FOQUS Documentation

Release 3.1.0

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Jun 19, 2019

Contents

CHAPTER 1

Installation

1.1 Install Python

Python 3.6 or higher is required to run FOQUS. Miniconda (https://docs.conda.io/en/latest/miniconda.html) or Anaconda (https://www.anaconda.com/download/) are convenient Python distributions, but the choice of interpreter is up to the user. One advantage of using Miniconda or Anaconda is that it is easy to create self-contained environments, which can help managing package version dependencies between different projects. This guide will walk through the installation process with a few optional steps for installing Miniconda and setting up an environment.

If you have a working version of Python 3.6 or greater, which you prefer over Anaconda, you can skip steps 1 to 4.

1. Get the correct version of Miniconda (https://docs.conda.io/en/latest/miniconda.html) for your platform, preferably Python >=3.6, but Python 3.x environments can be installed with the Python 2.7 version.
2. Install Miniconda by running the installer, and following a few simple prompts.
3. Set up a foqus environment; this environment will be referred to as "foqus" in the installation documentation, but you can use any name you like. If you would like to install multiple version of FOQUS (for example a stable version and the latest development version), this can be done with environments. In a terminal or, on Windows, in the Anaconda Prompt type `conda create -n foqus python=3 pip`
4. Activate the environment on Linux in a terminal type: `source activate foqus` on Windows in the Anaconda Prompt type: `conda activate foqus`

If you create an environment in which to install FOQUS, you will need to ensure that environment is active before installing FOQUS. On Windows, once FOQUS is installed a batch file is created that will activate the proper environment when running FOQUS. On Linux or Mac, you will need to activate the appropriate environment before running FOQUS.

1.2 Get FOQUS

There are 2 ways to get FOQUS either download it from the github page (https://github.com/CCSI-Toolset/FOQUS) or if you are a developer and would like to contribute, you can fork the repository and clone your fork.

6. Download FOQUS

- Get a tagged release here https://github.com/CCSI-Toolset/FOQUS/releases,
- Click the clone or download button here https://github.com/CCSI-Toolset/FOQUS to get the latest development version. or
- Use the git client to clone your fork of FOQUS (if you want to contribute).

7. If you downloaded a zip file extract the FOQUS source to a convenient location.

1.3 Install FOQUS

8. Open the Anaconda prompt (or appropriate terminal or shell depending on operating system and choice of Python), and change to the directory containing the FOQUS files.
9. If you set up a "foqus" conda environment activate it

- On Windows: `conda activate foqus`
- On Linux and OSX: `source activate foqus`

10. Install requirements: `pip install -r requirements.txt`
11. Install FOQUS. The in-place install will allow you to easily edit source code while the regular install will install FOQUS in the central Python library location, and not allow editing of the source code.

- Install in-place: `python setup.py develop`
- Regular install: `python setup.py install`

1.4 Run FOQUS Installation

12. Run foqus:

- On Windows a batch file (foqus.bat) is created in the source directory. This can be moved to any convenient location, and linked by a Windows shortcut if desired. Start FOQUS by running the batch file. The batch file should run FOQUS in the appropriate conda environment, if an Anaconda environment was used. If you encounter any trouble with the batch file, an additional batch file (foqus_debug.bat) is provided which will keep the cmd windows open after FOQUS quits allowing you to see any error messages which may be generated.
- On Linux or OSX launch foqus in a terminal. Activate the appropriate conda environment if necessary. since the script is installed you can run if by typing `foqus.py` in a terminal in any directory.

13. The first time FOQUS is run, it will ask for a working directory location. This is the location FOQUS will put any working files. This setting can be changed later. Files passed as command line arguments to FOQUS will be relative to where FOQUS is run. Once FOQUS starts, file paths will be relative to the FOQUS working directory.

1.5 Install Optional Software

There are several optional pieces of software which are not written in Python and not easily installed automatically. There are a couple packages which most users would want to install. The first is PSUADE, which provides FOQUS UQ functionality. The second is TurbineLite which requires Windows, and is used to interface with Excel, Aspen, and gPROMS software.

Other software listed below will enable additional features of FOQUS if available.

1.5.1 Install PSUADE (current version: 1.7.12)

PSUADE (Problem Solving environment for Uncertainty Analysis and Design Exploration) is a software toolkit containing a rich set of tools for performing uncertainty analysis, global sensitivity analysis, design optimization, model calibration, and more.

PSUADE install instructions are on the PSUADE github site (https://github.com/LLNL/psuade). For Windows users, there is an installer at https://github.com/LLNL/psuade/releases for your convenience.

1.5.2 Install Turbine and SimSinter (Windows Only)

- Install Microsoft SQL Server Compact 4.0 (https://www.microsoft.com/en-us/download/details.aspx?id=17876).
- Download and install the SimSinter (https://github.com/CCSI-Toolset/SimSinter/releases/) and TurbineLite (https://github.com/CCSI-Toolset/turb_sci_gate/releases/).
- Install SimSinter first, then TurbineLite.
- **After the install the Turbine Web API Service Will start automatically when Windows starts, but it will not start directly a**
  - Restart computer, or
  - Start the "Turbine Web API service": (1) open Task Manager, (2) go to the "Services" tab, (3) click the "Services" button (in the lower right corner), (4) right-click "Turbine Web API Service" from the list, and (5) click "Start"

1.5.3 Install ALAMO

ALAMO (Automated Learning of Algebraic Models for Optimization) is a software toolkit that generates algebraic models of simulations, experiments, or other black-box systems. For more information, go to http://archimedes.cheme.cmu.edu/?q=alamo.

Download ALAMO and request a license from the ALAMO download page (https://minlp.com/alamo-downloads).

1.5.4 Install NLopt

NLopt is an optional optimization library, which can be used by FOQUS. Unfortunately, the Python module is not available to be installed with pip. For installation instructions, see https://nlopt.readthedocs.io/en/latest/, or NLopt can be installed with conda as follows: `conda install -c conda-forge nlopt`

1.5.5 Install R

R is a software toolbox for statistical computing and graphics. R version 3.1+ are required for the ACOSSO and BSS-ANOVA surrogate models and the Basic Data's SolventFit model.

- Follow instructions from the R website (http://cran.r-project.org/) to download and install R.
- **Open R and type the following to install and load the prerequisite packages:**
  - `install.packages('quadprog')`
  - `library(quadprog)`
  - `install.packages('abind')`

  - `library(abind)`
  - `install.packages('MCMCpack')`
  - `library(MCMCpack)`
  - `install.packages('MASS')`
  - `library(MASS)`
  - `q()`
- The last command exits R. When asked to save workspace image, type “y”.
- Open FOQUS, go to the “Settings” tab, and set the “RScript Path” to the proper location of the R executable.

1.6 Optional FOQUS Settings

- Go to the FOQUS settings tab. - Set ALAMO and PSUADE locations. - Test TurbineLite config.

1.7 Automated tests

From top level of foqus repo type: `python foqus.py -s test/system_test/ui_test_01.py` or `foqus.bat -s test/system_test/ui_test_01.py`

1.8 Building a Local Copy of Documentation

In the FOQUS source directory go to the docs directory and type `make html`. This will build the docs which can be opened by opening build\html\index.html in a web browser.

CHAPTER 2

Introduction

The Framework for Optimization, Quantification of Uncertainty, and Surrogates (FOQUS) software provides a graphical interface and standard platform for several Carbon Capture Simulation Initiative (CCSI) tools. The primary feature of FOQUS is its ability to interact with commonly-used chemical engineering process modeling software. Models constructed using a variety of software can be combined into a larger composite model. CCSI tools SimSinter and the Turbine Science Gateway (TSG) provide connectivity to external process simulation software. SimSinter provides a standard library to enable interfacing with other software; TSG provides a simulation job queuing system that can be used on: (1) a single workstation, (2) networked workstations, (3) cluster, or (4) cloud computing resources.

In FOQUS, simulations can be connected in a meta-flowsheet, which enables parts of a process to be modeled using the most appropriate software and combines them into a single large model, possibly including recycle streams. For example, in studying a carbon capture system for a coal-fired power plant: a power plant may be modeled in Thermoflex; a solvent-based carbon capture system may be modeled in Aspen Plus; and a compression system may be modeled in gPROMS. To optimize the entire system, these models can be combined into a single large model. The resulting meta-flowsheet can be used for simulation-based optimization, uncertainty quantification (UQ), or generation of surrogate models.

This section provides brief overview and motivating examples, for different uses of FOQUS.

2.1 Simulation Based Optimization

Simulation-based optimization considers a process simulation to be a black box model, which is a model where the mathematical details are not known. In this case, models are evaluated using process simulation software; multiple models can be combined to form larger models. Due to the long run times and the limitations of the methods used, a limited set of optimization variables (usually less than 30) is considered. Simulation-based optimization has some advantages and disadvantages, compared to equation-based optimization methods. With simulation-based optimization, there is no need to provide simplified algebraic models, problem formulation is relatively simple, and a good solution can usually be obtained; however, a provably-global optimum cannot be found and it is impractical to deal with very large numbers of variables. Large numbers of variables may be found in superstructure and heat integration problems where the structure of a process is being optimized. Both simulation and equation-based optimization methods are used in CCSI.

Capture of CO_2 from a pulverized coal-fired power plant involves several very different systems including: a boiler, steam cycle, flue gas desulfurization, carbon capture, and CO_2 compression. It is convenient to separate many of these processes into smaller, more reliable simulations. The different processes may also be better simulated in different software packages. Although some process simulation software contains optimization features, there are several reasons these may not be practical for a large composite system. It may be hard to develop a large model of the entire system that reliably converges. Many optimization methods have a difficult time dealing with simulation errors, and many black box derivative free optimization solvers are better able to handle occasional simulation failures. It may not be practical to simulate the entire process accurately using a single tool. Derivatives are also difficult to estimate for many systems when models do not provide exact derivatives, making derivative-free methods a good option.

The motivating example used to demonstrate the optimization framework is fairly simple. The system consists of a series of bubbling fluidized bed (BFB) CO_2 adsorbers and regenerators modeled in Aspen Custom Modeler (ACM). The details of the BFB system are described in the CCSI BFB model documentation. A cost analysis for a 650 MW power plant and capture system is presented in an Excel spreadsheet. The simulation and spreadsheet files are provided in the examples directory in the FOQUS installation directory (see the tutorial in Section ref{tutorial.sim.flowsheet} for more information). The spreadsheet contains capital cost as well as operating and maintenance cost estimates, which are used to estimate the cost of electricity.

In this example, the objective function is the cost of electricity; the decision variables are design and operating variables in the ACM model. The cost of electricity is minimized while maintaining a 90 CO_2 percent capture rate. The BFB system model and the cost of electricity are contained in separate models connected in a FOQUS flowsheet, which enables the cost of electricity to be calculated in Excel, using data acquired from the ACM model. See Sections ref{tutorial.sim.flowsheet} and ref{sec.opt.tutorial} for more information about the optimization problem.

2.2 Uncertainty Quantification

The Uncertainty Quantification (UQ) module of FOQUS encompasses a rich selection of mathematical, statistical, and diagnostic tools for application users to perform UQ studies on their simulation models. The PSUADE tool provides most of the UQ functionality available in FOQUS *(Tong 2011)*. The recommended systematic multi-step approach consists of the following steps:

1. Define the objectives of the analysis (e.g., identify the most important sources of uncertainties).
2. Specify a simulation model to be studied. Acquire the model input files and the executable that runs the simulation (i.e., an executable that uses the specified inputs and generates model outputs). Identify the outputs of interest, identify all relevant sources of uncertainties, and ensure that they can be used as input variables to the simulation model.
3. Select some or all input parameters that have uncertainty attributed. Characterize the prior probability distribution of these selected parameters by specifying the upper/lower bounds. For non-uniform prior distributions (e.g., Gaussian), additional information (e.g., mean and standard deviation) is required to define the shape of the prior distribution. This prior distribution represents the user's best initial guess about the selected parameters' uncertainties.
4. Identify, if available, relevant data from physical experiments that can be used for model parameter calibration. Model calibration is a process that applies the observational data to update the prior distribution. The model calibration correlates the observational data to predict a distribution as a result.
5. Select a sample scheme and sample size. From this information, a set of input values are sampled from the prior distribution. The choice of sampling scheme (which affects how the samples populate the input space) depends on the UQ objective(s) specified in the first step.
6. "Run" the input samples. Running the input samples is the process where each sampled input value is fed to the simulation executable (specified in Step 2) and the corresponding output value is returned.
7. Analyze the results and make decisions on how to proceed.

Steps 1-4 are often done through expert knowledge elicitation and/or literature search. Steps 5-7 can be achieved through software provided in the FOQUS UQ module.

The FOQUS UQ module provides a number of sampling and analysis methods, including:

- Parameter screening methods: computes 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: evaluates how well a given response surface fits the data. This is important for choosing different response surfaces.
- Basic uncertainty analysis: propagates input uncertainty to output uncertainty.
- Sensitivity analysis methods: quantifies how much varying an input value can impact the resulting output value.
- Bayesian calibration: applies observational data to refine the estimate of input uncertainties.
- Visualization tools: views computed distributions and response surfaces.
- Diagnostics tools (mainly in the form of scatter plots): checks samples and model behaviors (e.g., outliers).

The adsorber 650.1 subsystem process model is used to demonstrate the UQ framework. The A650.1 process model was developed and is continuously refined by our Process Synthesis and Design Team. The model is based on their design and optimization of an initial full-scale design of a solid sorbent capture system for a net 650 MW (before capture) supercritical pulverized coal power plant. The A650.1 model describes a solid sorbent-based carbon capture system that uses the NETL-32D sorbent. NETL-32D is a mixture of polyethyleneamine (PEI) and aminosilanes impregnated into the mesoporous structure of a silica substrate. CO_2 removal is achieved through chemical reactions between the amine sites within the sorbent. The A650.1 model is implemented in Aspen Custom Modeler (ACM) and contains many components (e.g., adsorbers, regenerators, compressors, heat exchangers). For the UQ analyses, this manual focuses is on the adsorber units, which are responsible for the adsorption of CO_2 from the input flue gas.

In its original form, the A650.1 model consists of a deterministic simulation model, which means to consider all the parameters (e.g. chemical reaction parameters, heat and mass transfer coefficients) to have a fixed value (most likely fixed to a mean value, lower or upper bound for robustness). With the FOQUS UQ module, the model uncertainties can be addressed. Thus, UQ analysis of the A650.1 model would help to develop a robust design by addressing the following questions: * How accurately does each subsystem model predict actual system performance (under uncertain operating conditions)? * Which input parameters should be examined to improve prediction accuracy? * What is each input parameters' contribution to prediction uncertainty?

2.3 Optimization Under Uncertainty

The Optimization Under Uncertainty (OUU) module in FOQUS is an extension of simulation-based optimization by including the contribution of model parameter uncertainties in the objective function. OUU is useful when inclusion of uncertainties may significantly alter the optimal design configurations. A straightforward approach to include the effect of uncertainty is to replace the objective function with its statistical mean on an ensemble drawn from the probability distributions of the continuous uncertain parameters (other options are available in FOQUS). Alternatively, users can provide a set of 'scenarios', where each scenario is associated with a probability. The latter case is often called 'scenario optimization.' The FOQUS OUU accommodates both continuous and scenario-based uncertain parameters. OUU makes use of the flowsheet for evaluations of the objective function. Naturally, OUU requires more computational resources than deterministic optimization. However, the ensemble runs can be launched in parallel so ideally, the turnaround time remains about the same as that of deterministic optimization if high performance computing capability (such as the CCSI Turbine gateway) is used in conjunction with FOQUS.

2.4 Surrogate Models

Process simulations are often time consuming and occasionally fail to converge. For mathematical optimization, it is sometimes necessary to replace a simulation with a surrogate model, which is a simplified model that executes much faster. FOQUS contains tools for creating and quantifying the uncertainty associated with surrogate models.

2.4.1 ALAMO

While simulation based optimization can often do a good job of providing optimal design and operating conditions for a predetermined flowsheet, it cannot provide an optimal flowsheet. To obtain a more optimal flowsheet, a mixed integer nonlinear program must be solved. These types of problems cannot generally be solved using simulation based optimization. A solution is to generate relatively simple algebraic models that accurately represent the high fidelity models. FOQUS currently provides an interface for ALAMO *(Cozad et al. 2014)*, which builds surrogate model that are well suited for superstructure optimization.

2.4.2 ACOSSO

The Adaptive Component Selection and Shrinkage Operator (ACOSSO) surface approximation was developed under the Smoothing Spline Analysis of Variance (SS-ANOVA) modeling framework *(Storlie et al. 2011)*. As it is a smoothing type method, ACOSSO works best when the underlying function is somewhat smooth. For functions which are known to have sharp changes or peaks, etc., other methods may be more appropriate. Since it implicitly performs variable selection, ACOSSO can also work well when there are a large number of input variables. To facilitate the description of ACOSSO, the univariate smoothing spline is reviewed first. The ACOSSO procedure also allows for categorical inputs *(Storlie et al. 2013)*.

2.4.3 BSS-ANOVA

The Bayesian Smoothing Spline ANOVA (BSS-ANOVA) is essentially a Bayesian version of ACOSSO *(Reich 2009)*. It is Gaussian Process (GP) model with a non-conventional covariance function that borrows its form from SS-ANOVA. It tackles the high dimensionality (of inputs) on two fronts: (1) variable selection to eliminate uninformative variables from the model and (2) restricting the level of interactions involved among the variables in the model. This is done through a fully Bayesian approach which can also allow for categorical input variables with relative ease. Since it is closely related to ACOSSO, it generally works well in similar settings as ACOSSO. The BSS-ANOVA procedure also allows for categorical inputs *(Storlie et al. 2013)*.

CHAPTER 3

Flowsheets and Settings

This chapter provides general information about using FOQUS and constructing flowsheets. The FOQUS flowsheet provides the basis for other analysis tools.

3.1 Contents

3.1.1 Reference

Getting Started

Follow the installation instructions provided in the *Installation* chapter.

The first time FOQUS is started, the user is prompted to specify a working directory. The working directory preference is stored in %APPDATA%\.foqus.cfg on Windows (APPDATA is an environment variable). On Linux or OSX, the working directory is specified in $HOME/.foqus.cfg. Additionally the user can override the working directory when starting FOQUS by using the --working_dir <working dir> or -w <working dir> command line option. Log files, user plugins, and files related to other FOQUS tools are stored in the working directory. The working directory can be changed at a later time from within FOQUS. A full list of FOQUS command line arguments is available using the -h or --help arguments.

Home Menu

Session Information Display

FOQUS flowsheet information and settings are stored in a session. The session screen displays information about the current session. A menu is available by clicking the **Session** drop-down menu. The figure below shows the Home window.

Fig. 1: Home Screen

1. The buttons displayed at the top of the Home window, excluding **Help**, are tab-like buttons that change the window when selected. The depressed button indicates the currently displayed window.

A. **Session** displays the Session window, which contains a description of the session that is currently open. **Session** has a drop-down menu that displays the Session menu.

B. **Flowsheet** displays the meta-flowsheet editing window.

C. **Uncertainty** displays the interface for PSAUDE and UQ visualization.

D. **Optimization** displays the simulation-based optimization interface.

E. **OUU** displays the optimization under uncertainty interface.

F. **Surrogates** displays the surrogate model generation window.

G. **DRM-Builder** displays the dynamic reduced model builder, which can be used to develop reduced models for dynamic simulations.

H. **Settings** displays the main FOQUS settings window.

2. **Help** toggles the Help browser. The Help browser contains HTML help, licensing and copyright information, log messages, and debugging console.

3. The main Session window displays information about the current session and is divided into three tabs:

- **Metadata** displays information about the current FOQUS session. The **Session Name** provides a descriptive name for the session. This name is used by the data management framework and when running flowsheets remotely, so a name is required. Entering a name should be the first step in creating a FOQUS flowsheet. **Version** number can be used to keep track of changes to a FOQUS session. **Confidence** describes whether the FOQUS session is expected to produce reliable results or not. **ID** is a unique identifier to identify a particular saved version of the session. **Creation Time** is the date and time that the flowsheet was first saved. **Modification Time** is the time and date that the flowsheet was last saved.
- **Description** displays a detailed explanation of the purpose of the current session file, the problem being solved, and other useful information provided by the creator of the session file.
- **Change Log** displays a record of changes made to the file. If the **Automatically create backup session file, when saving changes** checkbox is selected in FOQUS **Settings**, a backup file should exist for entries in the **Change Log**. The backup can be matched to the **Change Log** by the unique identifier appended to the file name.

Session Menu

The figure below illustrates the **Session** menu.

Fig. 2: Home Window, Session Drop-Down Menu

1. **Add Current FOQUS Session to Turbine. . . *** upload the current FOQUS session to Turbine. This can be used run a flowsheet in parallel with turbine.
2. **Add\Update Model to Turbine** enables additional models to be uploaded to Turbine. Turbine provides simulation job queuing functionality so models cannot be run in FOQUS until they have been added to the Turbine server.
3. **New Session** clears all session information so that a new session can be started.
4. **Open Recent** shows a list of recently open FOQUS sessions that can be quickly reloaded for convenience.
5. **Open Session** opens a session that was previously saved to a file.

6. **Save Session** saves the current session with the current session file name. If the session has not been previously saved, the user will be prompted to enter a file name. **Save Session** commands the user to save two session files: (1) a file with the selected name and (2) if backup option is enabled, a backup file with a name constructed from the **Session Name** and **ID**. The Session **ID** is shown on the **Session, Metadata** tab. The backup file is saved to the working directory. This system prevents accidental saving over an important file. It also enables the user to open any previously saved session.
7. **Save Session As** is similar to **Save Session**; however, the user is prompted for a new file name.
8. **Exit FOQUS** exits FOQUS. The user is asked whether to save the current session before exiting.

Adding or Changing Turbine Simulations

Before running any flowsheet where a node is linked to a simulation, the simulation must be uploaded to the Turbine gateway. To use a simulation at least two things are required: (1) the simulation file (e.g., Aspen Plus file, Excel file) and (2) the SimSinter configuration. The SimSinter configuration file is a JavaScript Object Notation (JSON) formatted file that specifies the simulation, input, and output. Any additional files required to run the simulation must also be uploaded.

Fig. 3: Turbine Upload Dialog Box

1. **Create/Edit** enables use of the SimSinter configuration Graphical User Interface (GUI) to create a SimSinter configuration file. See the *SimSinter documentation* for more information.
2. **Browse** displays a file browser, which can be used to select an existing SimSinter configuration file. Once a SimSinter configuration file is selected, the **Application** type is filled in. The SimSinter **Configuration File** and simulation file are automatically added to the file upload table.
3. **Simulation Name** enables entry of a new name if uploading a new simulation. An existing simulation can be selected from the drop-down list if an existing simulation is being modified. After selecting a SimSinter configuration file, the simulation name is guessed from the SimSinter configuration file name, but it can be edited.
4. **Application** displays the application that will be used to run the simulation. This is filled in automatically based on information in the SimSinter configuration file, and cannot be edited.
5. **Add Files** enables uploading of any auxiliary files that may be required by the simulation. Multiple files may be selected at once.
6. **Remove Files** enables added files to be removed from the list of files to upload.
7. **File Table** displays a list of files to be uploaded to Turbine.
8. **Delete** allows the simulation with the name currently displayed in the **Simulation Name** drop-down list to be deleted from Turbine. Only simulations that have not been run can be deleted.
9. **Resource Relative Path** enables the user to set the path of resource files relative to the simulation working directory. To set the directory, select files in the **File Table**. Multiple files can be selected. Click **Resource Relative Path**, and type the relative path to assign to the selected resource files.
10. **Turbine Gateway Selection** enables the user to select the instance of Turbine to which to upload the simulation. **Current** is the Turbine instance currently set to run simulations. **Remote** is configured Remote instance. **Local** is the TurbineLite instance installed on the local computer. **Remote + Local** allows simulations to be uploaded to both the local and remote instances of Turbine. **Multiple/Custom** allows simulations to be uploaded to other Turbine instances by selecting Turbine configuration files.

Settings

The settings screen shows FOQUS settings that are related to the general FOQUS setup, and are unlikely to change between sessions. The settings screen is accessible by clicking the **Settings** button at the top of the Home window. The FOQUS settings can be stored in two locations: (1) "%APPDATA%.foqus.cfg" on Windows or "$HOME/.foqus.cfg" on Linux or OSX, (2) "foqus.cfg" in the working directory.

The Settings screen displays settings grouped into tabs. Figure *Settings, FOQUS Tab* shows **Settings, FOQUS** tab.

Fig. 4: Settings, FOQUS Tab

Options in the **Settings, FOQUS** tab are described below.

1. **Save settings to working directoy**, when checkbox is selected the settings file will be read from the specified working directory. This setting is useful for running multiple copies of FOQUS to ensure the settings do not conflict. When starting additional copies of FOQUS, it is best to start them from the Working Directory command line giving each copy of FOQUS its own independent working directory. If FOQUS is started more than once from the Windows start menu, each copy will use the same working directory. Starting FOQUS multiple times with the same working directory may cause unusual behavior in FOQUS.
2. **Use DMF if available**, when checkbox is selected the Data Management Framework (DMF) module will be loaded and the DMF options will be shown in the **Session** menu.
3. **Automatically create backup session file**, when checkbox is selected each time a FOQUS session is saved it will be saved twice. A backup copy with a universally unique identifier appended to the file name will be saved. This will allow the user to load any previous save point of the session.
4. **Smaller session files**, when checkbox is selected significant storage space is saved by excluding formatting from the session file; this makes the session files less human readable. A more readable session file can be useful for debugging.
5. **FOQUS Flowsheet Run Method** enables the user to select between running simulations on the same computer as FOQUS, or on a remote Turbine gateway. Running simulations remotely allows parallel execution. The default setting is "Local". If the user switches from "Local" to "Remote", a warning message will appear. The user will be informed that the models that have been uploaded to the Local Turbine may not be available in the Remote Turbine Gateway. Therefore, the user may need to upload these models into Turbine again in order to run the models remotely.
6. **Working Directory** is the path to the FOQUS working directory. The **Working Directory** is where FOQUS reads and writes files needed to function. When running multiple copies of FOQUS, the **Working Directory** can also be specified from the command line using the "-w" or "–workingDir" options. After changing the **Working Directory**, FOQUS should be restarted.
7. **PSUADE EXE** is the path to the PSUADE executable. PSUADE provides FOQUS's UQ features.
8. **SimSinter Home** is the path to the SimSinter interface for creating Sinter configuration files for simulations to be run with FOQUS. This setting is not required but it allows easy access to the SimSinter configuration GUI when uploading simulation to Turbine.
9. **iREVEAL Home** is the path the iREVEAL installation. This is required to use the iREVEAL surrogate model module.
10. **ALAMO EXE** is the path to the ALAMO executable. This is required to use the ALAMO surrogate model module.
11. **RScript Path** is the path to the RScript executable. This is required for surrogate model modules that use R as a platform.
12. **Java Home** is the path to the Java installation. The DMF and the iREVEAL surrogate modules require Java.

13. **Revert Changes** The settings changes are applied when the user navigates away from the settings screen. To undo changes made to settings the revert button can be clicked before changing to another screen.

The **Turbine** tab contains settings for configuring the local and remote instance of Turbine. Figure *Settings, Turbine Tab* shows the FOQUS Turbine settings.

Fig. 5: Settings, Turbine Tab

The first section in the **Turbine** tab is **TurbineLite (Local)**. This section contains settings related to the local installation of Turbine, and is only applicable when running FOQUS on the windows platform.

1. **Test** tests the connection to the local Turbine server to make sure it is configured and running properly.
2. **Start Service** starts the Turbine server service on Windows. The user must have permission to start services to use this button.
3. **Stop Service** stops the Turbine server service on Windows. The user must have permission to stop services to use this button.
4. **Change Port** can reconfigure the local Turbine server service on Windows to use a different port. This may be necessary if Turbine conflicts with another service.
5. **Aspen Version**, Aspen 7.3 is still in common use but the API differs slightly form newer versions. This option allows FOQUS to be used with Aspen 7.3.
6. **TurbineLite Home** is the location of the TurbineLite installation. For local simulation runs FOQUS needs to know where TurbineLite is installed so it can launch Turbine consumers to run simulations. This setting is not needed if simulations are only run remotely.
7. **Turbine Configuration (local)** is the path to the TurbineLite gateway configuration file for running simulations locally. If simulations are only run remotely, this setting is not needed. **New/Edit** displays a form to create or edit a Turbine configuration file. Having a setting for both local and remote Turbine allows easy switching between run methods.

The second section in the **Turbine** tab is **Turbine Gateway (Remote)**. This section contains settings related to a remote instance of Turbine.

1. **Test** tests the connection to the remote Turbine server to make sure it is configured and running properly.
2. **Turbine Configuration (remote)**, is the path to the Turbine gateway configuration file for running simulations remotely. If simulations are only run locally, this setting is not needed. **New/Edit** displays a form to create or edit a Turbine configuration file. Having a setting for both local and remote Turbine allows easy switching between run methods.
3. **Check Interval (sec)** is the number of seconds between checking the remote Turbine server for job results. This number should not be set too low to avoid overwhelming the Turbine server with requests.
4. **Number of Times to Resubmit Failed Jobs** is the number of times to resubmit jobs that fail. Jobs occasionally fail due to software bugs. This allows a job to be retried.

The **Logging** tab contains settings related to the FOQUS log files, which provide debugging information. The FOQUS log files are stored in the logs directory in the working directory. Figure *Settings, Logging Tab* show the FOQUS log settings. There are two log files (1) FOQUS and (2) Turbine Client.

Fig. 6: Settings, Logging Tab

1. The level sliders indicate how much information to send to the logs.
2. The **Log Files** section enables the user to specify where the log information is sent. The **File Out** checkboxes turn on or off the file output of logs. The **Std. Out** checkboxes enable or disable the output to the screen.

3. **Format** allows the format of the log messages to be changed. See the documentation for the Python 2.7 logging module for more information.
4. **Rotate Log Files** turns on or off log file rotation. When a log file reaches a certain size, a new log file is started and the contents of the old log are moved to a new file. There currently seems to be a bug in the log file rotation which occasionally makes the log file output stop; therefore, the **Rotate Log Files** option is labeled as an experimental feature.

Flowsheet

The meta-flowsheet defines connections between simulations. The flowsheet defines the order that simulations are performed and what data is transferred between them. Simulations are represented as nodes in the flowsheet. These simulations may be links to external simulation software through the Turbine gateway, or custom simulations or simulation wrappers written in Python. Directed edges in the flowsheet connect nodes. The edges also specify which variables in the simulations are equivalent.

If the flowsheet contains cycles, they are solved iteratively. Tear streams are selected by FOQUS based on two criteria: (1) minimize the maximum number of times any cycle is torn and (2) minimize the total number of tear edges (which only is considered when two tear sets have the same value for the first criteria).

FOQUS currently has two methods available for solving flowsheets with recycle: (1) direct substitution and (2) Wegstien *Wegstein 1958*. FOQUS will solve strongly connected components in the order they are encountered in the flowsheet. FOQUS flowsheets are generally not very complicated, so if a strongly connected component contains more than one tear stream, they are solved simultaneously. More advanced solution options will be added if a need arises. Figure *Flowsheet Recycle* shows how a simple flowsheet with recycle would be solved.

Fig. 7: Flowsheet Recycle

Flowsheet Editor

Figure *Flowsheet Editor* illustrates the main **Flowsheet Editor** screen and a description of the pieces. The toolbar on the left contains various flowsheet tools.

Fig. 8: Flowsheet Editor

The first three buttons are mouse mode buttons. The current mouse mode is shown by the depressed button. The remaining buttons on the toolbar perform an action. The flowsheet editing toolbar and flowsheet are described in detail below.

1. **Selection mode** enables the user to select nodes and edges. Multiple items may be selected by holding down the Shift key. To deselect everything, click an empty area of the flowsheet while not holding the Shift key. Selected items can be moved by dragging them. To move multiple items, hold down the Shift key while dragging. The last item selected becomes the current object to be edited in the **Node** or **Edge Editor**.
2. **Add node mode** enables the user to add a node by clicking anywhere on the flowsheet. Once a location is clicked, a dialog box opens where the new node name can be entered. If **Cancel** is selected, no node is added. The new node name cannot be "graph" and cannot match any existing node name.
3. **Add edge mode** enables edges to be added by selecting the node that the edge originates from, followed by the node the edge terminates at.
4. **Center flowsheet in display** centers the display on the flowsheet.

5. **Delete selected** deletes all selected nodes and edges. If a node is deleted, all edges connecting to that node are also deleted.
6. **Run a simulation** starts a single simulation run. This is primarily used to test a simulation before running optimization or UQ.
7. **Stop a simulation** is enabled when a simulation is running and stops any running simulation. The simulation may take several seconds to stop.
8. **Set inputs to defaults** returns all of the inputs to their default values.
9. **Determine tear edges** makes it easier to see where initial guesses are needed and makes it possible to edit the tear set before running the flowsheet. If tear streams are needed but not specified before running a flowsheet, they will be automatically specified, however inputs that will be used for the initial guess will not be known before running.
10. **Flowsheet solver settings** contains options related to tear solvers.
11. **Toggle node editor display** displays or hides the **Node Editor**. The user can change the node being edited by selecting from **Name** in the **Node Editor** or selecting it on the flowsheet in selection mode.
12. **Toggle edge editor display** displays or hides the edge editor. The user can change the edge being edited in the **Edge Editor**, or by selecting it in selection mode.
13. **Show results from all flowsheet runs** displays the results of all flowsheet runs in a table view. This can be exported to a spreadsheet.
14. **Node** represents a simulation or calculations.
15. **Edge** connects simulation data, represents data transfer between two nodes.

Node Editor

The **Node Editor** enables the assignment of simulations to a node, and editing variables. Figure *Node Editor Window* shows the Node Editor window with the input variables section of the toolbox displayed.

Fig. 9: Node Editor Window

1. **Apply** immediately applies any changes made in the **Node Editor**. This is not usually needed. Changes are applied when the current node is changed, the **Node Editor** is closed, or some other action is taken that requires the flowsheet, such as running the flowsheet.
2. **Revert** sets the node back to the version where the changes were last applied. This is usually the original state of the node when the editor was opened.
3. **Run** can be used to run the simulation represented by this node only. This can be used for testing to make sure the node is properly configured without running the whole flowsheet.
4. **Stop Run** is active when a simulation is currently running. It stops a single node run or a flowsheet run.
5. There are three tabs in the **Node Editor**: (1) **Variables** tab, shown in Figure *Node Editor Window*, (2) **Position** tab displays the coordinates of the node, and (3) **Node Script** tab enabling the entry of Python code to be executed after the simulation is run.
6. **Name** displays the name of the node currently being edited. The current node can be changed by selecting from existing nodes in the drop-down menu.
7. **Code** displays the error status code for the node.
8. **Message** displays a more detailed description of the error status of the node.

9. **Type** enables the user to select the type of model to run. The model types are none, Turbine, DMF Lite, DMF Server, or Python Plugin. None allows no model to be assigned to the node; this is useful when the node only executes a script entered directly into FOQUS. Turbine is used to execute Aspen, gPROMS, or Excel simulations. Python plugins are custom simulations or wrappers written by the user. Surrogate model methods may also produce Python plugin models.
10. **Model** enables selection of the models available on Turbine or loaded Python plugins.
11. **Input Variables** enables viewing and editing the node's input variables. Most of these variables are added automatically when a simulation is selected.
    a. **Add variable** enables the addition of an input variable. There are two reasons to add an input: (1) to use a variable to pass information to another simulation (even if the variable is not used in any node calculation, it can receive data from the previous simulation and be passed on to the next simulation) and (2) to use in a node script. For example, a variable could be added that provides output in different units of measure.
    b. **Remove variable** removes variables. If an input variable is removed that originally came from a Turbine simulation, the simulation will run with the default value.
    c. **Tags** displays a tag browser that lists commonly used variable tags.
    d. **Input Variables** table displays information about variables. Most attributes can be edited, except for the **Name** column within the **Input Variables** table. The rows for input variables are color coded depending on whether they are set by an edge from results in another node. White rows are not connected. Yellow rows are set by a tear edge. These variables serve as initial guesses but their value may change once the simulation has run. Red rows are set by an edge that is not a tear edge. The value set for these inputs does not matter and it may change once the simulation has run.
12. **Output Variables** is a variable table similar to the **Input Variables** table for node output variables. This area is displayed by clicking **Output Variables**.
13. **Settings** displays simulation settings. A description is provided for each setting. The available settings vary depending on simulation.

Node Variables

Variables in the node editor are grouped into two sections, inputs and outputs. The input and output variable tables are accessible as described in the previous section. The contents of the variable tables are described here.

The columns in the input variable list are:

- **Name** is the name of the variable,
- **Value** is the current value,
- **Unit** is the unit of measure,
- **Type** is the data type (float, int, or str),
- **Default** is the default value,
- **Min** is the minimum value,
- **Max** is the maximum value,
- **Description** is a description string,
- **Tag** is a list of strings that can be used to attach additional information to a variable
- **Distribution** is a distribution type,
- **Param1** is the first parameter of a parametric distribution the exact meaning depends on the selected distribution, and

- **Param2** is the second parameter of a parametric distribution the exact meaning depends on the selected distribution.

The minimum and maximum values for are not enforced when running simulations are not enforced. A value can be given outside the range. Optimization and UQ features make use of these values to set upper and lower bounds on decision variables or sampling. The distribution information is used when setting up sampling for UQ. In the future, this may also be used for things like optimization under uncertainty. Integer and string type variables cannot currently be used as optimization decision variables, or sampled with the UQ tool.

The rows of the input variable table are color coded. Some of the input variables may be set by connections to other nodes. White rows are variables who's values are not set by a connection. The variables that are red have values set by a connection, and the value given will be overwritten and does not matter. The values that are colored yellow are inputs set by a connection that is a tear stream. The values of these variables serves as an initial guess for solving recycles.

The output variable table is similar to the input table, however it only contains the columns: Name, Value, Unit, Type, Description, and Tags. The value of the outputs may not correspond to the inputs until the simulation has been run.

Node Script

There are three type of **Node Script** that can be used: (1) **Pre** runs before a node simulation, (2) **Post** runs after a node simulation, and (3) **Total** scripts how a node runs the simulation.

Figure *Node Script Tab* illustrates the **Node Script** tab of the **Node Editor** with calculations for an optimization test problem.

Fig. 10: Node Script Tab

Node scripts can be any valid Python code. The input and output variables for node scripts are stored in dictionaries x and f. The dictionary keys are the variable names. The f dictionary is used to update the node variables after the calculations are executed.

Edge Editor

The **Edge Editor** is illustrated in Figure *Edge Editor*. The **Edge Editor** can be used to set connections between node variables.

