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

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Presentation Outline

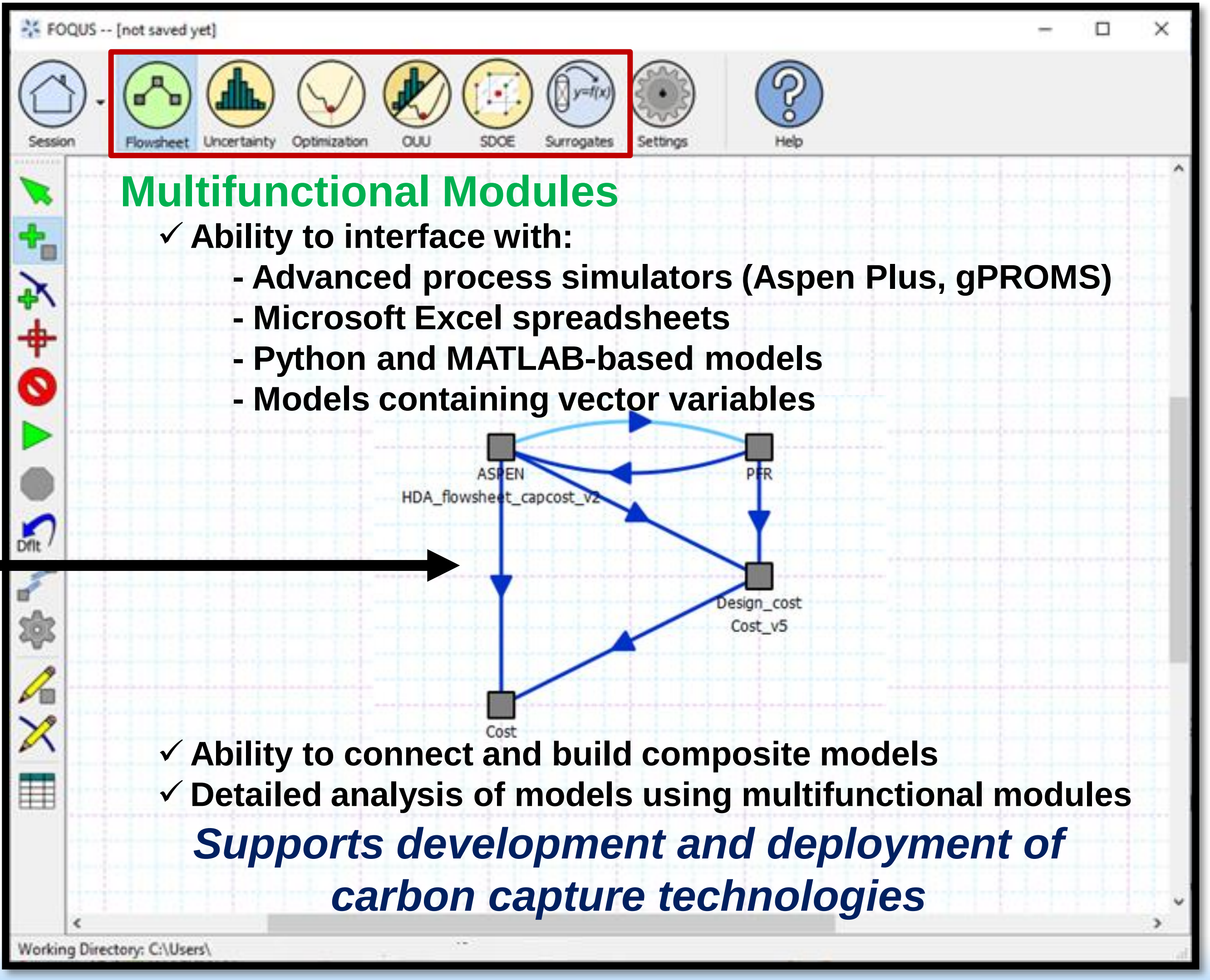
- Overview of FOQUS Software
- FOQUS Capabilities
- Applications of FOQUS in CCSI^2
  - SDoE Applied to Pilot-Scale Testing
  - Comprehensive Analysis: MEA Carbon Capture System
  - Economic Optimization of an Integrated Capture System
  - Analysis and Optimization of an Integrated Capture System
- Potential Support for Technology Commercialization
- Conclusion

