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

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Presentation Outline

- Motivation – CCSI^2 Toolset Development and Implementation.
- Overview of FOQUS Software.
- Overview of FOQUS Capabilities.
- Software Management Strategy.
- CCSI^2 Toolset and FOQUS for Carbon Capture Applications.
  - Comprehensive analysis of CCS systems.
  - Point source capture economic optimization.
  - Industrial carbon capture (flue gas from cement plant).
  - Support to pilot-scale testing campaigns – maximize learning with targeted experiments.
- CCSI^2 Toolset Remarks.

Motivation – CCSI² Toolset

CCSI² main goal: To accelerate the scale-up and commercial deployment of carbon capture technologies for industries.

Path toward achieving it: Leverage a comprehensive suite of tools and models for thorough analysis, scale-up, and optimization of carbon capture systems.

CCSI² Modeling and Optimization Activities

- Economic optimization of carbon capture systems.
- Modeling of new materials and capture processes (solvents, sorbents, membranes, etc.).
- Process modeling and technoeconomic analysis of hybrid and flexible carbon capture systems.
- Pilot-scale capture systems testing.

Main Challenges

- Composite models may be required to represent the overall system.
- Complex models – simulations, optimization can take a long time to converge.
- Advanced capabilities are required for comprehensive pilot system testing – design of experiments.
- System variables indexed by space and/or time.

Solution

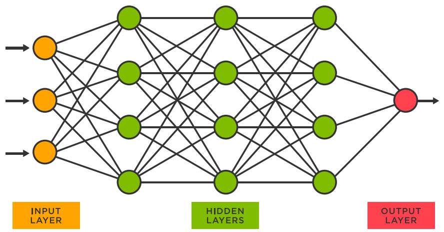
The **CCSI² toolset** contains different carbon capture models and **computational tools** capable of addressing these challenges.

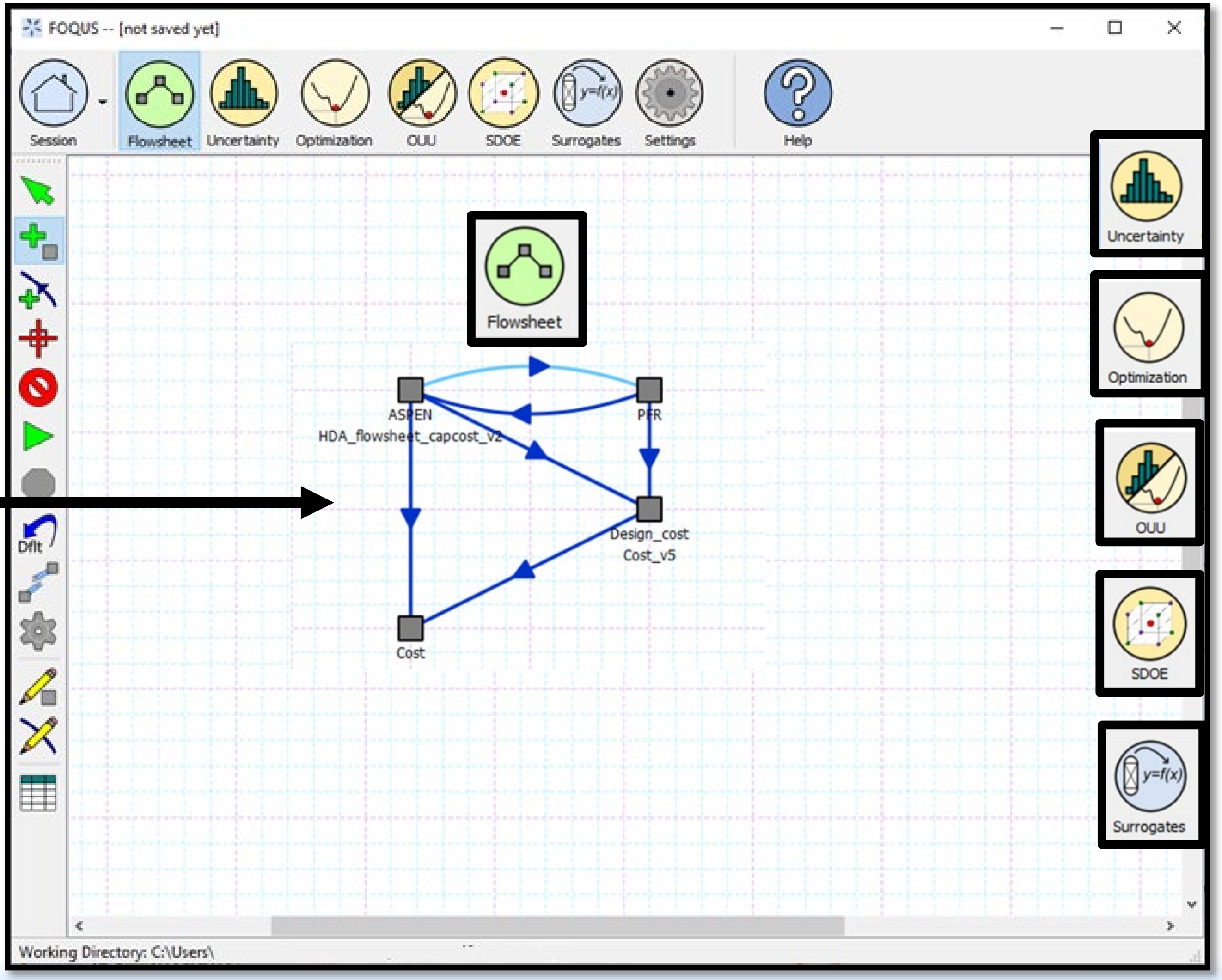
FOQUS is the central tool.