Fig. 11: Edge Editor

1. **Index** is the index of the current edge. The current edge can be changed by selecting an index from the drop-down menu, but since the index is not a very meaningful identifier it is usually more convenient to select the edge to edit with the graphical selection tool.
2. **Origin Node** is the node where an edge starts. This may be edited by selecting a different node from the drop-down menu.
3. **Destination Node** is the node to which the edge goes.
4. **Curve** can be a positive or negative number. The greater the magnitude of number, the more curved an edge will appear in the flowsheet. This setting is used to keep edges from overlapping in the flowsheet display.
5. **Tear** marks this edge as a tear. Before a simulation is run, if a valid tear set is not specified, FOQUS locates one.
6. **Active** specifies whether the edge is active or not. This allows connections to be temporarily disabled.

7. **Variable Connections** table displays which variables are connected. Inputs or outputs in the origin node can be connected to inputs in the destination node.
8. **Add connection** adds a new connection.
9. **Remove connection** deletes the selected connections.
10. **Auto** automatically connects variables having the same name. For example, in connecting a simulation to a spreadsheet to calculate costs there are a large number of variables for which it makes sense that the variables have the same name in the simulation and spreadsheet. **Auto** should be used with great care. Connecting variables with the same name is often not what is wanted. For example two simulations may have a variable named FlowAIn; however, it is very unlikely that they should be connected. It is more likely FlowAOut should be connected to FlowAIn.

Sample Results

Flowsheet evaluations that have been run in a FOQUS session can be viewed by clicking the table button in the flowsheet toolbar (#13 in Figure *Flowsheet Editor*. The results are displayed in a table, and the contents can be copied and pasted into a spreadsheet or exported to a CSV file. Figure *Flowsheet Results Table Window* show the Flowsheet Results Table window.

Fig. 12: Flowsheet Results Table Window

1. **Menu** contains a menu with four sub menus.
   1. **Import** data from files or the clipboard.
   2. **Export** data to files or the clipboard.
   3. **Edit** or delete data.
   4. **View** options for the table.
2. The **Current Filter** drop-down list enables the user to select a data filter, which can be used to filter and sort data.
3. **Edit Filters** enables the user to create or edit data filters.

Error Codes

Error codes are listed in the **Flowsheet Results** table for the whole flowsheet and for individual nodes. Table *Flowsheet Error Codes* shows the flowsheet error codes and Table *Node Error Codes* shows the node error codes. The most common flowsheet error is 1, a node calculation failed. The most common node error is 7, Turbine simulation error. These errors are typically caused by a simulation that fails to converge or has some other calculation error (e.g., ACM does not converge or an Excel spreadsheet simulation with a division by 0 error).

Table 1: Flowsheet Error Codes

Code	Meaning
-1	Did not run or finish
0	Success
1	A simulation/node failed to solve
2	A simulation/node failed to solve while solving tears
3	Failed to create a worker node
5	Unknown tear solver
11	Wegstein failed, reached iteration limit
12	Direct failed, reached iteration limit
16	Presolve node error
17	Postsolve node error
19	Unhandled exception during evaluation (see log)
20	Flowsheet thread terminated
21	Missing session name
40	Error connecting to Turbine
50	Error loading session or inputs
100	Single node calculation success
201	Cycle in determining calculation order (invalid tear set)

Table 2: Node Error Codes

Code	Meaning
-1	Did not run or finish
0	Success
1	Simulation error (see log)
3	Exceeded maximum wait time
4	Failed to create Turbine session ID
5	Failed to add Turbine job
6	Exceeded maximum run time
7	Turbine simulation error
8	Failed to start Turbine job
10	Failed to get Turbine jobs status
11	Flowsheet thread terminated
20	Error in node script
23	Could not convert Numpy value to list
27	Cannot read variable result (see log)

3.1.2 Tutorial

Example Files

Many of the tutorials in this manual make use of example files provided in the FOQUS examples. This tutorial helps the user find and copy the example files.

1. Locate the example files in the examples sub-directory of the FOQUS download.
2. Copy the example files directory to a convenient location for use in other tutorials.

Creating a Flowsheet

This tutorial provides information about the basic use of FOQUS and setting up a very simple flowsheet. A single node flowsheet will be created that performs a simple calculation using a square root so that simulation errors can be observed when a negative input value is provided.

1. Start FOQUS (see Section *Getting Started*).
2. In the session form enter the **Session Name** as “Simple_Flow” (Figure *Setting the Session Name*).

Fig. 13: Setting the Session Name

3. Set the session description.
    a. Select the **Description** tab (Figure *Setting the Session Description*).
    b. Type the description shown in Figure *Setting the Session Description*. The buttons above the **Description** tab box can be used to format the text.

Fig. 14: Setting the Session Description

4. Click the **Flowsheet** button at the top of the Home window (Figure *Flowsheet, Input Variables*).
5. Add a node named “calc.”
    a. Click the **Add Node** button in the toolbar on the left side of the Home window.
    b. Click a location on the gridded flowsheet area.
    c. Enter the node name “calc” in the dialog box.
6. Click the **Select Mode** button in the toolbar.
7. Open the Node Editor by clicking the **Node Editor** button in the toolbar.
8. Add input variables to the node. (When linking a node to an external simulation the input and output variables are populated automatically, and this step is not necessary.)
    a. Click **+** above the **Input Variables** table.
    b. Enter x1 in the variable **Name** dialog box.
    c. Click **+** above the **Input Variables** table.
    d. Enter x2 in the variable **Name** dialog box.
    e. Enter -2 and 2 for the **Min** and **Max** of x1 in the **Input Variables** table.
    f. Enter -1 and 4 for the **Min** and **Max** of x2 in the **Input Variables** table.
    g. Enter 1 for the value of x1.
    h. Enter 4 for the value of x2.

Fig. 15: Flowsheet, Input Variables

9. Add an output variable to the node. (When linking a node to an external simulation the input and output variables are populated automatically.)
    a. Click **Output Variables** to show the **Output Variables** table (Figure *Flowsheet, Output Variables*).
    b. Click **+** above the **Output Variables** table to add a variable.

c. Enter z in the output **Name** dialog box.

Fig. 16: Flowsheet, Output Variables

In this example, the node is not linked to any external simulation. The FOQUS nodes contain a section called node script, which can be used to do calculations before, after or instead of a simulation linked to the node. The node script can be used for things such as unit conversion, simple calculations, or simulation convergence procedures. The node scripts are written as Python. The **Input Variables** are contained in a dictionary named x and the **Output Variables** are contained in a dictionary named f. The dictionary keys are the variables names shown in the input and output tables. Only **Output Variables** can be modified by a node script.

10. Add a calculation to the node.

    a. Click the **Node Script** tab (Figure *Node Calculation*).

    b. Enter the following code into the Python code box:
    `f['z'] = x['x1']*math.sqrt(x['x2'])`

11. Click the **Variables** tab.

12. Click the **Run** button (Figure *Node Calculation*).

The flowsheet should run successfully and the output value should be 2. Rerun the flowsheet with a negative value for x2, and observe the result. The simulation should report an error.

Fig. 17: Node Calculation

13. Save the FOQUS session.

    a. Click the **Session** drop-down menu at the top of the Home window (Figure *Save Session*).

    b. Click **Save**. The exact location of save in the menu depends on whether or not the data management framework is enabled.

    c. The **Change Log** entry can be left blank.

    d. The default file name is the session name. Change the file name and location if desired.

Fig. 18: Save Session

Creating a Flowsheet with Linked Simulations

This tutorial is referenced by other tutorials. **Save the flowsheet in a convenient location for future use.**

This tutorial demonstrates how to link simulations to nodes, and how to connect nodes in a flowsheet. Two models are used: (1) a bubbling fluidized bed model in ACM and (2) a cost of electricity (COE) model in Excel. The COE model estimates the cost of electricity for a 650 MW (net before adding capture) supercritical pulverized coal power plant with solid sorbent post combustion CO_2 capture process added.

Before starting the tutorial, see Section *Example Files* to locate and copy the example files to a convenient location.

1. Start FOQUS. The Session window displays (Figure *Session Setup*).
2. Enter "BFB_opt" in **Session Name** (without quotes).
3. Click the **Description** tab. The problem description box displays and is shown in (Figure *Session Description*).

4. In the problem description box enter information about the problem being solved in the FOQUS session; this information can be more extensive than what is shown in the example.
5. Save the session file. Click **Save Session** from the **Session** drop-down menu. Enter change log information and a file name when prompted. The **Creation Time** in metadata page will be the time the session is first saved. The **Modification Time** will be the last time the session was saved. The **ID** is a unique identifier that changes each time the user saves the simulation. The **Change Log** tab provides a record of the changes made each time the session is saved.

Fig. 19: Session Setup

Fig. 20: Session Description

[subsec.opt.tutorial.flowsheet] There are two models needed for this optimization problem: (1) the ACM model for the BFB capture system and (2) the Excel cost estimating spreadsheet. These models are provided in the example files directory, under optimization/models (see Section *Example Files*). There are two SimSinter configuration files: (1) BFB_sinter_config_v6.2.json for the process model and (2) BFB_cost_v6.2.3.json for the cost model. The next step is to upload the models to Turbine.

6. Open the **AddUpdate Model to Turbine** dialog box (Figure *Open Upload to Turbine Dialog*).
7. In this case, the SimSinter configuration files have already been created. If a SimSinter configuration file needs to be created for the simulation, **Create/Edit** displays the SimSinter configuration GUI (see Figure *Upload to Turbine Dialog*). See the SimSinter documentation or Chapter *Simulation Standard Interface (SimSinter)* for more information.
8. Click **Browse** to select a SimSinter configuration file (Figure *Upload to Turbine Dialog*). Once the SimSinter configuration file is selected, the simulation file and sinterconfig file is automatically added to the files to upload. The application type is entered automatically. If there are additional files required for the simulation, those files can be added by clicking **Add File**.
9. Enter the simulation name in **Simulation Name**. This name is determined by the user, but will default to the SimSinter configuration file name. For this tutorial use BFB_v6_2.
10. Click OK to upload the simulation.
11. Repeat the upload process for the cost model. Name the model
BFB_v6_2_Cost.

Fig. 21: Open Upload to Turbine Dialog

The next step is to create the flowsheet. Figure *Flowsheet Editor* illustrates the steps to draw the flowsheet.

12. Click **Flowsheet** at the top of the Home window.
13. Click **Add Node mode**.
14. Add two nodes to the flowsheet. Name the first node “BFB” and the second node “cost”.
15. Click **Add Edge mode**.
16. Click the BFB node followed by the cost node.
17. Click **Selection mode** and select the BFB node.
18. Click **Toggle Node Editor**. The Node Editor displays as illustrated in Figure fig.tut.opt.nodeEditor.

Fig. 22: Upload to Turbine Dialog

Fig. 23: Flowsheet Editor

Each node must be assigned the appropriate simulation. Use the Node Editor to set the simulation type and the simulation name from simulation uploaded to Turbine. The Node Editor is illustrated in Figure fig.tut.opt.nodeEditor

19. Under **Model** and **Type**, set the simulation **Type** to Turbine. This indicates that the simulation is to be run with Turbine.
20. Under **Model**, set the simulation of the BFB node to BFB_v6_2.
21. The **Variables** and **Settings** are automatically populated from the SimSinter configuration file. Variable values, **Min/Max**, and descriptions can be changed; however, for this problem, the values taken from the SimSinter configuration should not be changed.
22. Repeat the process for the cost node, assigning it the BFB_v6_2_cost simulation.

The connections between variables in the BFB simulation and the cost estimation spreadsheet must be set, so that required information can be transferred from the BFB simulation to the cost simulation.

23. Click **Toggle Node Editor** to hide the Node Editor (Figure *Flowsheet Editor*).
24. Select the edge on the flowsheet with the **Selection** tool.
25. Click **Toggle Edge Editor** to show the Edge Editor. The Edge Editor is shown in Figure *Edge Editor*.
26. For convenience, all of the variables that should be connected from the ACM model to the Excel spreadsheet have been given the same names in their SimSinter configuration files. To connect the variables click **Auto** in the Edge Editor. **Auto** connects variables of the same name. Since this is often not desired, the **Auto** button should be used carefully. There should be 46 connected variables.

The flowsheet should now be ready to run. Test the flowsheet by executing a single evaluation before setting up the optimization problem.

27. Click **Run** in the Flowsheet Editor (Figure *Flowsheet Editor*).
28. The flowsheet may take a few minutes to run. The BFB simulation takes a significant amount of time to open in ACM. While running optimization, the evaluations take less time because the simulation remains opened. The simulation should complete successfully. A message box displays when the simulation is done. The status bar also indicates the simulation is running.
29. While the simulation is running, **Stop** is enabled.
30. Once the simulation runs successfully, **Save** the FOQUS session again, and **keep it for use in later tutorials**.

Flowsheets with Recycle

This section provides a tutorial on working with flowsheets containing recycle. Sections *Creating a Flowsheet* and *Creating a Flowsheet with Linked Simulations* provide tutorials for creating flowsheets, in this section a pre-constructed flowsheet is used.

1. From the example files, copy the RecycleMass_Bal_Test_02.foqus example file to a convenient location (see Section *Example Files*.
2. Open FOQUS.
3. Open the Mass_Bal_Test_02.foqus file.
    1. Open the **Session** drop-down menu on the right side of the **Session** button (Figure *Flowsheet with Recycle*).

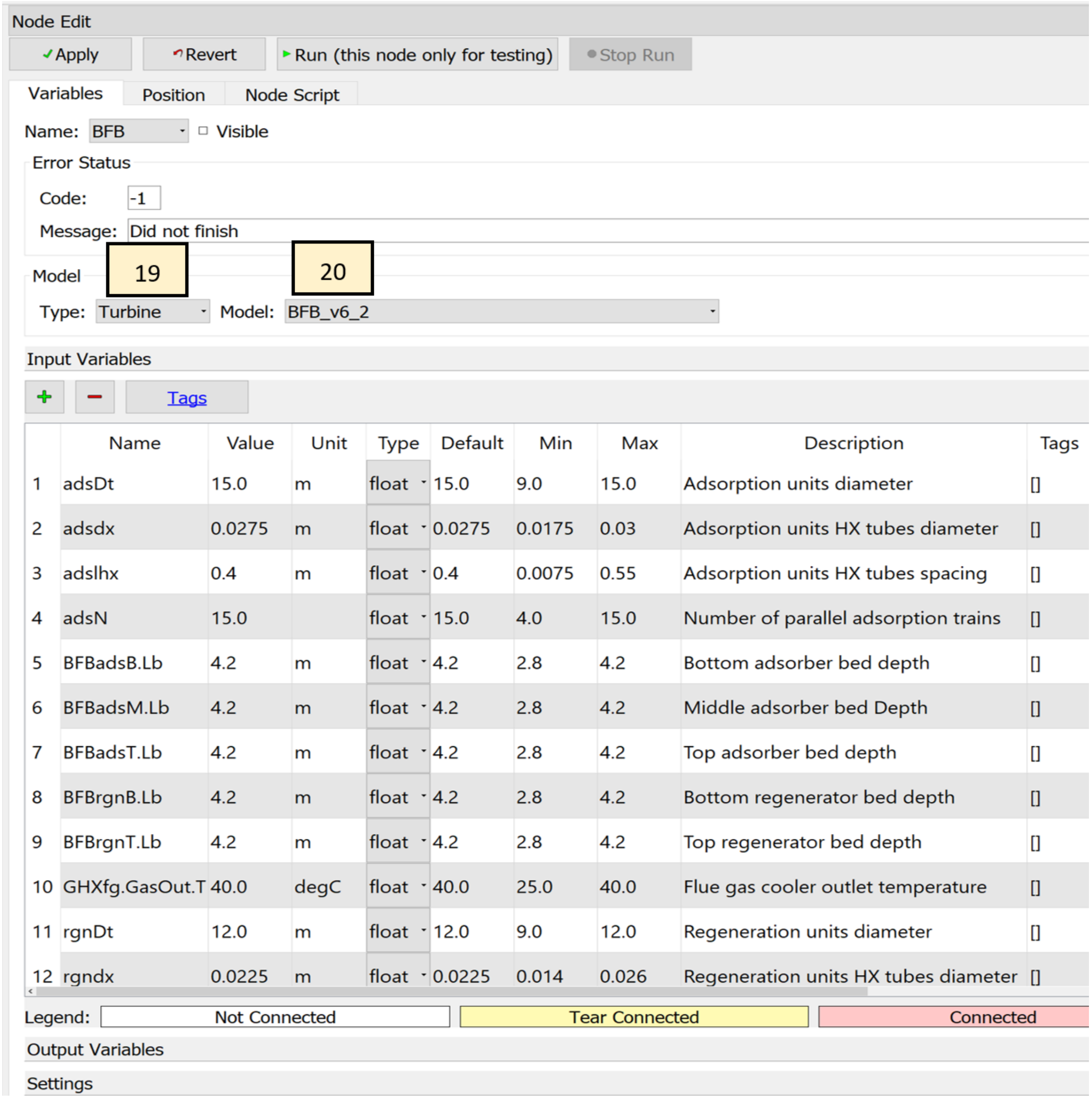

Fig. 24: Node Editor

Fig. 25: Edge Editor

   2. Select **Open Session** from the drop-down menu.
   3. Locate Mass_Bal_Test_02.foqus in the file browser, and open it.
4. Click **Flowsheet** button from the toolbar at the top of the Home window.

The flowsheet is shown in Figure *Flowsheet with Recycle*. The flowsheet consists of two reactors in recycle loops. The flowsheet contains mixers, reactors, separators, and splitters. Each node uses a set of simple calculations in the node script section. The tear edges are shown in light blue.

Fig. 26: Flowsheet with Recycle

5. Inspect a node.
   1. Make sure the Selection tool is selected (Figure *React_01 Node*.
   2. Open the Node Editor by clicking the **Node Edit** button in the left toolbar in the Flowsheet view.
   3. Click the "React_01" node.
   4. Click **Input Variables** table. Note: Some input rows are colored red. This denotes that their values are set by output of the previous flowsheet node by the edge connecting "Mix_01" to "React_01."
   5. Click the **Node Script** tab.
   6. Note the equations. **Input Variables** are stored in the x dictionary and **Output Variables** are stored in the f dictionary.
6. Click the gear icon in the left toolbar (see Figure *React_01 Node*. The tear solver settings are shown in Figure *Tear Solver Settings*.

Fig. 27: React_01 Node

Fig. 28: Tear Solver Settings

7. Remove the tear edges.
   1. Close the Node Editor.
   2. Open the Edge Editor. Click the **Edge Editor** icon in the left toolbar (see Figure *Edge Edit*.
   3. Click the edge between "React_01" and "Sep_01."
   4. In the Edge Editor, clear the **Tear** checkbox.
   5. Repeat for the other tear edge.
8. Close the Edge Editor.

There should now be no tear edges in the flowsheet. The user can select tear edges or FOQUS can automatically select a set. If there is not a valid set of tear edges marked when a flowsheet is run, tear edges will automatically be selected.

9. Automatically select a tear edge set by clicking the **Tear** icon in the left toolbar (see Figure *Edge Edit*).
10. Open the Node Editor and look at node "Sep_01." In the Input Variables table, notice that some of the input lines are colored yellow. The yellow inputs serve as initial guesses for the tear solver. The final value will be different from the initial value.
11. Click the **Run** button on the left toolbar. The flowsheet should solve quickly.
12. The results of the completed run are in the flowsheet. An entry will also be created in the Flowsheet Results data table (see Section *Flowsheet Result Data*.

Fig. 29: Edge Edit

Flowsheet Result Data

Flowsheet evaluation results are stored in a table in the FOQUS session. This data can be used for many purposes. The flowsheet evaluations may be single runs, part of an optimization problem, or part of a UQ ensemble. This tutorial provide information about sorting, filtering, and exporting data.

Copy the Data/Simple_flow.foqus file from the example files to a convenient location (see section *Example Files*). This file is similar to the one created in the tutorial Section *Creating a Flowsheet with Linked Simulations*, but it has been run an additional 100 times using a UQ ensemble (see *Uncertainty Quantification*).

1. Open FOQUS.
2. Open the Simple_flow.foqus session from the example files.
3. Click the **Flowsheet** button from the Home window.
4. Click **Flowsheet Data** in the toolbar on the left side of the Home window.

Fig. 30: Flowsheet Results Data Table, All Data

A data table should be displayed like the one shown in the figure below. There are 102 flowsheet evaluations. The first two evaluations are single runs, as can be seen in the **SetName** column, and the remaining 100 evaluation are from a UQ ensemble. The **Error** column shows several of the evaluations resulted in an error from a negative number being passed to the square root function.

This tutorial is broken up into mini-tutorials in the remaining subsections, which can be done independently. They each use the example data file described above.

Sorting Data

1. Open FOQUS.
2. Open the Simple_flow.foqus session from the example files.
3. Click **Flowsheet** in the main toolbar at the top of the FOQUS Home window.
4. Click **Flowsheet Data** in the toolbar on the left side of the Home Window.
5. Click **Edit Filters**.
6. Click **New Filter**.
7. Enter "Sort1" as the new filter name.
8. Click **New Filter**.
9. Enter "Sort2" as the new filter name.
10. Select "Sort1" from the **Filter** drop-down list.
11. Enter `["-result"]` as the **Sort by Column**. Include the square brackets. The square brackets indicate that there is a list of sort terms, although in this case there is only one. If multiple search terms are given, the additional terms will be used to sort results having the same value for the previous terms. The "-" in front of **result** indicates the results should be sorted in reverse. The names of the sort terms come from the column headings, and are case sensitive.
12. Click **Done** to save the filters and return to the results table.

Fig. 31: Sort1 Data Filter

14. Select "Sort1" from the **Current Filter** drop-down list.
15. The results are shown in below. The data should be sorted in reverse alphabetical order by **result**. Some of the columns are hidden to make the relevant results easier to see.

Fig. 32: Sort1 Data Filter Results

16. Click **Edit Filters**.
17. Select "Sort2" from **Filter** drop-down list.
19. Enter `["err", "-result"]` in the **Sort Term** field. This will sort the data first by **Error** code then by **result** in reverse alphabetical order.
20. Click **Done**.

Fig. 33: Sort2 Data Filter

21. Select "Sort2" in the **Current Filter** drop-down list.
22. The results are shown in below. The data should be sorted so all **Error** code zero results are first then sorted in reverse alphabetical order by **result**.

Filtering Data

1. Open FOQUS.
2. Open the Simple_flow.foqus session from the example files.
3. Click the **Flowsheet** button in the Home window.
4. Click the Results Data button (Table icon in left toolbar).
5. In the data table dialog, click **Edit Filters**.
6. Click **New Filter** and enter "Filter1" in the **Filter** field as the new filter name.

The filter expression is a Python expression. The `c("Comlumn Name")` function returns a numpy array containing the column data. The expression should evaluate to a column of bools where rows containing `True` will be included in the filtered results and rows containing `False` will be excluded. If combining multiple logical expressions the numpy logical functions https://docs.scipy.org/doc/numpy-1.15.1/reference/routines.logic.html should be used. Numpy is imported as `np`

8. In this example, results without errors in the "Single_runs" should be selected. In the filer expression field enter `np.logical_and(c("err") == 0, c("set") == "Single_runs")`

10. Click **Done**.
11. In the data table dialog, select "Filter1" from the **Current Filter** drop-down list.
12. The result is displayed in the Figure below.

Fig. 34: Sort2 Data Filter Result

Fig. 35: Filter1 Data Filter

Exporting Data

This tutorial uses a spreadsheet program such as Excel or Open Office. The exported data is subject to the selected filter. See the previous tutorials in this section for more information about sorting and filtering data to be exported.

Clipboard

FOQUS can export data directly to the Clipboard. The data can be pasted into a spreadsheet or as text. Copying data to the Clipboard eliminates the need for an intermediate file when creating spreadsheets.

1. Open FOQUS.
2. Open a spreadsheet program.
3. Open the Simple_flow.foqus session from the example files.
4. Click the **Flowsheet** button in the Home window.
5. Click the Results Data button (Table icon in left toolbar).
6. Click on the **Menu** drop-down list in the data table dialog.
7. Select “Export” from the **Menu** drop-down list.
8. Click **Copy Data to Clipboard**.
9. Select Paste in the spreadsheet program. The data table in FOQUS should paste into the spreadsheet. Filters can be used to sort or reduce the exported data.

CSV File

CSV (comma separated value) files can be read by almost any spreadsheet program, and are common formats readable by many types of software. FOQUS exports CSV files using the column headings from the data table as a header.

1. Open FOQUS.
2. Open a spreadsheet program.
3. Open the Simple_flow.foqus session from the example files.
4. Click the **Flowsheet** button in the Home window.
5. Click the Results Data button (Table icon in left toolbar).
6. Click the **Menu** drop-down list.
7. Select “Export” from the **Menu** drop-down list.
8. Click **Export to CSV File**.

Fig. 36: Filter1 Data Filter Result

9. Enter a file name in the file dialog.
10. In the spreadsheet program, open the CSV file exported in the previous step.

Using a Remote Turbine Instance

A remote Turbine instance may be used instead of TurbineLite. TurbineLite, used by default, runs simulations (e.g., Aspen Plus) on the user's local machine. The remote Turbine gateway has several potential advantages over TurbineLite, while the main disadvantage is the effort required for installation and configuration. Some reasons to run a remote Turbine instance are:

- Simulations can be run in parallel. The Turbine gateway can distribute simulations to multiple machines configured to run FOQUS flowsheet consumers. FOQUS consumers are basically additional instances of FOQUS running on remote systems which can run a FOQUS flowsheet.
- Simulations can be run on machines other than the user's, so as not to tie-up the user's machine running simulations.

Running Remote Turbine on Your Own Computer

To run remote turbine on you own computer (e.g., if your computer has multiple processors):

1. Navigate to the folder where your FOQUS working directory is located ("A" in Figure *FOQUS Working Directory and Folder*).

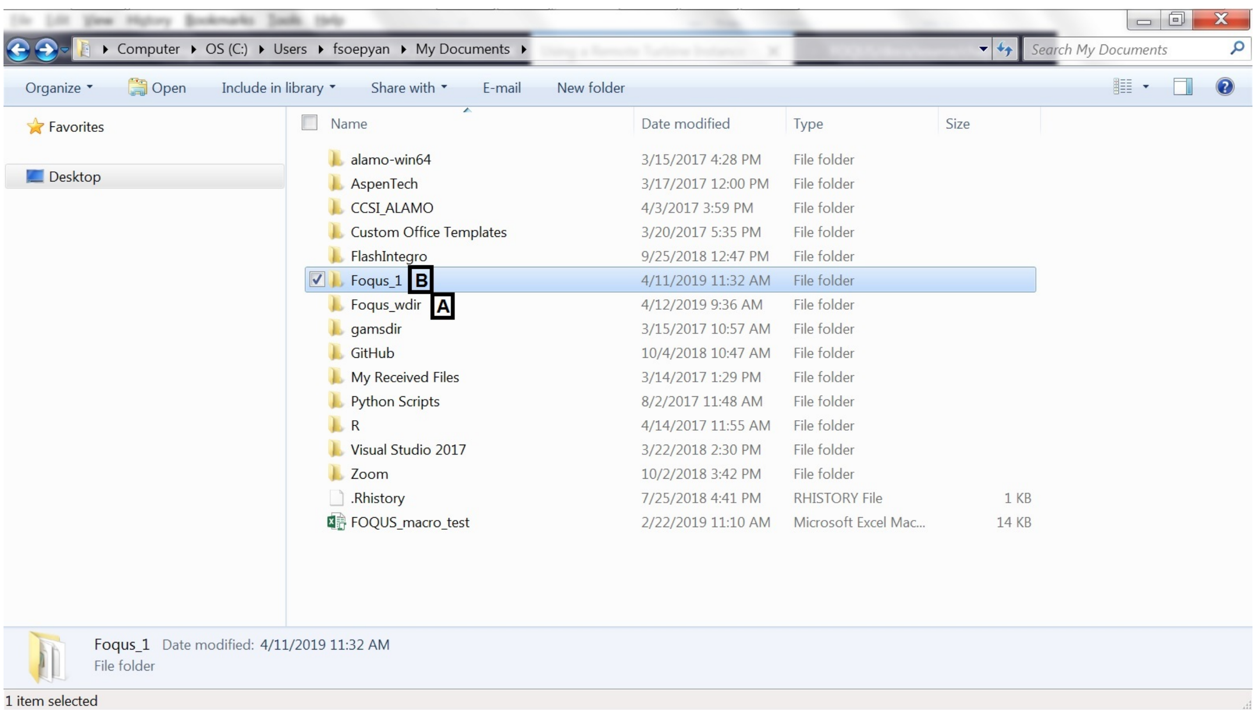

Fig. 37: FOQUS Working Directory and Folder

2. Create a blank folder ("B" in Figure *FOQUS Working Directory and Folder*). Here, this folder is called "Foqus_1".
3. Open the Anaconda prompt, and navigate to the folder where you downloaded FOQUS from GitHub (Please see Figure *The Anaconda Prompt for Remote Turbine*).

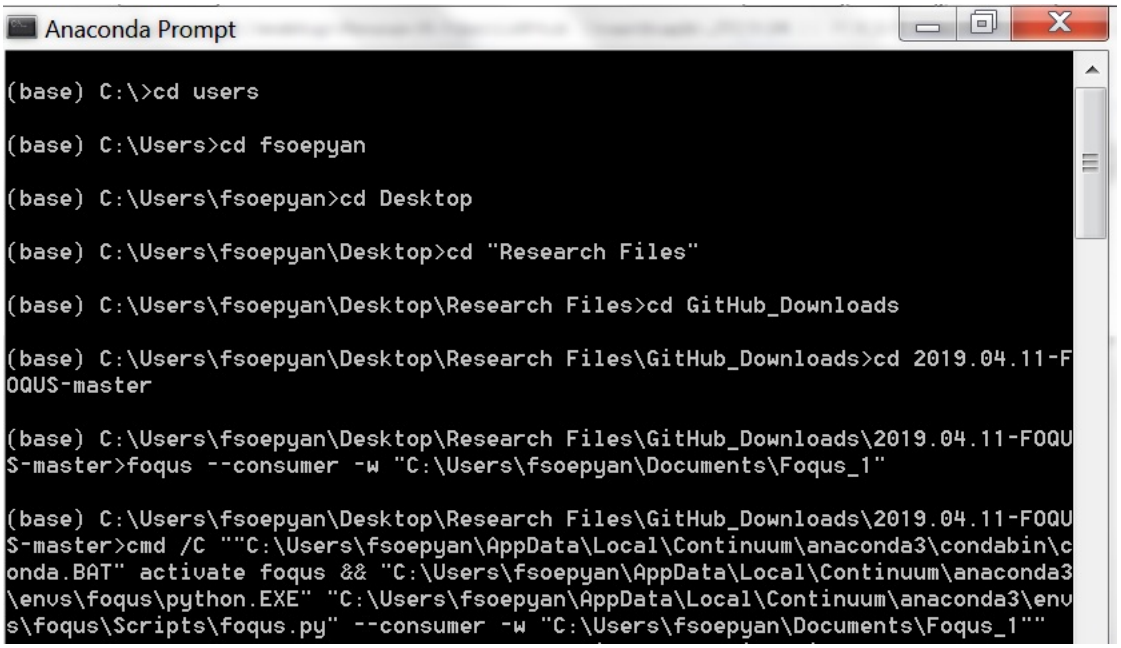

Fig. 38: The Anaconda Prompt for Remote Turbine

4. Once you navigate to the above-mentioned folder, type: "foqus –consumer -w" (without the quotes) and the location of the folder created in Step 2 (in quotes) (Please see Figure *The Anaconda Prompt for Remote Turbine*).
5. If successful, a message will appear (shown at the bottom of Figure *The Anaconda Prompt for Remote Turbine*).
6. If you have not done so already, open another Anaconda prompt, use it to open FOQUS.
7. Click "Settings" at the top menu ("C" in Figure *Remote Turbine Setting*).
8. Under "FOQUS Flowsheet Run Method", select "Remote" ("A" in Figure *Remote Turbine Setting*).
9. A message box will appear to warn the user that the simulations may need to be re-uploaded to Turbine. Click "OK" to continue ("B" in Figure *Remote Turbine Setting*).
10. Click the "Turbine" tab ("A" in Figure *Turbine Lite Setup for Running Turbine Remotely*).
11. If necessary, copy the item in "Turbine Configuration (remote)" ("C" in Figure *Turbine Lite Setup for Running Turbine Remotely*) to a convenient location (e.g., Notepad), just in case.
12. Make sure that the item under "Turbine Configuration (remote)" ("C" in Figure *Turbine Lite Setup for Running Turbine Remotely*) is the same as the item under "Turbine Configuration (local)" ("B" in Figure *Turbine Lite Setup for Running Turbine Remotely*). The reason you will be using Turbine Lite (instead of Turbine Gateway) is because you will be running the simulation remotely, but still in your own computer (instead of in other computers or in AWS - Amazon Web Service).
13. Run the flowsheet. The run should be successful (Figure *Example of Running the Flowsheet with Remote Turbine*). For this example, we used the "Simple_flow" example from "examplesSmoke Tests".

Running Remote Turbine on AWS (Amazon Web Service) or Multiple Computers

The steps below demonstrate how to set up FOQUS to run flowsheets remotely if the user would like to run FOQUS in parallel in AWS or on multiple computers (see Figure *Remote Turbine Settings*).

1. Obtain a user name, password, and URL from the site's Turbine administrator.

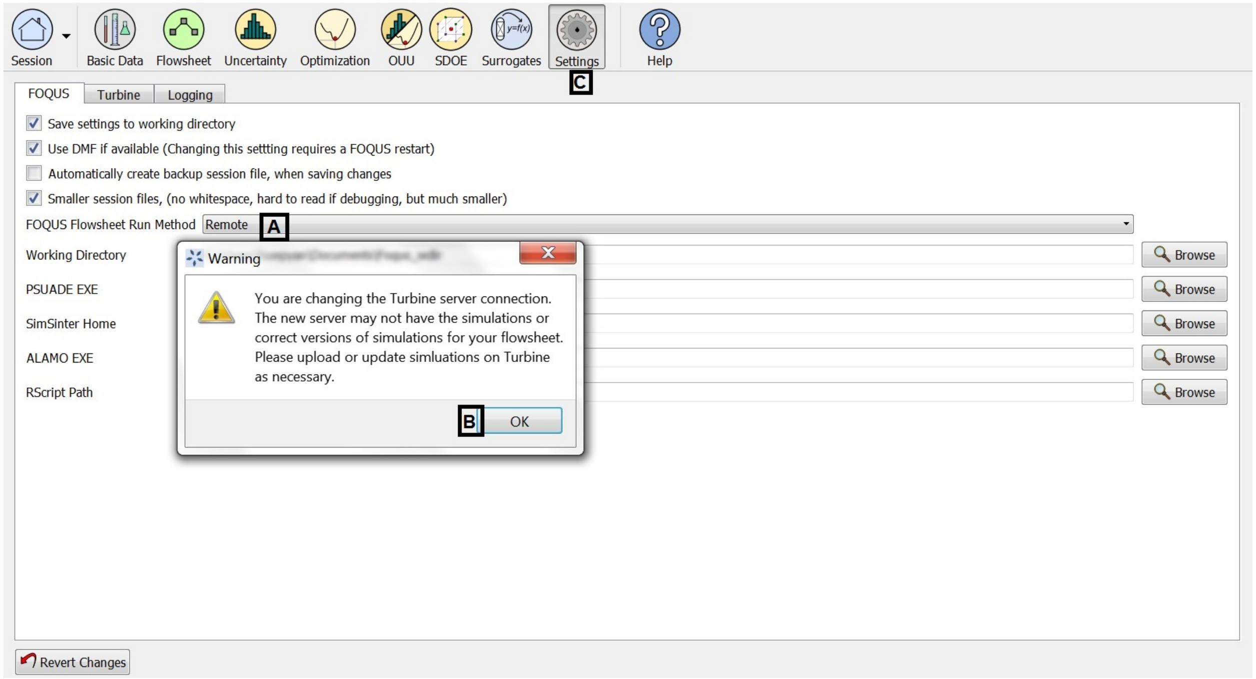

Fig. 39: Remote Turbine Setting

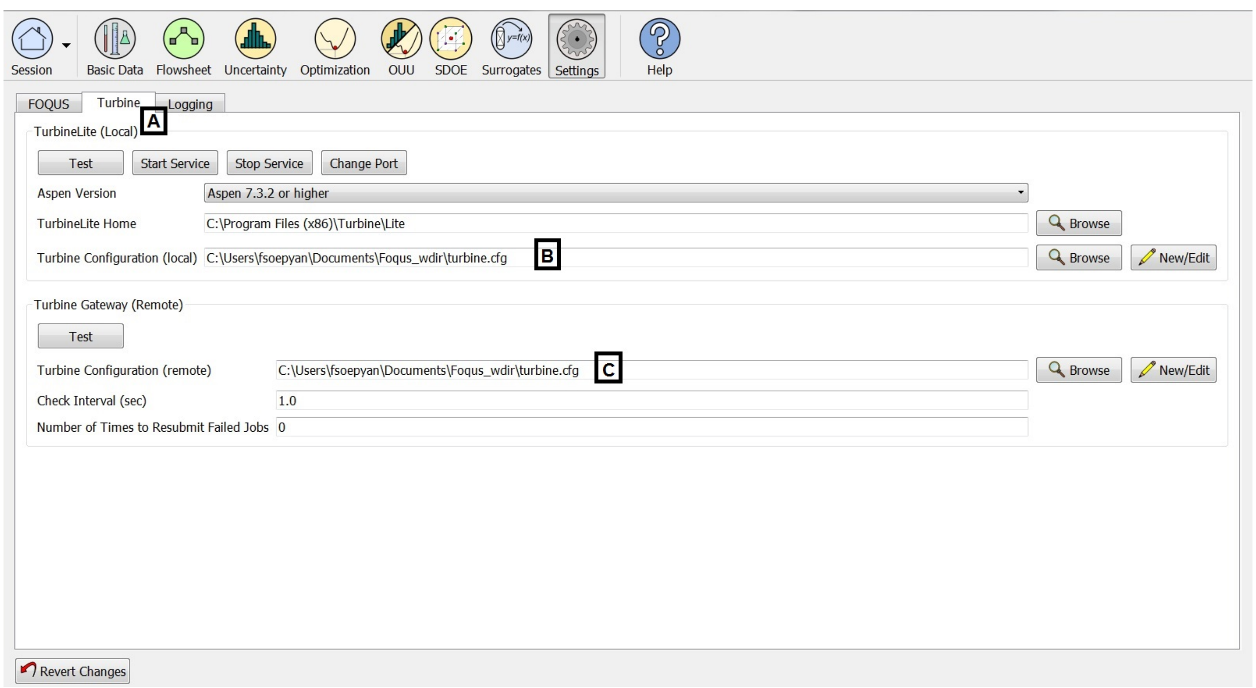

Fig. 40: Turbine Lite Setup for Running Turbine Remotely

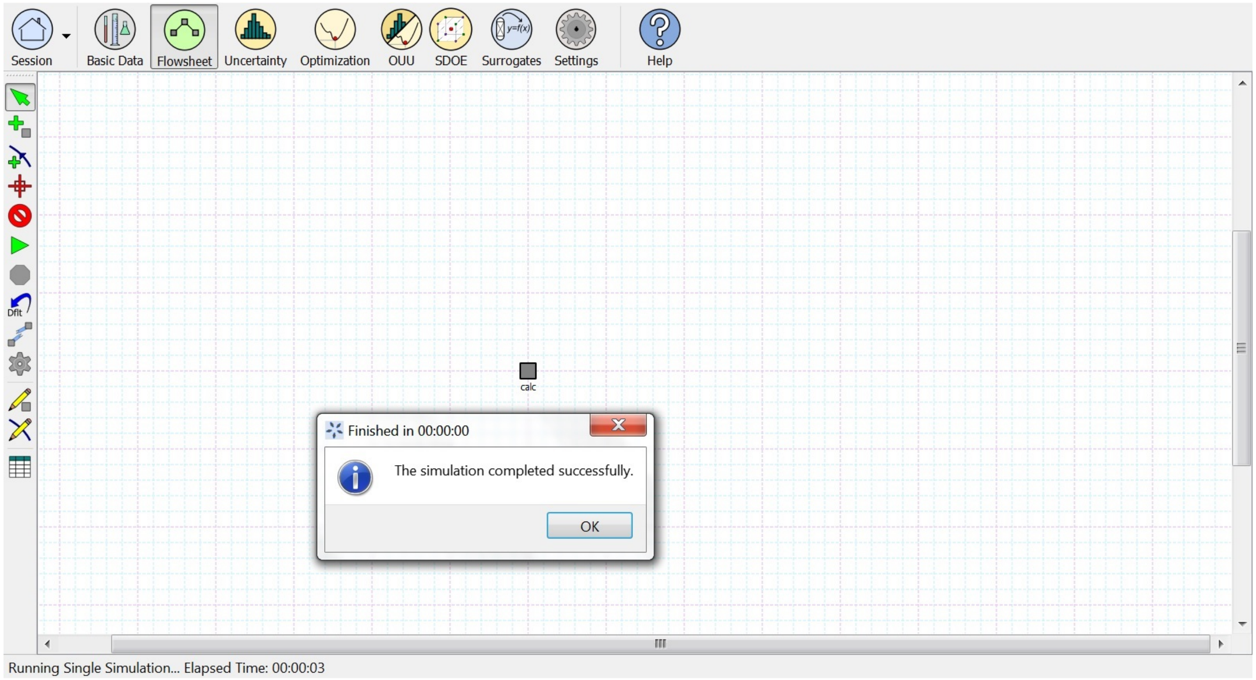

Fig. 41: Example of Running the Flowsheet with Remote Turbine

2. Open FOQUS.
3. Click **Settings** at the top right of the Home window (Figure *Run Method Settings*).
4. Select "Remote" from the **FOQUS Flowsheet Run Method** drop-down list. A message box will appear. The user will be warned that the models that have been uploaded to Turbine Local may not be available in Turbine Remote Gateway, which means that the user may need to upload the models into Turbine again (please see Step 7).
5. Click the **Turbine** tab; this displays the Turbine settings shown in Figure *Remote Turbine Settings*.