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

Overview of FOQUS Software

Core open-source computational tool within the CCSI-Toolset

Advanced Process Simulators and Modeling Environments



Multifunctional Modules

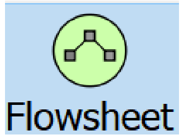
- ✓ **Ability to interface with:**
  - **- Advanced process simulators (Aspen Plus, gPROMS)**
  - **- Microsoft Excel spreadsheets**
  - **- Python and MATLAB-based models**
  - **- Models containing vector variables**
- ✓ **Ability to connect and build composite models**
- ✓ **Detailed analysis of models using multifunctional modules**

Supports development and deployment of carbon capture technologies

Comprehensive Analysis of Process Systems

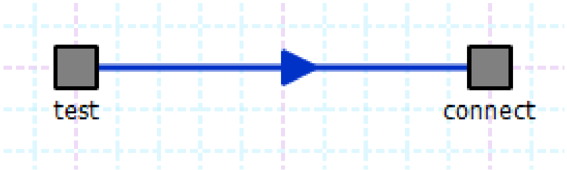
- Uncertainty Quantification
- Simulation-Based and Hybrid Optimization
- Surrogate Modeling
- Sequential Design of Experiments
- Optimization Under Uncertainty

Flowsheet



Features:

- Provides an interface for setting up and connecting models of interest



Nodes: Contain Individual Models

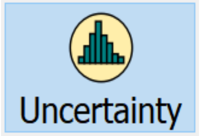
Edges: Transfer variables between nodes

- Nodes contain the required features for interfacing with the models
- **Single flowsheet simulations** can be implemented

Value:

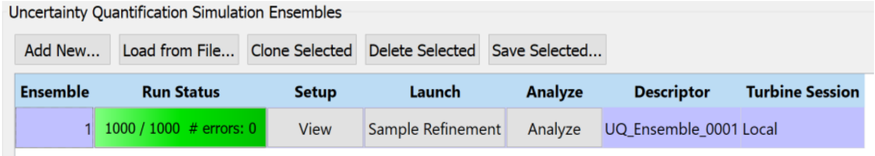
- Easy to interface and connect different types of models (Python, Aspen, etc.)
- Convenient to simulate the flowsheet for different sets of input variable values
- Flowsheet model—the foundation for implementing other FOQUS capabilities

Uncertainty Quantification



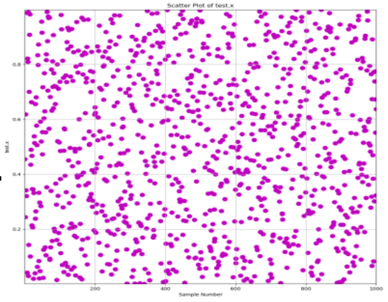
Features:

- Data Generation, Data Analysis, and Stochastic Parameter Estimation



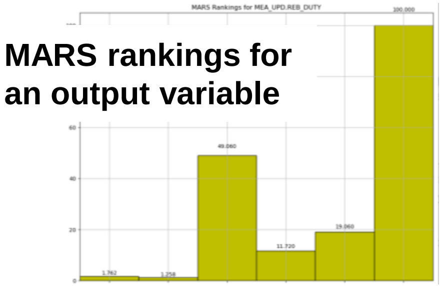
Visualization

Input Data



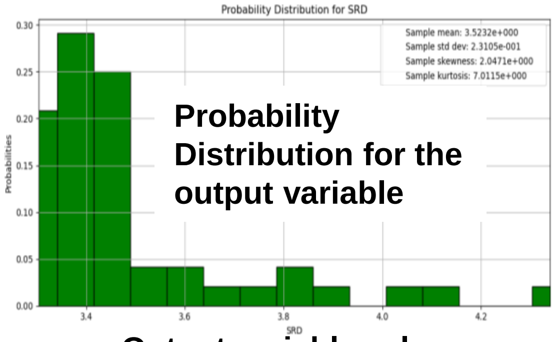
Sample Number

Parameter Screening



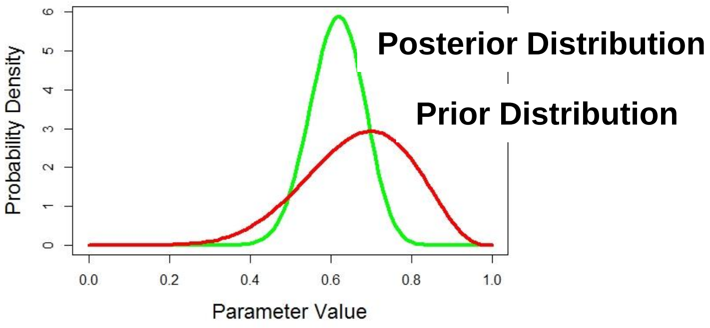
Input variables

Uncertainty Analysis



Output variable values

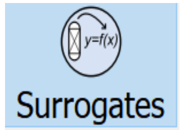
Bayesian Inference



Value:

- Automated framework for multiple simulation runs
- Wide range of data analysis options—helps in studying variability and uncertainty effects on the model
- Bayesian inference—incorporates experimental data for reducing model parameter uncertainties

Surrogate Modeling



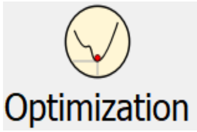
Features:

- Provides simplified representation of advanced simulator flowsheet models
- Interface with external tools for surrogate model development—ALAMO, ACOSSO, BSS-ANOVA
- Training data, variables of interest, and methods can be selected by the user

Value:

- Surrogate model plug-ins are developed for validation against test data and for implementation in flowsheet simulation
- Saves simulation time due to simplified model form
- Improves optimization time when used with the hybrid optimizer without compromising result accuracy

Optimization



Features:

- Provides the ability to set up deterministic optimization based on the flowsheet model
- Users can select decision variables, specify the objective function, constraints, and solver
- Provides an interface with derivative free optimizers (BFGS, NLOpt, SnobFit, OptCMA, SLSQP)
- Includes a hybrid simulation-based and mathematical optimizer

Value:

- Flexibility to modify the optimization problem as required
- Wide range of options to select the appropriate derivative free optimizer for the model of interest
- Flexibility to select simulation-based or hybrid optimization solvers depending on model complexity and allowable time expense

Optimization Under Uncertainty

Features:

- Stochastic 2-stage optimization
- Includes the contribution of parameter uncertainties in objective function

Value:

- Flexibility to modify the optimization problem in terms of parametric uncertainty
- Gives a realistic optimum point for models containing high-effect uncertainties

Sequential Design of Experiments

Features:

- Generate uniform and non-uniform space filling design
- Generate input response space filling design
- Design ordering

Value:

- Maximize learning through a systematic and concise set of experiments
- Reduce cost for pilot plant testing and model validation

Applications of FOQUS in $CCSI^2$

- Validation and improvement of carbon capture models based on pilot plant test campaigns

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

- Techno-economic evaluation and optimization of integrated carbon capture systems:
  - Supercritical pulverized coal power plant
  - Natural gas fired power plant
  - Cement production plant

SDoE Applied to Pilot-Scale Testing

Source: NCCC

National Carbon Capture Center (NCCC)

0.5 MWe test facility
Wilsonville, Alabama

Collaborated with CCSI[2] on aqueous monoethanolamine (MEA) test campaigns in 2014 and 2017

Source: TCM

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

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

Comprehensive Analysis: MEA Carbon Capture System

Process Modeling

Model Validation

UQ Analysis

Surrogate Model

Process Optimization

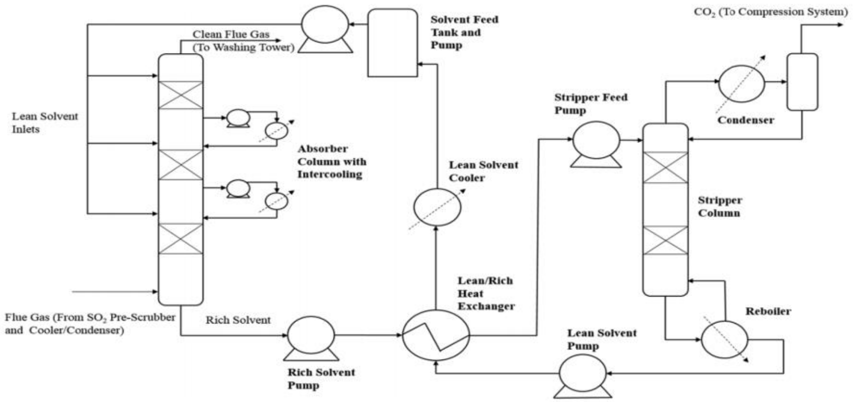


Figure: Schematic representation of the MEA carbon capture system

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. 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:

- Process model validation with 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

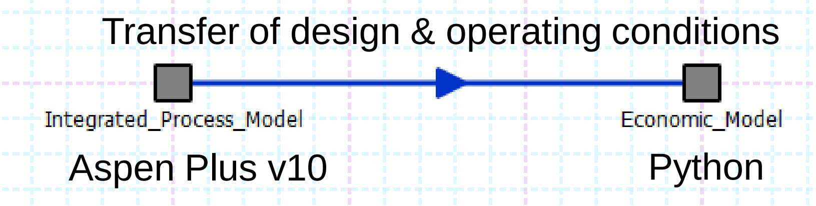
Figure adapted from: Development of a framework for sequential Bayesian design of experiments: Application to a pilot-scale solvent-based CO_2 capture process Morgan et al., *Appl. Energy*, 2020, 262, 114533

