Framework for Optimization, Quantification of Uncertainty, and Surrogates – Updated Capabilities

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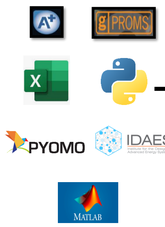
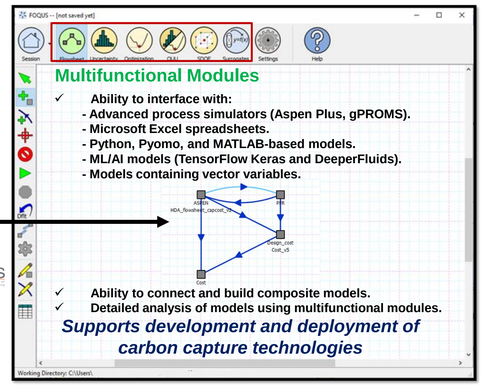
Overview of FOQUS Software

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.

Core open-source computational tool within the CCSI-Toolset

Advanced Process Simulators and Modeling Environments





Comprehensive, Efficient Analysis of Process Systems
- Uncertainty Quantification.
- Simulation-Based and Hybrid Optimization.
- Surrogate Modeling (primarily ALAMO).
- Sequential Design of Experiments.
- Optimization Under Uncertainty.
- Cloud computing through Amazon Web Services.

Machine Learning (ML) and Artificial Intelligence (AI) Plugin

Objectives:
- Developed a general FOQUS plugin for importing ML-based surrogates.
- Support Python-based Pymodel plug-ins (e.g., DeeperFluids or custom models) and integration with detailed process models (Aspen).

Features:
- Import user-trained TensorFlow Keras models into FOQUS for execution, optimization, and analysis.
- Automatically load models with custom neural network layers containing model variable labels and bound information.
- Define user-normalization for more accurate neural network models, leveraging built-in linear, logarithmic, and power scaling methods.

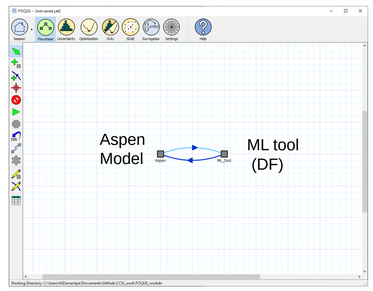
Final, trained, ML model (TensorFlow Keras) → **FOQUS Base Code** Access ML model and create flowsheet node plugin → **FOQUS Node Editor Interface**

Application: Interface Aspen Plus Solvent Column Model With Reduced Computational Fluid Dynamics Models With Novel Geometries (Deeper Fluids)

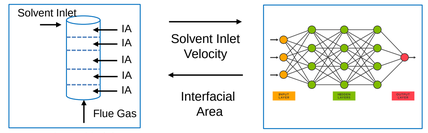
Objectives:
- Developed a FOQUS plugin for computational fluid dynamics PyTorch plugin developed by Lawrence Livermore National Laboratory.

Features:
- Builds surrogate model for MEA column system.
- Design inputs: packing type, column configuration.
- Operation inputs: solvent inlet velocity, solvent viscosity, solvent surface tension.
- Main output: gas-solvent interfacial area.

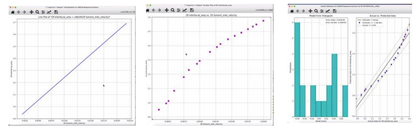
Define Node Class and Run Method



Connect Process and Surrogate Models



Results Analysis



FOQUS Support for Dynamic Process Models

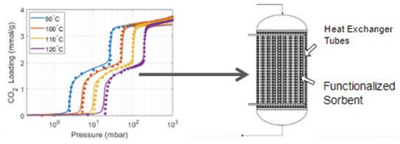
Vector Variable Support:
- Simulate and optimize models with process variables indexed over **space or time**.
- State variable/property profiles over a column.
- Vectorizing Python, MATLAB, SimSinter, and Aspen Custom Modeler models.
- Project applications:
  - RTI TCM Pilot Support.
  - Fluor Small Pilot Support.
  - Chevron Small Pilot/Advanced MOF.
  - TDA TCM Pilot.

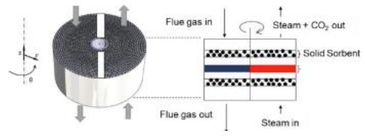
Support Metal-Organic Framework (MOF) Sorbent TEA Screening

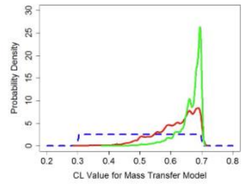
Objectives:
- Integration of dynamic process models into FOQUS for targeted carbon capture applications.
- Support for simulations leveraging kinetic, dynamic, and pseudo-steady-state scenarios.