Fig. 42: Run Method Settings

6. Create a Turbine configuration file; this contains your password in plain text, so it is very important that if you are allowed to choose your own password, you choose one that is not used for any other purpose.
    1. Click **New/Edit** next to the **Turbine Configuration (remote)** field. The Turbine Configuration window displays (see Figure *Remote Turbine Settings*).
    2. Select "Cluster/Cloud" from the **Turbine Gateway Version** drop-down list in the Turbine Configuration window.
    3. Enter the Turbine URL in the **Address** field.
    4. Enter the **User** name and **Password**.
    5. Click **Save as** and enter a new file name.
    6. Set the remote Turbine configuration file. Click **Browse** next to the **Turbine Configuration (remote)** field. Select the file created in Step 6e.

At this point the remote gateway is ready to use. The last step is to ensure that all simulations referenced by flowsheets to be run are uploaded to the remote Turbine gateway.

Fig. 43: Remote Turbine Settings

7. Upload any necessary simulations to Turbine (see Section *Adding or Changing Turbine Simulations* and the tutorial in Section *Creating a Flowsheet with Linked Simulations*)

Once all settings are specified there is no apparent difference between running flowsheets locally or on a remote Turbine gateway, and FOQUS can readily be switched between the two.

CHAPTER 4

Optimization

4.1 Contents

4.1.1 Reference

The simulation based optimization tool provides a plug-in system where different derivative free optimization (DFO) solvers can be used with FOQUS. Several solvers are provided with FOQUS. The CMA-ES solver *(Hansen 2006)* is a good global derivative free optimization (DFO) solver. The NLopt library provides access to several DFO solvers *(Johnson 2015)*. SLSQP and BFGS from the Scipy module are also provided *(Jones et al. 2015)*. Since FOQUS does not generally have access to derivative information the Scipy solvers rely on finite difference approximations, and should only be used with well-behaved functions. Due to convergence tolerances in process simulators, finite difference approximations may not be good for many of FOQUS's intended applications.

CMA-ES offers a restart feature, which can be used to resume an optimization if it is interrupted for any reason. Other solvers may use an auto-save feature, which does not provide the ability to restart, but will allow optimization to start from the best solution found up to the point the optimization was interrupted. Samples making up the population in CMA-ES can be run in parallel. The NLopt and Scipy plugins do not offer parallel computing for standard optimization. For any solver, parallel computation can be used for parameter estimation and optimization under uncertainty, where multiple flowsheet evaluations go into an objective function calculation.

Problem Set Up

See Chapter *[chpt.flowsheet]* for information about setting up a flowsheet in FOQUS. Once the flowsheet has been set up and tested, an optimization problem can be added. FOQUS allows multiple flowsheet evaluations to be used to calculate a single objective function value. This allows FOQUS to do parameter estimation and scenario based optimization under uncertainty. There are three types of variables used in the optimization problem: (1) fixed variables do not change during the optimization, (2) decision variables are modified by the optimization algorithm to find the best value of the objective function, and (3) sample variables, which are used to construct the multiple flowsheet evaluations that can go into an objective calculation. If no sample variables are defined, each objective function value will be based on a single flowsheet evaluation. Figure *Optimization Variable Selection* shows the **Variables** tab selection form.

Fig. 1: Optimization Variable Selection

1. The **Variables** tab contains the form for variables selection.
2. The **Variable** column shows the name of input variables in the flowsheet. If a variable is set by a connection to another variable through an edge, it is not shown in the table. The format for a variable name is {Node Name}.{Variable Name}.
3. The **Type** column allows the variables to be assigned as one of three types (1) fixed, (2) decision, or (3) sample.
4. The **Scale** column allows the scaling method to be set for each variable. Decision variables must be scaled. Scaling is ignored for other variables. In the FOQUS example files, there is a scaling spreadsheet that provides a demonstration of the different scaling methods. The upper and lower bound are used in the scaling calculations. Regardless of the scaling method, the optimizer sees the decision variables as running from 0 at their minimum to 10 at their maximum.
5. The **Min** and **Max** columns are used to define the upper and lower bounds for the variables. FOQUS requires that all optimization problems be bounded.
6. The **Value** column provides the starting point for the optimization. How the starting point is used depends on the optimization method. The starting point for sample variables is irrelevant. Fixed variables will remain at their starting point during the optimization.

The sample variables define a set of samples that will be used to calculate an objective function. For each objective function, the decision variables are fixed at values set by the optimization solver, and the flowsheet is evaluated for each row on the sample table. The results of the samples can be used to calculate the objective function. Using the **Samples** tab is optional. If no sample variables are set, each objective function value will be based on a single simulation. Figure *Optimization Sample Table* shows the Samples table form.

Fig. 2: Optimization Sample Table

1. The **Samples** tab contains the table used to define samples for objective function calculations. If there are no sample variables, the table should be empty.
2. **Add Sample** adds a row to the Samples table.
3. **Delete Samples** deletes the selected rows from the Samples table.
4. **Generate Samples** opens a dialog box that provides a selection of methods to generate samples or read samples from a file.
5. **Clear Samples** clears the Samples table.

Once the variables and (optionally) samples have been selected, the objective function and constraints can be defined. FOQUS is set up to handle multi-objective optimization, but no multi-objective optimization plug-ins are currently provided in the FOQUS installer, so some of the options may seem to be extraneous. There are two methods for entering the objective function and constraints into FOQUS: (1) Simple Python expressions and (2) a more extensive Python function. Python expressions are easier and sufficient for most cases. If the objective function is complicated it may be necessary to write a Python function, which can be as complex as needed.

The variables used in the Python code for the objective function or constraints are stored in two Python dictionaries, "f" for outputs and "x" for inputs. There are two ways to index the dictionaries depending on whether or not sample variables are used. For an input variable with sampling, the indexing is `x[Sample Index]['Node Name']['Variable Name'][Time Step Index]`. If no sample variables are defined, the sample index is not needed, so the indexing would be, `x['Node Name']['Variable Name'][Time Step]`. Node Name and Variable Name are strings so they should be in quotes. The sample and time step indexes are integers. For steady state simulations, the time step should be 0.

Figure *Optimization Simple Objective Function* shows the form for entering the objective function and constraints as Python expressions.

Fig. 3: Optimization Simple Objective Function

1. The **Objective/Constraints** tab contains the form used to enter the objective function and constraints.
2. The drop-down list enables the selection of either the "Simple Python Expression" or "Custom Python" form of the objective function.
3. **+** adds an objective function to the table. The solvers currently available are single objective and will only use the first objective function.
4. **-** removes the selected objective from the table.
5. The Python expression for the objective function can be entered in the **Expression** column.
6. The **Penalty Scale** column is intended for use with multi-objective solvers and allows the constraint violation penalty to be applied differently to objective functions with different magnitudes.
7. The **Value for Failure** column contains the value to be assigned to the objective function if the objective cannot be evaluated for any reason. The value should be higher than the expected highest value for a successful objective.
8. **+** adds an inequality constraint.
9. **-** removes selected inequality constraints.
10. The inequality constraints are in the form $g(\mathbf{x}) \leq 0$. The **Expression** column contains the Python expression for $g(\mathbf{x})$.
11. The **Penalty Factor** contains the coefficient a used in calculating the penalty for a constraint violation, see Equations *[eq.linear.constriant]* to *[eq.step.constriant]*.
12. The **Form** column contains a selection of different methods to calculate a constraint penalty.
13. **Check Input** checks the problem for any mistakes that can be detected before running the optimization.
14. **Variable Explorer** enables the user to browse the variables in the simulation. They can be copied and pasted into the Python expression. The variables are provided without the sample index.

The calculations for each type of constraint penalty are given in Equations *[eq.linear.constriant]* to *[eq.step.constriant]*.

$$\text{Linear penalty form: } p_i = \begin{cases} 0 & \text{if } g_i(\mathbf{x}) \leq 0 \\ a \times g_i(\mathbf{x}) & \text{if } g_i(\mathbf{x}) > 0 \end{cases}$$

$$\text{Quadratic penalty form: } p_i = \begin{cases} 0 & \text{if } g_i(\mathbf{x}) \leq 0 \\ a \times g_i(\mathbf{x})^2 & \text{if } g_i(\mathbf{x}) > 0 \end{cases}$$

$$\text{Step penalty form: } p_i = \begin{cases} 0 & \text{if } g_i(\mathbf{x}) \leq 0 \\ a & \text{if } g_i(\mathbf{x}) > 0 \end{cases}$$

If the Simple Python Expression method of entering the objective function does not offer enough flexibility, the Custom Python method can be used. The Custom Python method enables the user to enter the objective calculation as a Python function, which also should include any required constraint penalties.

Figure *Custom Objective Function* shows the Custom Python objective form. The top text box provides instructions for writing a custom objective function. The bottom text box provides a place to enter Python code. The numpy and math modules have been imported and are available as numpy and math. To use the Custom Python objective, the user must define a function called "onjfunc(x, f, fail)."" The three arguments are: (1) "x" is the dictionary of input variables, (2) "f" is the dictionary of output variables, and (3) "fail" is a boolean vector that indicates whether a particular sample calculation has failed. The "objfunc" function should return three values: (1) a list of objective function values for multi-objective optimization (in most cases with single objective optimization this will be a list with one value), (2) a list of constraint violations, and (3) the total constraint penalty. The constraint violation and penalty information are only used for debugging, so they are not required. It is safe to return [0] and 0 for the constraint information regardless of whether a constraint penalty has been added to the objective.

Fig. 4: Custom Objective Function

The code in Figure fig.opt.problem.objective2_code provides an example of a custom objective function for parameter estimation. The objective function minimizes the sum of the differences between simulation and empirical data. In this case the decision variables would be model parameters. The first line defines a function with three arguments. The "x" and "f" arguments are the input and output variables. The variable indexing is explained in the simple objective function section. The "fail" argument is a boolean vector where element "i" is true if sample "i" failed. If there are no sample variables, "fail" will only have one element.

The "if" in the function determines if any flowsheet evaluation failed, and assigns a bad objective function value if so. If all the flowsheet evaluations where successful, the results are used to calculate the objective function. In the objective function calculation, Python list comprehension is used to calculate the sum of squared errors. In this case, no constraint penalty is needed. The objective function is returned as a list with only one element. The last two return values are debugging information for constraints. In this case, the "zeros" are just place holders and have no real utility.

Solver Options

The **Solver** tab in the **Optimization** button tool enables the selection of the DFO method and setting of solver parameters. Figure *Optimization Solver Form* illustrates the solver form.

Fig. 5: Optimization Solver Form

Elements of the solver form are:

1. **Select Solver** drop-down list, which enables the user to select from available DFO solvers.
2. **Description** text box provides a description of the selected DFO solver.
3. **Solver Options** table contains the solver settings and a description of each option. The settings depend on the selected plug-in.

Running Optimization

The optimization monitor is displayed under the **Run** tab in the **Optimization** button tool. The optimization monitor, illustrated in Figure *Optimization Monitor Form*, is used to monitor the progress of the optimization as it runs.

Fig. 6: Optimization Monitor Form

Elements of the optimization monitor are:

1. **Start** starts the optimization.
2. **Stop** stops the optimization. The best solution found when optimization is stopped is stored in the flowsheet.

3. **Update delay** is how often the user interface communicates with the optimization thread to update the display.
4. **Optimization Solver Messages** displays output from the optimization solver.
5. **Best Solution Parallel Coordinate Plot** displays the values of the decision variables scaled. This plot is helpful in identifying when variables are at, or near, their bounds.
6. **Objective Function Plot** displays the objective function value at each iteration.
7. **Status Box** displays the current iteration, how many samples have been run, how many sample were successful, and how many failed.
8. **Clear** deletes solver messages from the solve message box.

As the optimization runs, the FOQUS flowsheet is updated to include the best solution found. If sampling is used, the first sample in the best objective function is stored in the flowsheet. If for any reason the optimization terminates, the best solution found is available in the flowsheet. The results for all flowsheet evaluations done for the optimization are available in the Results table in the Flowsheet Editor.

4.1.2 Tutorial

Optimization

This tutorial is a step-by-step walk through of simulation-based optimization. This tutorial builds on the tutorial in Section *Creating a Flowsheet with Linked Simulations*.

1. Open FOQUS.
2. Load the FOQUS session from the tutorial "Creating a Flowsheet with Linked Simulations" in Section *Creating a Flowsheet with Linked Simulations* or if that tutorial has not yet been completed, complete it first.

Problem Set Up

If the simulation runs successfully and the results are reasonable, proceed to define the optimization problem. There are four steps to setting up the optimization problem: (1) select the variables, (2) define samples (optional), (3) define the objective function, and constraints and (4) select and configure the solver.

3. Select the **Optimization** button from the toolbar at the top of the Home window (Figure *Optimization Problem Variables*). Select the **Variables** tab.
4. Select "Decision" from the drop-down list in the **Type** column as the variable type for all 17 variables shown. If more than 17 variables are shown, the edge connecting the "BFB" node to the "Cost" node was most likely not configured properly. The scale will automatically change to linear, which is acceptable for most problems.
5. The **Min**, **Max**, and **Value** columns can be changed. The **Min** and **Max** columns define the lower and upper bounds. The **Value** column specifies the initial point. For this example the defaults are acceptable.

Fig. 7: Optimization Problem Variables

If more than one flowsheet evaluation is used in the objective function calculation (e.g., parameter estimation or optimization under uncertainty), the next step is to setup the samples under the **Samples** tab. In this case only one evaluation is used to calculate an objective function value, so the sample setup is not needed. The next step is to define the objective function and constraints using the form under the **Objective/Constraints** tab as shown in Figure *Optimization Problem Objective*.

6. Select the **Objective/Constraints** tab (see Figure *Optimization Problem Objective*).

Fig. 8: Optimization Problem Objective

7. In the drop-down list, verify "Simple Python Expression" is selected.
8. Add an objective function by clicking **+** to the right of the Objective Function table.
9. The objective function is the cost of electricity from the cost spreadsheet. Enter:
   `f.Cost.COE`
   in the **Expression** column.
10. Enter 1 in the **Penalty Scale** column. This setting is used mostly for multi-objective optimization to apply the constraint penalty to different objectives.
11. Enter 500 in the **Value for Failure** column. This should be worse than the objective for any non-failed simulations.
12. Add a constraint by clicking **+** next to the Inequality Constraints table.
13. The constraint is that the fraction of CO_2 captured must be greater than or equal to 0.9. The constraint is in the form $g(\mathbf{x}) \leq 0$; therefore, in the **Expression** column enter:
    `0.9 - f.BFB.removalCO2.`
14. Enter 1000 for the **Penalty Factor**.
15. The constraint penalty **Form** should be linear.
16. The **Variable Explorer** button can be used to help select flowsheet variables.

Solver Settings

The last step before running the optimization is to select and configure the solver. The solver configuration form is shown in Figure *Optimization Solver Setup*.

Fig. 9: Optimization Solver Setup

17. Select the **Solver** tab (see Figure *Optimization Solver Setup*).
18. Select "OptCMA" from the **Select Solver** drop-down list.
19. The default options are acceptable. Solver options are described in the Solver Options table.

Running Optimization

The optimization run form is shown in Figure *Optimization Monitor*.

Fig. 10: Optimization Monitor

20. Click the **Run** tab to display the optimization run form (see Figure *Optimization Monitor*).
21. Click **Start**.
22. Once the optimization has run for while click **Stop**.

As the optimization run, the best result found is stored in the Flowsheet. If an optimization is run with sample variables the first sample in the set with the best objective function will be stored in the flowsheet. All simulation results can be viewed in the Flowsheet Results table.

The run form displays some diagnostic information as the optimization runs. The parts of the display labeled in Figure *Optimization Monitor* are described below.

23. The Optimization Solver Messages window displays information from the solver.
24. The **Best Solution Parallel Coordinate Plot** shows the value of the scaled decision variables, which is useful to see where the best solution is relative to the variable bounds.
25. The **Objective Function Plot** shows the best value of the objective function found as a function of the optimization iteration or sample number.
26. While the optimization is running, the status bar shows the amount of time that has elapsed since starting the optimization.

Parameter Estimation

Note: The NLopt solvers are used for the tutorial, but are an optional to the installation. See the install instructions for more information about installing NLopt.

This tutorial provides a very simple example of using the sampling with optimization. Sampling can be used to do optimization under uncertainty where there are several scenarios with differing values of uncertain parameters. Sampling can also be used to do parameter estimation, where estimated values must be compared against several data points. This tutorial will focus on parameter estimation.

At any point in this tutorial, the FOQUS session can be saved and the tutorial can be started again from that point.

The model is given by Equation *[eq.pe.tut]*. The unknown parameters are a, b, and c. The x and y data are given in Table *x-y Data*.

$$y = ax^2 + bx + c$$

Table 1: x-y Data

Sample	1	2	3	4	5
x	0	1	2	3	4
y	1	0	3	10	21

The first step is to create a flowsheet with one node. The node will have the input variables: a, b, c, x, and ydata; and output variable y.

1. Open FOQUS.
2. In the **Session Name** field, enter “PE_tutorial” (see Figure *Session Setup*).
3. Click the **Flowsheet** button in the top toolbar.

Fig. 11: Session Setup

4. Add a node to the flowsheet named “model.”
   1. Click **Add Node** in the left toolbar (see Figure *Adding Node and Inputs*).
   2. Click anywhere on the gridded flowsheet area.
   3. Select “model” in the **Name** drop-down list and then click **OK**.

5. Click the **Selection Mode** icon in the left toolbar (see Figure *Adding Node and Inputs*).
6. Click the **Node Editor** icon in the left toolbar (see Figure *Adding Node and Inputs*).
7. In the Node Edit input table, add the variables a, b, c, x, and ydata. The ydata variable will be used as an input for the known y sample point data, later in the tutorial.
    1. Click the **Add Input** icon (see Figure *Adding Node and Inputs*).
    2. Enter "a" for the variable name in the **Name** column.
    3. Enter -10 and 10 for the min and max in the **Min** and **Max** columns for a, b, c, and x.
    4. Repeat for all of the inputs.
    5. Enter 1 for the value of a, b, and c in the **Value** column.
    6. Enter 2 for the value of x in the **Value** column.
    7. The **Value**, **Min**, and **Max** for ydata do not matter.

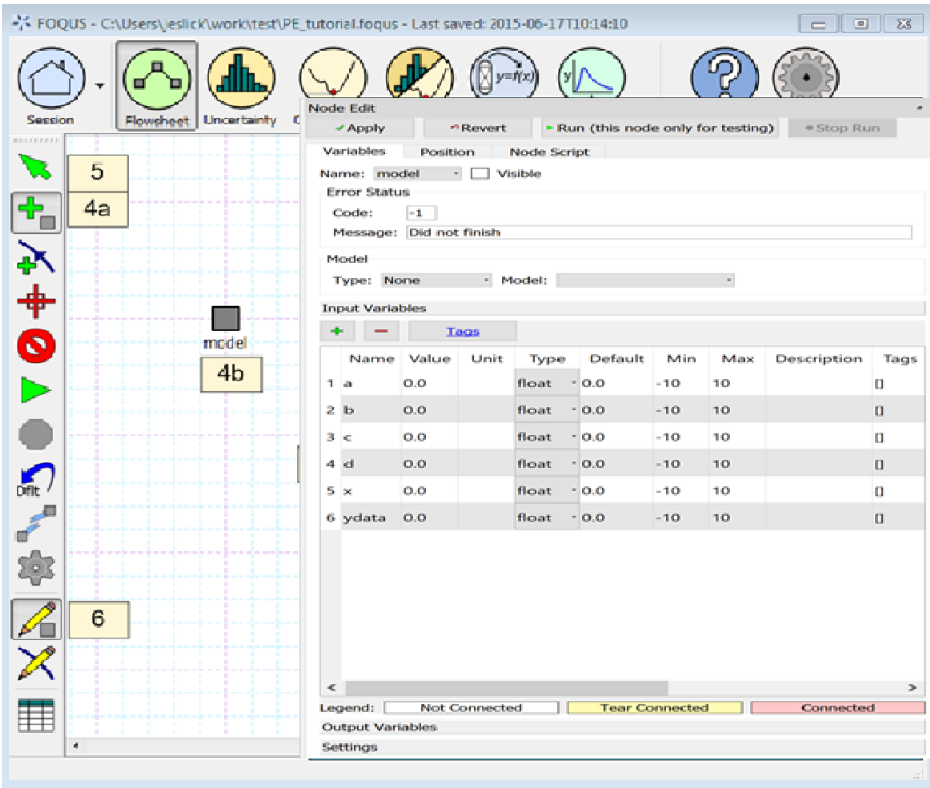

Fig. 12: Adding Node and Inputs

8. Click **Output Variables** (see Figure *Adding Outputs*).
9. Add the output variable y.
    1. Click the **Add Output** icon (see Figure *Adding Outputs*).
    2. Enter "y" for the variable name in the **Name** column.

Fig. 13: Adding Outputs

10. Add the model equation to the node.

    1. Click the **Node Script** tab.
    2. Enter the following code in the calculations box:

    ```
    f['y'] = x['a']*x['x']**2\
     + x['b']*x['x'] + x['c']
    ```

Fig. 14: Adding Node Calculation

11. Return to the Output Variables table in the Node Editor, by clicking on the **Variables** tab, and selecting **Output Variables**.
12. Click **Run** in the left toolbar in the FOQUS Home window, to test a single flowsheet evaluation and ensure there are no errors.
13. When the run is complete, there should be no error and the value of y should be 7 in the Output Variables table.

The next step is to setup the optimization. The objective function is to minimize the sum of the squared errors between the estimated value of y and the observed value of y. There are five data points in Table *x-y Data*, so there are five flowsheet evaluations that need to go into the calculation of the objective.

14. Click the **Optimization** button in the top toolbar of the Home window (see Figure *Optimization Variables*).
15. Select "Decision" in the **Type** column drop-down lists for "model.a," "model.b," and "model.c." The **Scale** column will automatically be set to linear.
16. Select "Sample" in the **Type** column drop-down lists for "model.x" and "model.ydata."

Fig. 15: Optimization Variables

The decision variables in the optimization problem will be changed by the optimization solver to try to minimize the objective, and the sample variables are used to construct the samples that will go into the objective function calculation.

17. Select the **Samples** tab (see Figure *Optimization Samples*).
18. Click **Add Sample** five times to add five samples.
19. Enter the data from Table *x-y Data* in the Samples table.
20. For larger sample sets, **Generate Samples** has an option to load from a CSV file.

Fig. 16: Optimization Samples

The objective function is the sum of the square difference between y and ydata for each sample in Table *x-y Data*. The optimization solver changes the a, b, and c to minimize the objective.

21. Click the **Objective/Constraints** tab.
22. Click the **Add Objective** icon on the right side of the Objective Function table (see Figure *Objective Function*).
23. In the **Expression** column, enter the following (without the line break):

    ```
    sum([(f[i]['model']['y'] - x[i]['model']['ydata'])**2
     for i in range(len(x))])
    ```

    The above expression uses Python list comprehension to calculate the sum of squared errors. The keys for x and f are: sample index, node name, variable name, time step.

24. Enter 1 for the **Penalty Scale**.
25. Enter 100 for the **Value for Failure**.
26. No constraints are required.

Fig. 17: Objective Function

Once the objective is set up, a solver needs to be selected and configured. Almost any solver in FOQUS should work well for this problem with the default values.

27. Click the **Solver** tab (see Figure *Optimization Samples*).
28. Select "NLopt" from the **Select Solver** drop-down list. NLopt is a collection of solvers that share a standard interface *(Johnson 2015)*.
29. Select "BOBYQA" under the Solver Options table in the **Settings** column drop-down list.

Fig. 18: Optimization Samples

30. Click the **Run** tab (see Figure *Running Optimization*).
31. Click the **Start** button.
32. The Optimization Solver Messages window displays the solver progress. As the solver runs, the best results found is placed into the flowsheet.
33. The **Best Solution Parallel Coordinate Plot** shows the scaled decision variable values for the best solution found so far.
34. The **Objective Function Plot** shows the value of the objective function as the optimization progresses.

Fig. 19: Running Optimization

The best result at the end of the optimization is stored in the flowsheet. All flowsheet evaluations run during the optimization are stored in the flowsheet results table.

35. Once the optimization has completed, click **Flowsheet** in the top toolbar.
36. Open the **Node Editor** and look at the **Input Variables** table. The approximate result should be a = 2, b = -3, and c = 1 (see Figure *Flowsheet, Input Variables Results*).

Fig. 20: Flowsheet, Input Variables Results

CHAPTER 5

Uncertainty Quantification

5.1 Contents

[sec:uq_overview]

5.1.1 Reference

The Uncertainty Quantification (UQ) module of FOQUS provides a multitude of analysis and visualization capabilities to facilitate the understanding of uncertainty's impact on a given system. In a generic UQ study, the workflow is usually comprised of the following steps:

1. Define the objectives of the analysis.
2. Specify and acquire the simulation model, which implements an input-to-output mapping from inputs to outputs.
3. Select the inputs that have uncertainty and characterize said uncertainty in the form of *prior* distributions.
4. Identify relevant data from physical experiments that can be used to refine these prior distributions on the inputs.
5. Generate a set of input samples according to the input distribution.
6. Propagate the set of input samples through the simulation model to get the corresponding output values.
7. Analyze the results to make informed decisions about subsequent analyses.

FOQUS UQ provides tools to perform Steps 5-7. With respect to Step 7, a variety of analysis capabilities are available. They include parameter screening methods, response surface construction/validation/prediction, uncertainty analysis, sensitivity analysis, and visualization.

In this chapter, components of the UQ user interface are first explained, then the use of these components for UQ analyses is illustrated.

UQ User Interface

The UQ module enables the user to perform UQ studies on a flowsheet. From the Uncertainty button on the Home window, the user can configure different simulation ensembles (different sets of samples generated using different sampling schemes), run them, and perform analyses. This screen is illustrated in Figure *[fig:uq_screen]*.

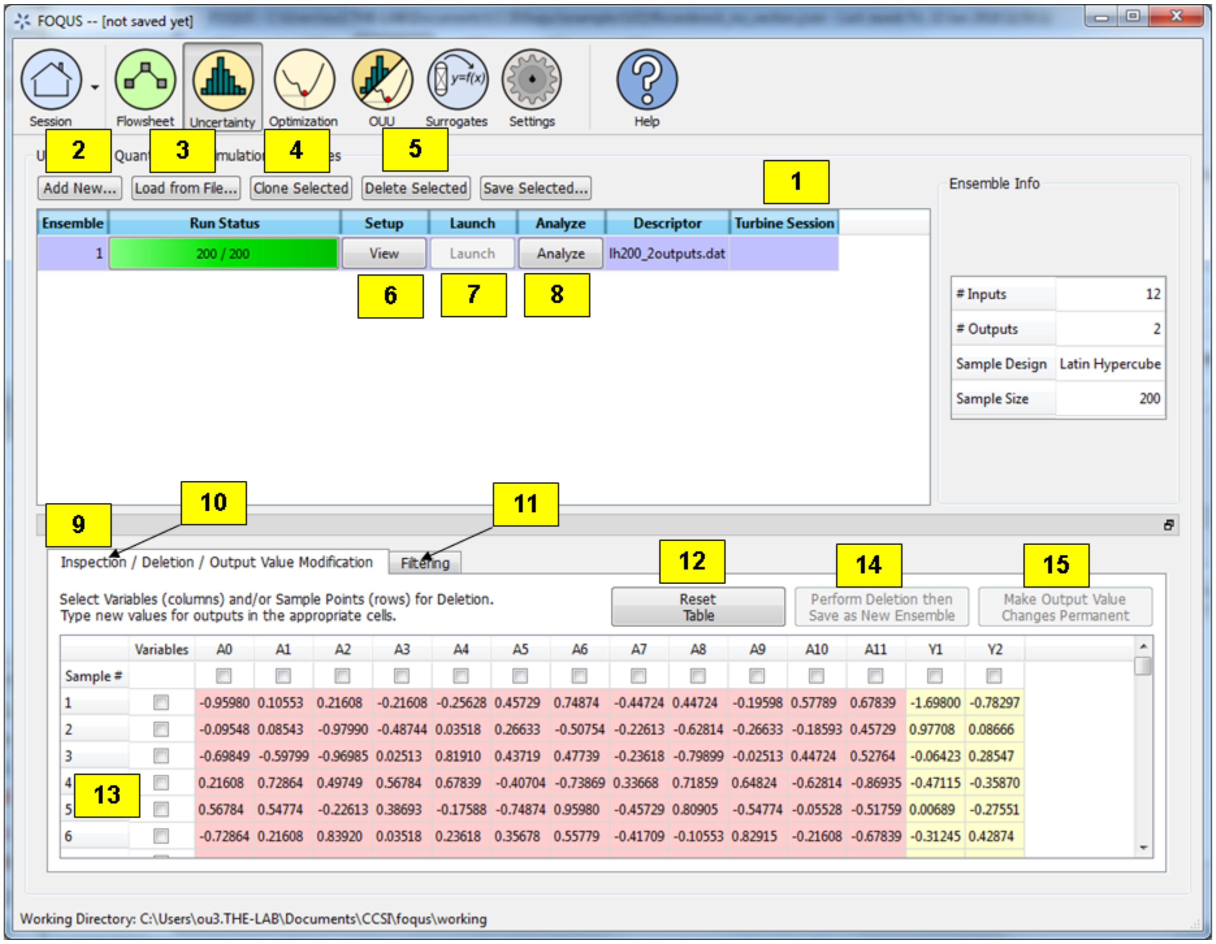

Fig. 1: Uncertainty Quantification Screen

[fig:uq_screen]

1. **Simulation Ensemble Table** displays all of the simulation ensembles: each ensemble being a row in the table. A simulation ensemble is a collection of sample points where each sample point has a different set of values for the uncertain variables. The values of these variables are generated based on the sampling scheme designated by the user. When launched, the output values of the sample points are calculated based on the generated sample input values. Subsequently, the corresponding simulation outputs can be analyzed. For each ensemble, the table displays the **Ensemble** index, **Run Status** (how many have been completed), **Setup** and **Launch** options (discussed below), and a **Descriptor**. The **Descriptor** contains the name of the corresponding node in the flowsheet or the name of the file if the ensemble was loaded from a file. Additional sample information such as **# Inputs**, **# Outputs**, **Sample Design**, and **Sample Size** are also displayed on the right.

2. **Add New** creates a simulation ensemble (a set of input samples) as a new row in the **Simulation Ensemble Table**. Once clicked, a dialog is displayed to prompt the user to choose between using (1) a flowsheet (an exact simulation model) or (2) a response surface (an approximate simulation model or an emulator) associated with the ensemble.

If using an emulator, the user must browse a PSUADE-formatted file that contains the training data for the emulator (in this version, the response surface type has been designated inside the sample file and can only be changed by editing the sample file) and select the output(s) to be evaluated by the trained emulator. Subsequently, a simulation setup dialog box is displayed for setting up the distributions of input variables and the sampling scheme to generate samples of the uncertain input variables. This **Simulation Ensemble Setup** dialog is explained in further detail in Section *1.1*.

3. **Load from File** loads a simulation ensemble from a sample file that conforms to the PSUADE full file format. (See Section *[ap:psuadefiles]* for details on the PSUADE full file format.) The user can click **Save Selected** to save an existing ensemble as a PSUADE full file, and load it by clicking **Load from File** to perform further analyses.
4. **Clone Selected** clones the selected simulation ensemble and adds the copy as a new row at the end of the table. This ensemble can then be edited (e.g., depending on whether the ensemble has been run, the user has different options for modifying the ensemble). This allows the user to create a new ensemble similar to the current ensemble without having to start from scratch (i.e., setting up the input parameters). For example: (1) **Clone Selected** can be used in conjunction with **Load from File** to clone an existing ensemble before input/output modification to prepare a new but similar ensemble for UQ analysis. (2) **Clone Selected** can also be used to prepare a fresh ensemble for evaluation via a different simulation model. In this case, the user should save the cloned ensemble, reload it by clicking **Add New**, associate it with a node, and then click **Launch** to start the runs.
5. **Delete Selected** deletes the currently selected simulation ensemble.
6. **Revise** enables a user to change a simulation ensemble before launching the run. If the ensemble was previously run or it is cloned from an already-generated sample, the corresponding button becomes **View** so the user can view the input samples in the simulation ensemble.
7. **Launch** starts the simulation process of the ensemble. (**Launch** is not enabled until the user has setup everything needed for simulations.) A simulation is launched for each sample point to compute the corresponding outputs.
8. **Analyze**, when enabled (after all simulation results are ready), enables the user to perform various UQ analysis to the ensemble. When clicked, a new dialog box displays, allowing the user to configure and run analysis.
9. **Data Manipulation** enables (1) the deletion of inputs, outputs, or samples, (2) the modification of output values for specific sample points, and (3) the range-based filtering of samples.
10. **Inspection/Deletion/Output Value Modification** serves three purposes: it enables the user to (1) view the numerical values of samples in table form, (2) delete variables and/or samples, and (3) edit the output values of specific samples. **Deletion** creates a new simulation ensemble as a new row in the simulation table that contains only those inputs/outputs and samples that were not selected for deletion. **Output Value Modification** changes the values within the ensemble itself.
11. **Filtering** enables the user to filter samples based on the values of an input or output. First, select the ensemble to be filtered from the **Simulation Ensemble Table**. Once filtering is complete, a new simulation ensemble is added as a new row in the simulation table. The new simulation ensemble contains only those samples that satisfy the filtering criterion (with input or output samples within the specified range).
12. **Reset Table** resets the table to default, meaning all variable and sample selections are unselected and output values within the table are reverted back to their original values, thus undoing any edits to the table.
13. The table displays the values of inputs and outputs for each sample. Inputs are highlighted in pink; outputs are highlighted in yellow. The user can select which variables (columns) to delete by selecting the checkboxes on top. Likewise, the user can select which samples (rows) to delete by selecting the checkboxes on the left. Multiple samples can also be selected/deselected by using (1) Shift+Click or Ctrl+Click to select multiple rows, or (2) right-clicking to bring up a menu to check or uncheck the checkboxes corresponding to the rows of the selected samples. In addition, the user can change any output value by editing the appropriate cell. These modified cells are highlighted green until changes are made permanent by clicking the appropriate button.

14. **Perform Deletion then Save as New Ensemble** creates a new simulation ensemble as a new row in the **Simulation Ensemble Table**. The new ensemble is without the variables and samples that were previously selected for removal.

15. **Make Output Value Changes Permanent** overwrites the output values in the current ensemble with those that are highlighted green in the table.

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    The **Filtering** tab is illustrated in Figure *[fig:uq_deltab]* and enables the user to filter samples based on the values of an input or output.

