Advanced PSE+ Stakeholder Summit** 

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Chational Laboratory West Virginia University





**Carnegie Mellon** 

# **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<sup>2</sup> 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)



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

$$CO_{2} \text{ Lean Loading (lean solvent)} = \frac{mol CO_{2}}{mol MEA}$$
Specific Reboiler Duty =  $\frac{Reboiler Duty}{Total rate of CO_{2} Recovered} [MJ/kg CO_{2}]$ 
\*CCSI-Toolset MEA Steady State Model – [https://github.com/CCSI-Toolset/MEA\\_ssm/releases/tag/3.2.1](https://github.com/CCSI-Toolset/MEA_ssm/releases/tag/3.2.1)

# **FOQUS Flowsheet Setup**



### Output:

- CO<sub>2</sub> 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 <sub>2</sub> free basis)	0.3
CO <sub>2</sub> Lean Loading	0.1
Stripper Pressure (kPa)	183.87
Flue Gas (FG) Flowrate (kg/hr)	2266.099
CO <sub>2</sub> conc. in FG (wt frac)	0.17314

### **Process Simulation Results**

Key output variables	Values
CO <sub>2</sub> Capture Rate (%)	99.98
Amount of CO <sub>2</sub> Recovered (kg/hr)	386.23
Reboiler Duty (W)	800781
SRD (MJ/kg CO <sub>2</sub> )	7.464





# 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





### Single Variable Sensitivity Study

### Run Simulation Ensemble – 1 process parameter changed at a time

Process Parameter	Range of Variation	Sampling	No of Points	Other input parameter values are the same as
CO <sub>2</sub> Lean Loading	0.1-0.3	LHS	20	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

Reboiler Duty vs. CO<sub>2</sub> 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



### Single Variable Sensitivity Study

### Run Simulation Ensemble – 1 process parameter changed at a time

Process Parameter	Range of Variation	Sampling	No of Points	Other input parameter values	
MEA Concentration	0.28-0.35	LHS	20	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

Reboiler Duty vs. 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





### 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 <sub>2</sub> Lean Loading	0.1–0.3
Stripper pressure (kPa)	180–200
Flue gas flowrate (kg/hr)	2000–3000
FG CO <sub>2</sub> concentration	0.17314–0.21

- Latin Hypercube Sampling
- Number of points:102

Data Visualization – 1 variable scatter plots







### Multi-variable Analysis

# Run Simulation Ensemble – 6 process parameters changed at a time

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Solvent Flowrate (kg/hr)	4500–7000
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FG CO <sub>2</sub> concentration	0.17314–0.21

- Latin Hypercube Sampling
- Number of points:102



Parameter Screening for CO<sub>2</sub> Capture %





### 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 <sub>2</sub> Lean Loading	0.1–0.3
Stripper pressure (kPa)	180–200
Flue gas flowrate (kg/hr)	2000–3000
FG CO <sub>2</sub> concentration	0.17314–0.21

- Latin Hypercube Sampling
- Number of points:102



Parameter Screening for Reboiler Duty



# **Surrogate Modeling**



## **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**



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

Surrogate Input Variables
Lean solvent flowrate (kg/hr)
MEA Concentration (wt frac)
CO <sub>2</sub> Lean Loading
Stripper Pressure (kPa)
Flue Gas (FG) Flowrate (kg/hr)
CO <sub>2</sub> conc in FG (wt frac)

### **Surrogate Output Variables**

CO<sub>2</sub> Capture Rate (%) Reboiler Duty (W)

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	

### **ALAMO Settings**

	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**



### h(x) represents Process Model:

- Mass, energy balances
- Stream connections
- Design specification (CO<sub>2</sub> Capture Rate = 90 %)

**Objective Function f(x):** SRD **Decision Variables (x):** CO<sub>2</sub> Lean Loading

Other Process Parameters – fixed at default values

DFO Solver: NLopt (default settings)

### **Result:**

### **Objective Function (SRD)\* = 3.465**

Process Parameter	Туре	Range of Variation	Initialization (default values)	Optimum Value
CO <sub>2</sub> 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: <u>https://github.com/CCSI-Toolset/SimSinter/releases/tag/3.0.0</u>



# 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<sub>2</sub> capture
- FOQUS capabilities are interconnected flexible to use
- Each capability provides valuable information enables decision making for the path forward



# **CCSI<sup>2</sup> Toolset Resources**

### CCSI<sup>2</sup> Additional Information

https://www.acceleratecarboncapture.org/

CCSI<sup>2</sup> 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



# **Acknowledgements**

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# Carbon Capture Simulation for Industry Impact

For more information <u>https://www.acceleratecarboncapture.org/</u>

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### Single Variable Sensitivity Study

### Run Simulation Ensemble – 1 process parameter changed at a time

Process Parameter	Range of Variation	Sampling	No of Points	Other input parameter values same as defaul
Stripper pressure	180-200	LHS	20	



CO<sub>2</sub> Capture Rate (%) vs. Stripper Pressure

**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

Reboiler Duty vs. Stripper Pressure



**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



### Single Variable Sensitivity Study

### Run Simulation Ensemble – 1 process parameter changed at a time

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

Reboiler duty vs. Lean solvent flowrate



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





### Single Variable Sensitivity Study

Run Simulation Ensemble – 1 process parameter changed at a time

Process Parameter	Range of Variation	Sampling	No of Points	Other input parameter values
Flue gas flowrate	2000-3000	LHS	20	same as default



CO<sub>2</sub> Capture Rate (%) vs. FG Flowrate

**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

Reboiler Duty vs. FG Flowrate



**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



### Single Variable Sensitivity Study

### Run Simulation Ensemble – 1 process parameter changed at a time

Process Parameter	Range of Variation	Sampling	No of Points	Other input
FG CO <sub>2</sub> concentration	0.17314-0.21	LHS	20	same as default



**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<sub>2</sub> 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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