Overview of FOQUS Software

Core open-source computational tool within the CCSI-Toolset

Advanced Process Simulators and Modeling Environments





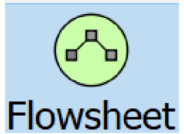
Comprehensive Analysis of Process Systems

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

Support development and deployment of carbon capture technologies.

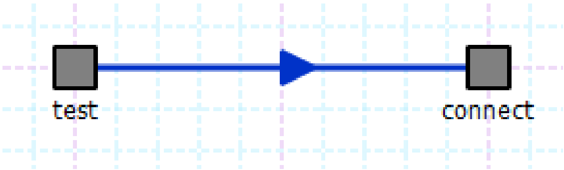
CCSI[2]
Carbon Capture Simulation for Industry Impact

Flowsheet



Features:

- Provides a platform to interface with, connect, and simulate different types of models (Python, Aspen, MATLAB etc.).



Nodes: Contain individual models.

Edges: Transfer variables between nodes.

Value:

- Ability to interface with:
  - Advanced process simulators (Aspen Plus, ACM, gPROMS).
  - Microsoft Excel spreadsheets.
  - Python and MATLAB models.
  - Machine Learning and Artificial Intelligence models (TensorFlow Keras, DeeperFluids).
- Ability to set up and simulate composite models.
- Foundation for implementing other FOQUS capabilities.

Uncertainty Quantification (UQ)

Features:

- **Automated Framework for Multiple Simulation Runs**

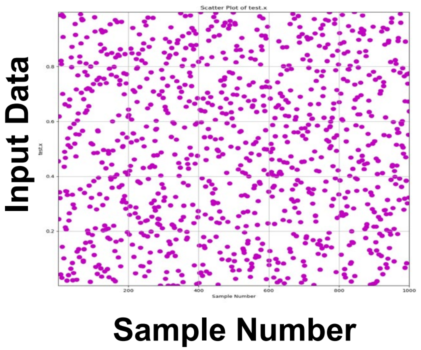
Uncertainty Quantification Simulation Ensembles

Add New... | Load from File... | Clone Selected | Delete Selected | Save Selected...