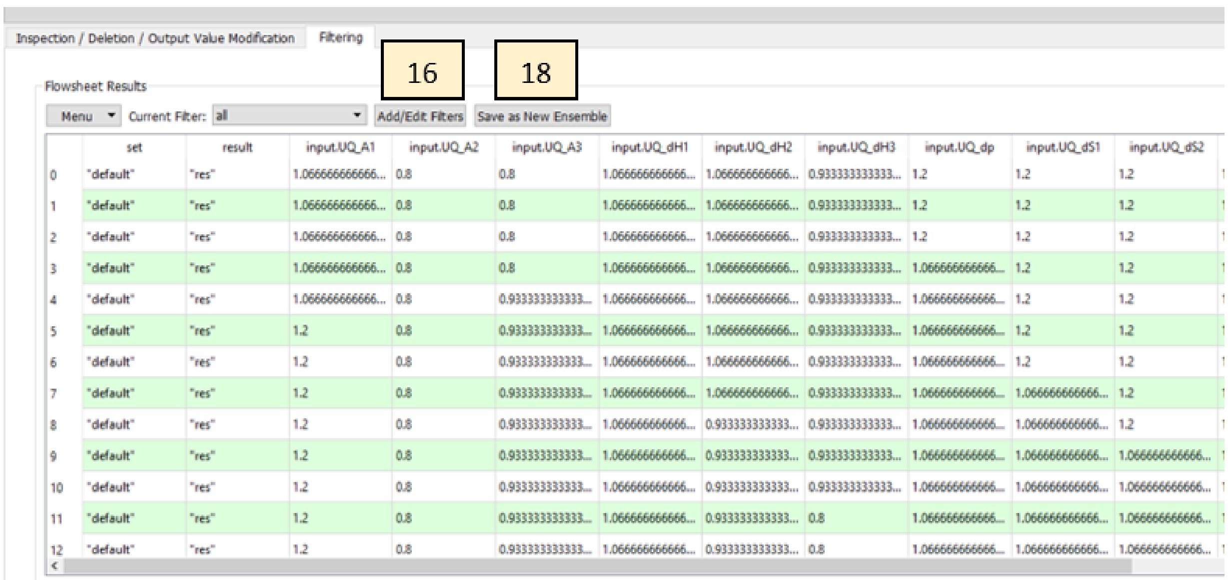

Fig. 2: Filtering Tab

[fig:uq_deltab]

enumerate

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16. Click on Add/Edit Filters, in the Flowsheet Results window within the "Filtering Tab"

17. 1. Within the Filter Dialog Box, Click on "New Filter" to add a filter
    2. Enter a filter expression in python format. Variables can be dragged into the expression, from the "Columns", click Done.

18. Select a "Current Filter" after which the the filtered ensemble can be saved by clicking on " Save as New Ensemble"

    The single-output **Analysis of Ensemble** dialog, which is displayed when **Analyze** is clicked for the selected ensemble, has two modes, as shown in Figure *[fig:uq_analysisW]* and Figure *[fig:uqt_rsaeua]*.

    [fig:uq_analysisW]

    enumerate

19. Select **Wizard** or **Expert** mode. The **Wizard** mode provides more detailed guidance on how to perform UQ analysis. For users familiar with UQ analysis techniques, the **Expert** mode provides more functionality and flexibility but with less guidance on its use. For example, users will be able to customize the input distributions, as well as run more advanced uncertainty analysis that handles both epistemic and aleatory uncertainties.

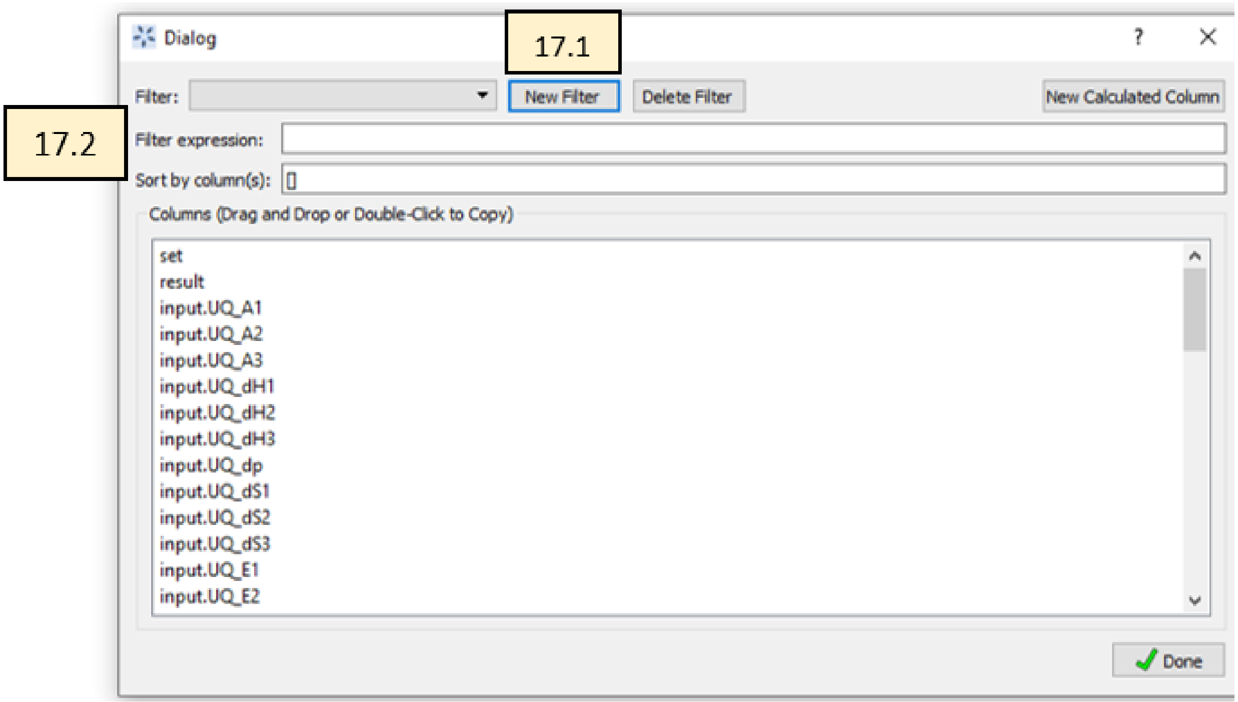


Fig. 3: Filtering Dialog Box

20. The **Analyses Performed** section provides the user a history of previous analyses that were performed. The results of these analyses are cached, so the user can plot the analysis results without having to recompute them.
21. The **Analysis Table** populates as the user performs analyses. It lists previous analyses that the user has performed, along with some of the main analysis settings (analysis type, inputs and outputs analyzed, etc.)
22. Depending on the type of analysis performed, the **Additional Info** button displays any additional settings or parameters set by the user in the selected analysis that were not shown in the **Analysis Table**.
23. The **Results** button will display the results of the selected analysis.
24. The **Delete** button will delete the selected analysis from the history of previous analyses. Once deleted, the user will need to perform the analysis again to see its results.
25. The **Qualitative Parameter Selection** (top part of the **Analysis of Ensemble** dialog) houses the controls for parameter selection analysis. Parameter selection is a qualitative sensitivity analysis method that identifies a group of dominant input parameters that are recommended for inclusion in subsequent UQ analyses, as they are the ones that most impact the output uncertainty. The parameter screening results are shown as bar graphs so that the user can rank the uncertain parameters visually.
26. Before performing parameter selection, the user must select a single output for identifying parameter sensitivities from the **Choose output to analyze** drop-down list.
27. There are several methods of parameter selection. The list of parameter selection methods available depends on the sample scheme of the selected ensemble. Select the appropriate method from the **Choose Parameter Selection Method** drop-down list. Then click **Compute input importance** to start the analysis.
28. The **Ensemble Data** radio button directs FOQUS to perform analyses on the raw ensemble data.
29. To view plots of the raw ensemble data, choose the desired input(s) from the **Select the input(s)** drop-down lists. Then click **Visualize**. If multiple inputs are selected, each must be unique.
30. To perform an analysis, select the desired analysis ("Uncertainty Analysis" or "Sensitivity Analysis") from the

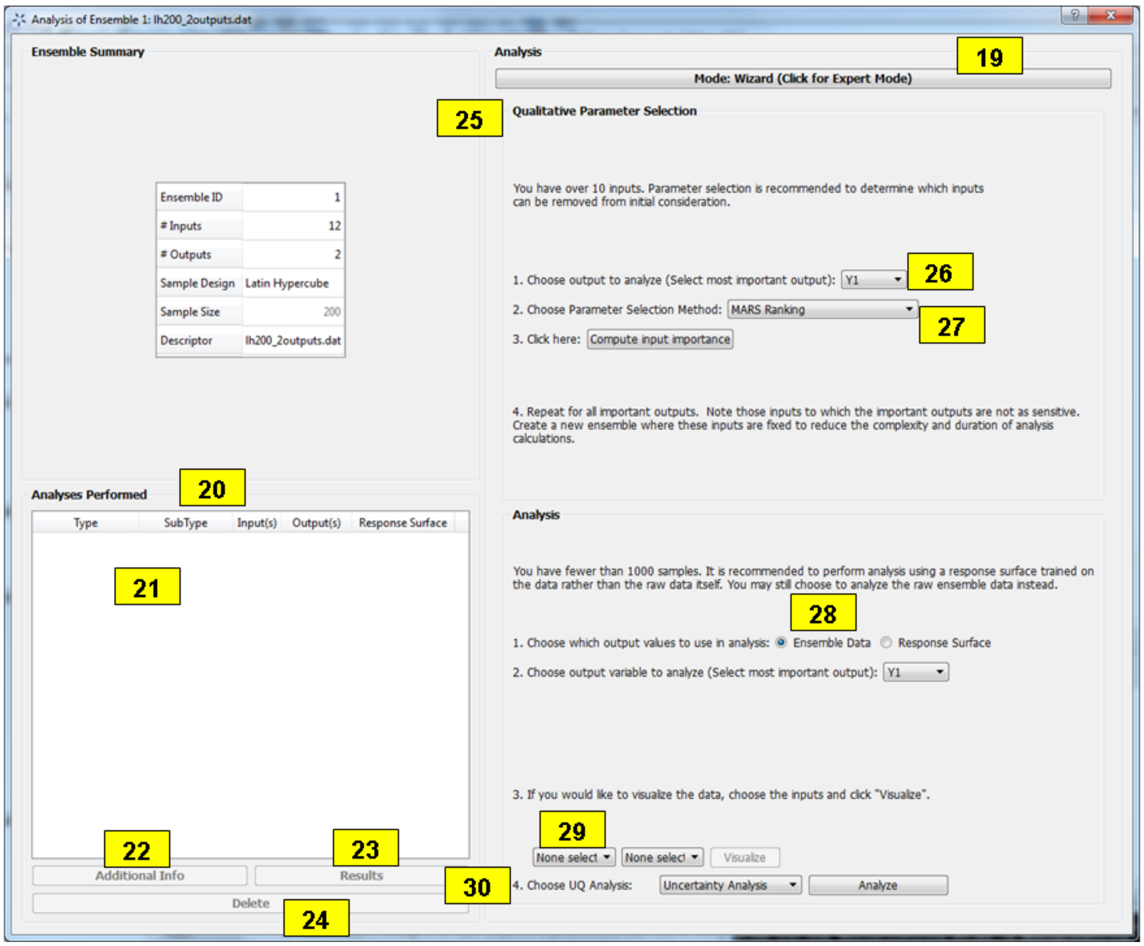


Fig. 4: Analysis Dialog, Ensemble Data Analysis, Wizard Mode

Choose UQ Analysis drop-down list. Uncertainty Analysis computes and displays the probability distribution of the single selected output parameter and displays its sufficient statistics, such as mean, standard deviation, skewness, and kurtosis. Sensitivity Analysis computes and displays each uncertain input parameter's contribution to the total variance of the output. If Sensitivity Analysis is selected, choose the type of sensitivity analysis desired in the next drop-down list. There are three options for Sensitivity Analysis: (1) first-order, (2) second-order, and (3) total-order.

- First-order analysis examines the effect of varying an input parameter alone.
- Second-order analysis examines the effect of varying pairs of input parameters.
- Total-order analysis examines all interactions' effect of varying an input parameter alone and as a combination with any other input parameters.

Click **Analyze** to run the analysis. (Note: Raw ensemble data analysis may not be suitable if the sample size is small. It may be useful if the data set has tens of thousands of sample points or if an adequate response surface cannot be constructed. Otherwise, response surface-based analyses are recommended.)

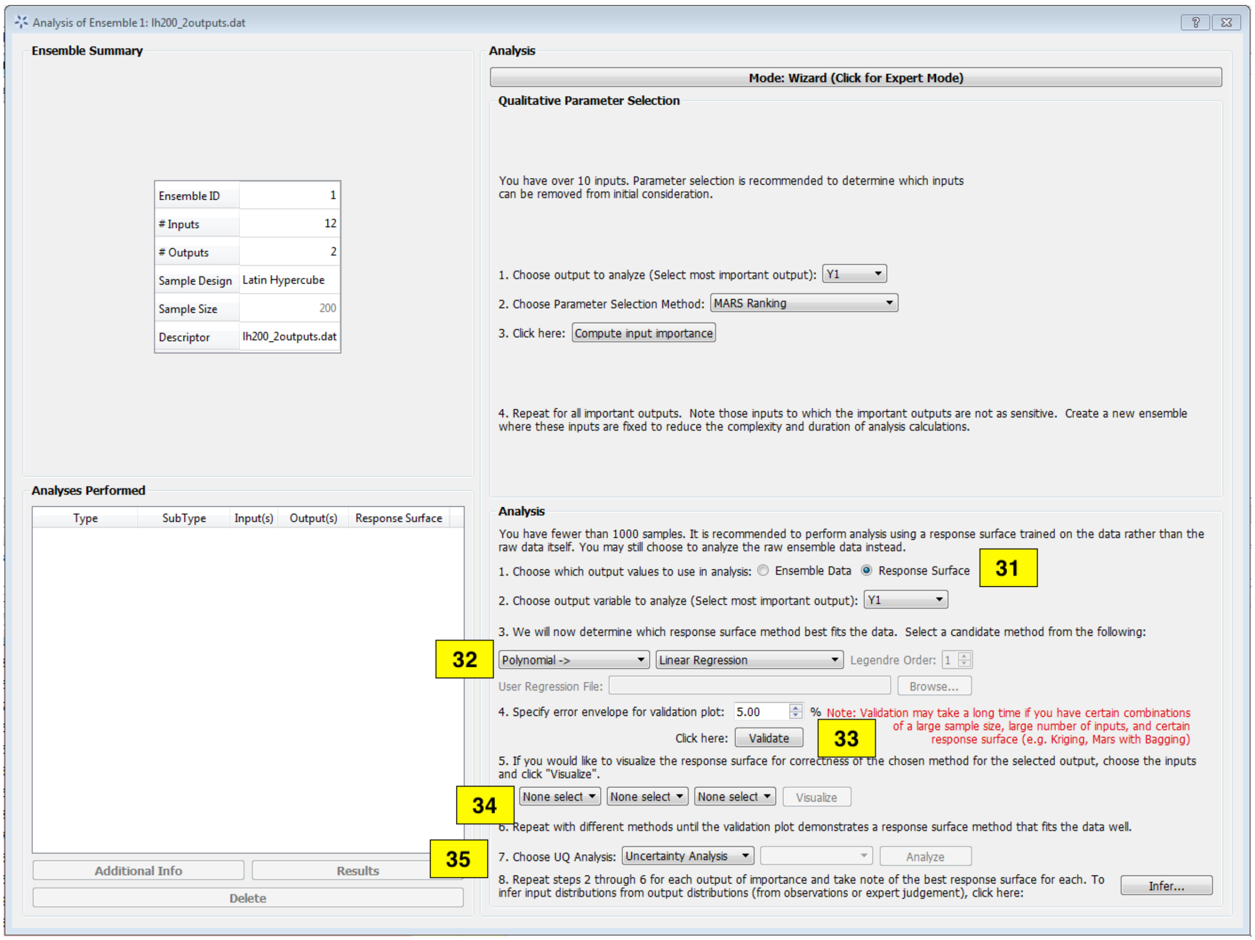


Fig. 5: Analysis Dialog, Response Surface Analysis, Wizard Mode

[fig:uq_analysisW2]

[itm:uq_analysis]

31. **Response Surface** enables the user to perform all analyses related to response surfaces. A response surface is an approximation of the input-to-output relationship. This is an inexpensive way to approximate the values of outputs given different input values when the actual simulation of output values is computationally intensive.

FOQUS uses the data (i.e., input-output samples) to fit a response surface scheme. The first step in this analysis is to select which output to analyze.

32. Select the **Response Surface Model** to be used to approximate the input-to-output mapping. Selection of "Polynomial" or "MARS" requires one further selection in the second drop-down list. If "Polynomial" is chosen in the first drop-down list and "Legendre" is chosen in the second drop-down list, the user needs to specify a number for the **Legendre polynomial order** before analysis can proceed. [itm:uq_rs]
33. The response surface selected must be validated before further analyses can be performed. The user can specify the error envelope for the validation plot. When **Validate** is clicked, the resulting plots display the best fit between the response surface (based on the model selected) and the actual data.
34. **Choose UQ Analysis** enables the user to perform response-surface-based UQ analyses. Select the analysis in the first drop-down list. If the desired analysis is Sensitivity Analysis, select the desired type of sensitivity analysis in the second drop-down list and then click **Analyze**. **Uncertainty Analysis** and **Sensitivity Analysis** compute and display the same quantities as in item #*[itm:uq_analysis]*. However, the results displayed are based on samples drawn from the trained response surface, not the simulation ensemble itself. Moreover, if the selected response surface has uncertainty, the resulting plots also reflect this uncertainty information.
35. FOQUS also provides visualization capabilities, enabling the user to view the response surface as a function of one or multiple inputs. Up to three inputs can be visualized at once. Click **Visualize** to view. A 2-D line plot displays if only one input parameter is selected. A 3-D surface plot and a 2-D contour plot display if two input parameters are selected. A 3-D isosurface plot with a slider bar displays if three input parameters are chosen. For the isosurface plot, the user can use the slider to selectively display the 3-D input parameter space that activates a particular range in the output parameter.

    Finally, the **Bayesian Inference of Ensemble** dialog (shown in Figure *[fig:uq_inf]*) is used to calculate the posterior distributions (prior distributions integrated with data) of the uncertain input parameters. Inference utilizes Markov Chain Monte Carlo (MCMC) to compute the posterior distributions, using response surfaces that serve as fast approximations to the actual simulation model.

    [fig:uq_inf]

    enumerate

36. Inference uses a response surface to approximate the input-to-output mapping. In **Output Settings**, select the observed outputs and select the response surface type that works best with each observed output. As in item (*[itm:uq_rs]*), further selections may be required based on the response surface chosen. The simulation ensemble is used as the training data for generating the response surfaces.
37. The user can specify which inputs are fixed, design (fixed per experiment, but changes between experiments), or variable using the **Input Settings Table**. In addition, the user can specify which inputs are displayed in the resulting plots of the posterior distributions. By default, once inference completes, all inputs will be displayed in the plots. To omit specific inputs, clear the checkboxes from the **Display** column of the table. Finally, in **Expert** mode, this table can also be used to modify the input prior distributions. The default prior is the input distribution specified in the simulation ensemble. To change the prior distribution type, use the drop-down list in the **PDF** column and enter corresponding values for the PDF parameters. To change the range of a uniform prior, scroll all the way to the right to modify **Min/Max**.
38. The **Observations** section enables the user to add experimental data in the form of observations of certain output variables. At least one observation is required. Currently, the observation noise model is assumed to be a normal distribution. Other distributions may be supported in the future. To specify the observation noise model, enter the mean (and standard deviation, if standard inference is selected) for each output observation. For convenience, the **Mean** and **Standard Deviation** fields have been populated with the statistics from the ensemble uncertainty analysis. If any inputs are selected as design inputs, their values will also be required here.
39. **Save Posterior Input Samples to File** checkbox, when selected, saves the posterior input samples as a PSUADE sample file (format described in Section *[ap:psuadefiles]*). This file characterizes the input uncertainty as a set of

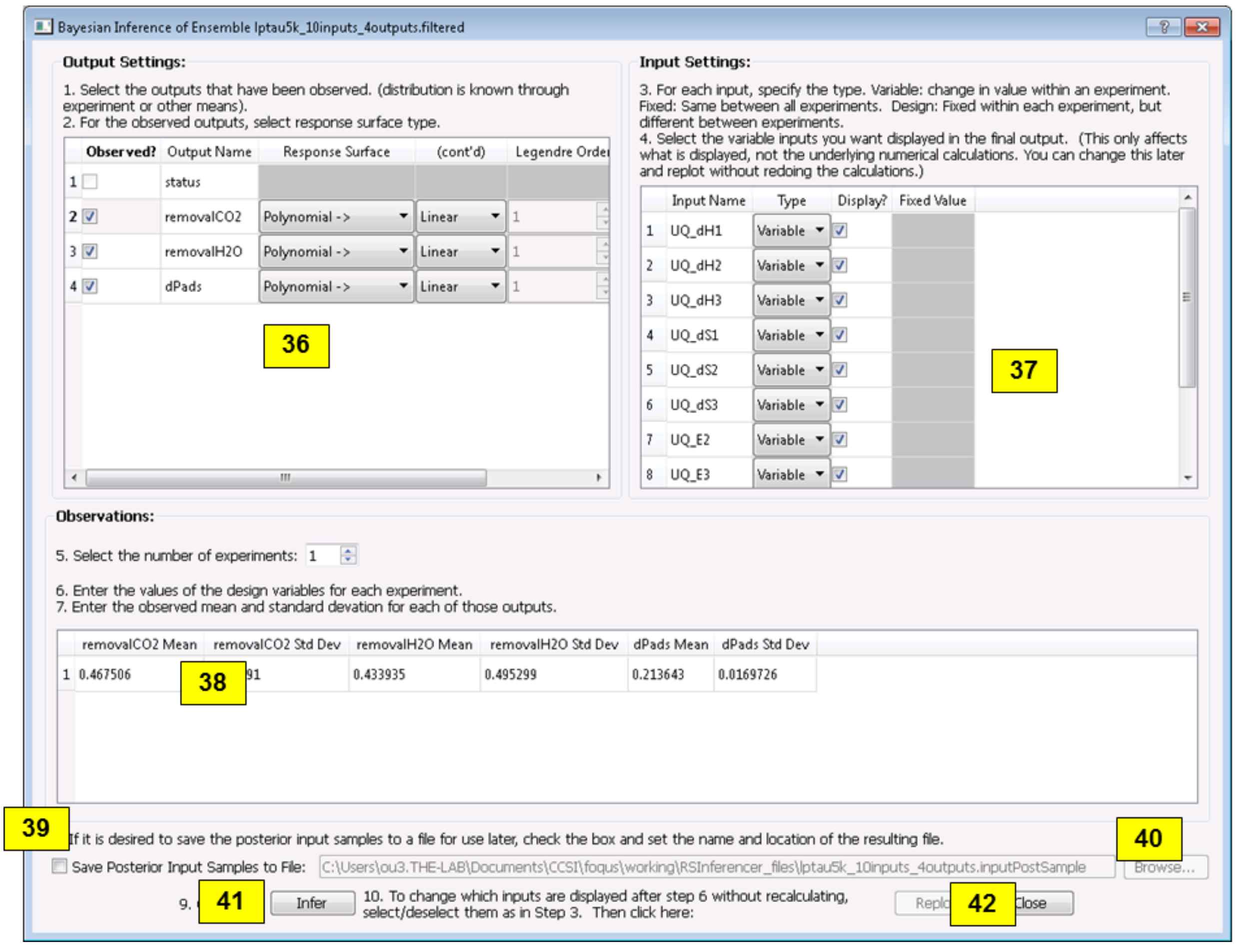


Fig. 6: Bayesian Inference Dialog

samples, which can be re-used in the **Simulation Ensemble Setup** dialog, to evaluate the outputs corresponding to these posterior input samples.

40. If saving posterior samples to a file, click **Browse** to set the name and location of where this file is saved.
41. Click **Infer** to start the analysis. (Note: If the inference returns an invalid posterior distribution (i.e., one with no samples), it usually means the prior distributions or that the observation data distributions are not prescribed appropriately. In this case, it is recommended that the user experiment with different priors and/or data distribution means and/or standard deviations.)
42. Inference calculations often take a very long time. If inference has run to completion, use Replot to generate new plots (e.g., to only display a subset of the input posterior graphs) from the cached inference results.

Simulation Ensemble Setup Dialog

The **Simulation Ensemble Setup** dialog (shown in Figure *[fig:uq_sim_dist]*) is used to create a new simulation ensemble. This is done by: (1) setting up distribution parameters and generating samples, or (2) loading samples from a file. This dialog is displayed when selecting **Add New** on the UQ window (Figure *[fig:uq_screen]*).

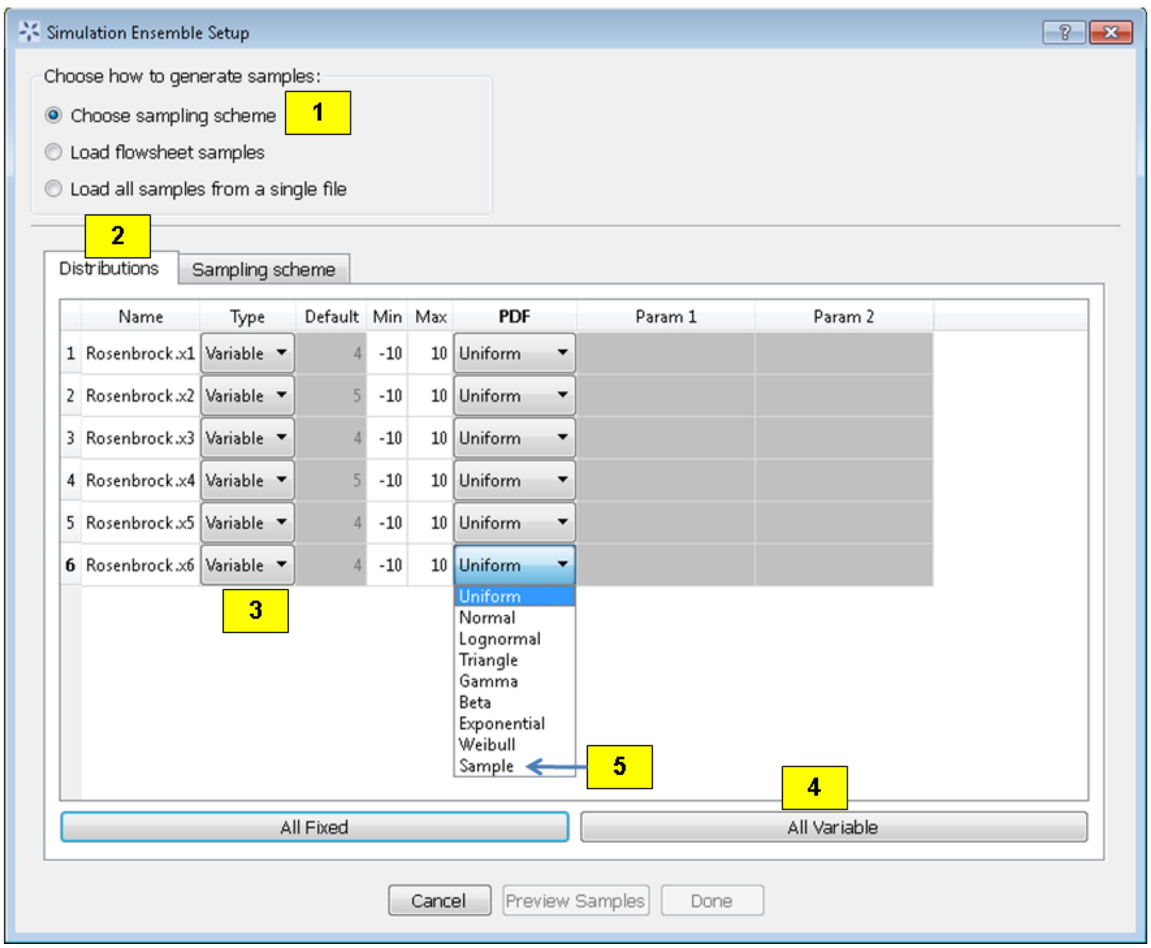


Fig. 7: Simulation Ensemble Setup Dialog, Distributions Tab

[fig:uq_sim_dist]

1. Choose how to generate samples. There are three options: (1) **Choose sampling scheme** (default), (2) **Load flowsheet samples**, or (3) **Load all samples from a single file**. The option 3 is explained in item

(*[itm:uq_sim_last]*). [itm:uq_sim_first]

2. If **Choose Sampling Scheme** is selected, the **Distributions** tab is displayed. The user specifies the input uncertainty information.
3. The **Distributions Table** is pre-populated with input variable information gathered from the flowsheet node. Under the **Type** column drop-down list, the user can select "Fixed" or "Variable". Selecting "Fixed" means that the input is fixed at its default value for all the samples. Changing the type to "Variable" means that the input is uncertain; therefore, its value varies between samples. With any fixed input, the only parameter that can be changed is the **Default** value (i.e., all samples of this input are fixed at this default value). With any variable input, the **Min/Max** values, as well as the probability distribution function (**PDF**), for that input can be changed. Some PDFs have their own parameters (e.g., mean and standard deviation for a normal distribution), which are required in the columns right of the distribution column. See the PSUADE manual for more details on the different PDFs.
4. **All Fixed** and **All Variable** are convenient ways to set all the inputs to variable or fixed.
5. Note: A "Sample" PDF refers to sampling with replacement (i.e., input samples would be randomly drawn, with replacement, from a sample file). If the selected distribution for any input is "Sample", then the following parameters are required: (1) the path of the sample file (which must conform to the sample format specified in Section *[ap:psuadefiles]*); (2) the output index that designates which output is to be used.
6. In the **Sampling scheme** tab (Figure *[fig:uq_sim_samplescheme]*), specify the sampling scheme, the sample size, and perform sample generation.

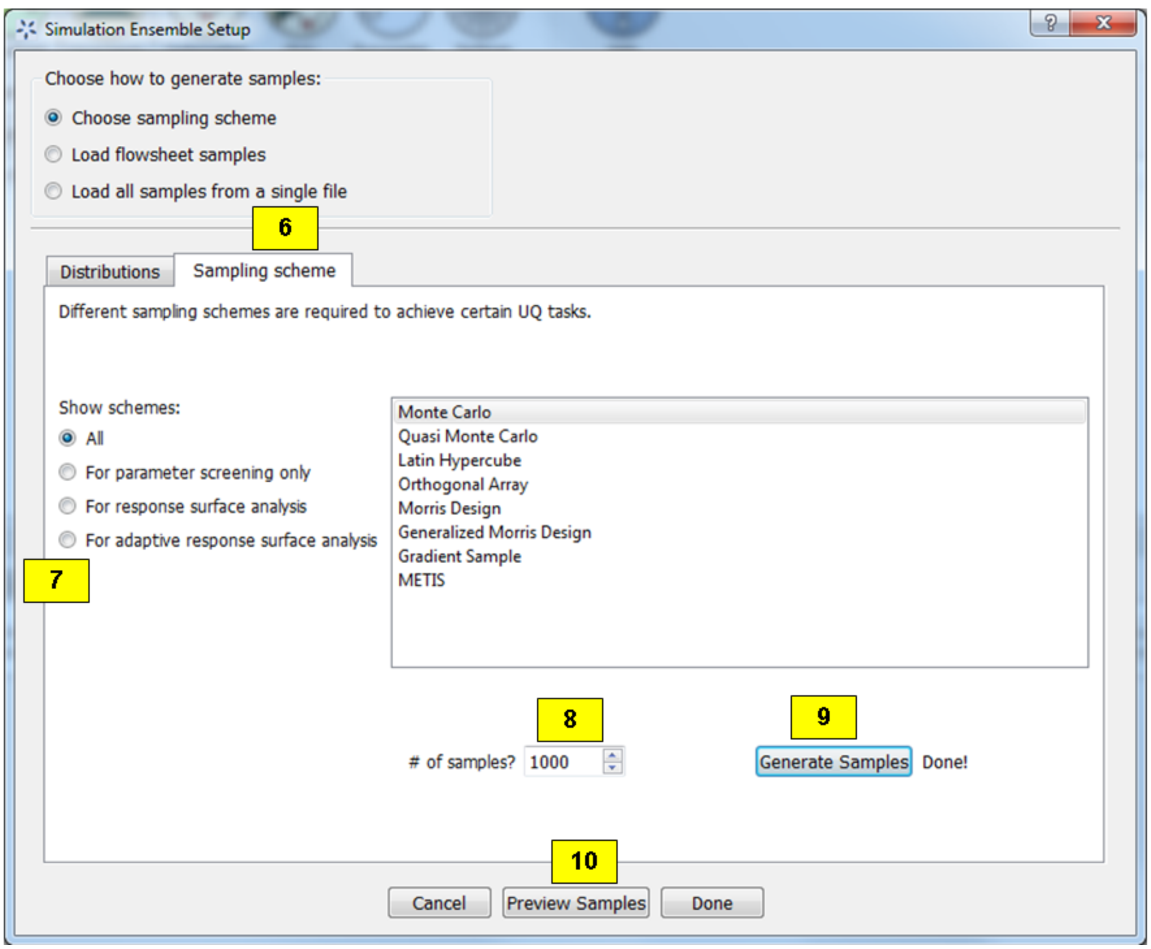


Fig. 8: Simulation Ensemble Setup Dialog, Sampling Scheme Tab

[fig:uq_sim_samplescheme]

7. Each radio button displays a different list of sampling schemes on the right. The radio buttons serve as a guide to help in the selection of the appropriate sampling schemes for target analyses. A sampling scheme must be selected from the list on the right to proceed.
8. Set the number of samples to be generated from the **# of samples** spinbox.
9. When all parameters are set, click **Generate Samples**. This generates the values for all the input variables, based on the sampling scheme selected.
10. Once samples have been generated, click **Preview Samples** to view the samples that were generated. This displays the sample values in table form, as well as graphically as a scatter plot.
11. From item (*[itm:uq_sim_first]*), if the user elects to load all samples from a single file, click **Browse** to select the file containing the samples (Figure *[fig:uq_sim_loadsample]*). This file must conform to the PSUADE full file format, the PSUADE sample format, or CSV file (all formats described in Section *[ap:psuadefiles]*). Note: This is the only place where all the formats are supported. Once the file is loaded, the file name displays in the text box. These samples can now be used in the same way as an ensemble that was newly generated (as described above).

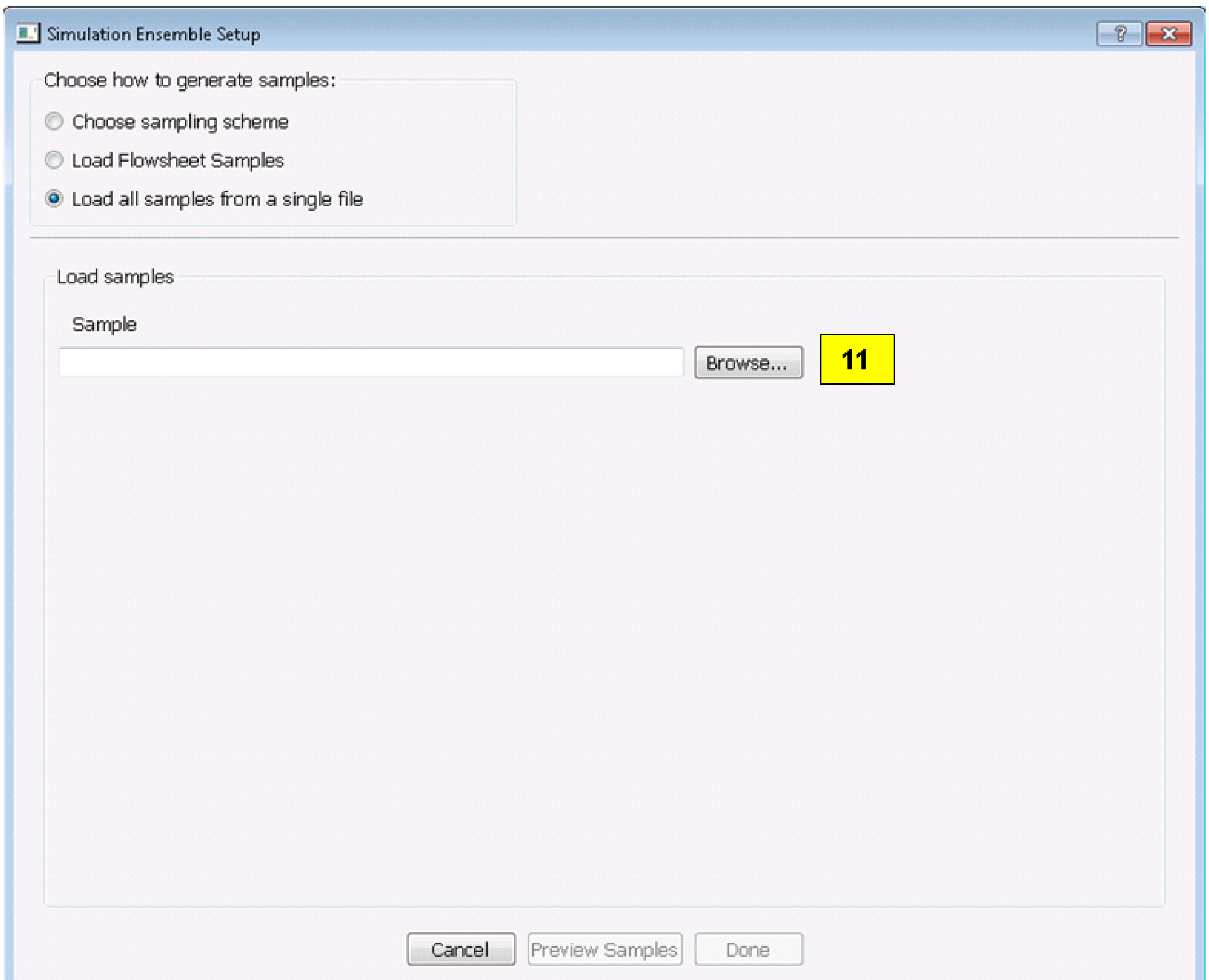


Fig. 9: Simulation Ensemble Setup Dialog, Load Samples Option

[fig:uq_sim_loadsample]

[itm:uq_sim_last]

5.1.2 Tutorial

This section contains five tutorials that illustrate the use of FOQUS UQ to facilitate the UQ workflow discussed above.

Each tutorial will refer to example files located in the examples directory of the FOQUS download.

Simulation Ensemble Creation and Execution

In this tutorial, a simulation ensemble is created and run.

1. From the FOQUS main screen, click the **Session** button and then select **Open Session** to open a session. Browse to the examples folder, go into the UQ subfolder, and then select the "Rosenbrock_novectors.foqus" problem (Figure *Home Screen*).

