Framework for Optimization, Quantification of Uncertainty, and Surrogates, and CCSI² Toolset Capabilities

CCSI²
Carbon Capture Simulation for Industry Impact

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FOQUS Overview

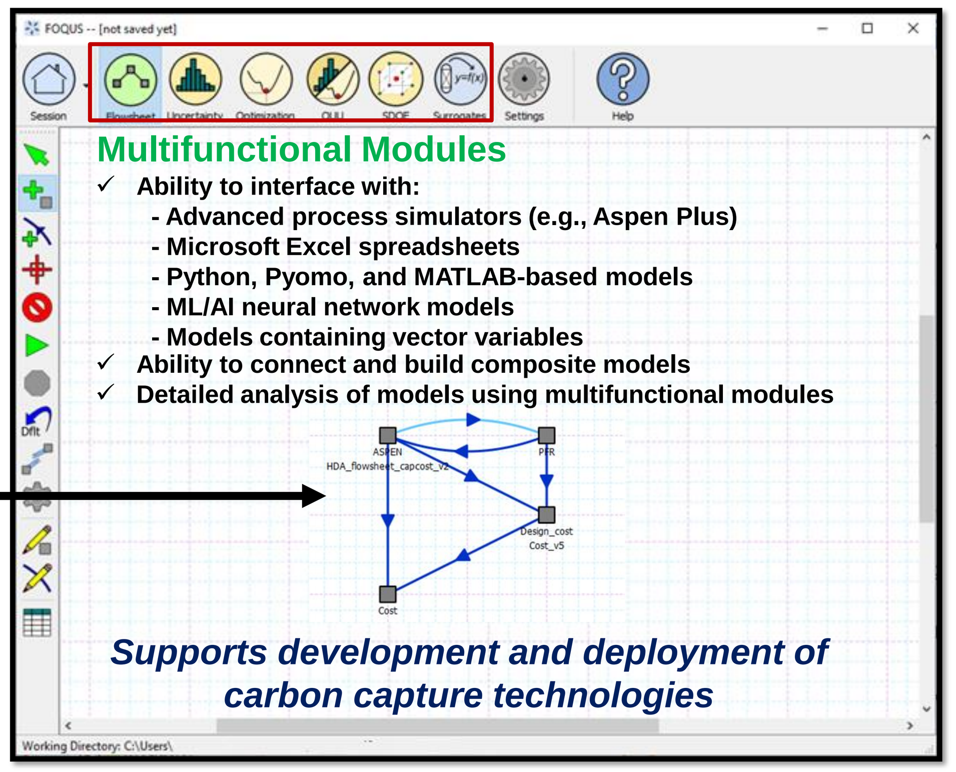
Value:

- Easy to interface and connect models developed in different platforms (Python, Aspen, etc.)
- Flowsheet model—the foundation for implementing other FOQUS capabilities
- Convenient to simulate the flowsheet for different sets of input variable values
- Regular development supports feature generation and addresses user feedback

Core open-source computational tool within the CCSI Toolset

Advanced Process Simulators and Modeling Environments

PYOMO IDAES



Comprehensive, Efficient Analysis of Process Systems

- Uncertainty quantification
- Simulation-based and hybrid optimization
- Surrogate modeling (ALAMO, ML/AI)
- Sequential design of experiments
- Optimization under uncertainty
- Cloud computing through Amazon Web Services

Machine Learning, Artificial Intelligence & Surrogate Modeling Plugins

Motivation:

- Develop a general plugin for importing ML-based surrogates into FOQUS
- Support externally-trained, multi-input/multi-output neural network models

Features:

- Imports user-trained models for execution, optimization, and analysis
- Supports TensorFlow Keras, PyTorch, Scikit-learn, Surrogate Modeling Toolbox
- Automatically loads models with custom neural network layers containing model variable labels and bound information
- Defines user normalization for more accurate neural network models, leveraging built-in linear, logarithmic, and power-scaling methods