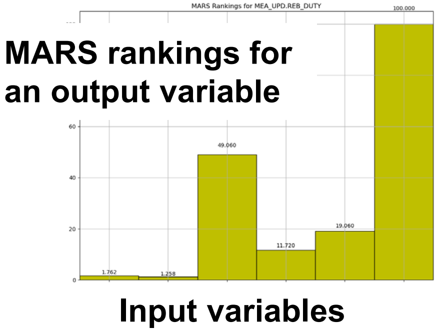
Ensemble	Run Status	Setup	Launch	Analyze	Descriptor	Turbine Session
1	1000 / 1000 # errors: 0	View	Sample Refinement	Analyze	UQ_Ensemble_0001	Local

- **Data Analysis and Stochastic Parameter Estimation**

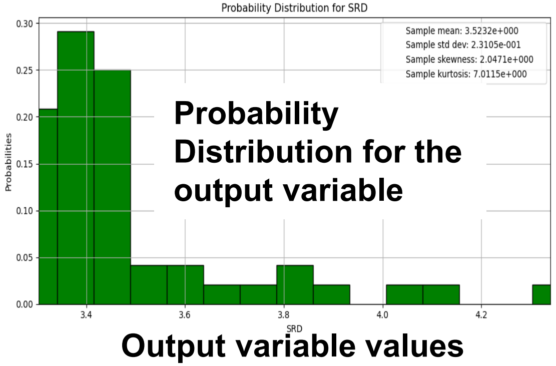
Visualization



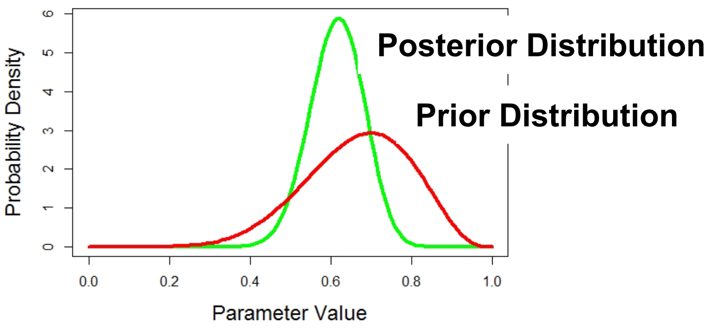
Parameter Screening



Uncertainty Analysis



Bayesian Inference



Value:

- Wide range of data analysis options—enables sensitivity analyses, quantification of model form, and parametric uncertainty.
- Bayesian inference—incorporates experimental data for reducing model parameter uncertainties.

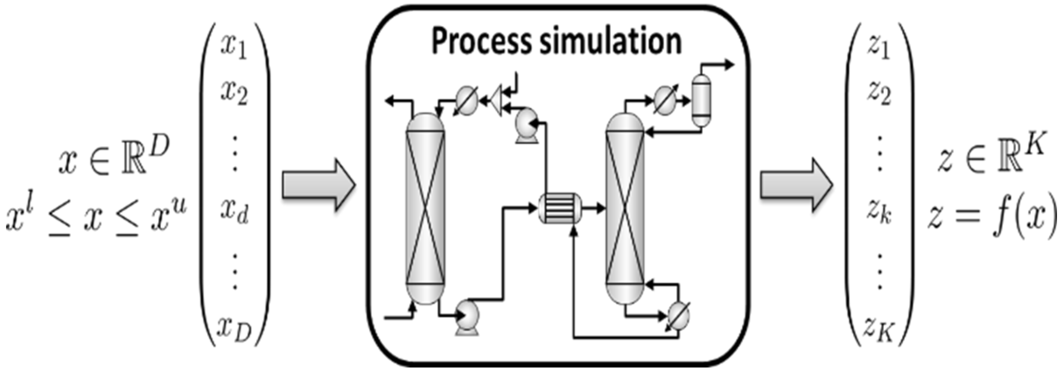
Surrogate Modeling

Features:

- Interfaces with external tools—ALAMO, ACOSSO, BSS-ANOVA—for surrogate model (SM) development.
- Training data, variables of interest, and methods for the SM can be selected by the user.

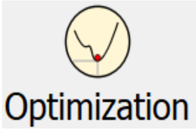
Value:

- Simplified representation of advanced simulator models saves simulation and optimization time.



- Surrogate model plugins are created for:
  - Validation against test data.
  - Implementation in flowsheet simulation.

Optimization



Features:

- Implementation of deterministic optimization based on the FOQUS flowsheet.

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

s.t.

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

$f(\tilde{x})$ is the objective function

$\tilde{x}$ is the set of decision variables.