Economic Optimization of an Integrated Capture System

EEMPA solvent-based capture system connected with supercritical pulverized coal power plant

Work done:

- Set up the required model in FOQUS flowsheet



- Simulation-based optimization—Optimization module

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

$f(\tilde{x})$ is cost of CO_2 capture 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%

Accomplishments:

- ✓ Determined optimum design of absorber and regenerator in the capture system
- ✓ Minimum cost of CO_2 capture: 51.3 \$/ton CO_2
- ✓ Ongoing extension of this work with NGCC power plant

References for economic model:

[1] Systematic study of aqueous monoethanolamine (MEA)-based CO2 capture process: Techno-economic assessment of the MEA process and its improvements. Li et al. (2016), *Applied Energy*, 165: 648-659

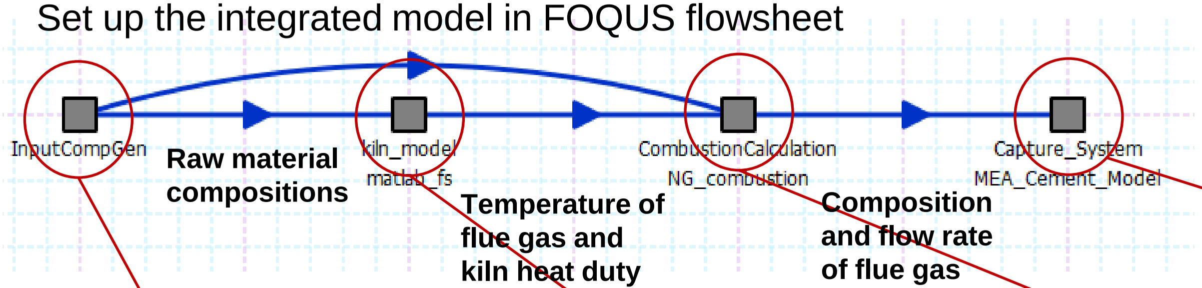
[2] NETL, Cost and Performance Baseline for Fossil Energy Plants Volume 1a: Bituminous Coal (PC) and Natural Gas to Electricity Revision 3, DOE/NETL-2015/1723

Analysis and Optimization of an Integrated Capture System

MEA solvent-based capture system connected with cement production plant

Workflow:

- 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 3.18–3.25 MJ/kg CO_2 at 90% CO_2 capture rate

Potential Support for Technology Commercialization

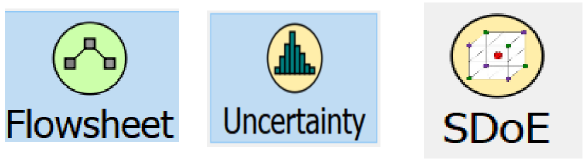
Transitioning a Technology From Concept to the Market

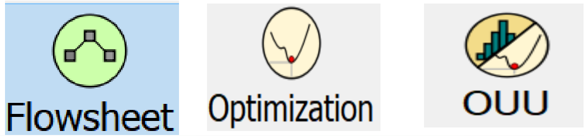
Key Aspects

- **Systematic, disciplined approach**
- **Effectiveness and reliability of the transition**
- **Good speed of transition**
- **Continuous improvement for sustaining the technology in the market**

These requirements can be mapped to the FOQUS capabilities

Process analysis and characterization	*Essential for scaling up the technology*	
Quantifying process uncertainties	*Essential for understanding the risks associated with uncertain parameters*	
Selecting the optimum process configuration		
Process optimization	*Essential for techno-economic analysis to determine commercial feasibility*	





Summary

- FOQUS facilitates interfacing with advanced process simulation platforms
  - Aspen Plus, Python, MATLAB, gPROMs, Excel
- Enables and simplifies advanced analysis of complex carbon capture processes
  - Uncertainty quantification, optimization, optimization under uncertainty, surrogate modeling
- Demonstrates comprehensive analysis of carbon capture systems integrated with point source
  - Supercritical pulverized coal, natural gas combined cycle power plant, and cement factory with carbon capture
- Provides meaningful insights into carbon capture technology development and deployment
- Enables analysis and evaluation of novel technologies and materials to accelerate technology commercialization

Future Work:

- Enable the connection with computational fluid dynamics software (e.g., COMSOL) and machine learning and artificial intelligence models

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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