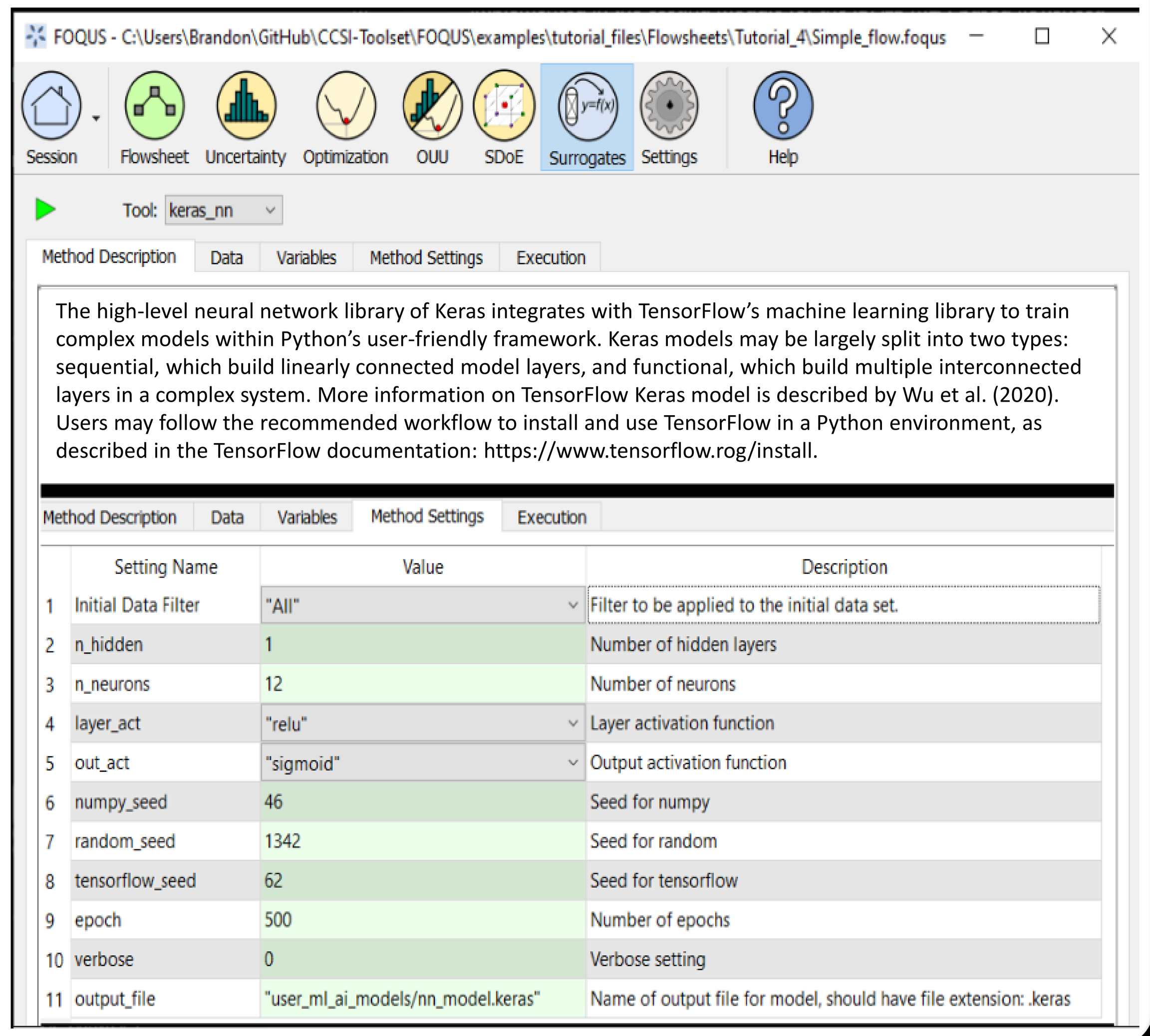
Final Trained ML Model → **FOQUS Base Code** (Access ML model and create flowsheet node plugin) → **FOQUS Node Editor Interface**

Motivation:

- Extend the existing Surrogates Toolbox to support training neural network models in FOQUS and automatically export generated user models

Features:

- Loads external datasets for neural network training and validation
- Supports TensorFlow Keras, PyTorch, and Scikit-learn, in addition to non-neural network surrogate training in ALAMO
- Enables users to set training parameters directly inside the FOQUS interface (network width, depth, activation functions, epochs)
- Has an execution window for training output and automatic user model export



