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

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Presentation Outline

• Motivation – CCSI² Toolset Development and Implementation.
• Overview of FOQUS Software.
• Overview of FOQUS Capabilities.
• Software Management Strategy.
• CCSI² 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.
• CCSI² 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

- A+ PROMS
- IDAES
- PYOMO
- MATLAB

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

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

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• 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.
- 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.

\[
\begin{align*}
\min_{\bar{x}} \quad & f(\bar{x}) \\
\text{s.t.} \quad & \bar{x}^L \leq \bar{x} \leq \bar{x}^U \\
& h(\bar{x}) = 0 \\
& g(\bar{x}) \leq 0
\end{align*}
\]

- $f(\bar{x})$ is the objective function
- $\bar{x}^L$ and $\bar{x}^U$ are the lower and upper bounds of the decision variables, respectively.
- $h(\bar{x})$ denotes equality constraints (e.g., heat and material balance in process models).
- $g(\bar{x})$ 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.
Features:
• Stochastic single- and two-stage optimization formulations are supported.

Single stage (without recourse)
\[
\min_{z_1} \phi_{z_3, z_4} [F(z_1, z_3, z_4)]
\]

Two stage (with recourse)
\[
\min_{z_1, z_3, z_4} \phi_{z_3, z_4} [\min_{z_2} F(z_1, z_2, z_3, z_4)]
\]

- \(z_1\): Set of design/decision variables.
- \(z_2\): Set of recourse/operating variables.
- \(z_3\): Set of discrete uncertain variables.
- \(z_4\): Set of continuous uncertain variables.
- \(F\): Simulation Model.

\(\Phi\): 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.
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 + CO₂ 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:
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 CCSI²

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.

• 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.

Discussed Further…
Comprehensive Analysis of Carbon Capture Systems

Model Scale: ~ 0.5 Mwe.
Property Method: ELECNRTL.

Input variables of interest:
1. CO₂ Lean Loading.
2. Lean Solvent Flowrate.
3. Monoethanolamine (MEA) concentration in lean solvent.
4. Stripper pressure.
5. Flue gas flowrate.
6. Flue gas CO₂ concentration.

Output variables of interest:
1. CO₂ 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% CO₂ 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 CO₂ at 90% CO₂ capture rate.

Figure adapted from: Development of a framework for sequential Bayesian design of experiments: Application to a pilot-scale solvent-based CO₂ capture process Morgan et al., Appl. Energy, 2020, 262, 114533
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.

\[
\begin{align*}
\min_{\bar{x}} f(\bar{x}) \\
\text{s.t.} \\
\bar{x}_L &\leq \bar{x} \leq \bar{x}_U \\
h(\bar{x}) &= 0 \\
g(\bar{x}) &\leq 0
\end{align*}
\]

- \( f(\bar{x}) \) is the Levelized Cost of Electricity (LCOE) in $/MW-hr.
- \( h(\bar{x}) \) denotes constraints directly included in Aspen model.
- \( g(\bar{x}) \) 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.

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

**PNNL:** Pacific Northwest National Laboratory

References for economic model:
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 CO₂ at a 90% CO₂ capture rate.
National Carbon Capture Center (NCCC)

0.5 MWe test facility
Wilsonville, Alabama

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

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 CO₂ 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 CO₂ 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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