$h(\tilde{x})$ denotes equality constraints (e.g., heat and material balance in process models).

$g(\tilde{x})$ denotes inequality constraints for key output variables.
(e.g., product quality, gas emissions, other performance indicators in process models).

- Provides an interface with derivative free optimizers (BFGS, NLOpt library, SnobFit, OptCMA, SLSQP).
- Includes a hybrid simulation-based and mathematical optimizer.
- Users can select decision variables and specify the objective function, inequality constraints, and solver.

Value:

- Flexibility to select from a wide range of optimizers depending on **model complexity** and **expected solution time**.

Optimization Under Uncertainty

OUU

Features:

- Stochastic single- and two-stage optimization formulations are supported.

Single stage (without recourse)

$$\min_{z1} \phi_{z3,z4} \, [F(z1, z3, z4)]$$

Two stage (with recourse)

$$\min_{z1,z3,z4} \phi_{z3,z4} \, [\min_{z2} \mathrm{F}(\mathrm{z1}, \mathrm{z2}, \mathrm{z3}, \mathrm{z4})]$$

z1: Set of design/decision variables.
z2: Set of recourse/operating variables.
z3: Set of discrete uncertain variables.
z4: Set of continuous uncertain variables.
F: Simulation Model.

Φ: Statistical metric for the objective function.

Value:

- Produces optimal solutions that **rigorously account for operation and epistemic uncertainty**.
- Gives a **realistic optimum point** for models containing high-effect uncertainties.

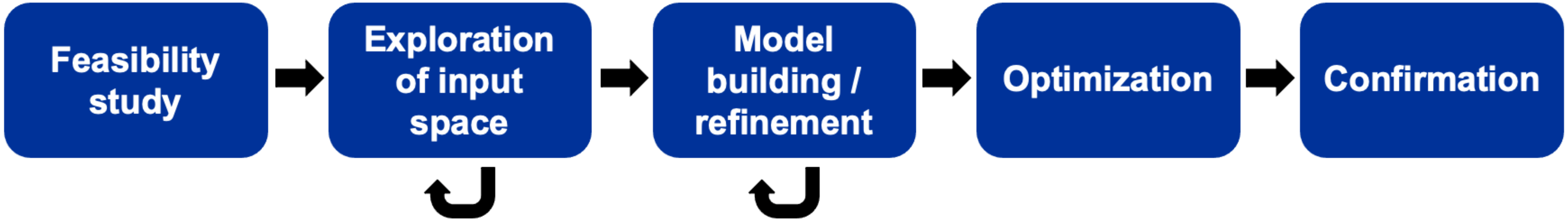
Sequential Design of Experiments

Features:

- Generates uniform, non-uniform, and input response space filling designs.
- Robust Optimality-Based Design of Experiments.
- Graphical tools for design evaluation and comparison.
- Design ordering algorithm.

Value:

- Maximizes learning through a systematic and concise set of experiments.
- Extracts maximum information in pilot testing with fixed budget of resources.
- Enables uncertainty reduction of process models through experimental data collection.
- Supports different data collection objectives.



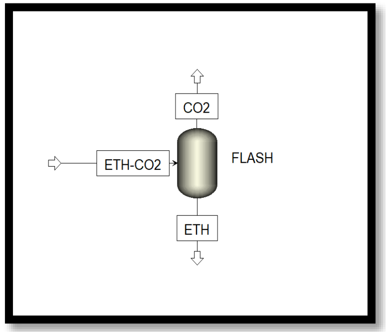
Cloud Computing in FOQUS

Amazon Web Services is used to run flowsheet simulations remotely.

Advantage:

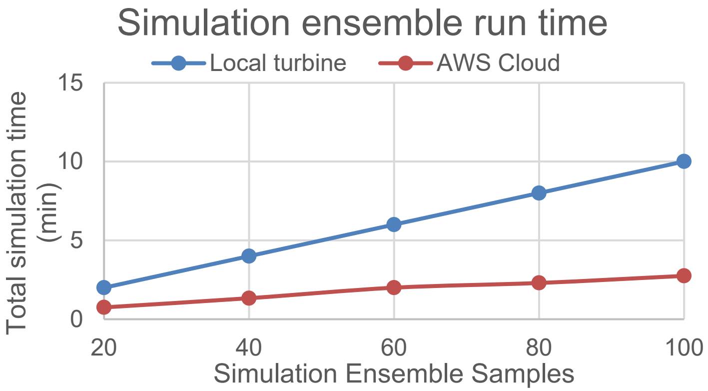
Saves time while running multiple simulations (UQ ensemble) and instances of optimization problems.