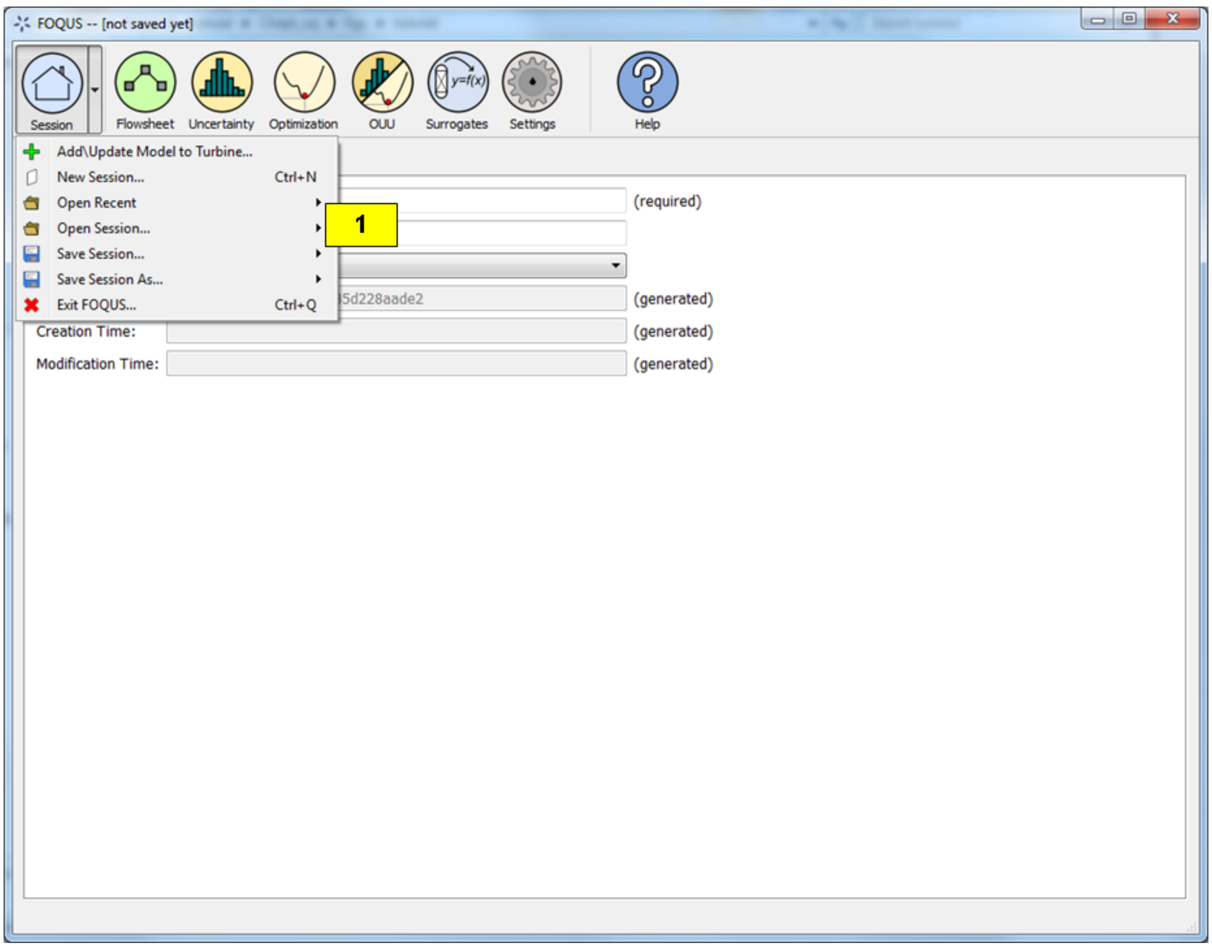


Fig. 10: Home Screen

2. Opening this file loads a session that has a flowsheet with one node (Figure *Flowsheet for Rosenbrock Example*). See Section *Creating a Flowsheet* for a detailed example of creating a flowsheet.

3. Click the **Uncertainty** button (Figure *Uncertainty Quantification Screen*).

4. Click Add New to create a new simulation ensemble.

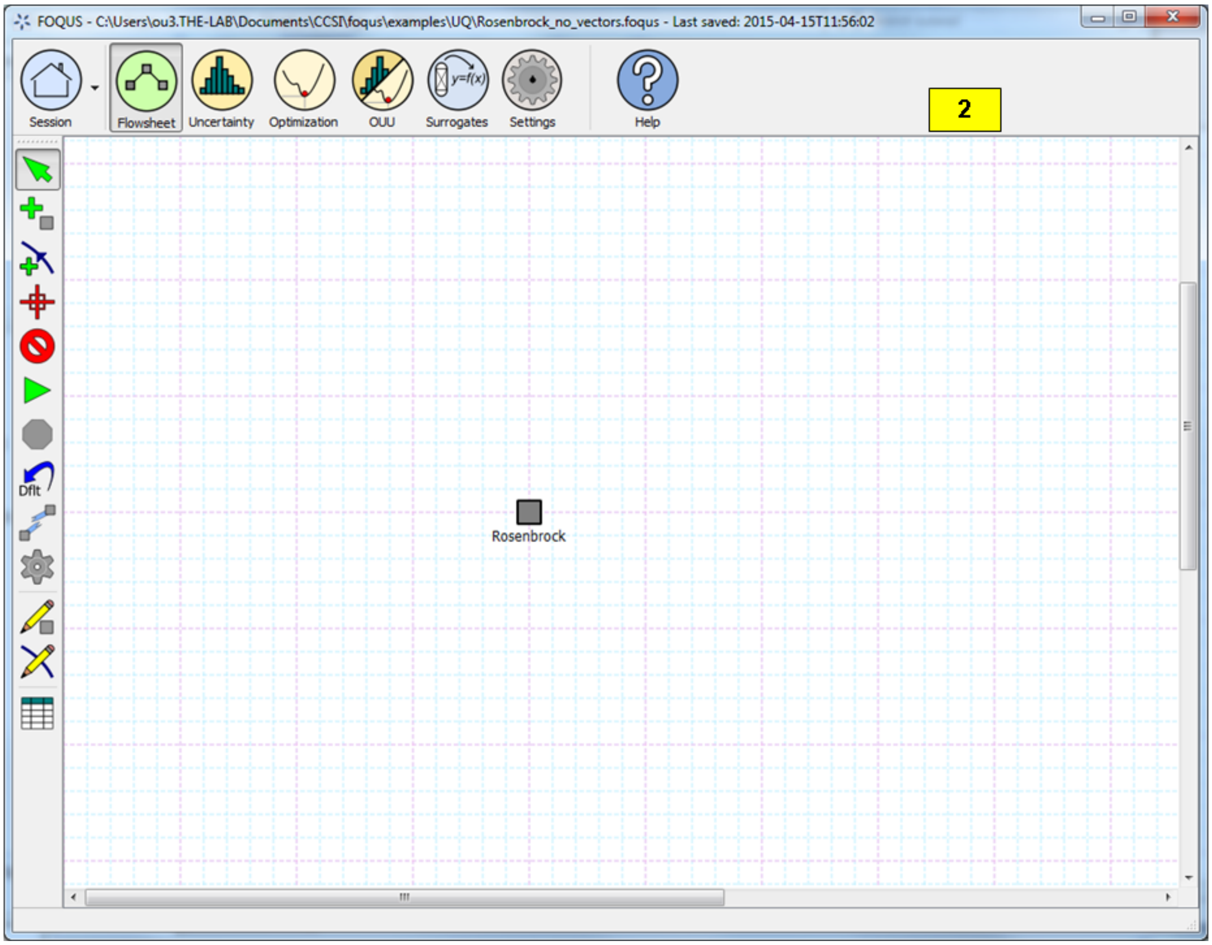


Fig. 11: Flowsheet for Rosenbrock Example

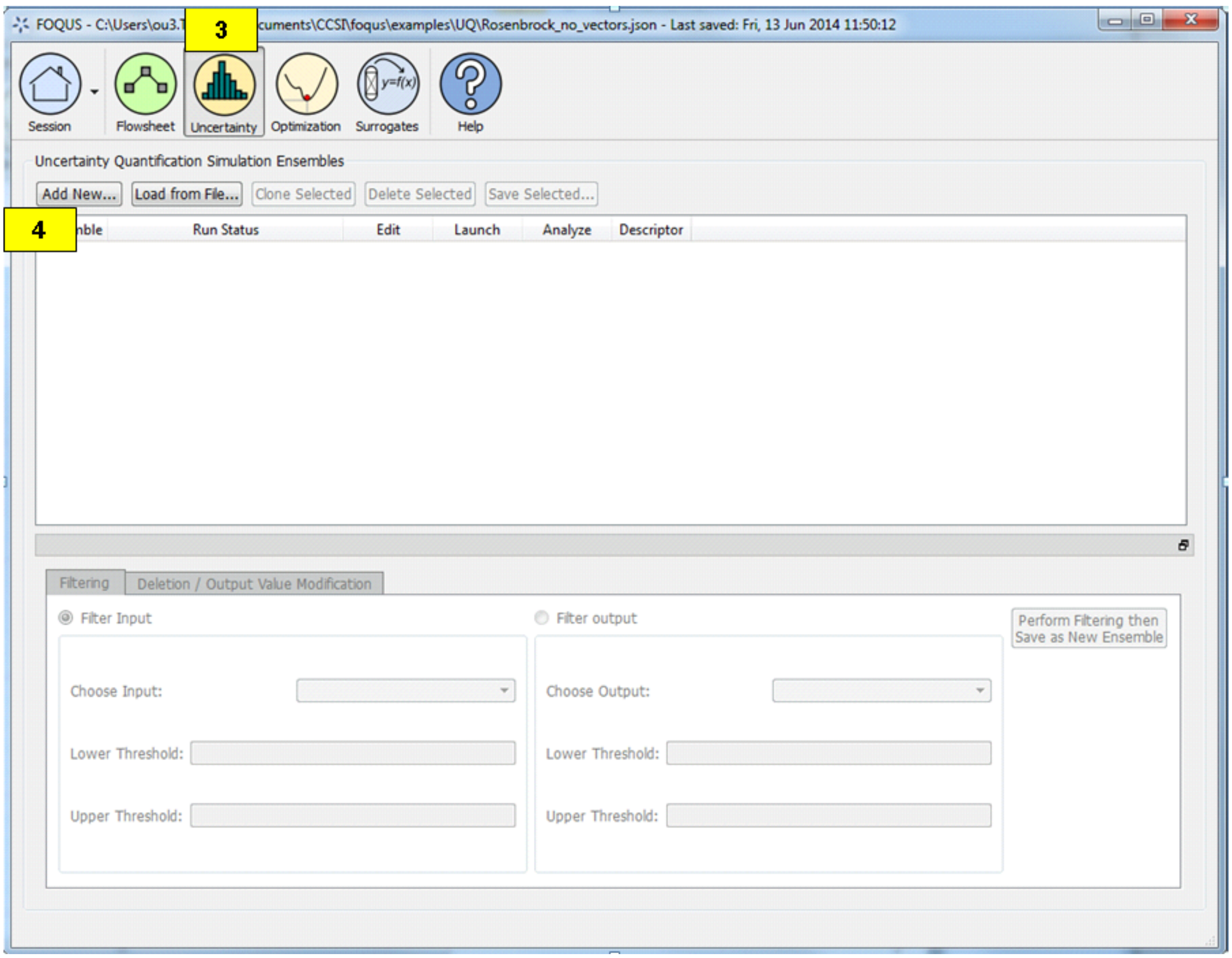


Fig. 12: Uncertainty Quantification Screen

5. The Add New Ensemble dialog displays (Figure *Add New Ensemble Dialog, Flowsheet Option*). The "Use flowsheet" option should be enabled.

6. *This item describes additional features and is provided for information only. It is not intended to be followed as part of the step-by-step tutorial.*

   An alternative is to use an emulator by selecting "Use emulator." This alternative is preferred if the actual simulation model is too computationally expensive to be practical for a large number of samples. This option enables the user to trade off accuracy for speed by training a response surface to approximate the actual simulation model. If this option is selected (Figure *Add New Ensemble Dialog, Emulator Option*), the user needs to provide a training data file containing a small simulation ensemble generated from the actual simulation model. This training data file is be in the PSUADE full file format (Section *[ap:psuadefiles]*).

   - Click Browse and select the training data file with which to train the response surface. The inputs, outputs and response surface type is read from the training data and populated accordingly on this dialog box.
   - Select Output(s) of Interest. To select multiple outputs, the user can use Shift + Click to select a range, or use Ctrl + Click to select/deselect individual outputs.

7. Click OK.

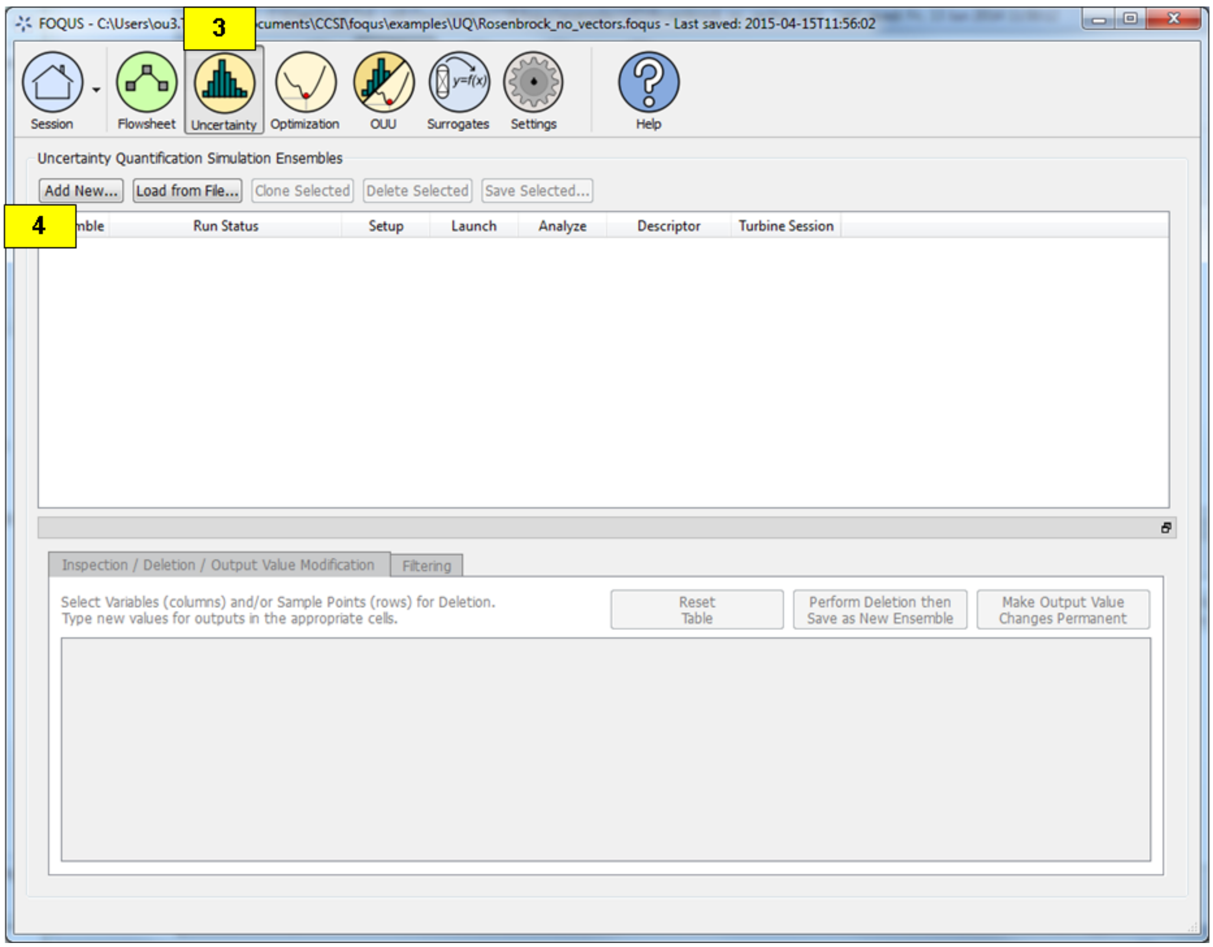


Fig. 13: Add New Ensemble Dialog, Flowsheet Option

enumerate

8. This displays the Simulation Ensemble Setup dialog box (Figure *Simulation Ensemble Setup Dialog, Distributions Tab*) that prompts the user for options specific to the creation of input samples.

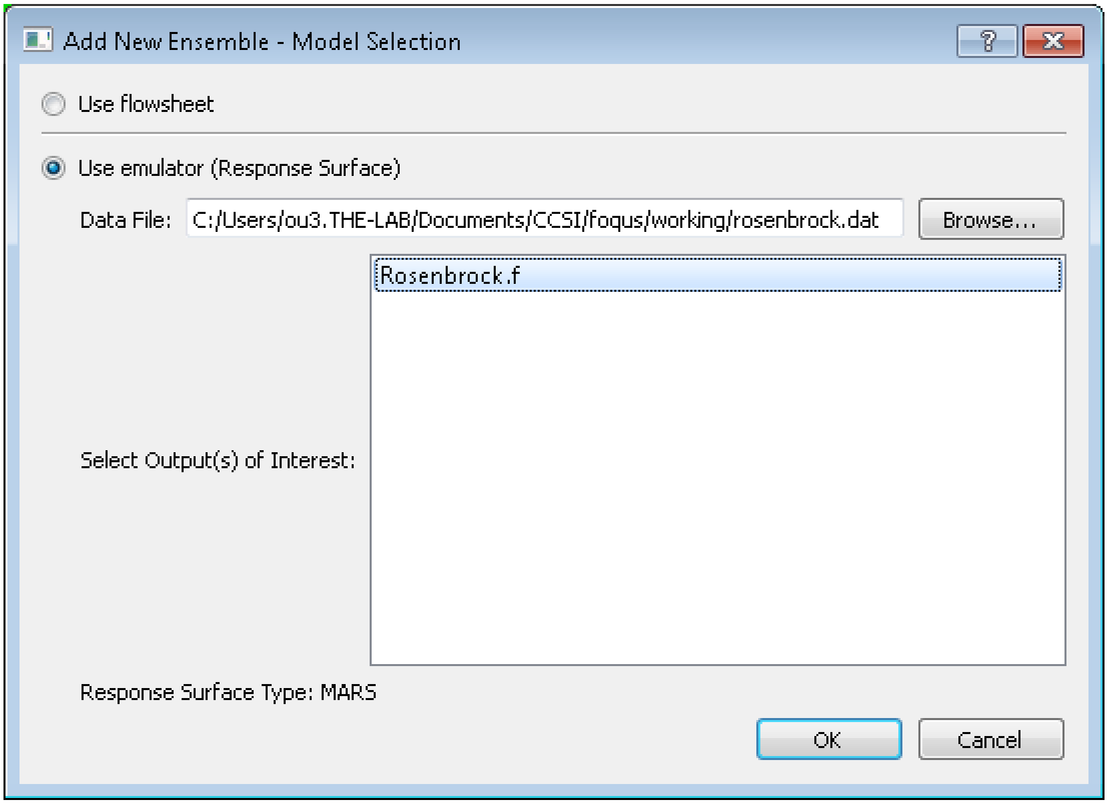


Fig. 14: Add New Ensemble Dialog, Emulator Option

9. Within the Distributions tab, the Distributions Table has all the inputs from the flowsheet node, each displayed in its own row.

   1. Click the All Variable button.
   2. Change the Type of "x2" to "fixed."
   3. Enter 5 into the Default column for "x2."

   Subsequently, other cells in the row are enabled or disabled according to the type selection.

   enumerate

   In this dialog, extra options that are available related to simulation ensemble setup are discussed.

   - Change the PDF of "x6" by exploring the drop-down list in the **PDF** column of the **Distributions Table**. The drop-down list is denoted by box (9c) in Figure *Simulation Ensemble Setup Dialog, Distributions Tab, PDF Selection*. If any of the parametric distributions are selected (e.g., "Normal", "Lognormal", "Weibull"), the user is prompted to enter the appropriate parameters for the selected distribution. If non-parametric distribution "Sample" is selected, the user needs to specify the name of the sample file (a CSV or PSUADE sample format is located in Section *[ap:psuadefiles]*) that contains samples for the variable "x6." The user also needs to specify the output index to indicate which output in the sample file to use. The resulting simulation ensemble would contain "x6" samples that are randomly drawn (with replacement) from the samples in this file.
   - Alternatively, select Choose sampling scheme (box (8) of Figure *Simulation Ensemble Setup Dialog, Distributions Tab*), and try selecting "Load all samples from a single file." With this selection, a new dialog box prompts the user to browse to a PSUADE full file, a PSUADE sample file, or CSV file (all formats are described in Section*[ap:psuadefiles]*) that contains all the samples for all the input variables in the model.

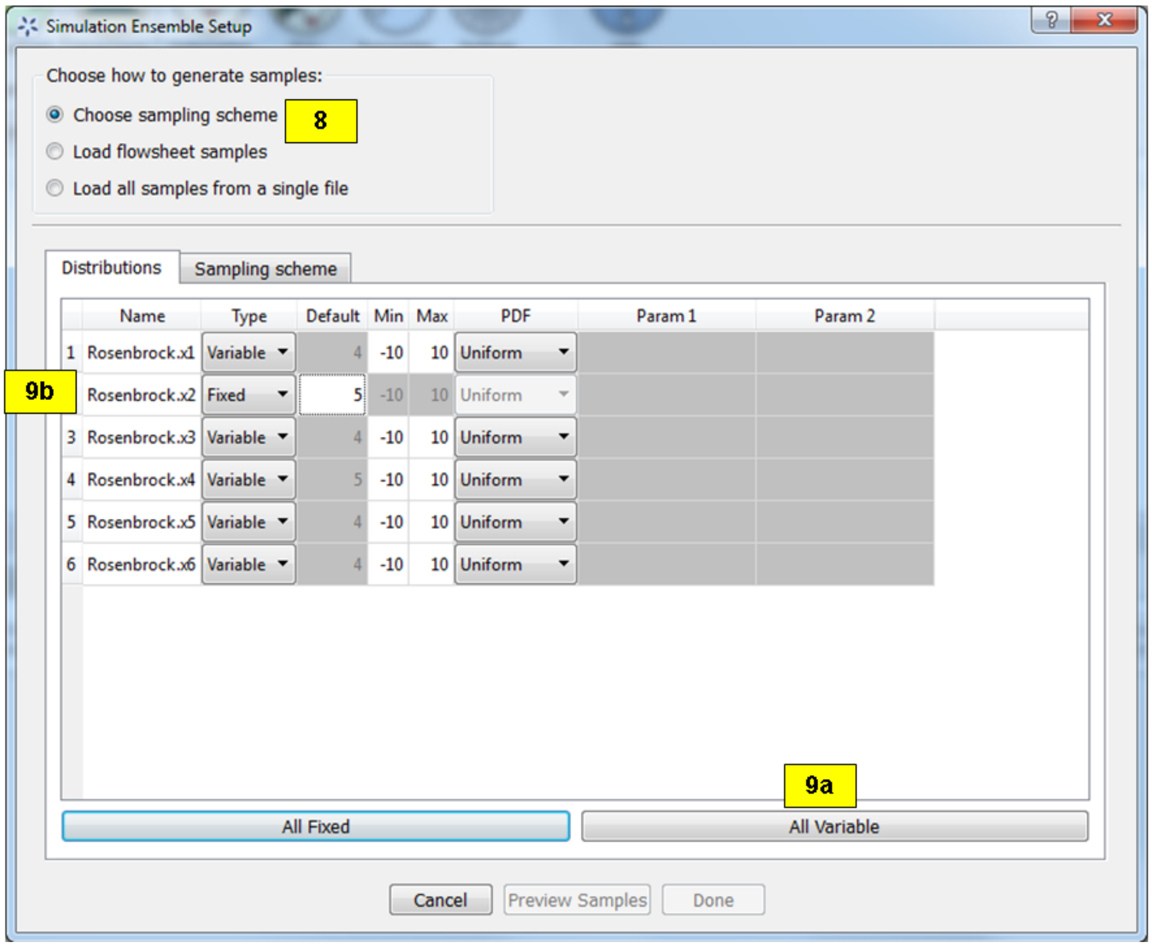


Fig. 15: Simulation Ensemble Setup Dialog, Distributions Tab

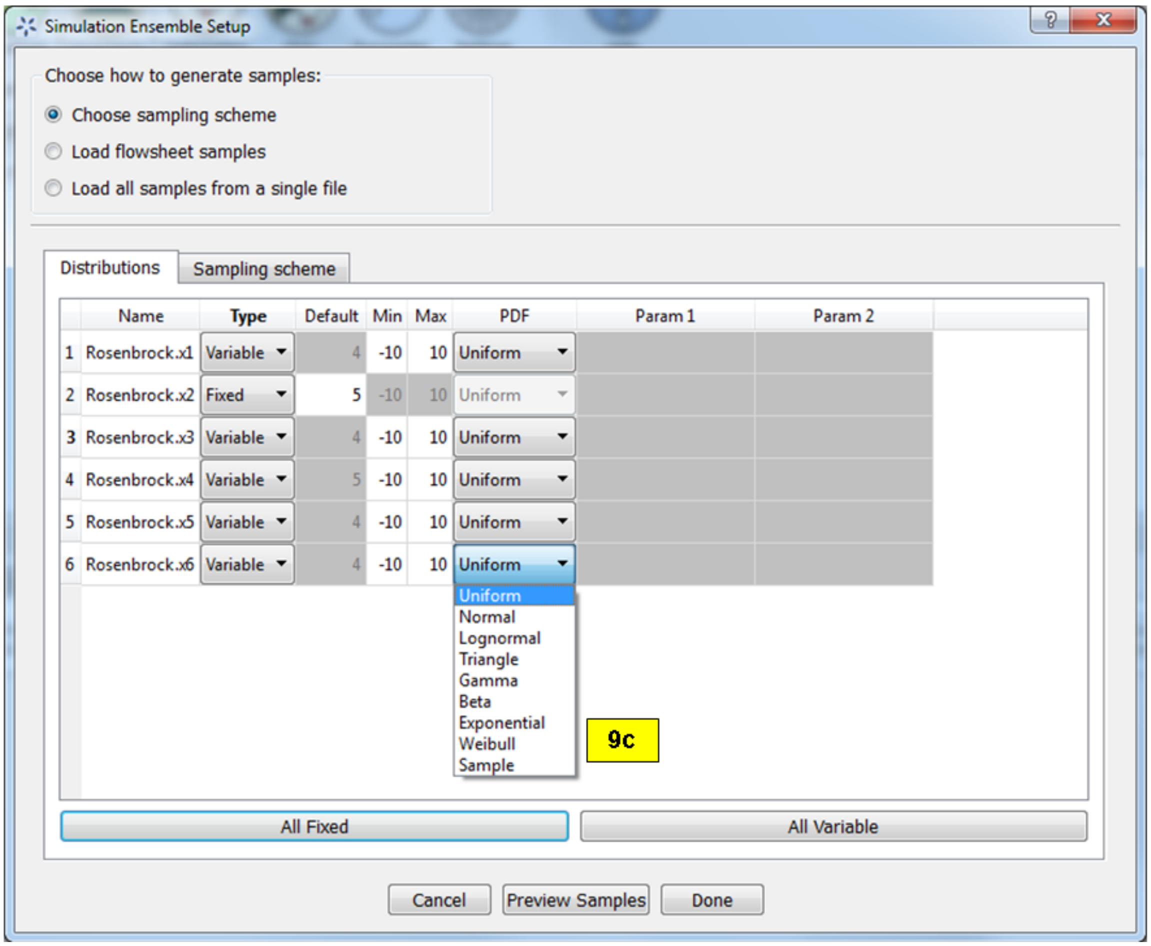


Fig. 16: Simulation Ensemble Setup Dialog, Distributions Tab, PDF Selection

Both of these options offer the user additional flexibility with respect to characterizing input uncertainty or generating the input samples directly.

enumerate

10. Once complete, switch to the Sampling Scheme tab (Figure *Simulation Ensemble Setup Dialog, Sampling Scheme Tab*).

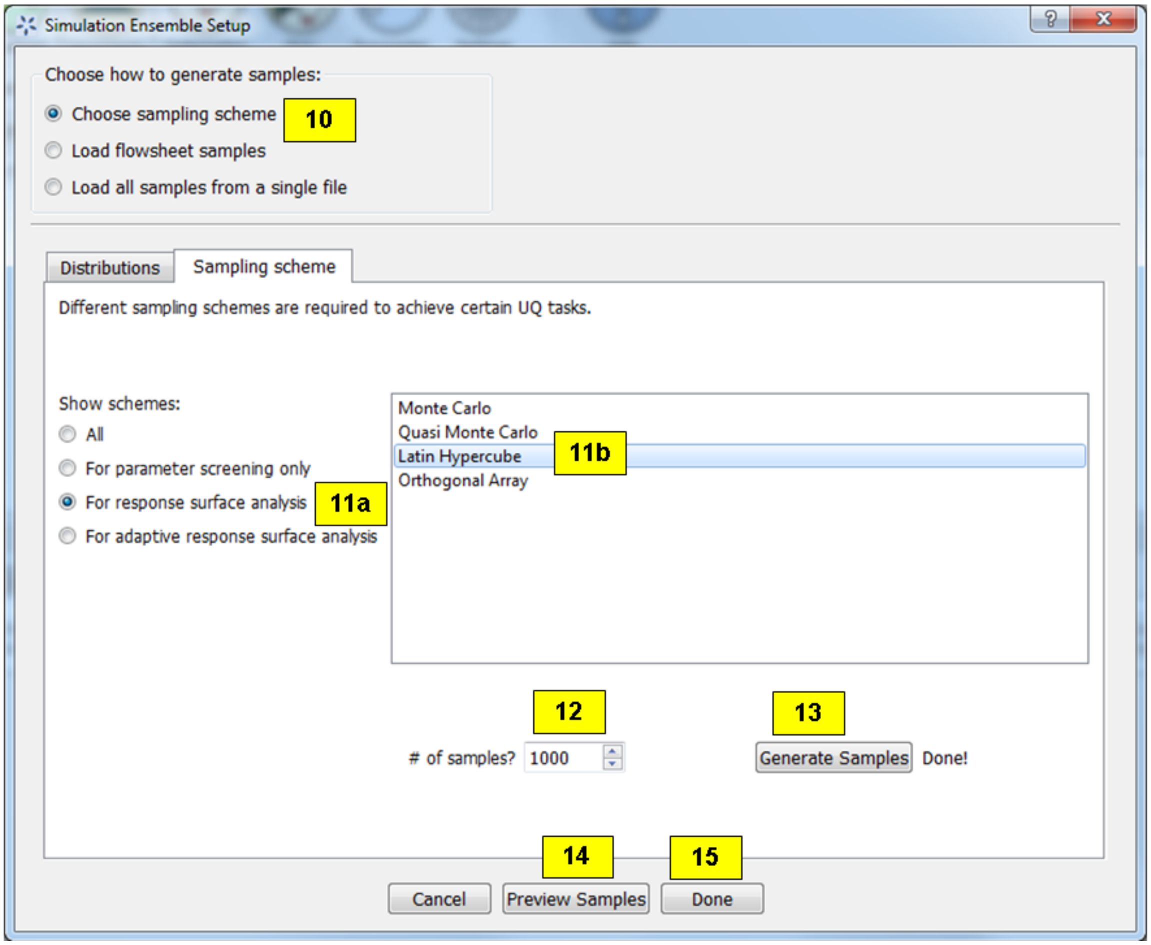


Fig. 17: Simulation Ensemble Setup Dialog, Sampling Scheme Tab

11. Select a sampling scheme with the assumption that the user is unsure which sampling scheme to use, but wants to perform some kind of response surface analysis. This example helps the user find a suitable one.
    1. Click For response surface analysis. Note the list on the right changes accordingly.
    2. Select "Latin Hypercube" from the list on the right.
12. To generate 500 samples, change the value in "# of samples." Some sampling schemes may impose a constraint on the number of samples. If the user has entered an incompatible sample size, a pop-up window displays with guidance on the recommended samples size.
13. Click Generate Samples to generate the sample values for all the variable input parameters. On Windows, if the user did not install PSUADE in its default location (C:Program Files (x86)psuade_project 1.7.1binpsuade.exe) and the user did not update the PSUADE path in FOQUS settings (refer to Section *Settings*), then the user is prompted to locate the PSUADE executable in a file dialog.
14. Once the samples are generated, the user can examine them by clicking Preview Samples. This displays a table

of the values, as well as the option to view scatter plots of the input values. The user can also select multiple inputs at once to view them as separate scatter plots on the same figure.

15. When finished, click Done.

16. The simulation ensemble should be displayed in the Simulation Ensemble Table. If the user would like to change any of the parameters and regenerate a new set of samples, simply click the Revise button.

17. Next, calculate the output value for each sample. Click Launch. The user should see the progress bar quickly advance, displaying the status of completed runs (Figure *Simulation Ensemble Added*).

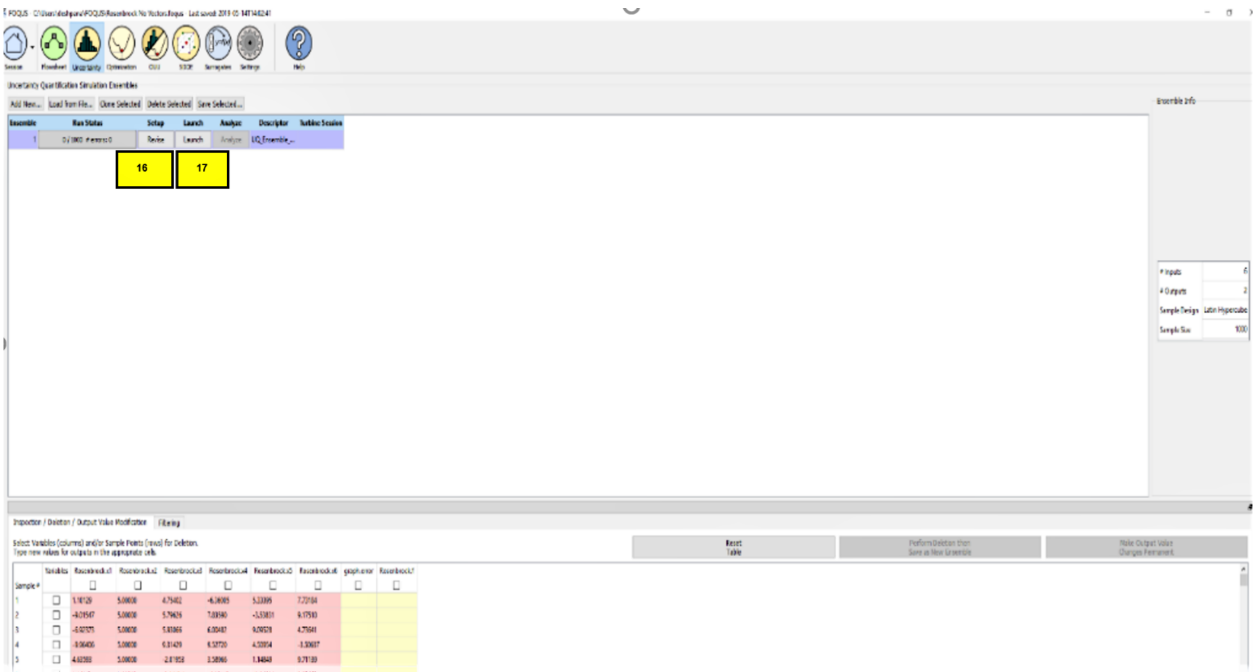


Fig. 18: Simulation Ensemble Added

18. Next, look at the output.

1. Click Analyze for "Ensemble 1" (Figure *Simulation Ensemble Evaluation Complete*).
2. Step 1 of "Analysis" (bottom page), the user selects Ensemble Data (Figure *Simulation Ensemble Analysis*).
3. Step 2 of "Analysis" is to select "Rosenbrock.f" (Figure *Simulation Ensemble Analysis*).
4. Step 3 of "Analysis" is to keep the analysis method as "Uncertainty Analysis" and then click Analyze. The user should see two graphs displaying the probability and cumulative distributions plots (Figure *Uncertainty Analysis Results*). Users should keep in mind these figures are intended to show what type of plots they would get, but they should not expect to reproduce the exact same plots.

Prior to this, the "Rosenbrock" example was selected to illustrate the process of creating and running a simulation ensemble because simulations complete quickly using this simple model. But from this point on, the adsorber subsystem of the A650.1 design is used as a motivating example to better illustrate how one would apply UQ within the context of CCSI.