Metal Organic Framework Fixed Bed:
- Isotherm, kinetic, process modeling and techno-economic analysis of fixed-bed MOF carbon capture systems—pilot support through model testing and analysis.
- Modeling for direct air capture and novel sorbent materials such as monolith and hollow fibers in carbon capture systems.

Process Model Development, Uncertainty Quantification, and Optimization







FOQUS-MATLAB Plugin

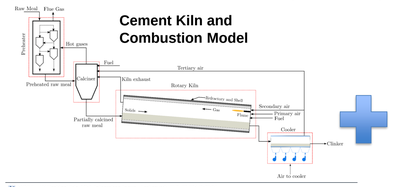
Objectives:
- Support simulation, detailed analysis of unit models developed in MATLAB.

Project Applications:
- Membrane Technology Research Membrane TCM Pilot.
- Absorber Intensification Modeling.
- Industrial Capture Modeling and Pilot Support.

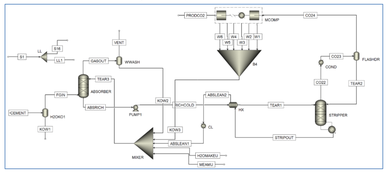
Features:
- Support the integration and use of MATLAB process models in FOQUS.
- Support the implementation of CFD simulations in FOQUS through COMSOL-MATLAB interface via LiveLink.
- Support detailed analysis of unit models developed in MATLAB as part of a larger manufacturing process (e.g., reactor or kiln).

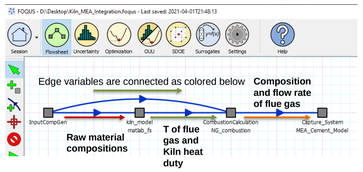
Application – Industrial Carbon Capture Analysis:

Cement Kiln and Combustion Model



Carbon Capture System (MEA based)





Cement-MEA Integrated Model:
- For a given cement quality, determined the optimized CO_2 composition to be approximately **17.7 mol%.**
- The optimized integrated model has **SRD** similar to the MEA standalone model, which is approximately **3.2 MJ/kg CO_2** captured.

Feed compositions node
Inputs:
- Lime saturation factor.
- Silica ratio.
- Alumina ratio.
- Limestone ratio.

Output:
- Mass fraction of $CaCO_3$, CaO, SiO_2, Al_2O_3, and Fe_2O_3.

MATLAB Kiln model node
Inputs:
- Mass compositions of raw materials
- Peak gas temperature.
- Location of peak gas temperature.
- Solid flow rate.
- Temperature of gas at inlet.

Output:
- Compositions of clinker.
- Emission of CO_2 from calcination reaction.
- Heat required by kiln.

Combustion Aspen model node
Inputs:
- Temperature of flue gas.
- Heat duty (heat required by the kiln for clinker production).
- Limestone ratio.

Output:
- Flue gas flow rate.
- Mole composition of flue gas.
- Flow rate of required fuel.

MEA Aspen model node
Inputs:
- Flue gas flow rate.
- Mole composition of flue gas.
- Absorber packing height.
- Stripper packing height.
- Lean loading.
- Heat exchange pinch point.

Output:
- Stripper reboiler duty.
- Other.

FOQUS Interface To AWS For Cloud Optimization

Objectives:
- Run multiple simulations or ensembles via remote turbine and Amazon Web Services (AWS).
- Reduce time required to solve complex flowsheets.

Features:
- Saves time running multiple simulations (e.g., Uncertainty Quantification, optimization).
- Ability to scale up hundreds of compute nodes for cloud storage.

Application 1: NGCC-EEMPA Economic Optimization
- Minimize overall levelized cost of electricity.

Variables included in $\tilde{x}$

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

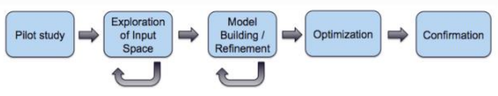
$f(\tilde{x})$: levelized cost of electricity
$h(\tilde{x})$: constraints in Aspen model
$g(\tilde{x})$: 80% maximum allowable flooding in columns

Variable	Initial Value	Minimum	Maximum
Absorber Packing Height (m)	21.6	12.0	25.0
Absorber Diameter (m)	12.6	9.0	16.0
Stripper Packing Height (m)	12.2	8.0	25.0
Stripper Diameter (m)	3.7	2.0	14.0
Lean Solvent Loading (mol CO_2/mol EEMPA)	0.08	0	0.1
Rich Solvent Temperature Exit from Lean/Rich Heat Exchanger (ºC)	87.5	37.0	94.0

Solver: CMA-ES (derivative free optimizer)
LCOE = 74 $/MW-hr
(24 simulations, 4 iterations)

Turbine Option	Solution Time
Local	~ 3 hrs
FOQUS Cloud	~ 1 hr (expected)

Application 2: Parallelized Sequential Design of Experiments:
- Faster design construction from simultaneous search.
- Allows for fewer constraints on candidate set size.



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