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A framework for optimization and quantification of uncertainty and sensitivity for developing carbon capture systems

John C. Eslick,[a,b] Brenda Ng,[c] Qianwen Gao,[a] Charles H. Tong,[c] Nikolaos V. Sahinidis,[b] David C. Miller[a,]*

[a]*National Energy Technology Laboratory, Pittsburgh, PA USA*
[b]*Carnegie Mellon University, Pittsburgh, PA USA*
[c]*Lawrence Livermore National Laboratory, Livermore, CA USA*

Abstract

Under the auspices of the U.S. Department of Energy's Carbon Capture Simulation Initiative (CCSI), a Framework for Optimization and Quantification of Uncertainty and Sensitivity (FOQUS) has been developed. This tool enables carbon capture systems to be rapidly synthesized and rigorously optimized, in an environment that accounts for and propagates uncertainties in parameters and models. FOQUS currently enables (1) the development of surrogate algebraic models utilizing the ALAMO algorithm, which can be used for superstructure optimization to identify optimal process configurations, (2) simulation-based optimization utilizing derivative free optimization (DFO) algorithms with detailed black-box process models, and (3) rigorous uncertainty quantification through PSUADE. FOQUS utilizes another CCSI technology, the Turbine Science Gateway, to manage the thousands of simulated runs necessary for optimization and UQ. This computational framework has been demonstrated for the design and analysis of a solid sorbent based carbon capture system.

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Keywords: Optimization; Uncertainty Quantification; Simulation; Surrogate Model; Carbon Capture

* Corresponding author. Tel.: +1-412-386-6555
E-mail address: david.miller@netl.doe.gov

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1. Introduction

The U.S. Department of Energy initiated the Carbon Capture Simulation Initiative (CCSI) to develop computational tools and models to accelerate the development and scale up of carbon capture technologies by (1) enabling promising concepts to be more quickly identified through rapid computational screening of processes and devices, (2) reducing the time to design and troubleshoot new devices and processes by using optimization techniques to focus development on the best overall process conditions and by using detailed equipment models to better understand and improve the internal behavior of complex equipment, and (3) quantifying the technical risk in taking technology from laboratory-scale to commercial-scale by understanding the sources and effects of model and parameter uncertainty [1]. To support the objectives of CCSI, the Framework for Optimization, Quantification of Uncertainty and Sensitivity (FOQUS) was developed to enable the required large-scale process optimization and rigorous uncertainty quantification (UQ) of detailed models within process simulators [2].

In order to effectively evaluate new concepts and materials for carbon capture, it is essential that the comparison be made in the context of a complete process that has been rigorously optimized. In addition, the underlying models and costing methodologies must be based on a common set of assumptions. Finally, the uncertainty associated with these model predictions must be accurately quantified in order to know whether a potential technology is truly superior to another. If the uncertainty is too large, identifying the sources of uncertainty can allow additional data collection to improve the model and increase confidence in order to enable effective decision making. This paper describes how FOQUS supports the design, optimization, and uncertainty quantification of carbon capture processes.

2. Framework for Optimization, Quantification of Uncertainty and Sensitivity

2.1. FOQUS structure

FOQUS consists of several parts: a meta-flowsheet to connect models and external simulation software to the framework, the ALAMO code to generate algebraic surrogate models, a simulation-based optimization tool to perform derivative-free optimization (DFO) of interconnected high fidelity process models, and the PSUADE UQ engine. The structure of FOQUS is shown in Fig. 1, where the FOQUS Engine manages information and data flow among the components.