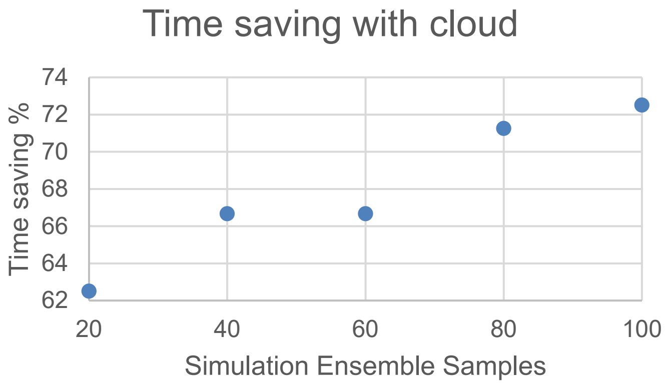
Solution time improvement analysis:



Ethanol - CO_2 Flash Unit Aspen

- Ethanol + CO_2 mixture (50 %)
- Inlet Flow = 100 kg/hr
- Inlet T, P = 25°C, 100 bar
- FLASH P= 1 to 10 bar
- UQ Ensemble = Latin Hypercube





Reference:

https://foqus.readthedocs.io/en/latest/chapt_flowsheet/tutorial/remote.html

Software Management Strategy

Base Code Maintenance and Release Management

- Open-source collaboration and contribution from different software developers.
- Rigorous use of software development tools (Git and GitHub).
- Continuous Integration: automated tests, coverage, static analysis, coding standards.
- Regular (quarterly) release schedule.

Communication, Feedback from Tech Team, Stakeholders, and Users

- Outreach and support of our users and stakeholders and understanding their requirements and expectations to drive fixes, improvements, and new capabilities.
- Annual stakeholder meetings: highlight new capabilities and applications.
- User experience: improving the FOQUS GUI usability via user case studies.

Applications of FOQUS in CCSI^2

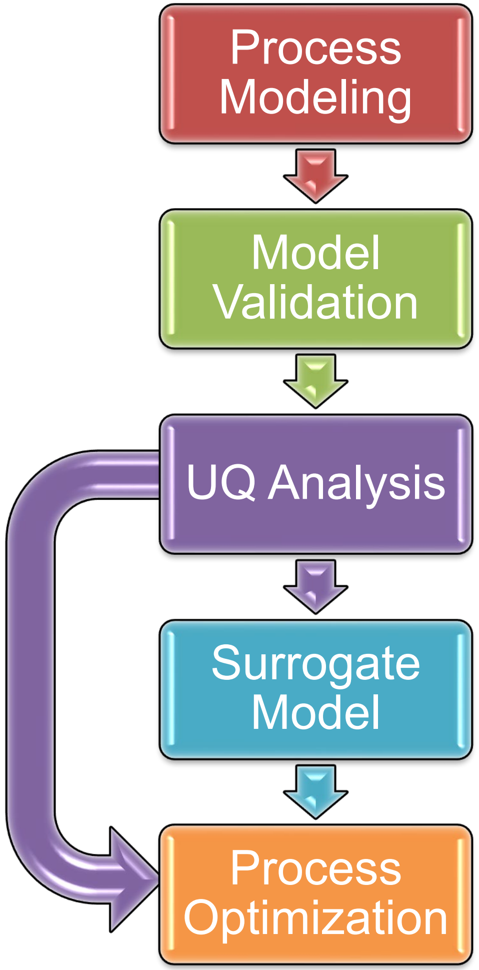
FOQUS – Central tool to support and implement various R&D projects.

- Comprehensive technical analysis and optimization of various carbon capture systems:
  - Solvent.
  - Sorbent.
  - Membrane.
  - Hybrid.