A quick recap on our motivating example: The A650.1 design consists of two coupled reactors: (1) the two-stage bubbling fluidized bed adsorber and (2) moving bed regenerator, in which the output (outlet of sorbent stream) from one reactor is the input (inlet) for the other. The performance of the entire carbon capture system is obtained by solving these two reactors simultaneously, accounting for the interactions between the reactors. However, it is also necessary to study the individual effects of the adsorber and the regenerator without the side effects of their coupling since the two reactors display distinct characteristics under different operating conditions. Thus, the Process Design/Synthesis

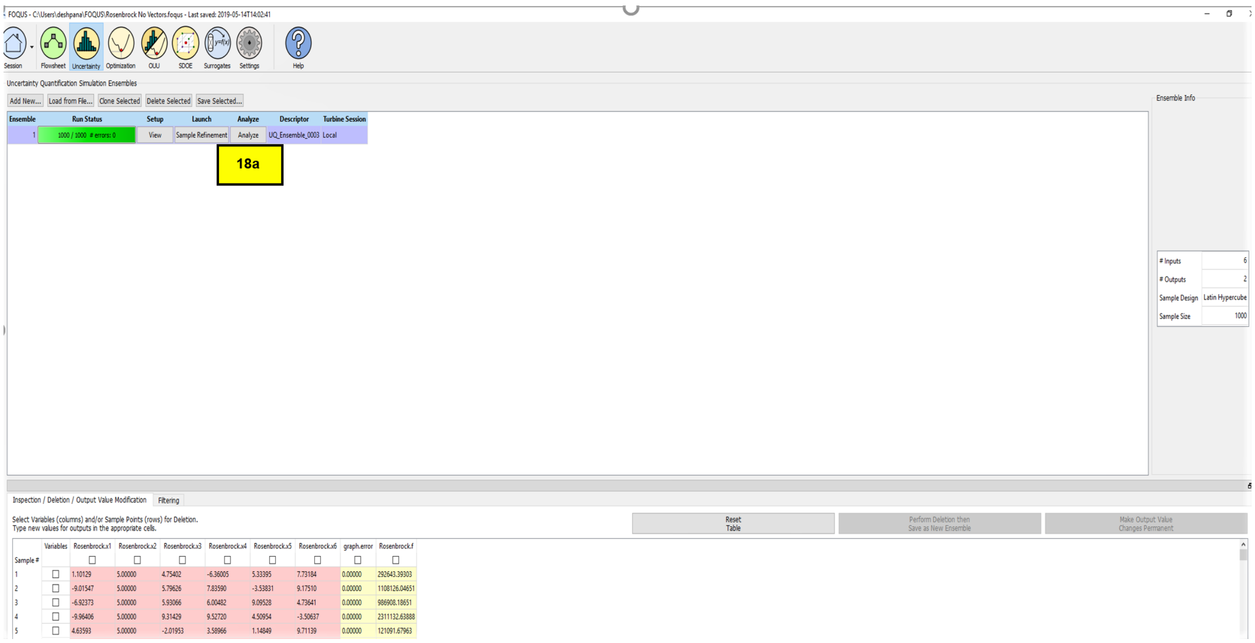


Fig. 19: Simulation Ensemble Evaluation Complete

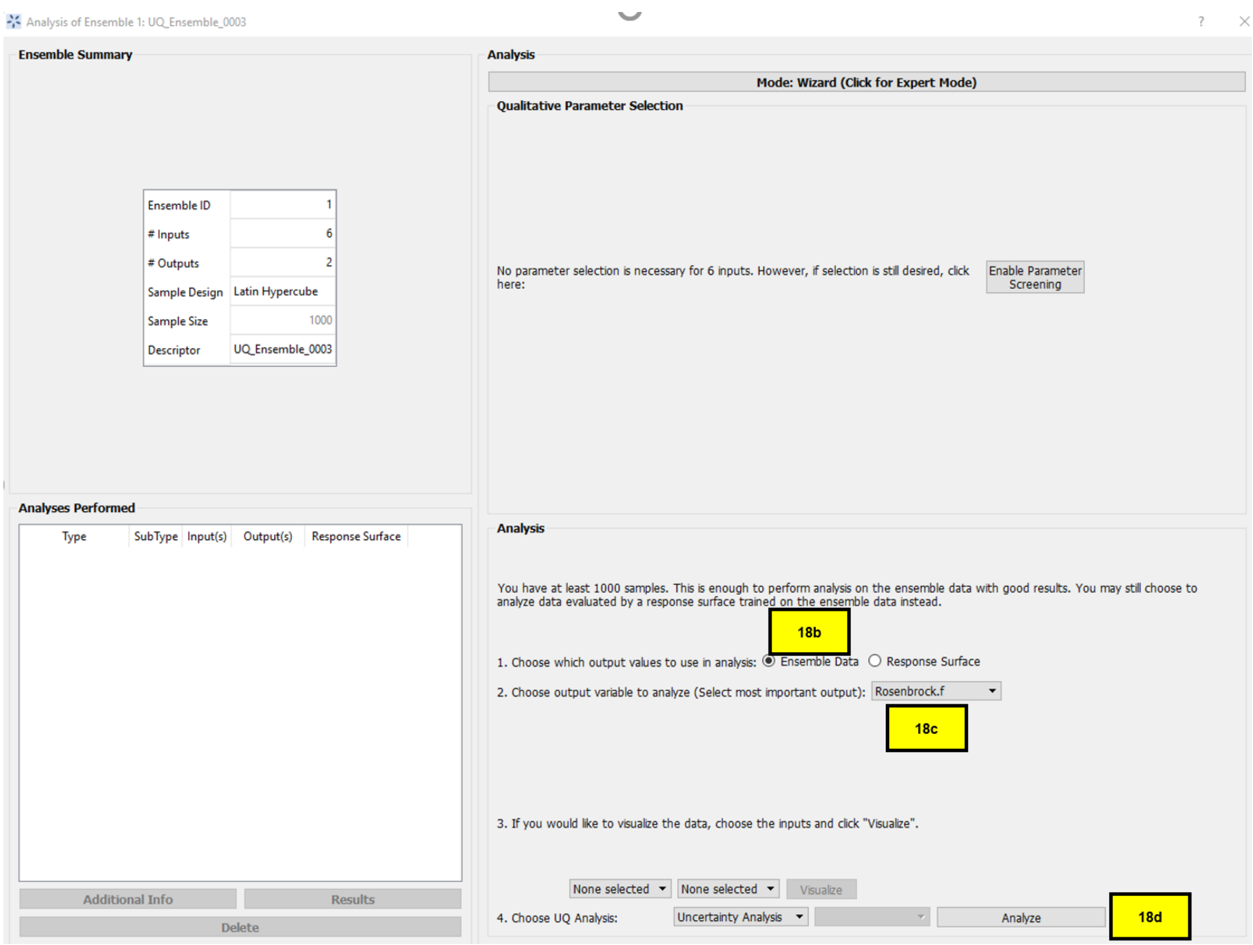


Fig. 20: Simulation Ensemble Analysis

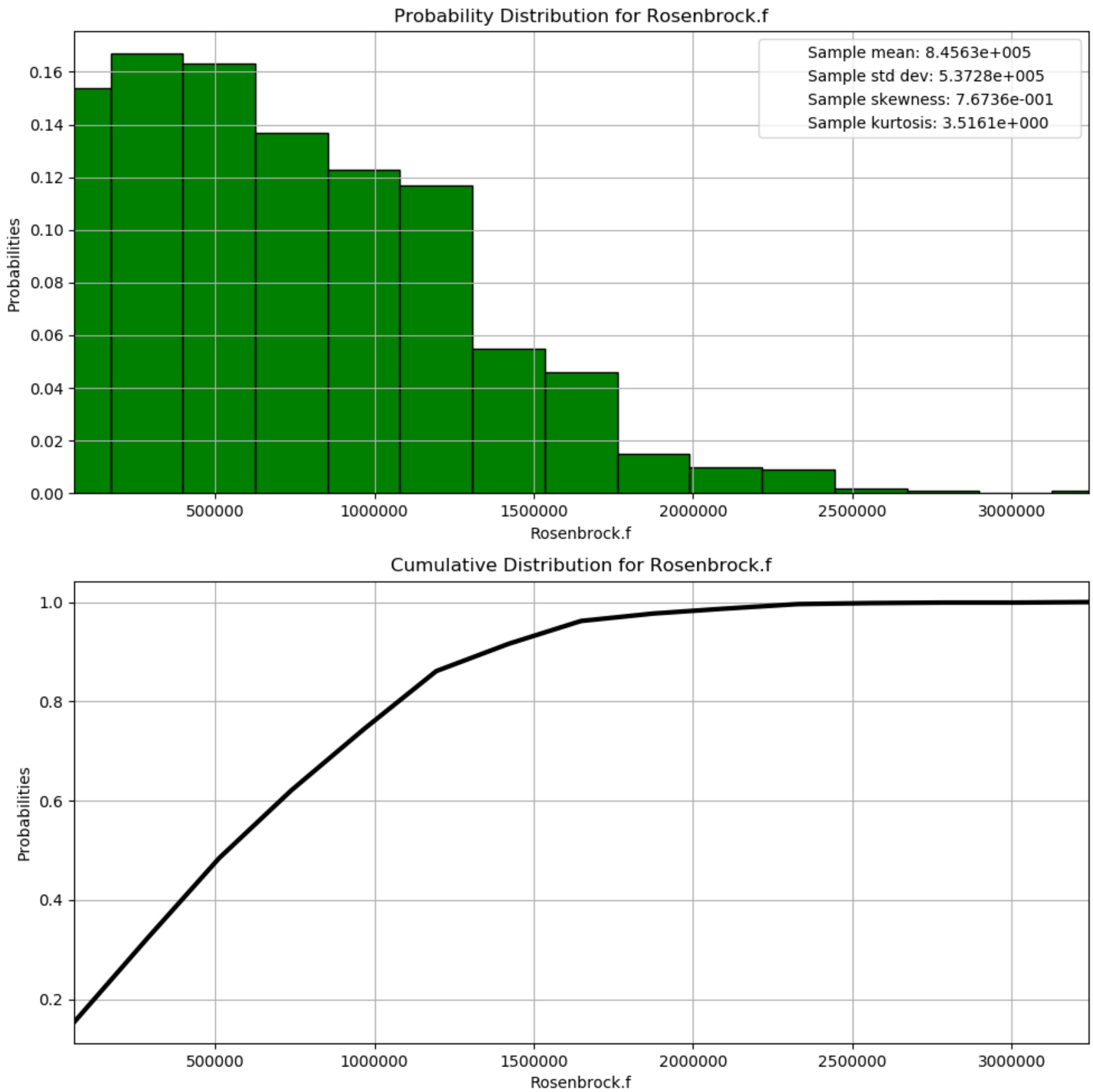


Fig. 21: Uncertainty Analysis Results

Team has given us a version of the A650.1 model that can be run in two modes: (1) coupled and (2) decoupled. In this section, analysis results are presented from running the A650.1 model using the decoupled mode and examining the adsorber in isolation from the regenerator.

Data Manipulation

In this tutorial, instructions to change the data before analysis are described. Current capabilities include sample filtering, input/output variable deletion, and output value modification.

Filtering

Filtering involves selecting out samples whose values of a certain input or output fall into a certain range. Typically, when runs are returned from the Turbine gateway, there could be simulations that failed to converge in Aspen, thus the simulation samples corresponding to these failed runs should be excluded from analysis. Follow the steps below to filter out the samples due to failed runs:

1. Click Load from File on the UQ window (Figure*[fig:uqt_data_filter]*).

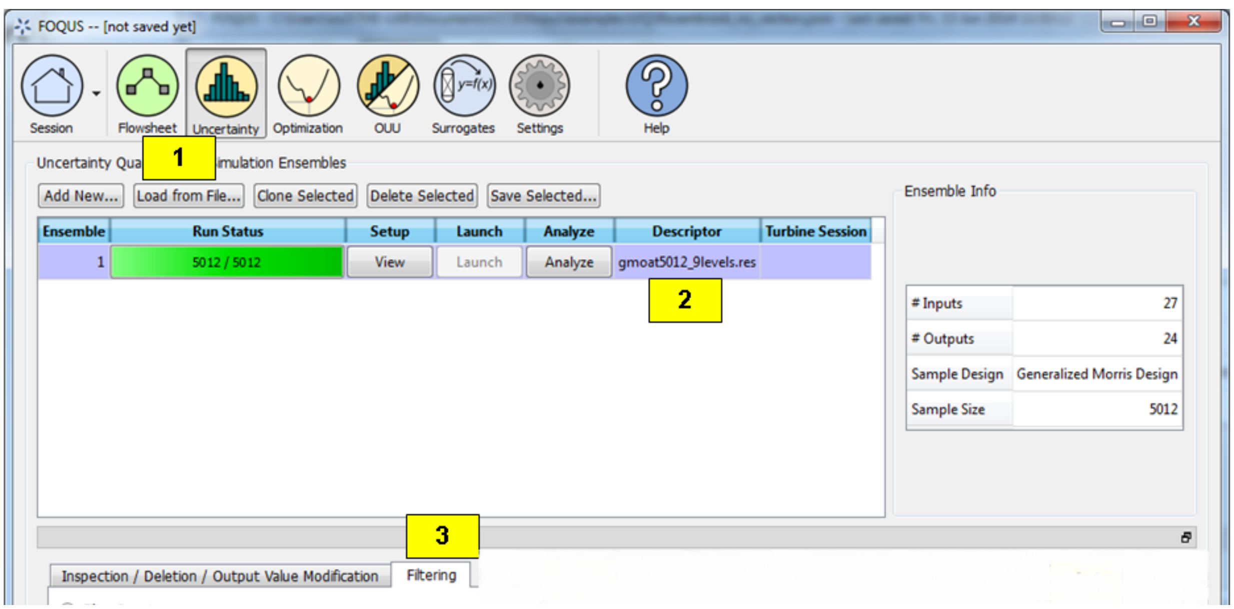


Fig. 22: Data Manipulation, Filtering Tab
[fig:uqt_data_filter]

2. Select the file "gmoat5012_9levels.res" in the examplesUQ folder. This file is an actual simulation ensemble that has already been run on the Turbine gateway. To find this file, the user may need to change the file filter to "All files."

3. Select the Filtering tab.

4. Filtering the loaded simulation ensemble based on output values is performed.

   1. Click on "New Filter", and create a filter named "f1"
   2. Add the Filter Expression c("output.status") == 0, since the user should keep only the samples in which the output parameter status is "0."
   3. Click "Done"

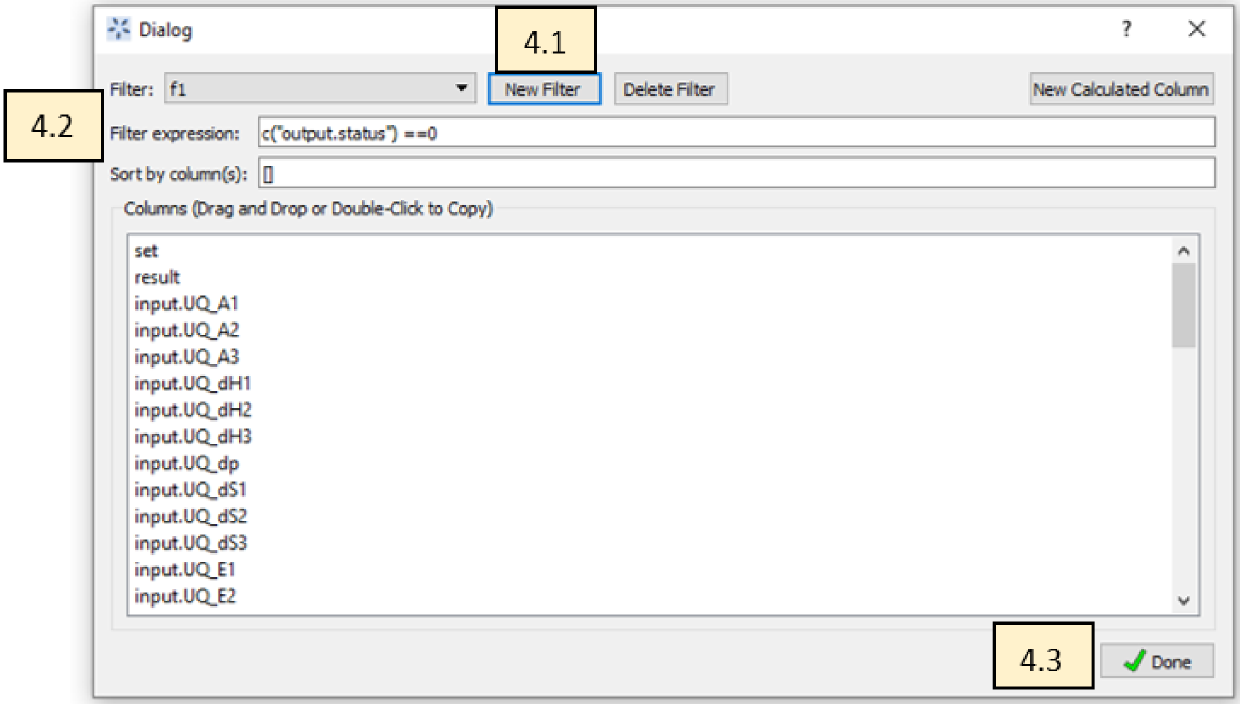


Fig. 23: Data Manipulation, Filtering Dialog Box

4. Select 'f1' as the " Current Filter" in the Flowsheet Result window within "Filtering Tab"
5. Once the Filtering is complete, click on "Save as New Ensemble" and a new row should be added to the simulation table

Data Manipulation, Applying the filter

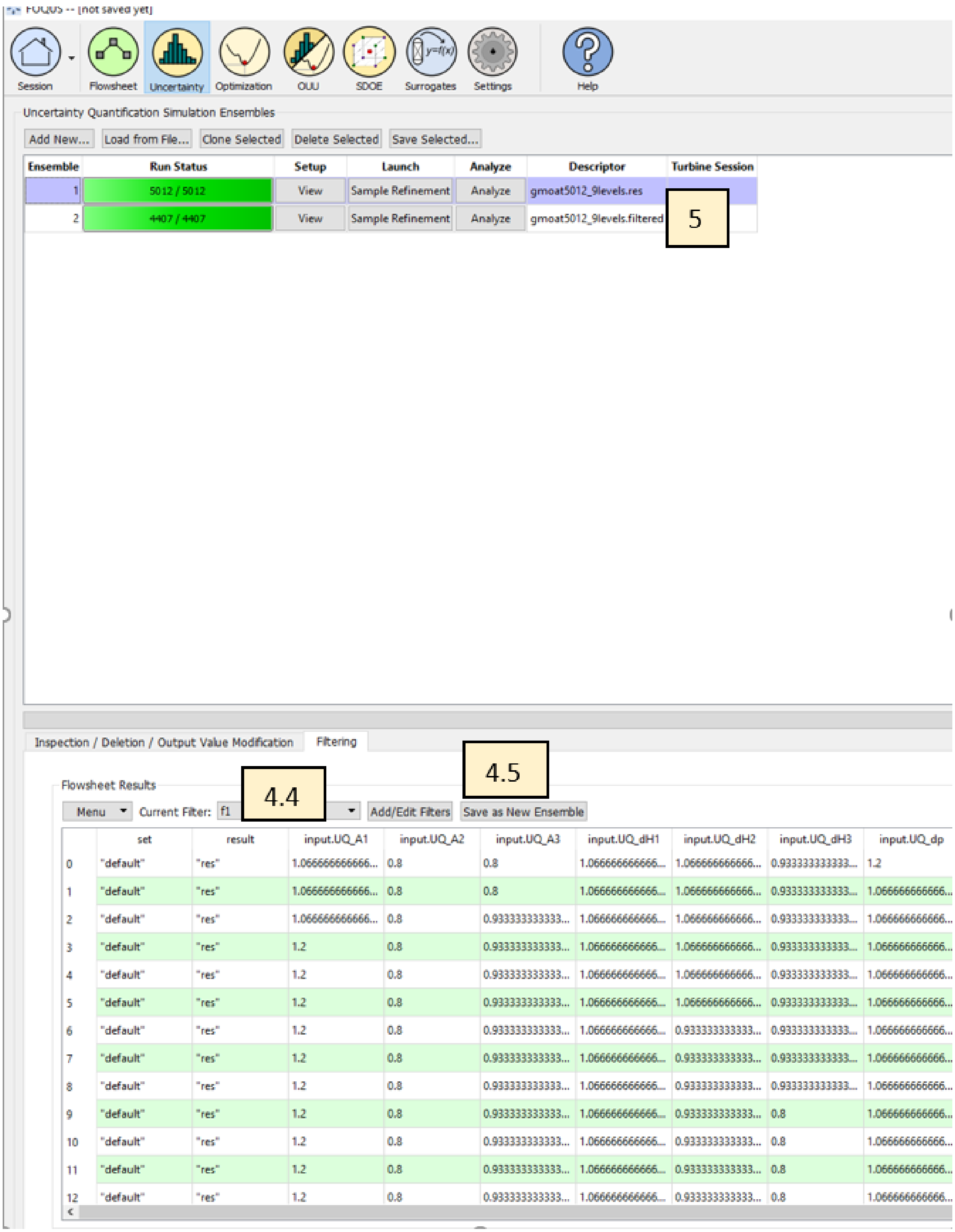
1. Once filtering is complete, a new row should be added to the simulation table (Figure *[fig:uqt_data_filter_results]*). This ensemble contains only those samples that have a status value of "0." Analysis can now be performed on this new ensemble because this ensemble contains only the valid simulations (i.e., those with output status value of 0), in which Aspen calculations have properly converged.

   [fig:uqt_data_filter_results]

Variable Deletion

If an input or output variable is to be removed from consideration for analysis, this can be done in the **Inspection/Deletion/Output Value Modification** tab. Delete the status output from the previous filtering as it is no longer needed for further analysis.

1. Verify that the ensemble that resulted from filtering is selected. If not, select that ensemble.
2. Click the Inspection/Deletion/Output Modification tab.
3. Scroll to the right of the table to the outputs, which are colored yellow.
4. Select the checkbox corresponding to the "status" output (the first output).
5. Click Perform Deletion then Save as New Ensemble.


FOQUS -- [not saved yet]
Session
Flowsheet
Uncertainty
Optimization
OUU
SDOE
Surrogates
Settings
Help
Uncertainty Quantification Simulation Ensembles
Add New...
Load from File...
Clone Selected
Delete Selected
Save Selected...
Ensemble
Run Status
Setup
Launch
Analyze
Descriptor
Turbine Session
5012 / 5012
View
Sample Refinement
Analyze
gmoat5012_9levels.res
4407 / 4407
gmoat5012_9levels.filtered
5
Inspection / Deletion / Output Value Modification
Filtering
Flowsheet Results
4.4
4.5
Menu
Current Filter: f1
Add/Edit Filters
Save as New Ensemble
set
result
input.UQ_A1
input.UQ_A2
input.UQ_A3
input.UQ_dH1
input.UQ_dH2
input.UQ_dH3
input.UQ_dp

The results are illustrated in Figure *[fig:uqt_data_mod]*. Note: The output count has decreased by one for the new ensemble. The user can verify that the "status" output was removed in the new ensemble by viewing this in the **Inspection/Deletion/Output Value Modification** tab again. Deletion of an input can be performed similarly by selecting its checkbox and clicking the **Perform Deletion then Save as New Ensemble** button.

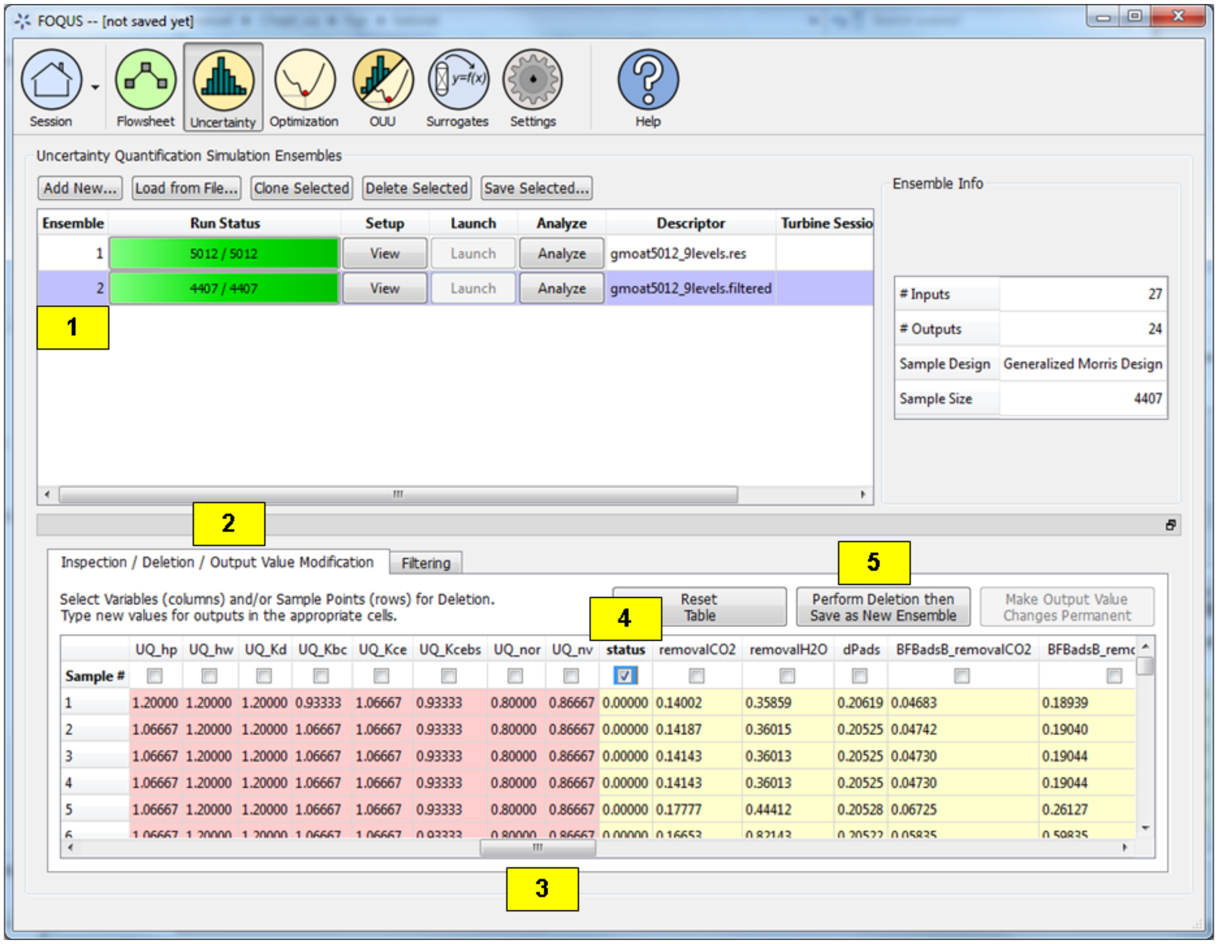


Fig. 24: Data Manipulation, Inspection/Deletion

[fig:uqt_data_mod]

Output Value Modification

To change the value of an output for a sample or several samples, follow steps below:

1. Select an ensemble.
2. Click the Inspection/Deletion/Output Value Modification tab.
3. Scroll to the right to the outputs.
4. Click on a cell for one of the outputs and enter a new value. Do the same for another cell. Notice that the modified cells turn green. This indicates the cells that have been modified.
5. Click Make Output Value Changes Permanent to permanently change the values. The modified cells will turn yellow, indicating the permanent change. If the user wishes to reset the table and start over before making changes permanent, click the Reset Table.

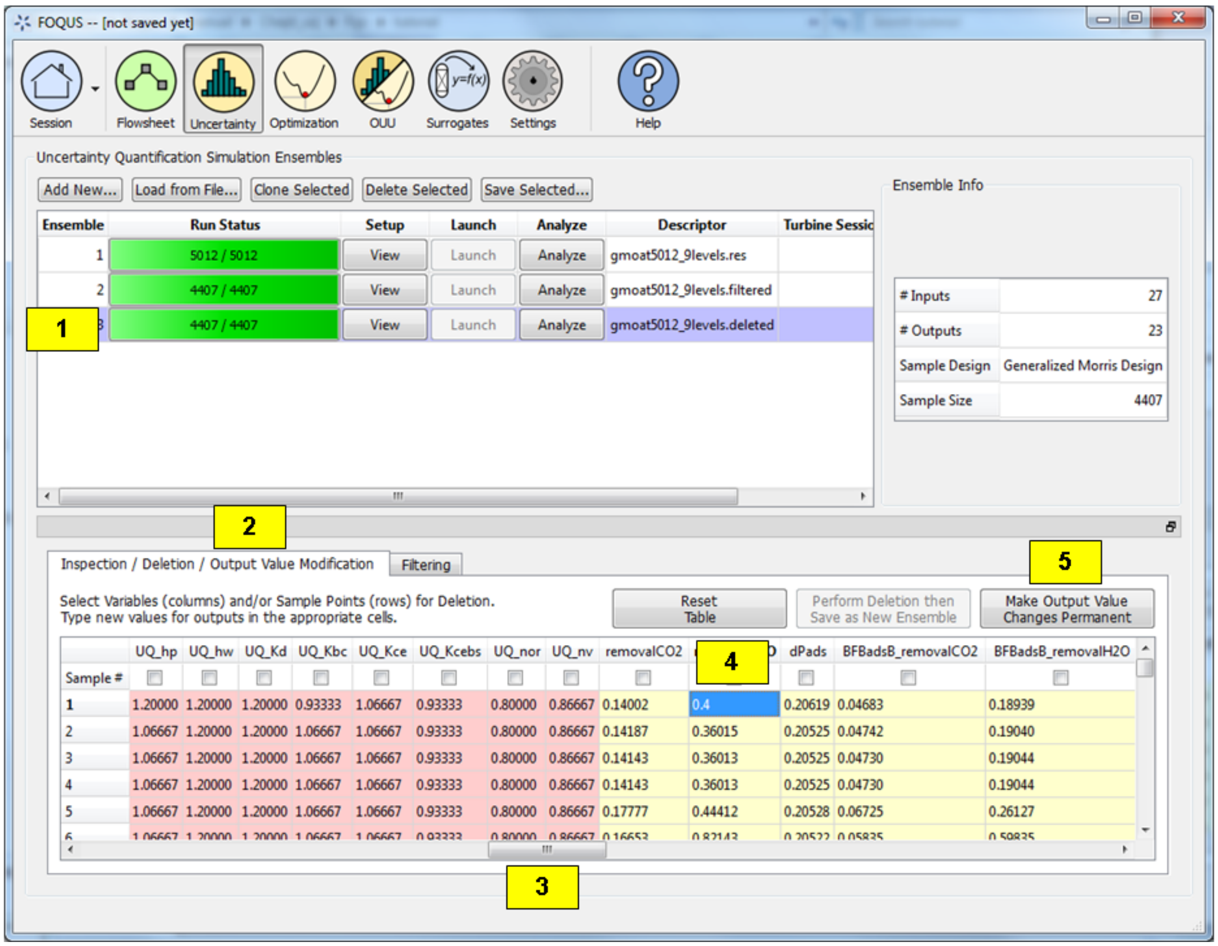


Fig. 25: Data Manipulation, Value Modification

[fig:uqt_data_mod_output]

Single-Output Analysis

From the Single-Output Analysis Screen, the user can perform analyses that are specific to a particular output of interest. Here, the “removalCO2” output parameter is discussed.

Parameter Selection

For simulation models that have a large number of input parameters, it is common practice to down-select to a smaller subset of the most important input parameters that are most relevant to the output of interest. This is done so subsequent detailed studies can be performed more efficiently. By using a smaller set of inputs, a smaller set of samples may be needed.

1. From the UQ window, load the file “gmoat5012_9levels.filtered” in examplesUQ. (This file contains the same set of samples that resulted from data filtering. They are included here to make each demo self-inclusive.)
2. Click **Analysis**. A new page is displayed (Figure *[fig:uqt_analysis_param]*).

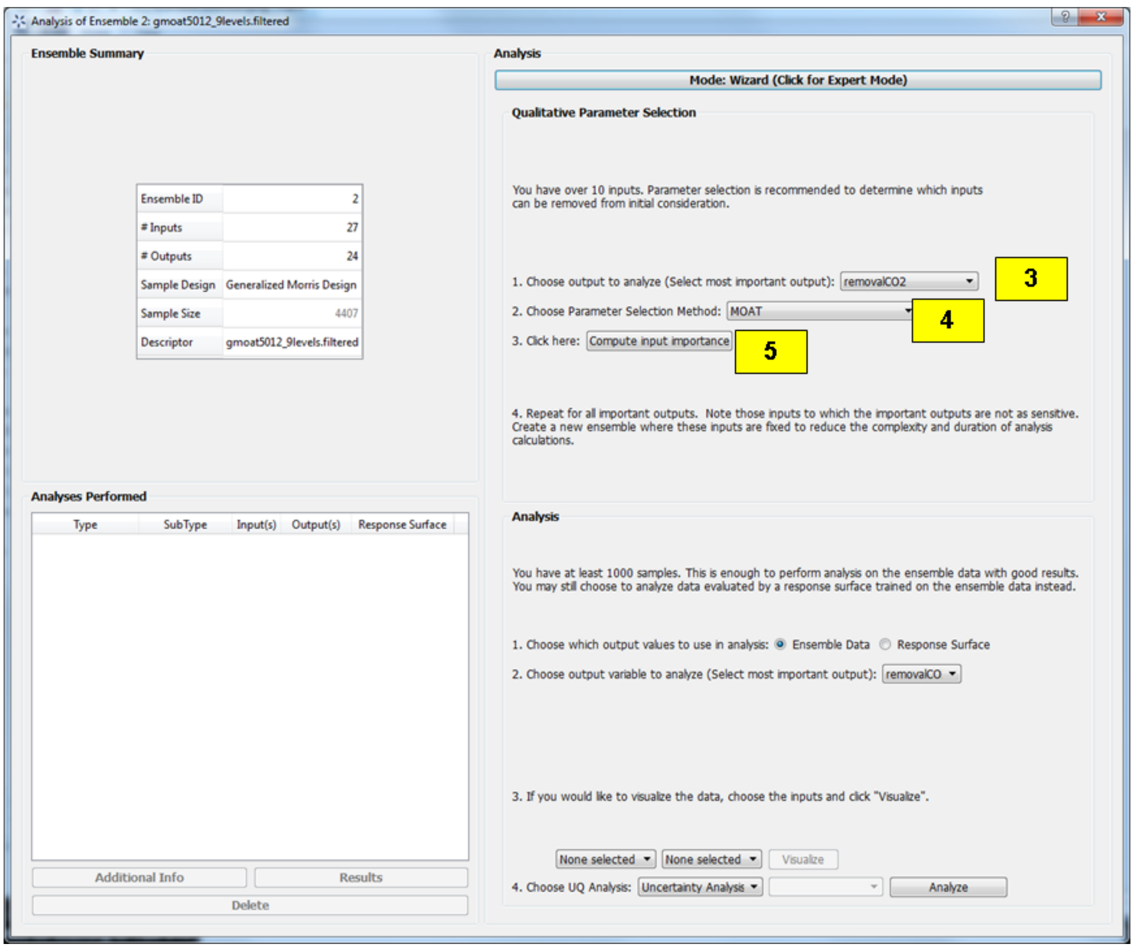


Fig. 26: Analysis Dialog, Parameter Selection

[fig:uqt_analysis_param]

3. Under the Qualitative Parameter Selection section, select “removalCO2” as the output.
4. Select “MOAT” as the method to be used.

5. Click **Compute input importance**. A graph should appear with the results (Figure *[fig:uqt_param_results]*).

   [fig:uqt_param_results]

The bars in the plot represent the importance of a particular input in determining the value of the output. For example, the values of dH3 and dS3 are very important in determining the value of removalCO2, whereas Hce and hp have no affect (the y-axis displays the average changes in the model output as a result of changing the inputs in their respective ranges. For example, from Figure *[fig:uqt_param_results]*, changing dH2 in its range results in an average change in CO_2 removal as much as about 57 percent with a margin of +/- 3 percent). Thus, it would be safe to exclude any inputs that have negligible bar lengths from analysis. Next, down-select the ten most important inputs based on these results. See Section *[subsubsec:uqt_vardel]* for details. Change the number of samples and scheme as desired and then generate new samples. Click **Launch** to run these samples to obtain another simulation ensemble that can be analyzed.

Ensemble Data Analysis

If the user is interested in the output uncertainty of "removalCO2" based on the uncertainties from the ten most important input parameters, perform uncertainty analysis, which would compute the probability distribution and sample statistics of "removalCO2."

1. Load "lptau20k_10inputs_4outputs.filtered" from the examples\ UQ folder. Assume this is the file that the user would receive after running the cloned simulation ensemble in which the user has down-selected the ten most important inputs, set the Sampling Scheme to "Quasi-Monte Carlo (LPTAU)", set the sample size to 20K, and performed data filtering to retain only the samples with the status output equal to "0."
2. Click Analyze. A new page displays (Figure*[fig:uqt_analysis_ua]*).
3. Select "Ensemble Data" to indicate that analysis is to be directly performed on the raw sample data.
4. Select "removalCO2" as the output variable to analyze.
5. Select "Uncertainty Analysis" and then click Analyze.

   [fig:uqt_analysis_ua]

   Once uncertainty analysis is complete, results display (Figure *[fig:uqt_ua_results]*) illustrating the probability distribution function (PDF), cumulative distribution function (CDF), and the sufficient statistics (e.g., mean, standard deviation) of "removalCO2" (top left corner of the PDF plot). This is used to evaluate if the output uncertainty is acceptable. If the output uncertainty is too great or the user prefers the system to operate within a higher percentage of capture, pursue further analyses to understand the relationships between the inputs and outputs, and investigate what can be done to reduce the output uncertainties by reducing the input uncertainties.

   [fig:uqt_ua_results]

   Next, the user may apply variance-based sensitivity analysis to quantify each input's contribution to the output variance:

   enumerate

6. From the bottom of the "Analysis" section, select "Sensitivity Analysis."
7. There are three options for sensitivity analysis: (1) first-order, (2) second-order, and (3) total-order. First-order analysis examines the effect of varying an input parameter alone. Second-order analysis examines the effect of varying pairs of input parameters. Total-order analysis examines all interactions' effect of varying an input parameter alone and as a combination with any other input parameters. For this demonstration, select "Total-order" and click Analyze. The total sensitivity indices display in a graph. Note: If the simulation ensemble has more than ten inputs, "Total-order" is disabled (since any reasonable sample size is not sufficient). Additionally, since quantitative sensitivity analysis in general requires large ensembles with many samples (thousands or more), ensemble sensitivity analysis (without the use of response surfaces) is often less practical and accurate than response surface based analyses. The result is illustrated in Figure*[fig:uqt_sa_results]*.