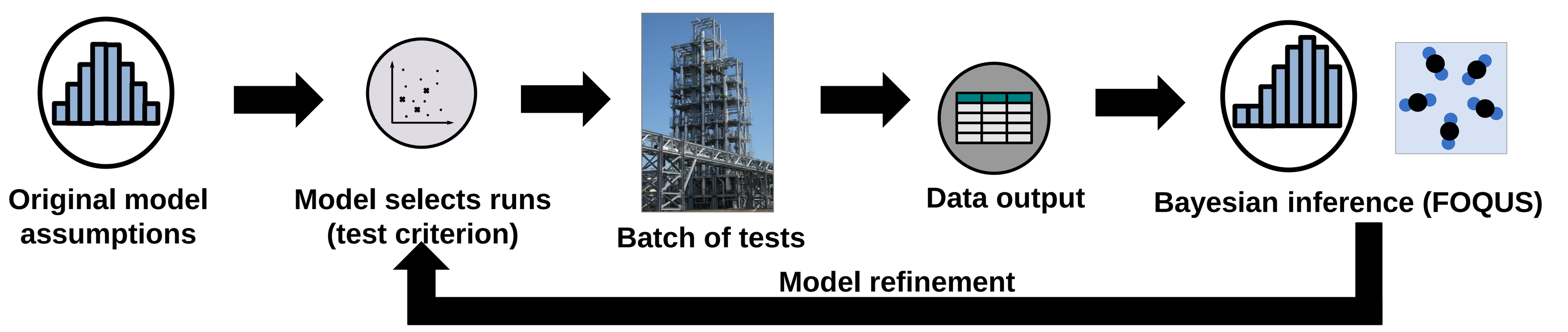
FOQUS Sequential Design of Experiments

Motivation:

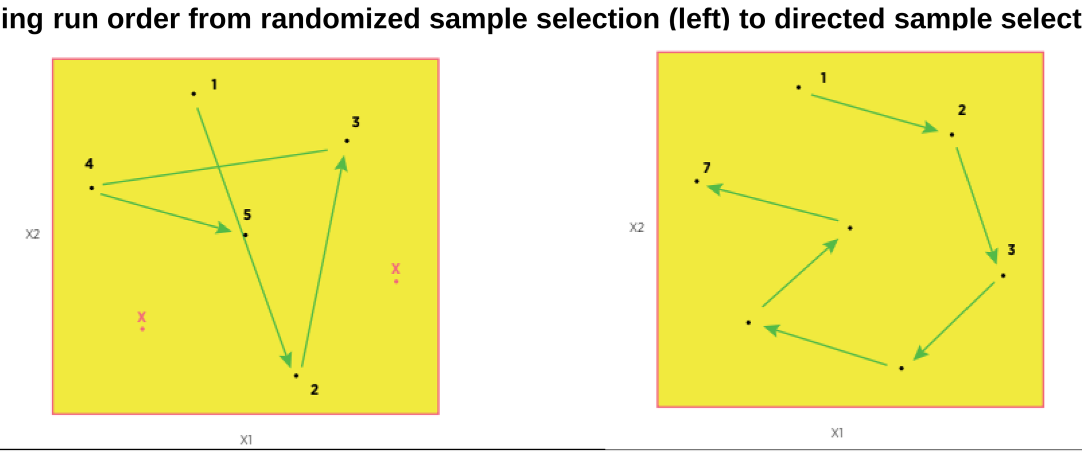
- Expand sequential design of experiments capabilities in FOQUS to support of ongoing pilot planning and testing, and incorporate science-based methodology

Features:

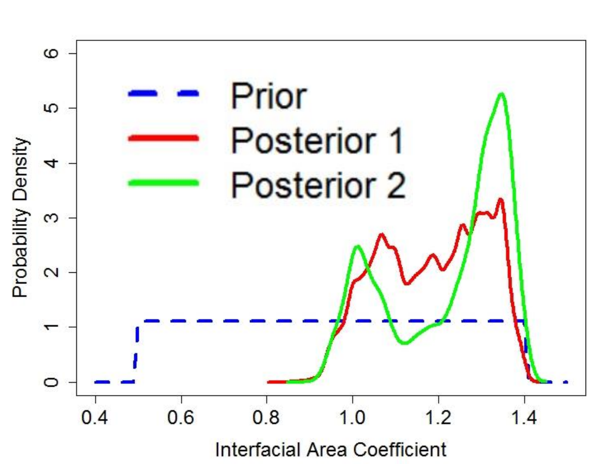
- Uniform space-filling (USF) parallelizes implementation, providing the same result as the original algorithm with a 2.5x runtime improvement across platforms
- Nonuniform space-filling (NUSF) parallelizes implementation, providing the same result as the original algorithm with a 3.5x runtime improvement on Windows
- New ordering capabilities incorporating hard-to-change factors into sample generation to improve performance and convergence

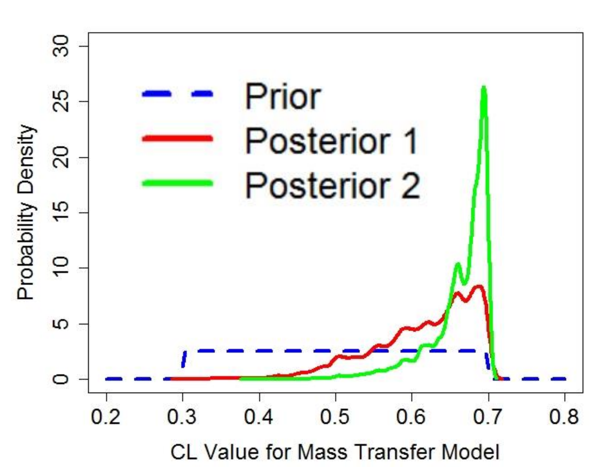


Optimizing run order from randomized sample selection (left) to directed sample selection (right)



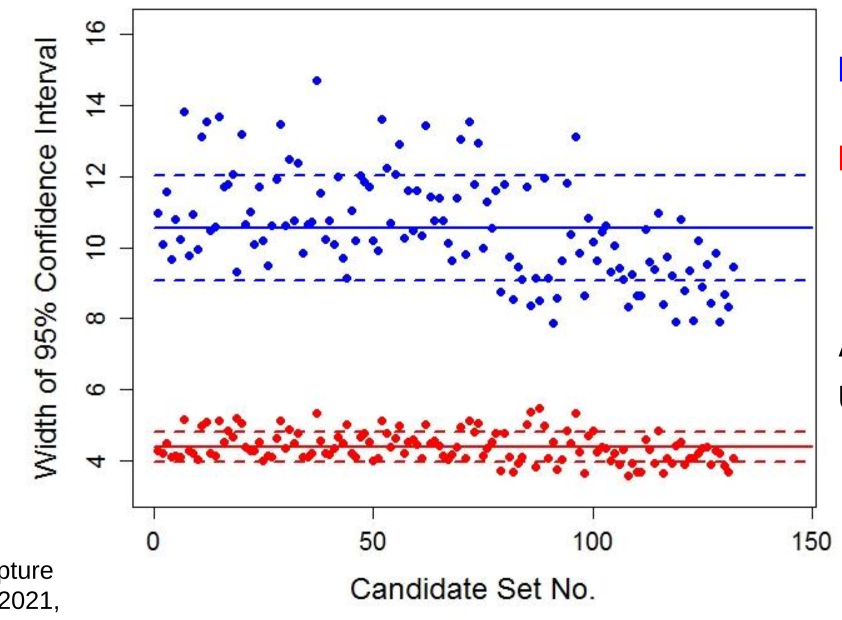
Example: Technology Centre Mongstad Pilot Model Improvements





Candidate set includes variation in:

- Solvent circulation rate
- Flue gas flowrate and CO_2 concentration
- Reboiler steam flowrate