Discussed Further…

- Technoeconomic evaluation and optimization of integrated carbon capture systems:
  - Supercritical pulverized coal power plant (SCPC).
  - Natural gas-fired power plant (NGCC).
  - Cement production plant.
- Validation and improvement of carbon capture models based on pilot plant test campaigns.

Comprehensive Analysis of Carbon Capture Systems



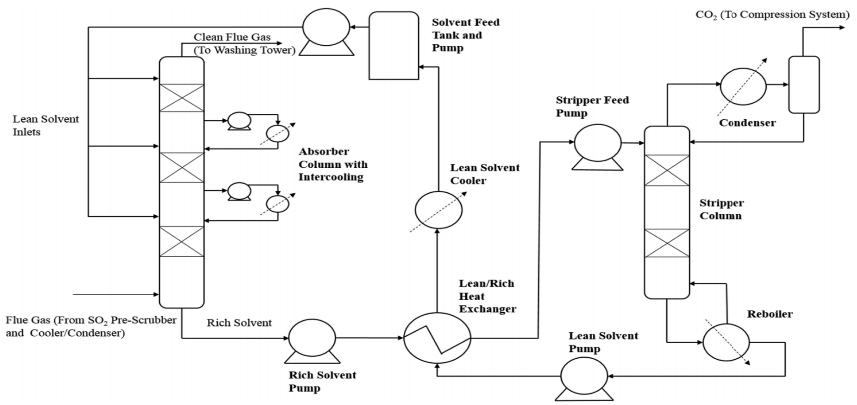


Figure: Schematic representation of the MEA carbon capture system.

Model Scale: ~ 0.5 Mwe.
Model Platform: Aspen Plus v10.
Property Method: ELECNRTL.
Input variables of interest:

1. CO_2 Lean Loading.
2. Lean Solvent Flowrate.
3. Monoethanolamine (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).

Work done:

- Set up the model in FOQUS flowsheet.
- Process model validation with National Carbon Capture Center (NCCC) pilot plant data.
- Parameter screening and sensitivity study.
- Process optimization for minimizing SRD at 90% CO_2 capture rate.

Accomplishments:

✓ The MEA carbon capture model was successfully validated with plant data.
✓ The cause-effect relationship between the input and output parameters was clearly established.
✓ The minimum value of SRD was found to be ~ 3.47 MJ/kg CO_2 at 90% CO_2 capture rate.

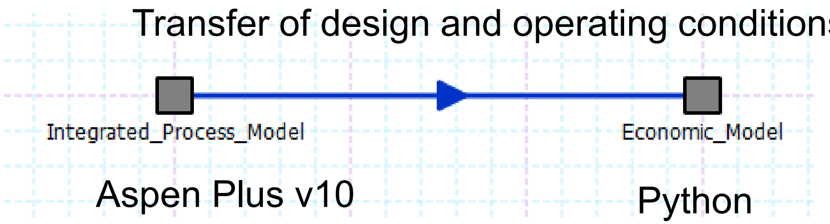
Figure adapted from: Development of a framework for sequential Bayesian design of experiments: Application to a pilot-scale solvent-based CO_2 capture process Morgan et al., *Appl. Energy*, 2020, 262, 114533

Point Source Capture Economic Optimization

Optimized an integrated natural gas combined cycle power plant with a solvent-based carbon capture system. Study performed for economic evaluation of a new solvent (EEMPA) developed by PNNL.

Work done:

- Set up the required model in FOQUS flowsheet.



- Simulation-based optimization using NLopt DFO solver.

$$\min_{\tilde{x}} f(\tilde{x})$$
$$\underline{\text{s.t.}}$$
$$\tilde{x}^L \leq \tilde{x} \leq \tilde{x}^U$$
$$h(\tilde{x}) = 0$$
$$g(\tilde{x}) \leq 0$$

$f(\tilde{x})$ is the Levelized Cost of Electricity (LCOE) in \$/MW-hr.

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

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

Accomplishments:

✓ Determined the minimum LCOE and optimum design of absorber and regenerator in the capture system.

Ongoing work: Process modeling and optimization improvements.