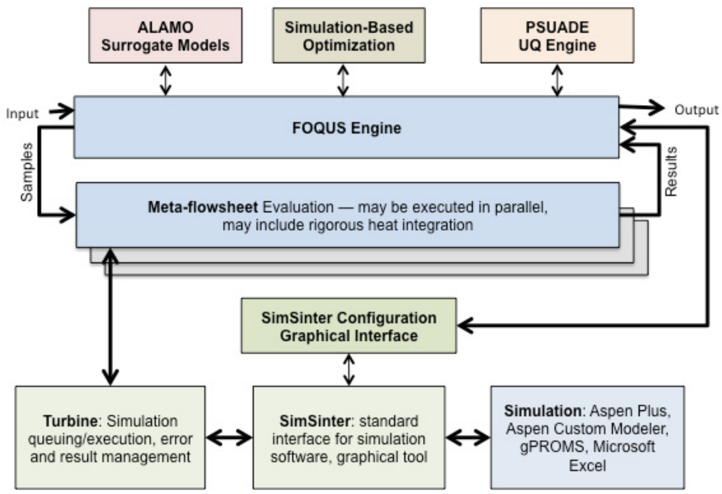

Fig. 1: Structure of the parts of FOQUS

The meta-flowsheet portion of FOQUS allows process models created in different software packages to be connected to each other. In a large project, models are typically developed by different authors using specialized simulation packages. Combining these models into a single, comprehensive simulation of a full process can be challenging. Often different software may be particularly well suited to different types of processes; for example, a commercial, general purpose chemical process simulation package may be best for modeling a carbon capture process, but more specialized software may be more appropriate for modeling the power plant. FOQUS allows these different types of models to be linked together. Fig. 2 shows an example of two nodes in the FOQUS flowsheet editor linking a bubbling fluidized bed (BFB) model with a model to estimate the capital and operating costs.

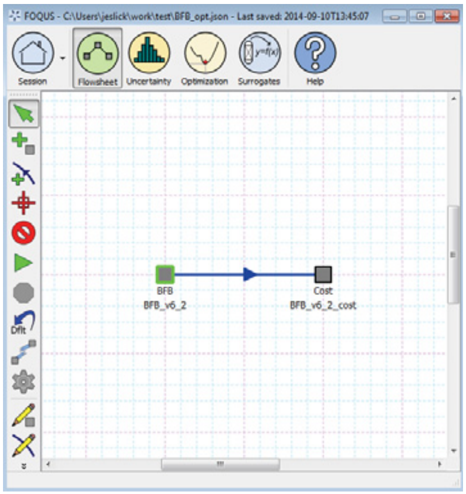

Fig. 2: FOQUS Meta-Flowsheet Editor

The meta-flowsheet in FOQUS provides greater ability to use common models in the analysis of different technologies, by making it easier to reuse smaller models. The FOQUS graphical user interface (GUI) makes linking small models to create an overall process model a relatively simple task. The meta-flowsheet supports recycle loops among nodes. These are solved by an iterative sequential modular method. SimSinter provides standard .NET programming interfaces to several simulation packages including Aspen Plus, Aspen Custom Modeler, gPROMS, and Excel. Support for new modeling packages can be added by writing a backend interface for SimSinter. SimSinter also allows the inputs, outputs, and settings for a simulation to be defined in a format common to all supported software via the SimSinter configuration GUI.

The Turbine Science Gateway handles the logistics of launching and running the thousands of simulations required for generating surrogate models, optimization and uncertainty quantification [3]. Turbine works on workstations, clusters, and cloud computing. With sufficient licenses and computing resources, thousands of simulations can be run in parallel, significantly reducing the time required for simulation-based optimization and UQ analysis.

FOQUS provides a standard way for several components to interface with process models. ALAMO builds simple algebraic surrogate models well suited for rigorous superstructure optimization [4] from the more detailed, high fidelity process models connected to the framework. A simulation based optimization tool is available, which uses derivative free optimization (DFO) methods with black box models. FOQUS has a system for DFO plug-ins allowing easy addition of various DFO methods. Uncertainty Quantification (UQ) is performed using the PSUADE software [5]. The UQ portion of FOQUS allows for sampling, sensitivity analysis, and propagation of uncertainty through the system being studied. Each of the tools will be described in detail in the next sections.

2.2. Surrogate models for superstructure optimization

The first step in developing an optimal process is to determine the process configuration, i.e., the selection of specific unit operations and their interconnections. A widely used approach is superstructure-based optimization. Following the determination of a process configuration, further process optimization and quantification of uncertainty occur utilizing rigorous process models such as those developed for bubbling fluidized bed (BFB) reactors [6].