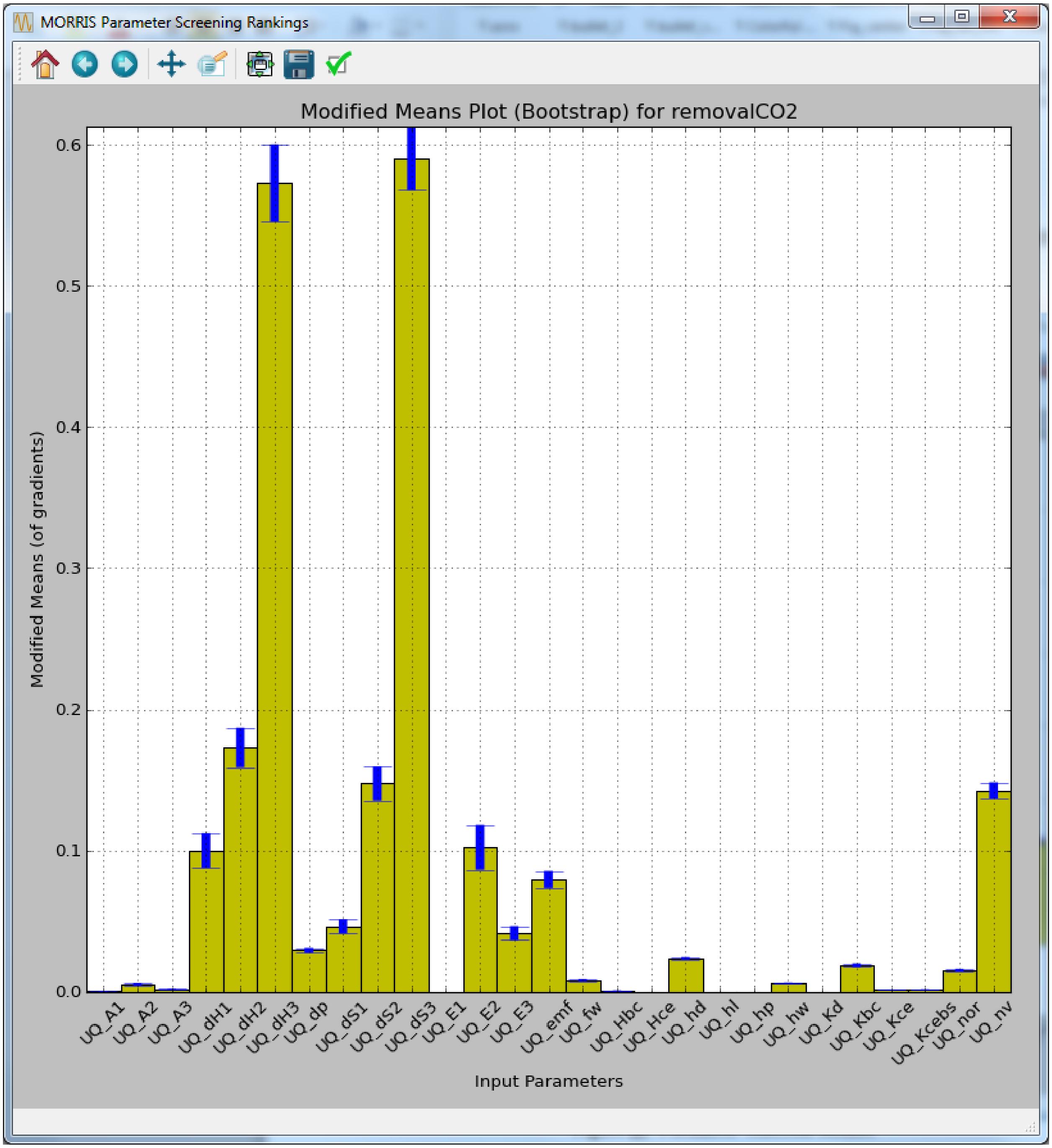


Fig. 27: Parameter Selection Results

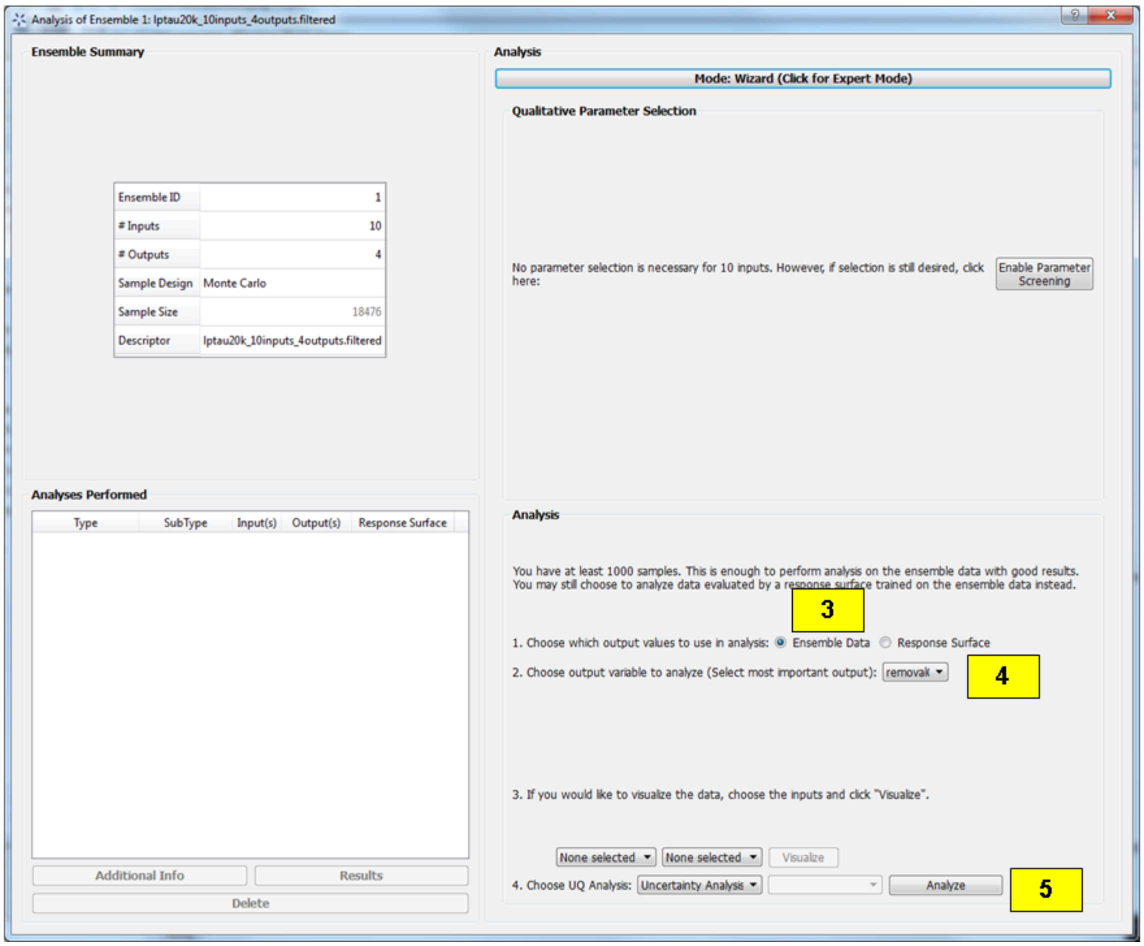


Fig. 28: Analysis Dialog, Ensemble Data Uncertainty Analysis

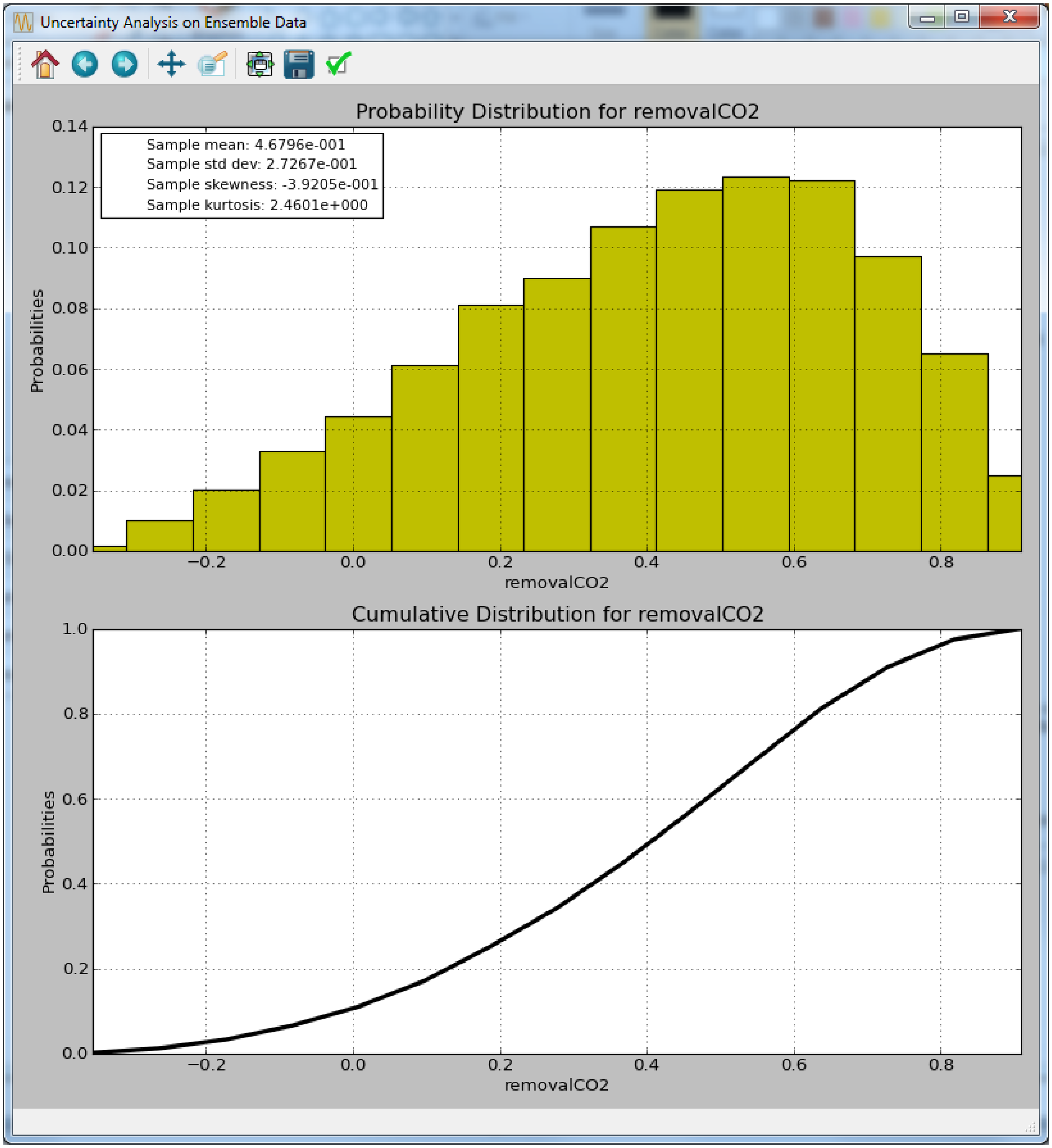


Fig. 29: Ensemble Data Uncertainty Analysis Results

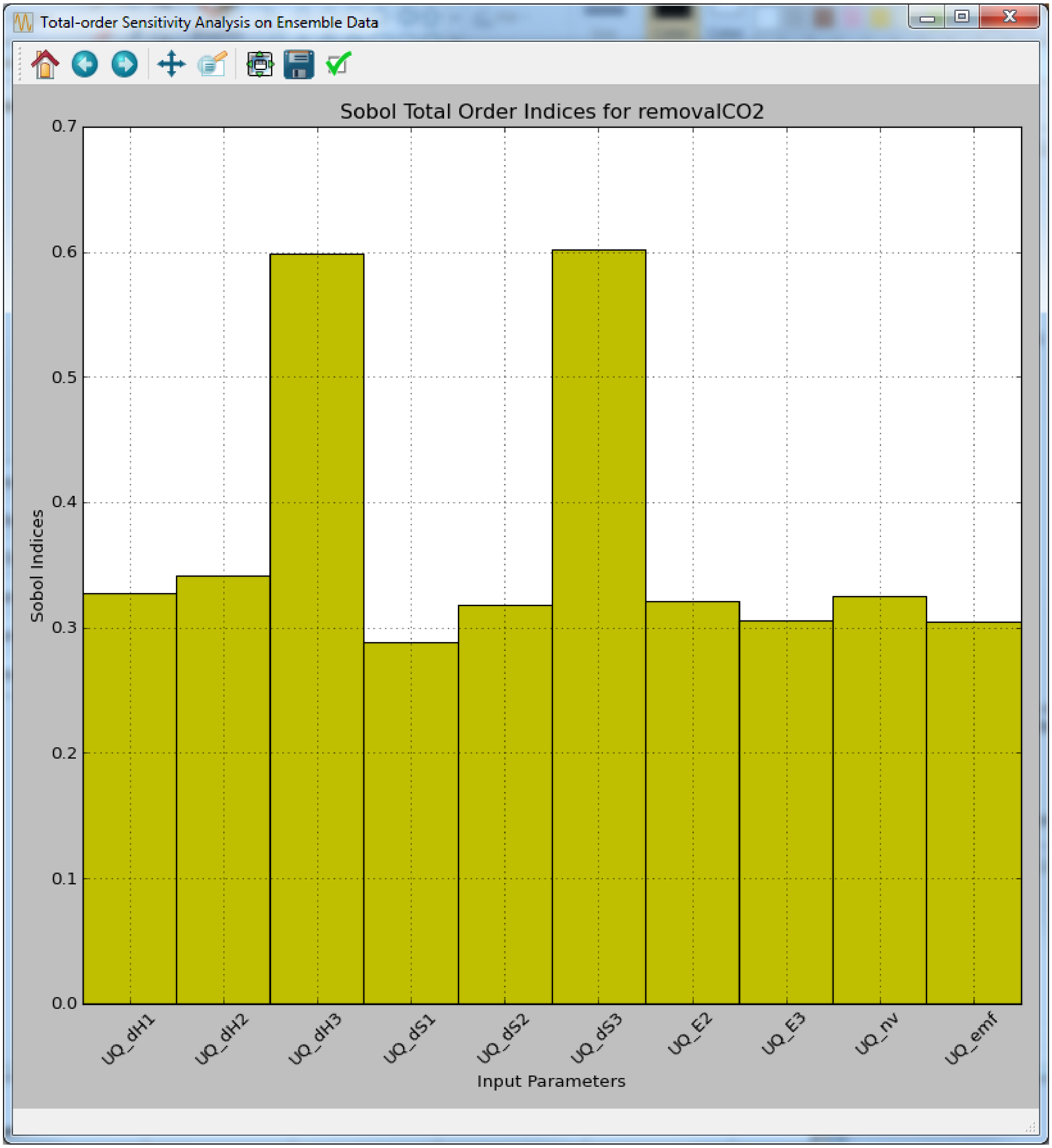


Fig. 30: Ensemble Data Total-order Sensitivity Analysis Results

[fig:uqt_sa_results]

These results confirm that "removalCO2" is more sensitive to "dH3" and "dS3" than other inputs. (The y-axis displays an approximate percentage of output variance attributed to each individual parameter. Since total sensitivity includes higher order interaction terms with other parameters, the sum of these total sensitivity indices usually exceeds 1.)

Ensemble Data Visualization

1. In this release, ensemble data visualization is only available in "Expert" mode. At the top of the "Analyze" page, toggle the bar to expert mode and select "removalCO2" as the output. Next, to "Visualize Data," choose an input (e.g., "UQ_dH1") and click **Visualize** for a 2-D scatter plot of "removalCO2" versus that input (Figure *[fig:uqt_splot1_results]*).

   [fig:uqt_splot1_results]

2. Next, select a second input (e.g., "UQ_dH2") and click **Visualize** for a 3-D scatter plot of "removalCO2" versus the two inputs. (Note: The input selections must be unique for the **Visualize** button to be enabled.) Figure *[fig:uqt_splot2_results]* shows the results.

   [fig:uqt_splot2_results]

   The plot in Figure *[fig:uqt_splot2_results]* can be rotated by clicking and dragging.

Response Surface Based Analysis

For simulation models that are expensive to run, response surface analysis can be a resourceful option. To construct a response surface, a space-filling sampling design is desired. For example, quasi-Monte Carlo (LPTAU) or Latin hypercube sampling schemes are recommended. Additionally, there are several possibilities for curve fitting methods. If the sample size is relatively small, polynomial regression or Gaussian process (if installed as part of PSUADE) is preferred. Alternatively, if the sample size is large enough (one hundred or more), cubic splines (if installed) may also be feasible.

Response Surface Model Validation

To proceed with response surface based analysis, the user needs to find a suitable response surface with which to approximate the input-to-output mapping. Validation is performed to see how well a particular response surface can predict a subset of the withheld data.

1. Load "lptau100_10inputs_4outputs.dat" from the examplesUQ folder. Note: This is an extremely small simulation ensemble, as this is used to highlight the differences (in validation results) between a good response surface and a bad one.
2. Click Analyze for the current ensemble. A new dialog page displays (Figure*[fig:uqt_rs_validate]*).
3. Under "Analysis" (bottom section), under Step 1, select "Response Surface."

   [fig:uqt_rs_validate]

4. Under Step 2, select "removalCO2" as the output for analysis.
5. Under Step 3, select "Polynomial" for response surface method.
6. There are multiple types of polynomial response surfaces, with increasing complexity as the user navigates down the list. For now, select "Linear" in the next drop-down list.
7. Insert 5.00 as the error envelope for the validation plot. Click Validate. The result is illustrated in Figure*[fig:uqt_rs_validate_results]*.

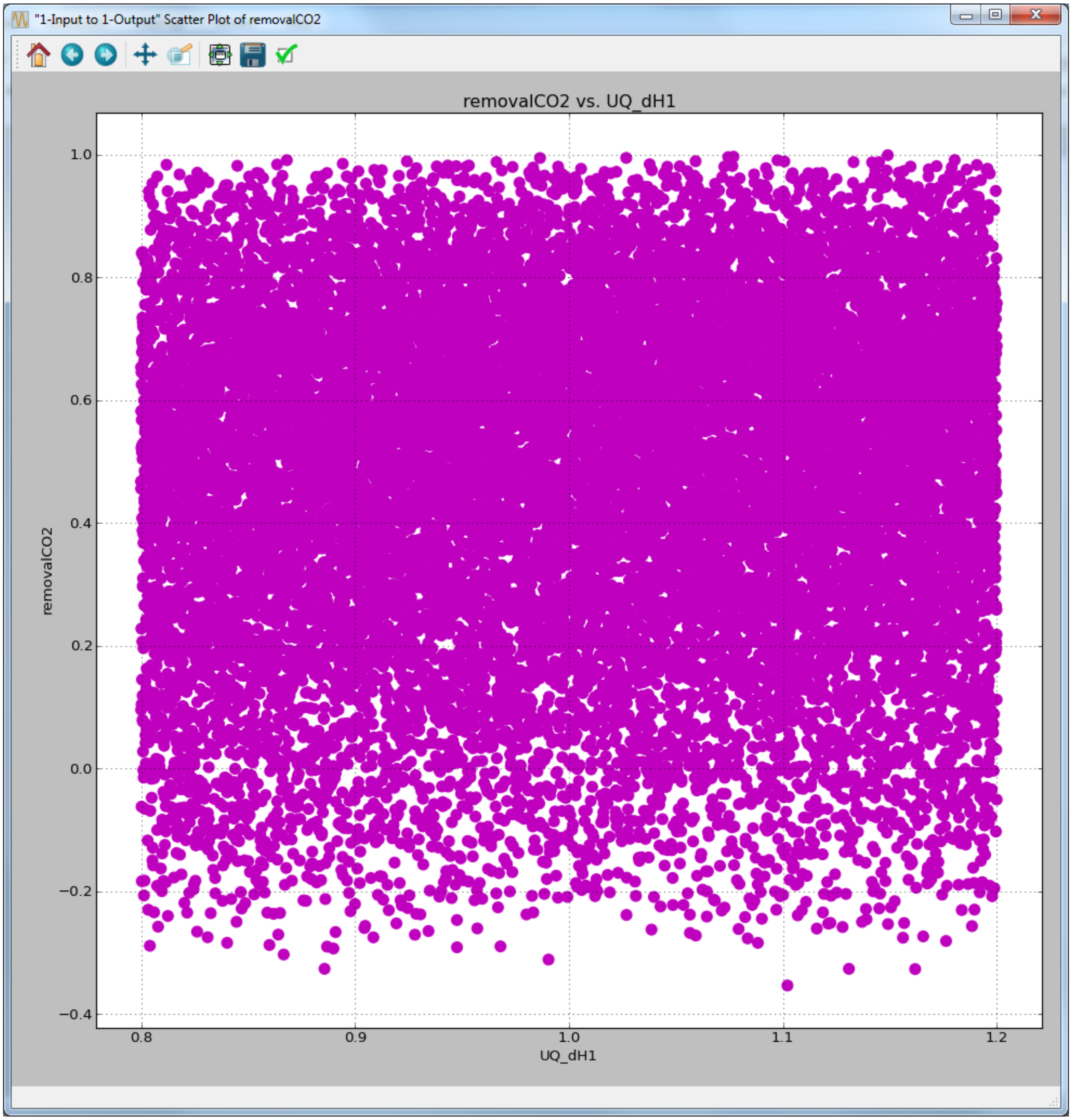


Fig. 31: Ensemble Data Visualization of One Input

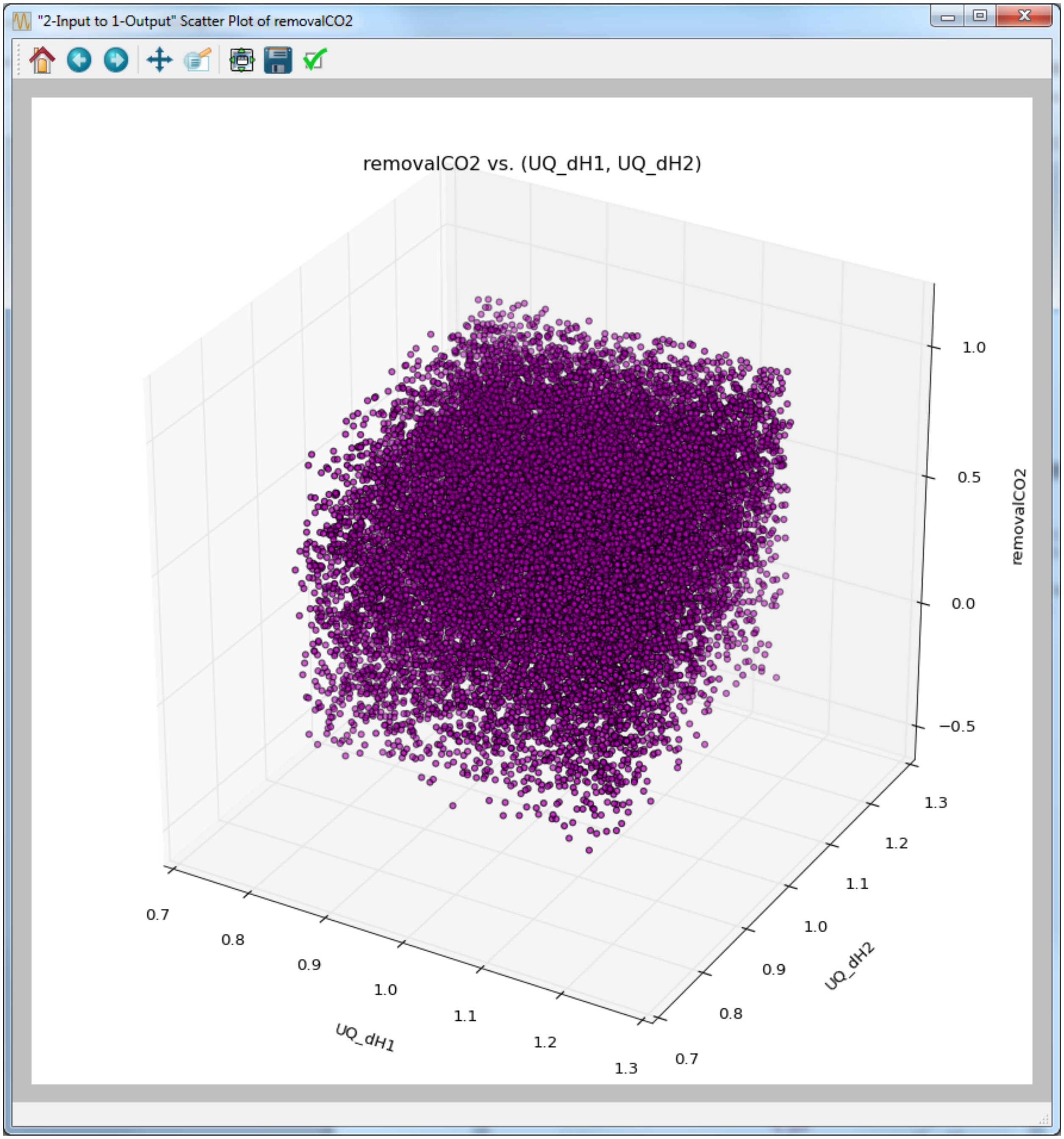


Fig. 32: Ensemble Data Visualization of Two Inputs

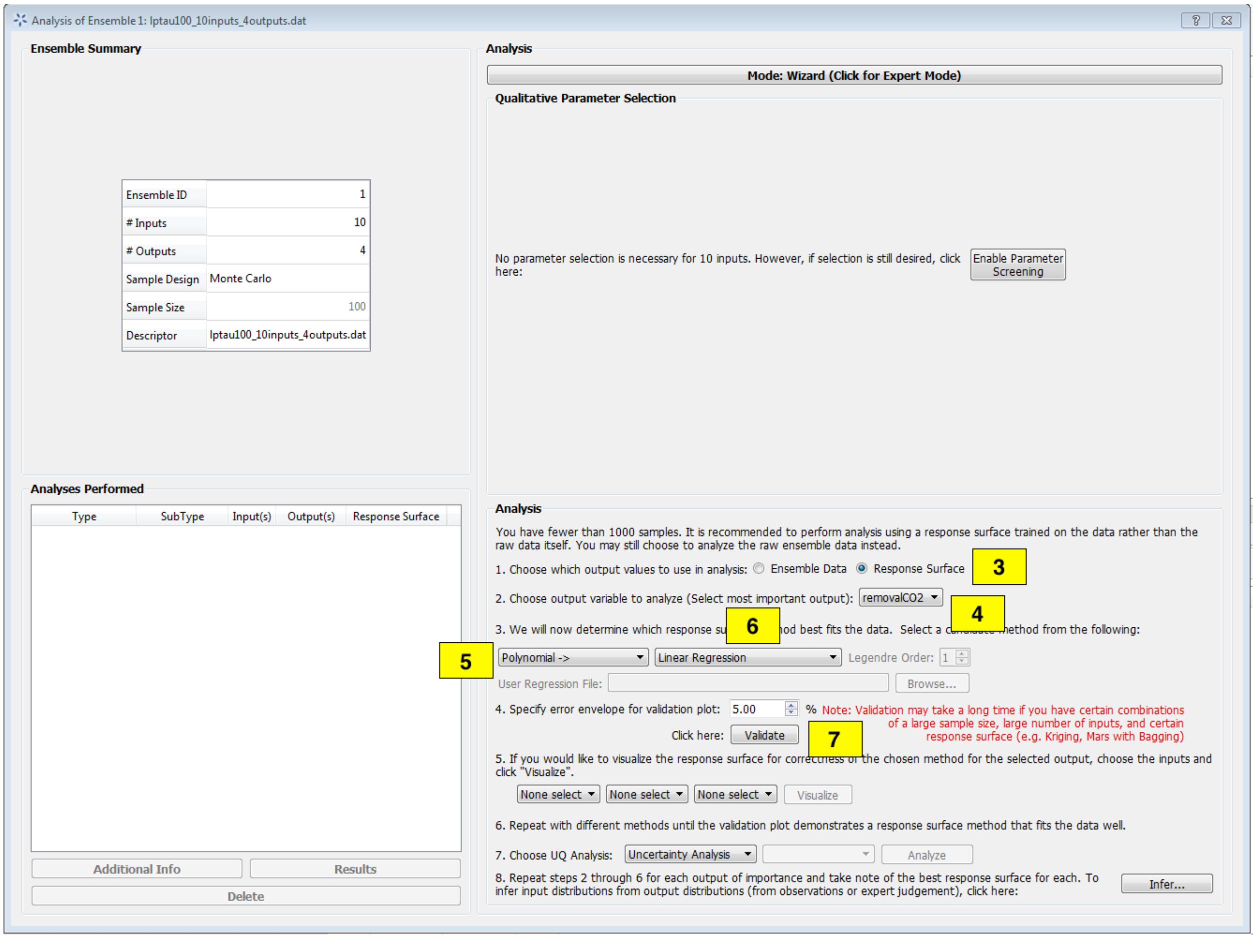


Fig. 33: Analysis Dialog, Response Surface Validation of Linear Model

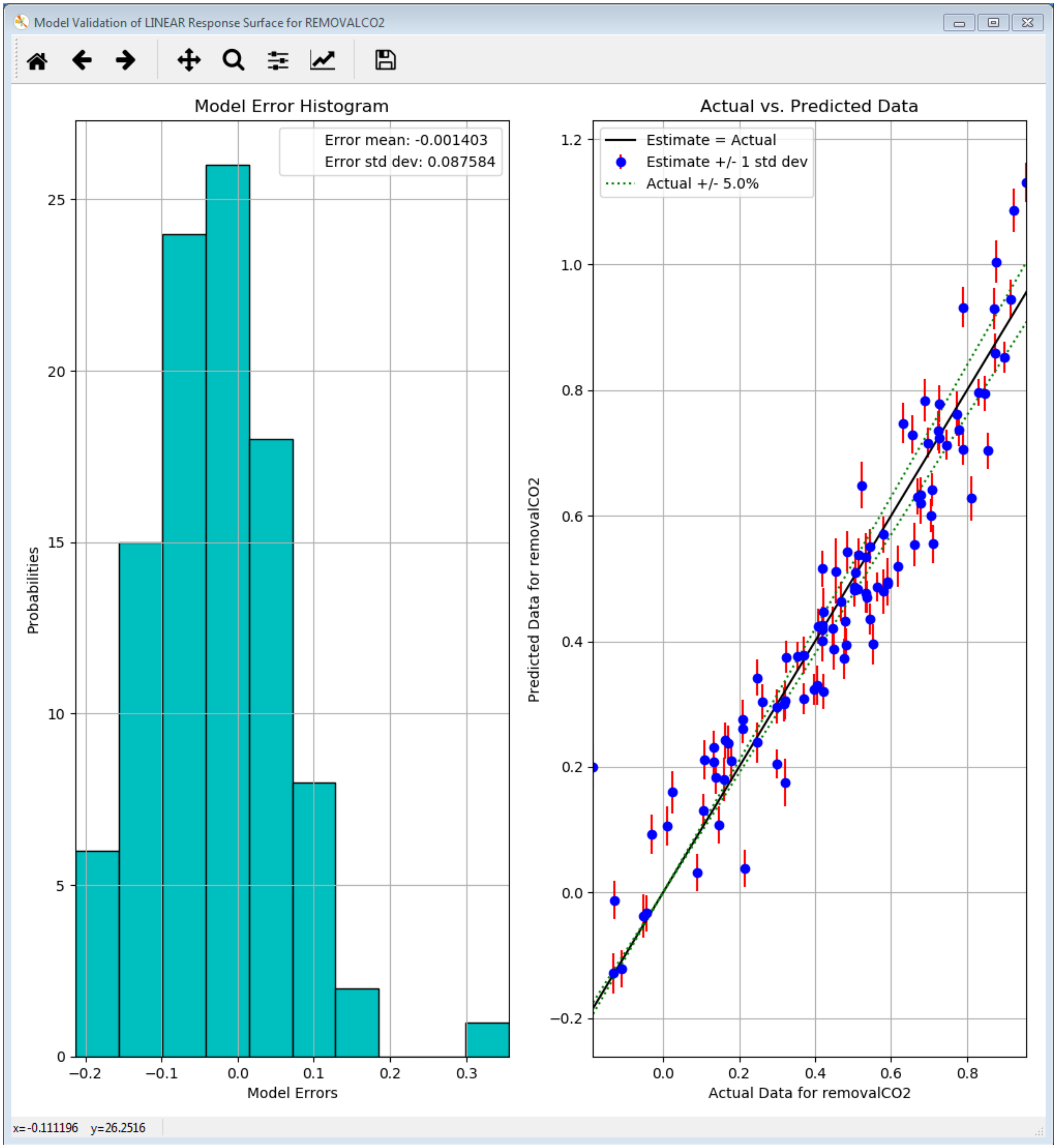


Fig. 34: Linear Response Validation Results

[fig:uqt_rs_validate_results]

The cross-validation results for the linear regression model are displayed as a histogram of errors to the left and a plot of predicted values versus actual values to the right. The histogram displays the cross validation error distribution, which provides the user information on what the errors are like overall. If this distribution is not centered on zero, there may be a systematic bias in the response surface model. If the distribution is too wide, it is not a good fit. As for the plot of predicted values versus actual values, the more closely the points are to the diagonal, the better the fit. Most response surface models, with the exception of MARS, also provide uncertainty information about the response surface. The vertical error bars on the left plot reflect the uncertainty in the linear response's predictions.

In summary, these two figures should provide sufficient information for the user to judge how good the fit is. As is apparent in the figures, the linear model consistently overestimates and thus is an ill-suited response surface to model our data. In general, the user may use a few response surface methods to see which method gives the best fit.

Response Surface Based Uncertainty Analysis

These capabilities are similar to those for ensemble data analysis. The difference is that the results are now derived from a much larger ensemble that is computed from the response surface. With the 100 samples from the ensemble data, a response surface is trained and is used to generate 100K samples internally to compute the results for uncertainty and sensitivity analyses. (Note: Validation must be performed before these analyses are available.)

After the response surface validation step, select "Uncertainty Analysis" to be the UQ analysis in Step 7 of "Analysis" (Figure *[fig:uqt_rs_validate]*). Click **Analyze** and a distribution representing the output uncertainty will be displayed (Figure *[fig:uqt_rsua_results]*).

[fig:uqt_rsua_results]

Compare the response surface based uncertainty results (Figure *[fig:uqt_rsua_results]*) to the results from ensemble data analysis (Figure *[fig:uqt_ua_results]*). The two main differences are easily seen.

- Two PDFs on top plot: A response surface (in this case, linear regression) is used to predict the output values corresponding to the input samples. From the validation step (left plot of Figure*[fig:uqt_rs_validate_results]*). Note: There is error associated with the response surface's predictions. This error is propagated in uncertainty analysis, in the form of standard deviations around the predicted output values (i.e., the means). Accordingly, two histograms are presented: The "mean PDF" represents the output probability distribution computed from the response surface's predicted output values only, without consideration for the uncertainties surrounding these predicted values. The "ensemble PDF" represents the output probability distribution that encompasses the uncertainties surrounding these predicted values. In most cases, the ensemble PDF should have a larger spread because it is accounting for more uncertainties (i.e., those that stem from the approximations inherent in the response surface).
- Multiple cumulative distribution functions (CDFs) on bottom plot: The "mean CDF" is constructed from a cumulative sum on the mean PDF in the top plot. Since each predicted output value (i.e., the mean) has an associated standard deviation, this information is used to construct other PDFs that correspond to output values that are +/- 1, 2, and 3 standard deviations from the mean. These PDFs are then converted to CDFs and shown as colored lines. These colored lines provide an uncertainty "envelope" around the mean CDF.

Response Surface Based Mixed Epistemic-Aleatory Uncertainty Analysis

In "Expert Mode", the user can perform more advanced uncertainty analysis that handles both epistemic and aleatory uncertainties. To do so, the user will need to designate the uncertainty type (epistemic or aleatory) for each uncertain input. In general, epistemic uncertainties are reducible uncertainties that arise due to lack of knowledge, such as simplifying assumptions in a mathematical model. Therefore, epistemic uncertainty is often characterized by upper and lower bounds. On the other hand, aleatory uncertainties are irreducible uncertainties that represent natural,

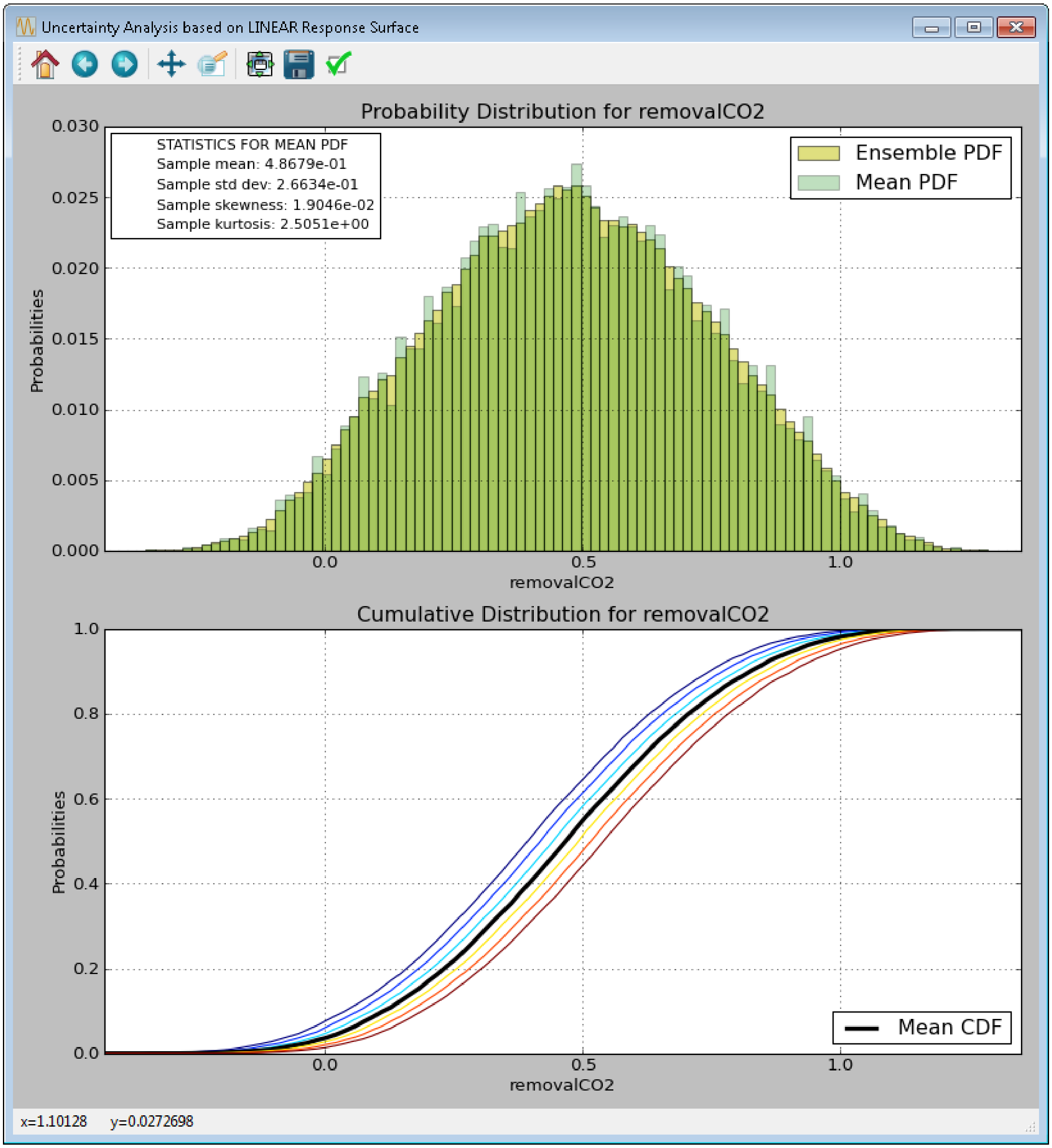


Fig. 35: Response Surface Based Uncertainty Analysis Results

physical variability in the phenomenon under study. As such, aleatory uncertainties are often characterized by distributions. Hence, the user is required to provide a PDF for each aleatory input. (In FOQUS, with the exception of mixed epistemic-aleatory uncertainty analysis, all uncertain inputs are treated as aleatory inputs.)

To perform mixed epistemic-aleatory uncertainty (Figure *[fig:uqt_rsaeua]*), switch to "Expert Mode" by clicking the **Mode** button that toggles between the analysis modes. After response surface validation, select "Uncertainty Analysis" in the first **Choose UQ Analysis** drop-down list, then "Epistemic-Aleatory" in the secondary drop-down list, for the UQ analysis. In the input table, designate the parameter **Type** ("Epistemic", "Aleatory" or "Fixed") and the corresponding information for each input. Once complete, click **Analyze**. In this tutorial we consider dH1 & dH2 as epistemic uncertain parameters, and rest of them are aleatory.