References for economic model:
[1] 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 improvements. Applied Energy 165: 648-659.
[2] 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

EEMPA: N-[2-ethoxyethyl]-3-morpholinopropan-1-amine

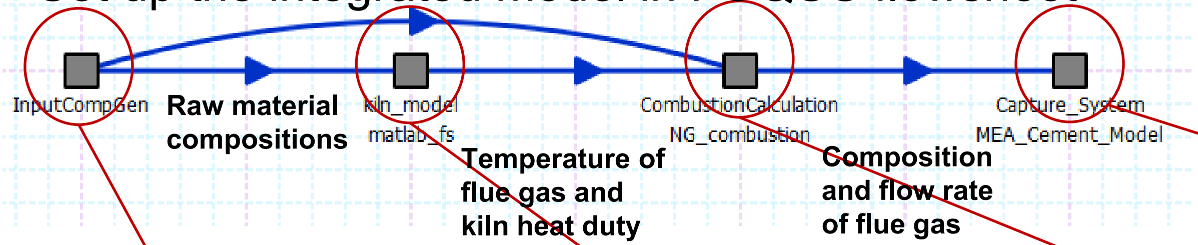
PNNL: Pacific Northwest National Laboratory

Analysis and Optimization of Industrial Capture Systems

Optimized integration of MEA solvent-based capture system with cement production plant.

Work done:

- Set up the integrated model in FOQUS flowsheet



Feed Compositions
Inputs: Cement raw material quality.
Output: Cement raw material composition.

MATLAB Model – Cement Kiln
Inputs: Cement raw material composition.
Output: Kiln heat duty and temperature.

Natural Gas Combustion Aspen Model
Inputs: Kiln heat duty and temperature, cement raw material composition.
Output: Flue gas flowrate and composition.

MEA Carbon Capture System Aspen Model
Inputs: Flue gas details, capture system design, operating conditions.
Output: Stripper reboiler duty.

- **UQ module:** Implemented parameter screening and sensitivity analysis of the model.
- **Optimization module:** Implemented process optimization to minimize specific reboiler duty associated with the capture system.

Accomplishments:

✓ Successfully demonstrated a detailed process analysis of the integrated model.
✓ Achieved a minimum specific reboiler duty in the range of 3.18 to 3.25 MJ/kg CO_2 at a 90% CO_2 capture rate.

CCSI²
Carbon Capture Simulation for Industry Impact

CCSI² Support to Pilot-Scale Testing Campaigns

Rigorous implementation of Sequential Design of Experiments

Source: NCCC

National Carbon Capture Center (NCCC)

0.5 MWe test facility
Wilsonville, Alabama

Collaborated with CCSI² on aqueous MEA test campaigns in 2014 and 2017.

Source: TCM

Technology Centre Mongstad (TCM)

12 MWe test facility
Mongstad, Norway

Collaborated with CCSI² on aqueous MEA test campaign in 2018.

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

Test Campaign Phases

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.
Phase 3 Determine input combinations to minimize the maximum model prediction variance in the design space.	Phases 4–5 Minimize solvent regeneration energy requirement.

Accomplishments

- ✓ Maximized learning from pilot plant testing within the allowable budget and schedule.
- ✓ Model was improved through the refinement of mass transfer and interfacial area parameters.
- ✓ Average reduction of ~ 58% in the uncertainty of CO_2 capture percentage predicted by the model.

CCSI² Toolset Remarks

- FOQUS facilitates interfacing with advanced process simulation platforms.
- Enables advanced analysis of complex carbon capture processes.
  - Uncertainty Quantification, Optimization, Optimization Under Uncertainty, Surrogate Modeling, and Sequential Design of Experiments.
- Demonstrates comprehensive analysis of carbon capture systems integrated with various point sources.
  - SCPC, NGCC power plants, and cement plant with carbon capture.
- Enables techno-economic analysis and evaluation of novel technologies and materials to accelerate technology commercialization.

Ongoing development work:

- Technical enhancements of the interface with machine learning and artificial intelligence models.
- Improvements to the cloud computing capability.
- Sequential Design of Experiments – new capabilities and enhancements.

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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CCSI²

Carbon Capture Simulation for Industry Impact

For more information

https://www.acceleratecarboncapture.org/

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