Novel equipment models were developed, as part of the CCSI project, for the solid sorbent capture system [6-10]. Once these equipment models are available, the next step is design of the complete capture process. An important part of this process design is superstructure optimization. Superstructure optimization characterizes structural alternatives for a process that achieves certain task. The process will combine mass and heat exchange units that can be arranged in different configurations. A designer is particularly interested in identifying a configuration that minimizes a cost function which balances capital and operating costs. A systematic approach is taken to this design problem by using binary variables to model the presence of different capture and heat exchange units in a flowsheet. Different operating conditions are evaluated by their energy and capital requirements. For this project, the superstructure optimization problem is setup and solved using GAMS. GAMS (General Algebraic Modeling System) is a modeling language designed to facilitate setting up large optimization problems and has numerous advanced optimization solvers [11]. Due to the large number of integer and continuous variables required for superstructure optimization, it cannot be done directly with process models. Relatively simple algebraic surrogate models are required.

ALAMO is a tool available through the FOQUS interface that allows creation of the simplified algebraic surrogate models [4]. These surrogate models are combined into an algebraic mixed-integer nonlinear optimization model that is solved to provide an optimal equipment configuration, along with optimal operating conditions. The ALAMO tool in FOQUS can generate algebraic surrogate models for any FOQUS meta-flowsheet. ALAMO starts by compiling a large set of potential basis functions that may be used to construct the surrogates. ALAMO then relies on Bayes information criterion (and other similar subset selection metrics) in order to determine a subset of basis functions and corresponding regression coefficients that best fit the model without overfitting. A regularization step reduces the number of potential basis functions and increases the likelihood of successful completion of modern integer programming algorithms for subset selection. Once an initial dataset has been used to identify a promising surrogate model, ALAMO uses DFO methods to find areas of the parameter space with the largest model mismatch in order to guide additional sample generation. This adaptive sampling procedure provides model validation and dynamic design of experiments that maximize the amount of information gained from a small number of simulated points. As a result, ALAMO is able to generate simple models that are accurate over a specified range of problem variables. FOQUS's ability to evaluate samples in parallel can greatly accelerate the process of sample simulation for surrogate model development. Once the algebraic models have been generated, the superstructure optimization [7] problem can be formulated, which enables an algorithmic approach for determining an optimal process configuration, i.e., the selection of specific unit operations and their interconnections.

2.3. Simulation-based optimization

While the use of surrogate models facilitates large-scale, superstructure optimization to determine the best process configuration, once the structure is determined, simulation-based optimization, which works directly with the high-fidelity process models, is useful to verify and further refine the resulting process. Because accurate derivatives are usually not available for complicated process models, DFO methods are employed [12, 13]. Current DFO methods typically are best suited to problems having less than 30 decision variables [13]. For larger numbers of variables, surrogate models may be required.

FOQUS includes a plug-in system for DFO solvers. This makes it relatively easy to implement new DFO solvers. FOQUS handles inequality constraints by applying a penalty for constraint violations to the objective function. Input variables are automatically scaled by FOQUS so the DFO solvers see all the variables ranging from 0 at their minimum to 10 at their maximum; this accounts for large variations in the magnitudes of decision variables.

Variables can be scaled by several methods depending on what is most appropriate for the problem. The DFO plug-in provides samples to the FOQUS engine, which are run by Turbine.

Many DFO methods are readily able to make use of parallel sample evaluation. Since process models often take minutes to evaluate, simulation based optimization problems run in FOQUS can take several days to finish when samples are run in series. Parallel computing can significantly reduce the amount of time required. FOQUS can also save the state of the optimization, and it can be restarted if execution stops for any reason. Currently, a DFO plug-in is available based on CMA-ES [3] that supports parallel computing and restart. This plug-in has been tested with carbon capture system models for amine-based solvents and solid sorbents.