Prior CI Width: (10.5 ± 1.5)%

Posterior CI Width: (4.4 ± 0.4)%

Average reduction in uncertainty: 58.0 ± 4.7%

Morgan, J., Omell, B., Matuszewski, M., Miller, D., et al. Application of Sequential Design of Experiments (SDoE) to Large Pilot-Scale Solvent-Based CO_2 Capture Process at Technology Centre Mongstad (TCM) (March 24, 2021). *Proceedings of the 15th Greenhouse Gas Control Technologies Conference* 15-18 March 2021, Available at SSRN: https://ssrn.com/abstract=3811695 or http://dx.doi.org/10.2139/ssrn.3811695

CCSI² Process Model Bundle

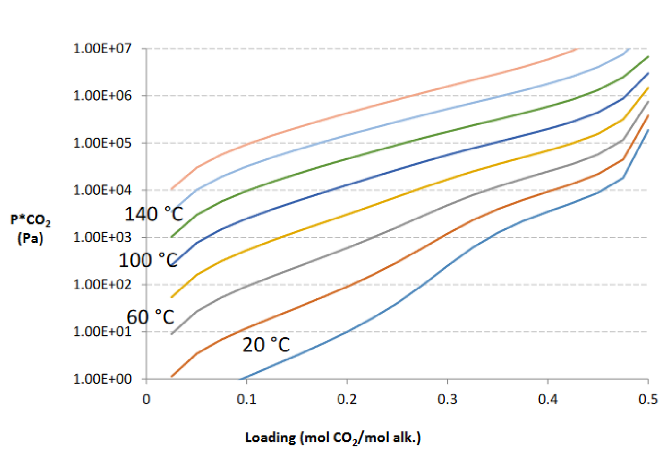
Motivation:

- Provide a suite of process models supporting detailed simulation for CO_2 capture systems

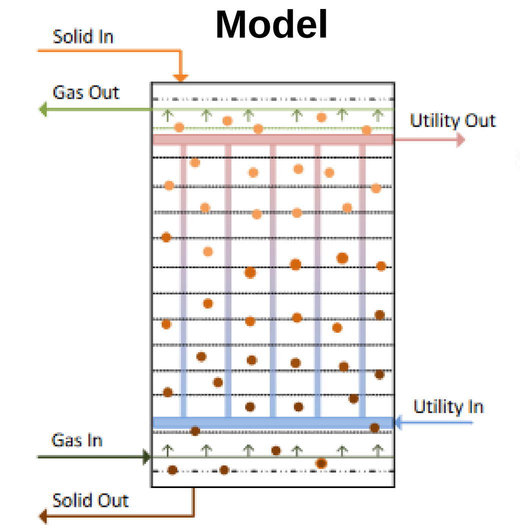
Subset of Available Models:

- Solvent Crossflow Heat Exchanger Calculator: Optimizes equipment sizing and log-mean temperature to minimize capital and operating expenses
- Bubbling Fluidized Bed Reactor, Moving Bed Reactor, and Membrane Separation Models: Process synthesis & design to facilitate rapid screening of new CO_2 capture concepts and technologies
- 2MPZ: Complex thermodynamics, techno-economic assessments, pilot plant data reconciliation, and process design uses 8 molal 2-methylpiperazine, an alternative solvent to monoethanolamine

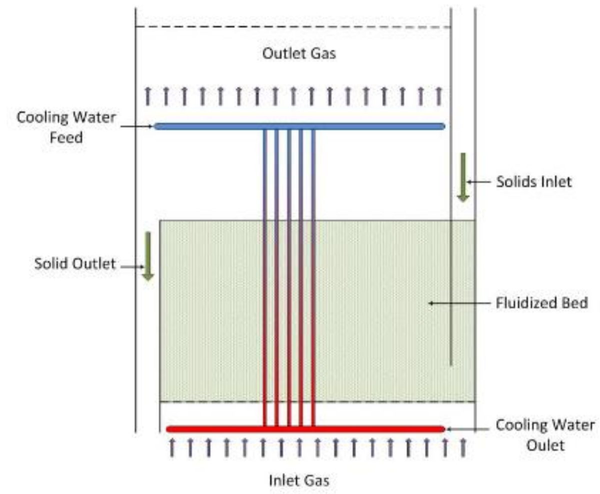
2MPZ Model, CO_2 Solubility Prediction



Moving Bed Model



Bubbling Fluidized Bed Model



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