Fig. 3 shows the optimization problem setup dialog. There are three sections. The first section shows the inputs for the FOQUS flowsheet that are not set by connections to other variables. The checkboxes indicate whether the variables are to be included as decision variables in the optimization problem. The scale column shows the scaling method used to scale the variables. All decision variables must be scaled so that they range between 0 and 10. The min and max columns set the bounds on variables, while the value column provides the initial guess. The next section defines the objective function. Multiple objective functions can be defined for use with multi-objective optimization methods. For single objective methods, only the first is used. The objective is defined as a Python expression using the input and output variables defined in the previous section. The penalty scale is a multiplier for constraint violation. This is useful for multi-objective optimization where different objective functions may have different magnitudes. The last column is a value to assign to the objective function if a simulation fails to converge. This value should be worse than any expected valid objective function value and is used to discourage the optimization algorithm from looking in regions of the search space where the simulation fails. The last section defines the set of inequality constraints in the same format as the objective function. The constraint expression (g(x)) should be less than or equal to zero when the constraint is not violated and positive for a constraint violation. The penalty factor sets the magnitude of the penalty that is added to the objective function for constraint violations. The penalty form sets the method of calculating the penalty for a constraint. The penalty is 0 if $g(x) \leq 0$. If g(x) is positive, the penalty is calculated by one of three functions: linear, quadratic or step.

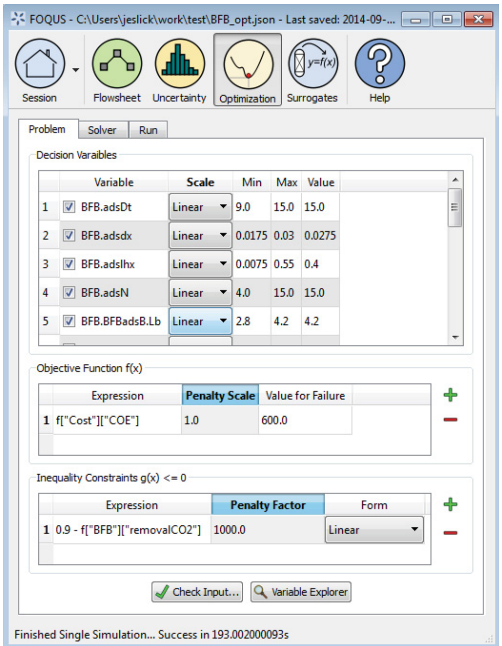

Fig. 3: FOQUS DFO problem definition page

2.4. Uncertainty quantification

Quantifying uncertainty is critical for process modeling since process models may comprise a number of interconnecting building blocks each of which can be a simplified physics model representing complex multi-physics. The pervasive use of these simplified models for keeping computational cost manageable mandates the rigorous and thorough assessment of the effect of the errors and uncertainties introduced in the modeling and simplification processes. The tasks of quantifying uncertainties thus consist of first identifying and characterizing (defining ranges and probabilities) all relevant sources of uncertainties. Then, mathematical and statistical computational tools are applied to propagate and analyze the effect of input uncertainties on the model outputs of interest. One can further compare the relative uncertainty contributions from the uncertainty sources via sensitivity analysis. Uncertainties in the experimental data for calibrating/validating the simulation model can be incorporated to the model uncertainty characterization via parameter inferences. The UQ component within FOQUS encompasses a rich selection of mathematical, statistical, and diagnostic tools for application users to perform UQ studies on their simulation models. The underlying statistical engine, PSUADE [5], provides most of the UQ functionality available in FOQUS. The capabilities provided by FOQUS UQ include:

- *Parameter screening methods* compute the importance of input parameters to identify which are important (to be kept in subsequent analyses) and which to ignore (to be weeded out).
- *Response surface (used interchangeably with surrogate) construction* approximates the relationship between the input samples and their outputs via a smooth mathematical function; this response surface or surrogate can then be used in place of the actual simulation model to speed up lengthy simulations.
- *Response surface validation methods* evaluate how well a given response surface fits the data; this is important for choosing between different response surfaces.
- *Basic uncertainty analysis* propagates input uncertainty to output uncertainty.
- *Sensitivity analysis methods* quantify how much varying an input value can impact the resulting output value.
- *Bayesian inference* applies observational data to refine the estimate of input uncertainties.
- *Visualization tools* to view computed distributions and response surfaces
- *Diagnostics tools* (to date, mainly in the form of scatter plots) to check samples and model behaviors (e.g. outliers)

The FOQUS front end provides user with convenient access to these UQ functionalities. For example, after a process flowsheet has been created via the meta-flowsheet module, the UQ interface allows users to select uncertain parameters and prescribe their uncertainty (probability) distributions. Subsequently, the front end can guide a user through generating a sampling design and propagating the ensemble (a collection of sampling locations in the parameter space) through the flowsheet using Turbine. After the simulation results have been returned by Turbine, various statistical analyses as listed above can be performed on the sample data set. Fig. 4 below shows a snapshot of the FOQUS UQ front end in which a pre-evaluated sample for a carbon capture process simulation model has been loaded. Upon launching the parameter screening capability, the relative importance of each input parameter will be displayed, as shown in Fig. 5. A new data set can be generated that varies only the important input parameters. After loading this new sample data and launching the uncertainty analysis capability, statistical data as well as the corresponding output distribution plots will be displayed, as shown in Fig. 6 for the lean loading calculated by a regenerator model. If a user wishes to see a breakdown of the output uncertainty with respect to its contribution from each uncertain parameter (uncertain parameters for this model are chemical kinetics parameters), a global sensitivity analysis may be launched which will then display the corresponding results where the height of the bars represents the relative contribution of the parameters toward the overall output uncertainty, as shown in Fig. 7. This statistical information may be useful for process designers to predict process performance with confidence bounds in view of the incomplete knowledge of the process physics.

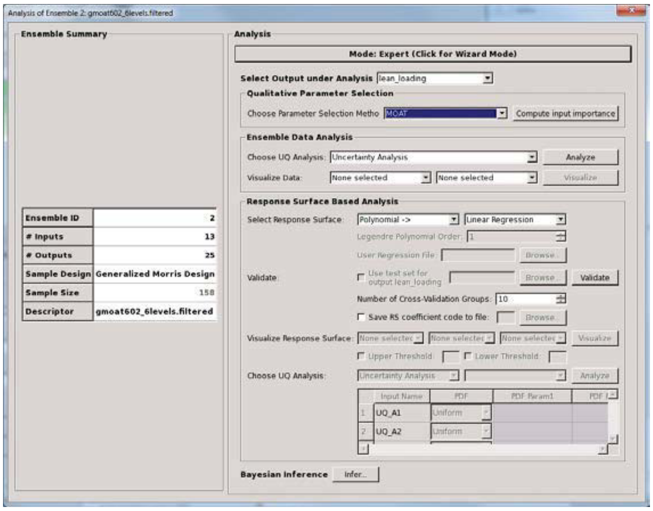

Fig. 4: FOQUS UQ user interface for parameter screening

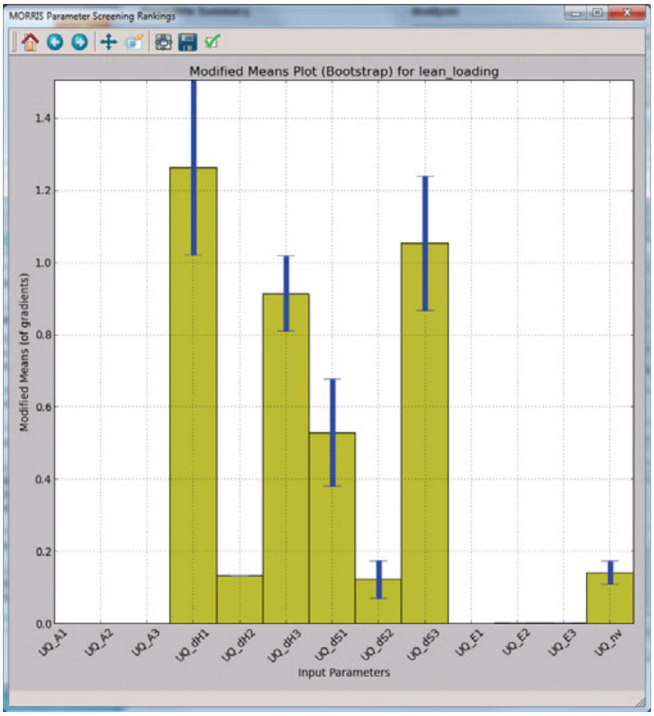

Fig. 5: FOQUS UQ parameter screening results of lean loading

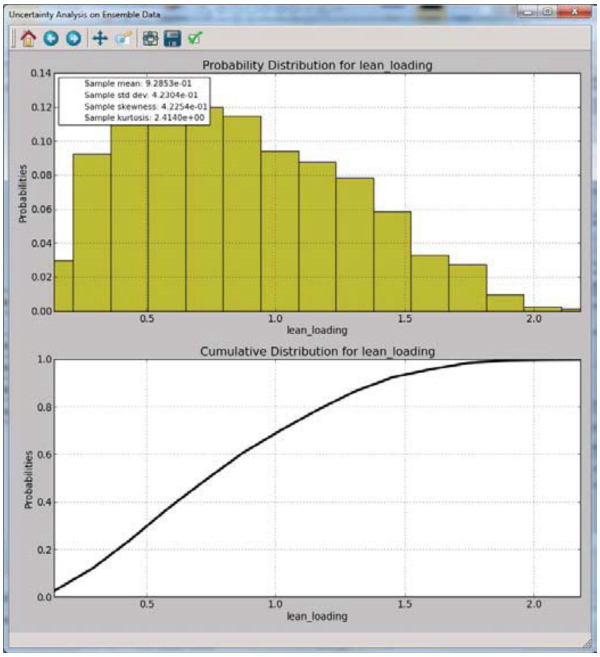

Fig. 6: FOQUS UQ analysis result – uncertainty analysis of lean loading

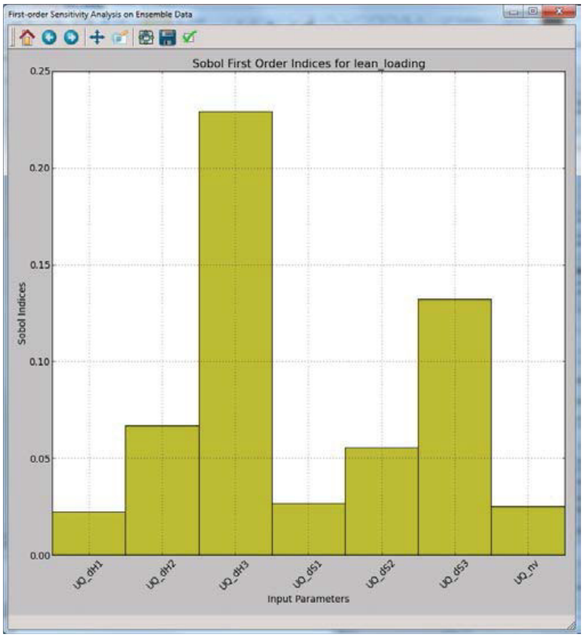

Fig. 7: FOQUS UQ analysis result – output sensitivity analysis for chemical kinetics parameters

3. Summary

In summary, FOQUS provides new capabilities for integrating multi-scale models with advanced optimization and uncertainty quantification techniques

(1) To rapidly synthesize complete, optimized, and integrated processes (such as integrating a power plant with a carbon capture system and a CO_2 compression system, or designing an integrated manufacturing facility);

(2) To identify the most promising concepts (such as a new high-tech membrane separation material) in the context of a complete process so the technical and economic performance characteristics can be appropriately evaluated;

(3) To assess the sources and effects of model and parameter uncertainty to guide experimental- and pilot-scale testing to focus on acquiring the most important types of data to minimize risk.

FOQUS enables this by providing the capability to link simulation modules built in different simulation packages together with its built-in capabilities for large-scale optimization, process integration, and UQ.

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