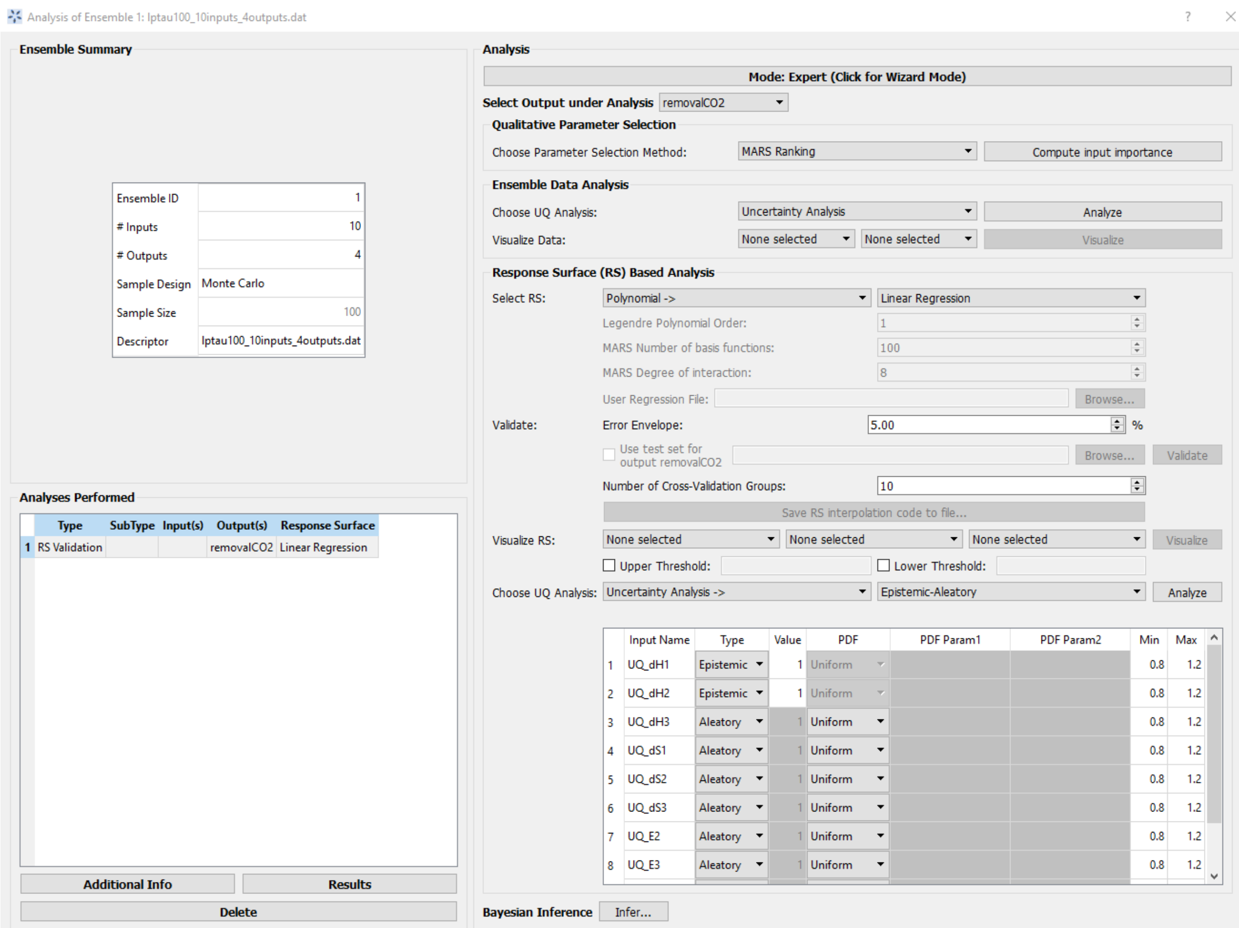


Fig. 36: Response Surface Based Mixed Epistemic-Aleatory Uncertainty Analysis

[fig:uqt_rsaeua]

The results of mixed epistemic-aleatory uncertainty analysis is a plot (Figure *[fig:uqt_rsaeua_results]*) containing multiple CDFs. In the mixed analysis, the epistemic inputs are sampled according to their lower and upper bounds. Each sample point spawns a response surface based uncertainty analysis, in which the epistemic inputs are fixed at their sampled value and the aleatory input uncertainties are propagated to generate a CDF that represents the output uncertainty. A slider is provided for the user to extract the probability range corresponding to a particular value of the output.

[fig:uqt_rsaeua_results]

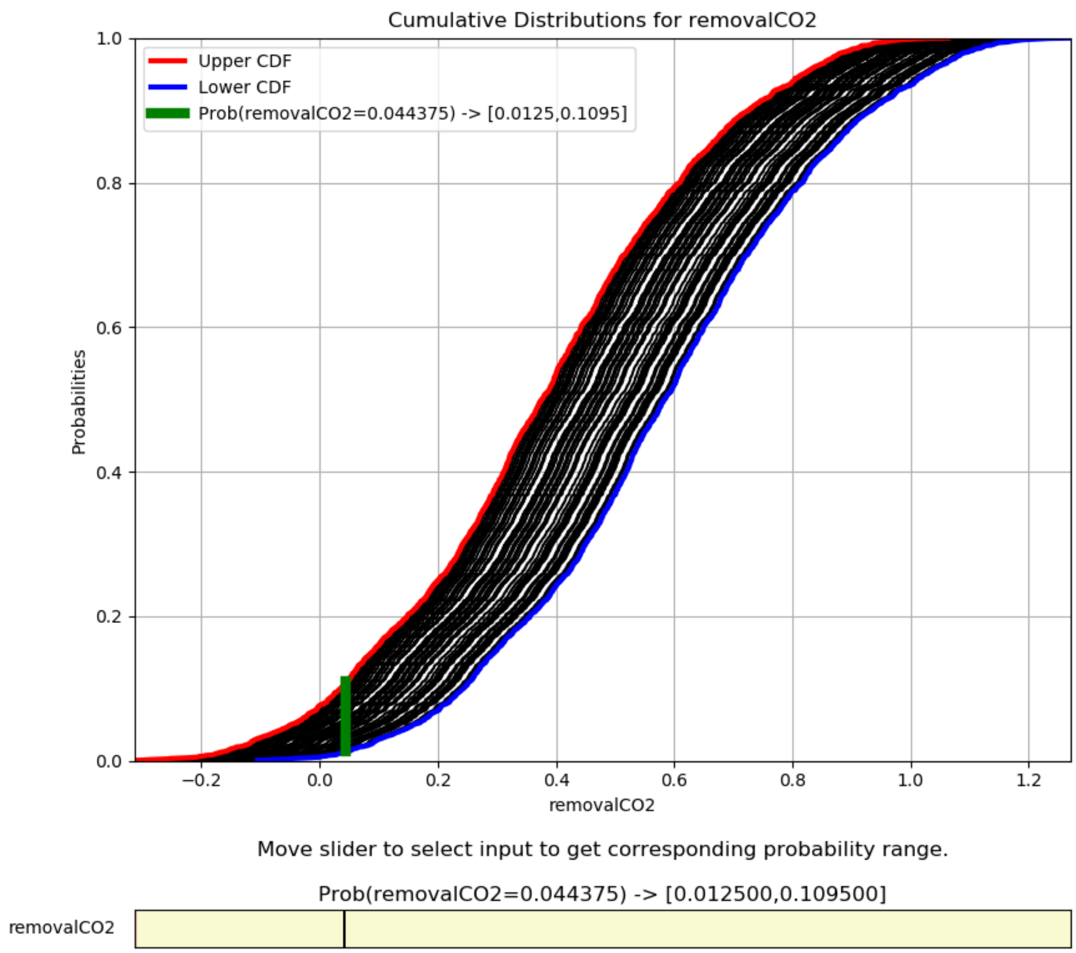


Fig. 37: Response Surface Based Mixed Epistemic-Aleatory Uncertainty Analysis Results

Response Surface Based Sensitivity Analysis

For quantitative sensitivity analysis, follows these steps:

1. In the Choose UQ Analysis drop-down list (Step 6 of "Analysis"), select "Sensitivity Analysis."
2. In the next drop-down list, select "First-order" and click Analyze. (This analysis may take a long time depending on the sample size and the response surface used.)

Prediction errors are associated with the response surface's predictions of the output values (left plot of Figure *[fig:uqt_rs_validate_results]*). Earlier, it was observed that the response surface error contributed to the output uncertainty, leading to a larger spread in the output PDF (top plot of Figure *[fig:uqt_rsua_results]*). In Figure *[fig:uqt_rssa_results]*, the response surface error contributed to uncertainty (shown as blue error bars) surrounding each input's contribution to the output variance (shown as yellow bars).

[fig:uqt_rssa_results]

Response Surface Based Visualization

The response surface that has been validated can also be visualized.

1. Select one input next to "Visualize Response Surface."
2. Click **Visualize** to display a 2-D line plot that displays "removalCO2" versus the selected input.

   [fig:uqt_rs1_results]

3. Select another input next to the first one for a 2-D response surface visualization.
4. Click **Visualize** to display a figure with a 3-D surface plot and a 2-D contour plot (Figure *[fig:uqt_rs2_results]*).

   [fig:uqt_rs2_results]

5. Select another input next to the second one for a 3-D response surface visualization.
6. Click **Visualize** to display a 3-D isosurface plot. Move the slider to see the points in the 3-D input space that fall within the small range of "removalCO2" (Figure *[fig:uqt_rs3_results]*).

   [fig:uqt_rs3_results]

Bayesian Inference

For each output variable, the user specifies an observed value (from physical experiments) with the associated uncertainties (in the form of standard deviation), if applicable. Whether standard inference or SolventFit is selected, the tool will launch a Markov Chain Monte Carlo (MCMC) algorithm to compute the posterior distributions of the uncertain input parameters. These input posterior distributions represent a refined hypothesis about the input uncertainties in light of what was previously known (in the form of input prior distributions) and what was observed currently (in the form of noisy outputs).

1. Load the file "lptau5k_10inputs_4outputs.filtered" from the examplesUQ folder.
2. Click **Analyze** for the current ensemble and a new dialog box displays (Figure *[fig:uqt_analysis_infer]*).

   [fig:uqt_analysis_infer]

3. Select "Response Surface" in the "Analysis" section.
4. Select "Output variable to analyze" to be "removalCO2."
5. Select "Linear Regression" as the response surface.

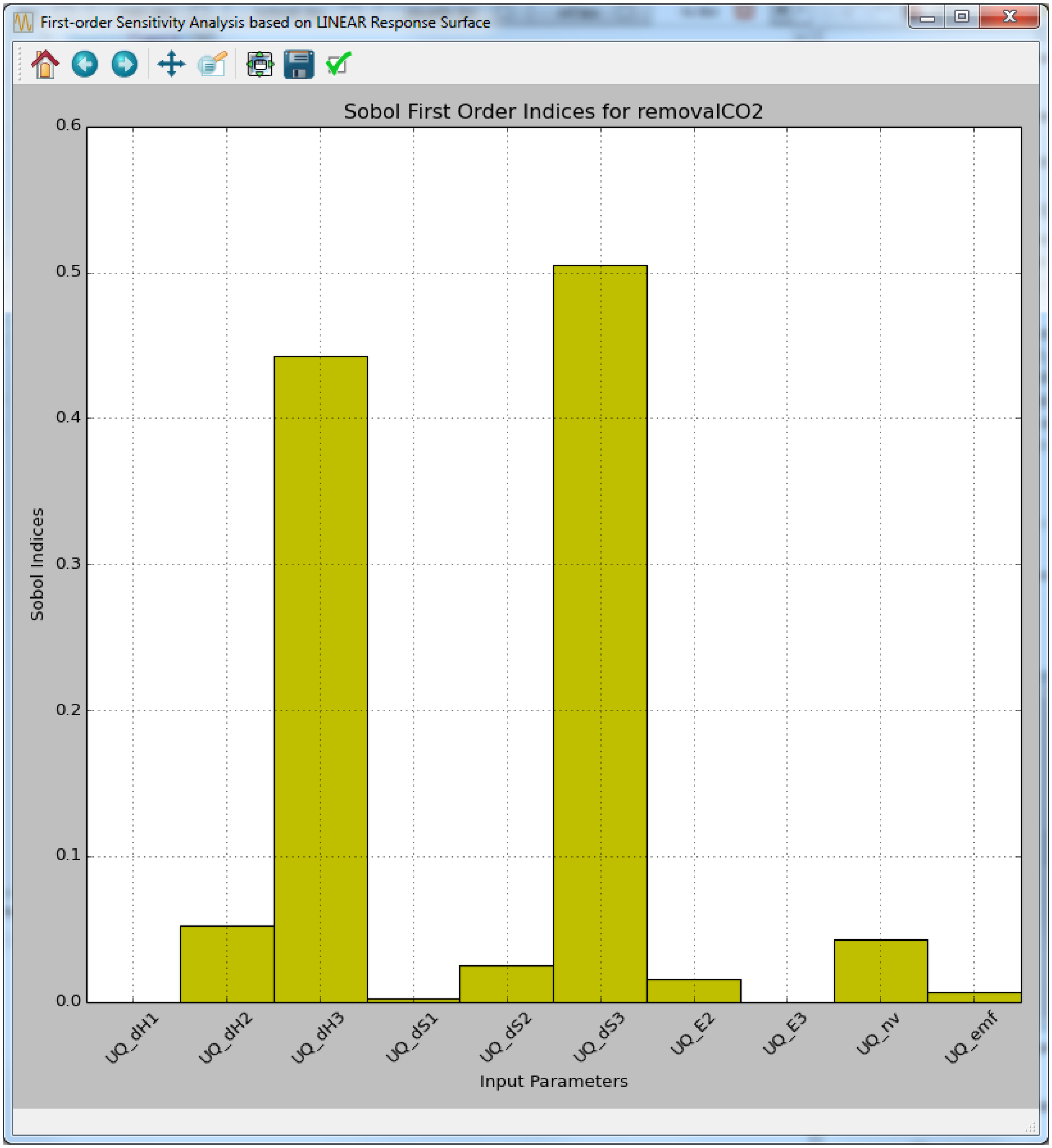


Fig. 38: Response Surface Based First-order Sensitivity Results

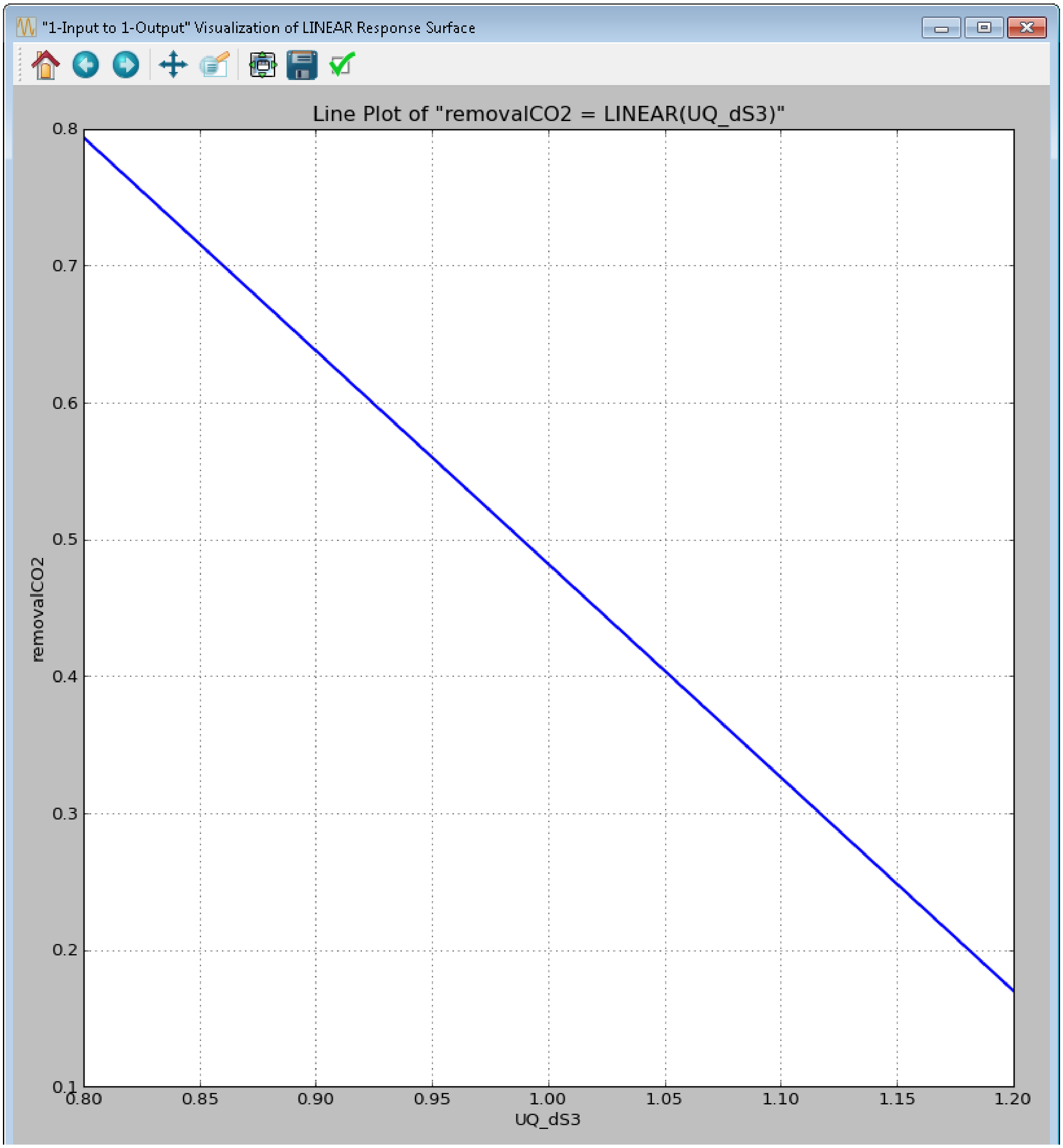


Fig. 39: 1-D Response Surface Visualization

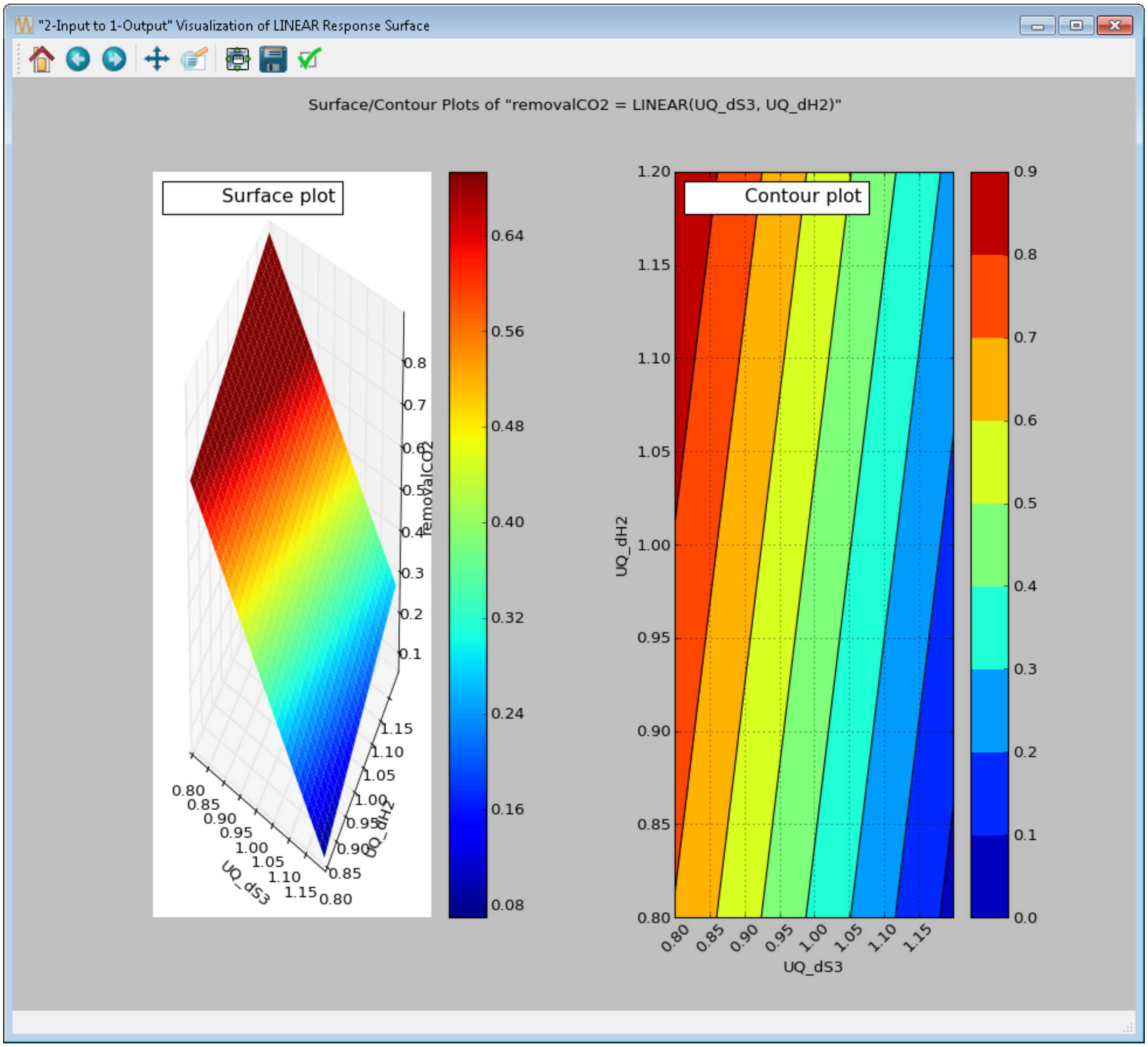


Fig. 40: 2-D Response Surface Visualization

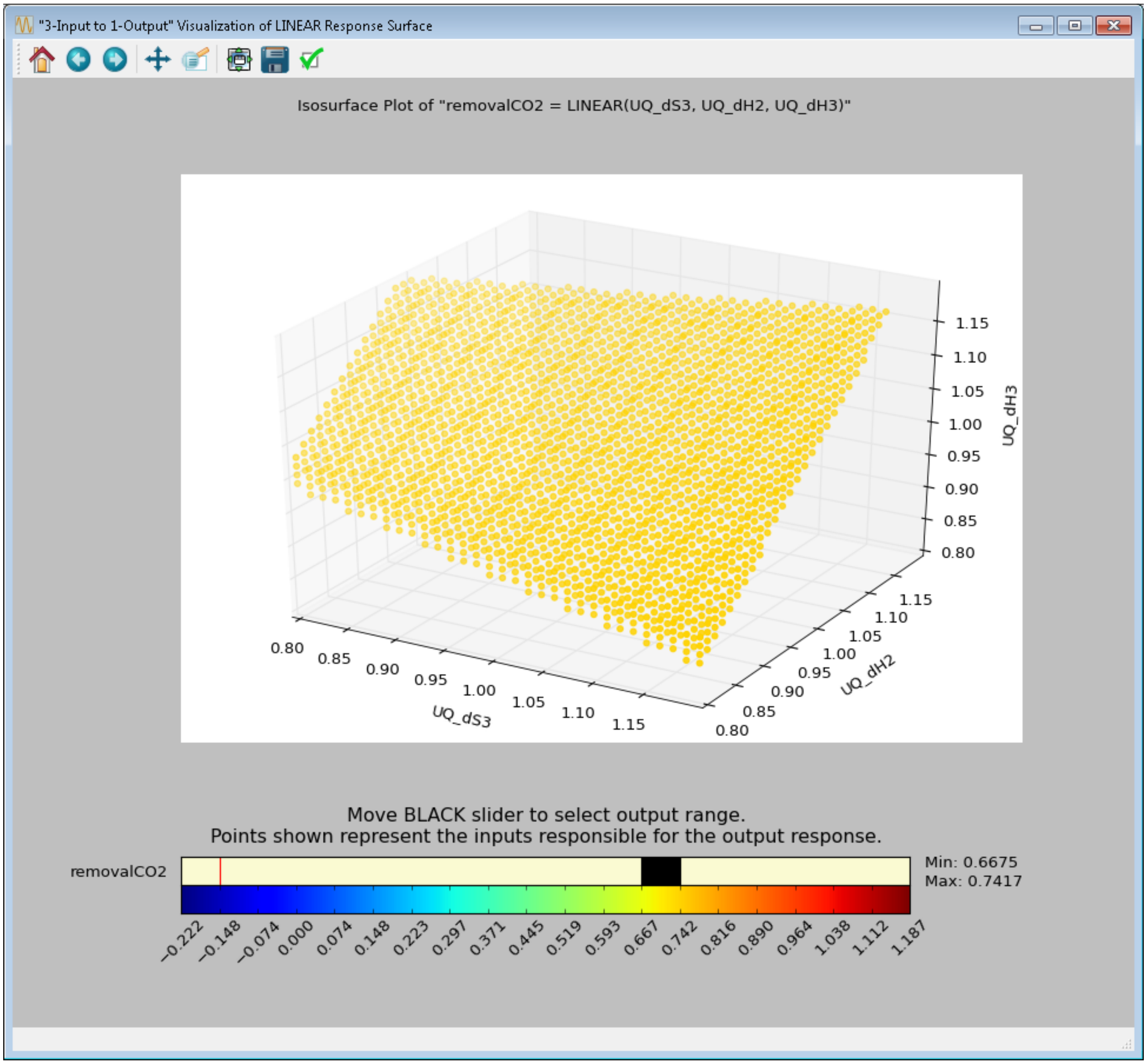


Fig. 41: 3-D Response Surface Visualization

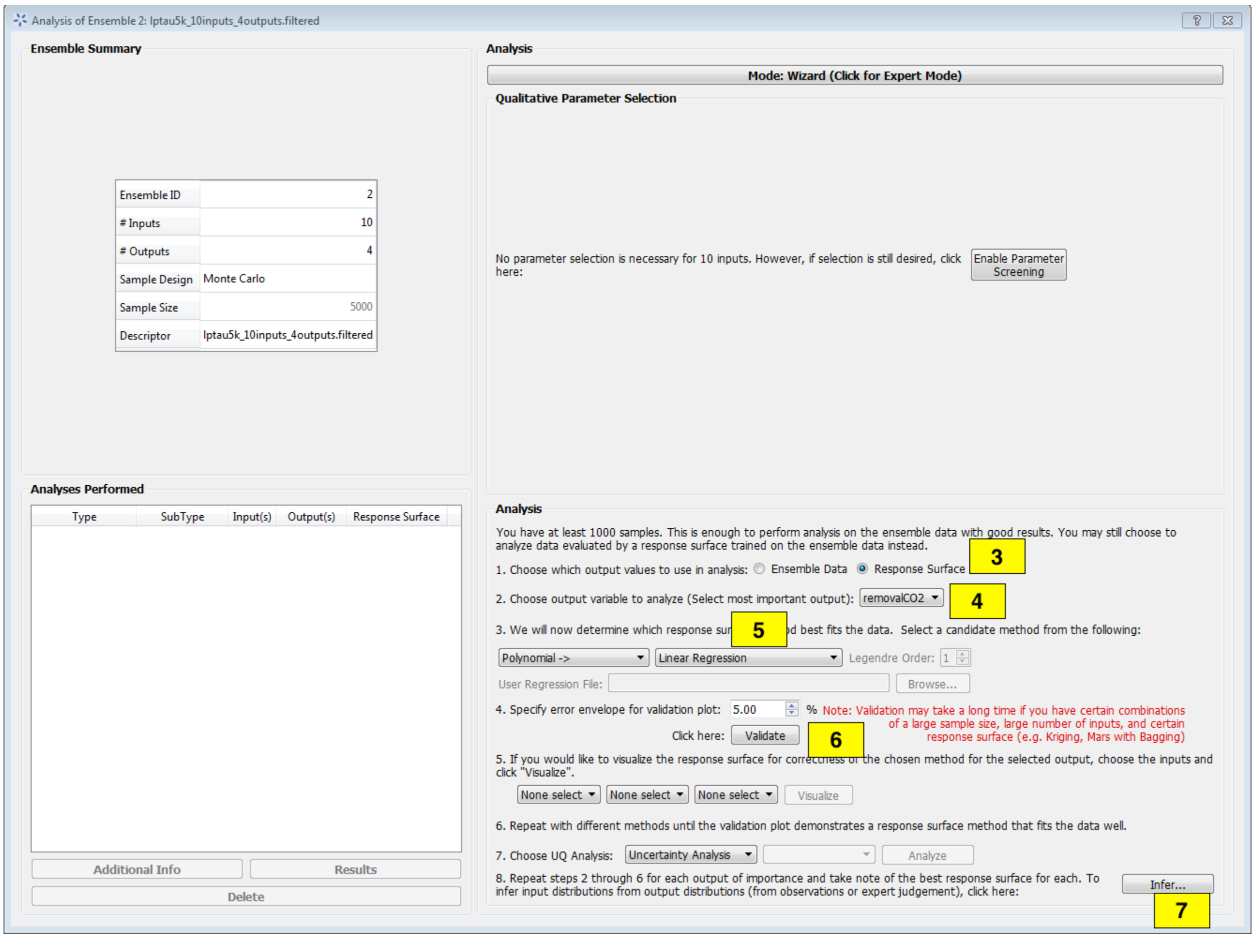


Fig. 42: Analysis Dialog, Bayesian Inference

6. Insert 5.00 as the error envelope for the validation plot. Click Validate. The GUI allows the user to proceed with Bayesian inference after one input has been validated; however, the user may want to validate all outputs since they are all used in the inference.

7. Once validation is completed, click Infer at the lower right corner, which displays a new dialog box (Figure*[fig:uqt_infer]*).

8. In the Output Settings table (on the left), select the second, third, and fourth outputs as the observed outputs. The user can experiment with using different response surface models (for example, linear polynomials) to approximate the mapping from inputs to each of the outputs.

9. In the Input Settings table (on the right), designate input types (variable, design, or fixed) and if necessary, switch to Expert Mode to revise the prior distribution on the input parameters. The prior distribution represents knowledge that the user possesses about the inputs before observational data (from experiments) has been incorporated into this knowledge. If the user does not have any updated knowledge about the simulation ensemble, it is OK to leave the table as is.

10. In the **Observations** table (in the middle), select the number of experiments from which the user can get observational data. In essence, if the user has N observations, then N should be set as the number of experiments. The table will then populate columns for design inputs (if any) and observed outputs. Currently, only normal distribution is supported as the noise model for observations. Enter the mean and standard deviation for each of these observations. For convenience, the mean and standard deviation values are prepopulated with the results from uncertainty analysis. These values have been provided as a sanity check for the user, in case the observation for a particular output is way out of range from these distributions.

    [fig:uqt_infer]

11. To save an input sample drawn from the posterior distribution, select the Save Posterior Input Samples to File checkbox and select a location and file name to store the sample.

12. Click Infer to start the analysis. Inference can take a long time; thus, a stop feature has been implemented. Once inference starts, the Infer button changes to Stop. To stop inference calculations, click Stop which changes the button back to Infer, allowing the user to restart the calculations from scratch. If inference is allowed to run its course, its results are interpolated to produce heat maps (off-diagonal subplots in Figure*[fig:uqt_infer_results]*) for visualization. This interpolation step can take a few minutes and while it is running, Infer is disabled.

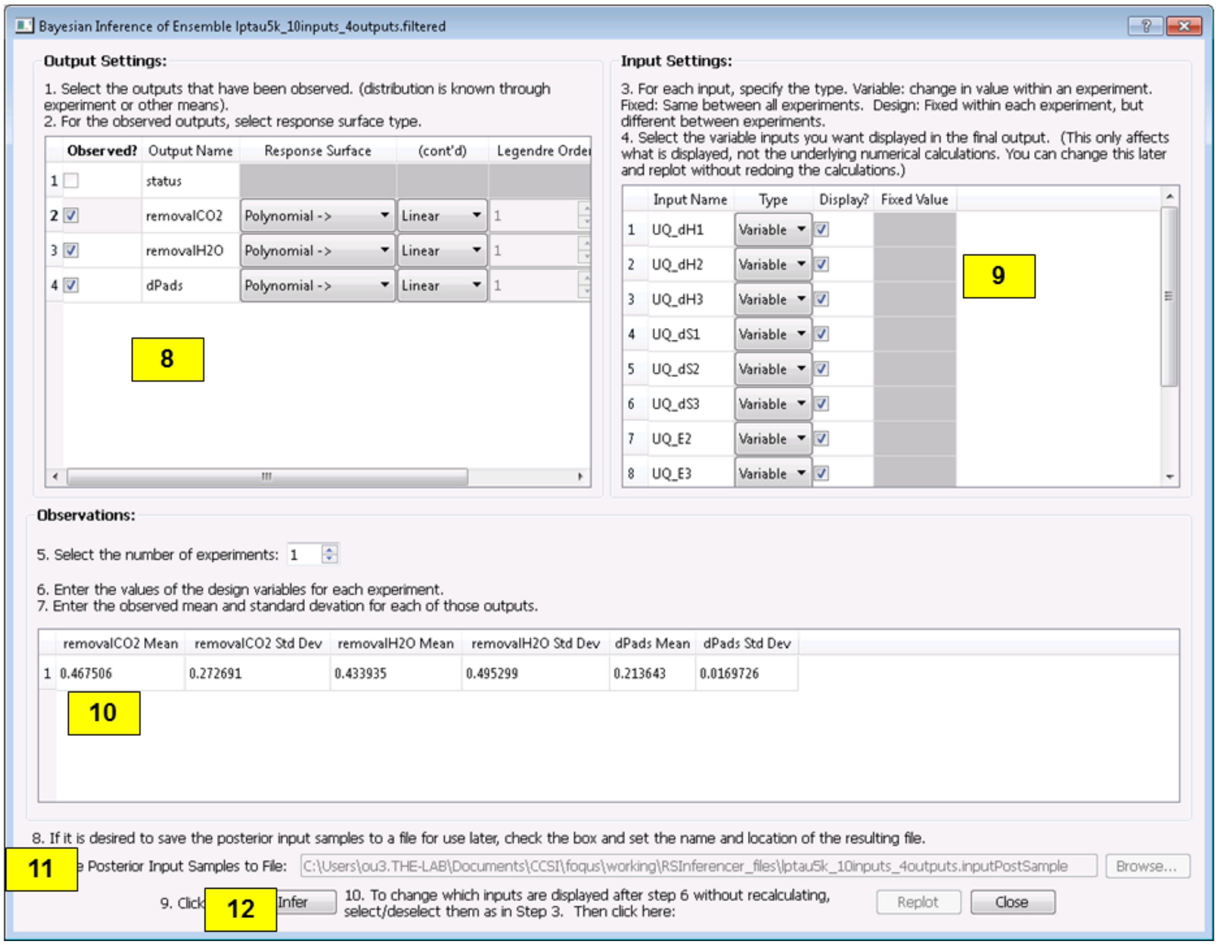
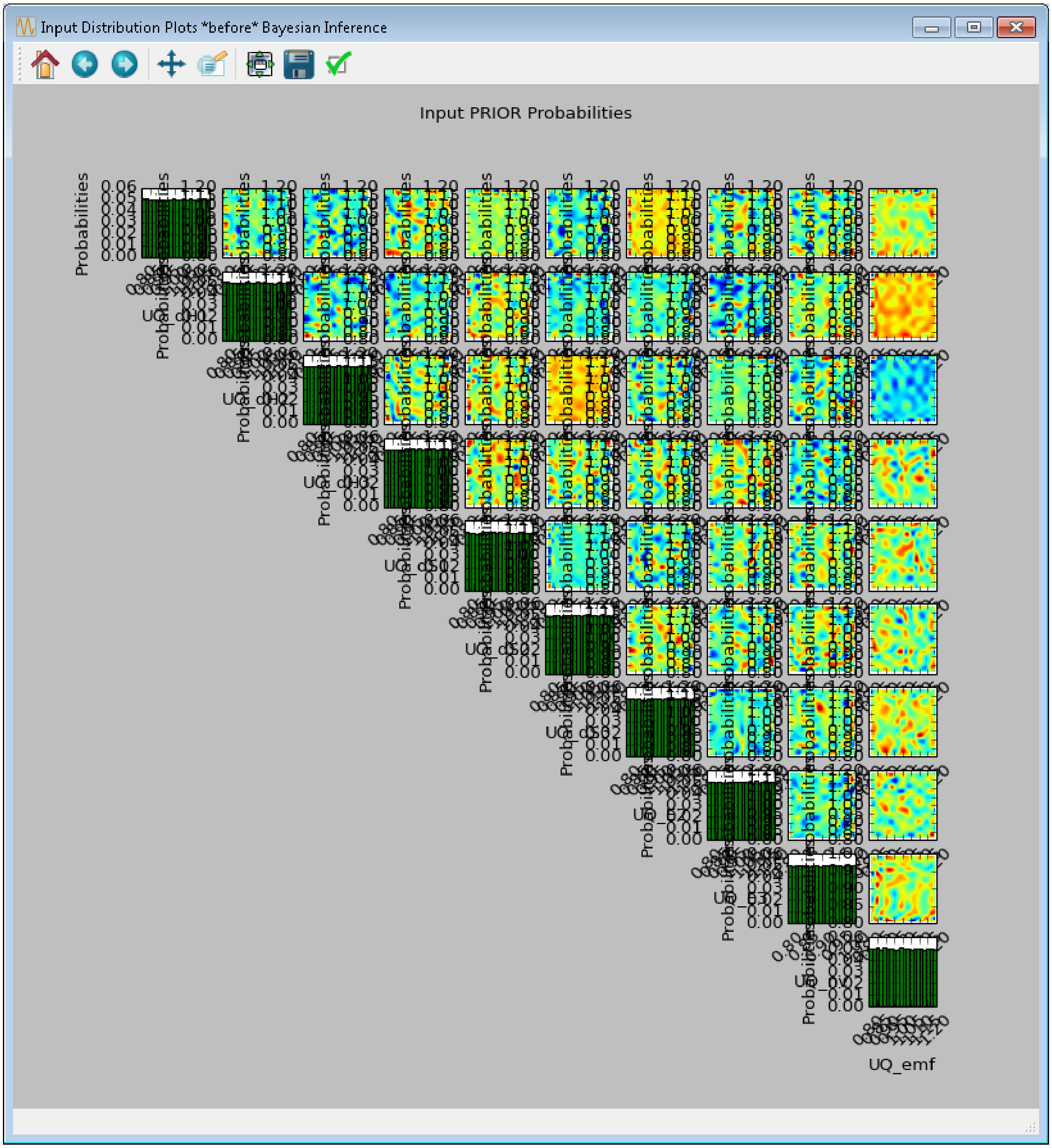
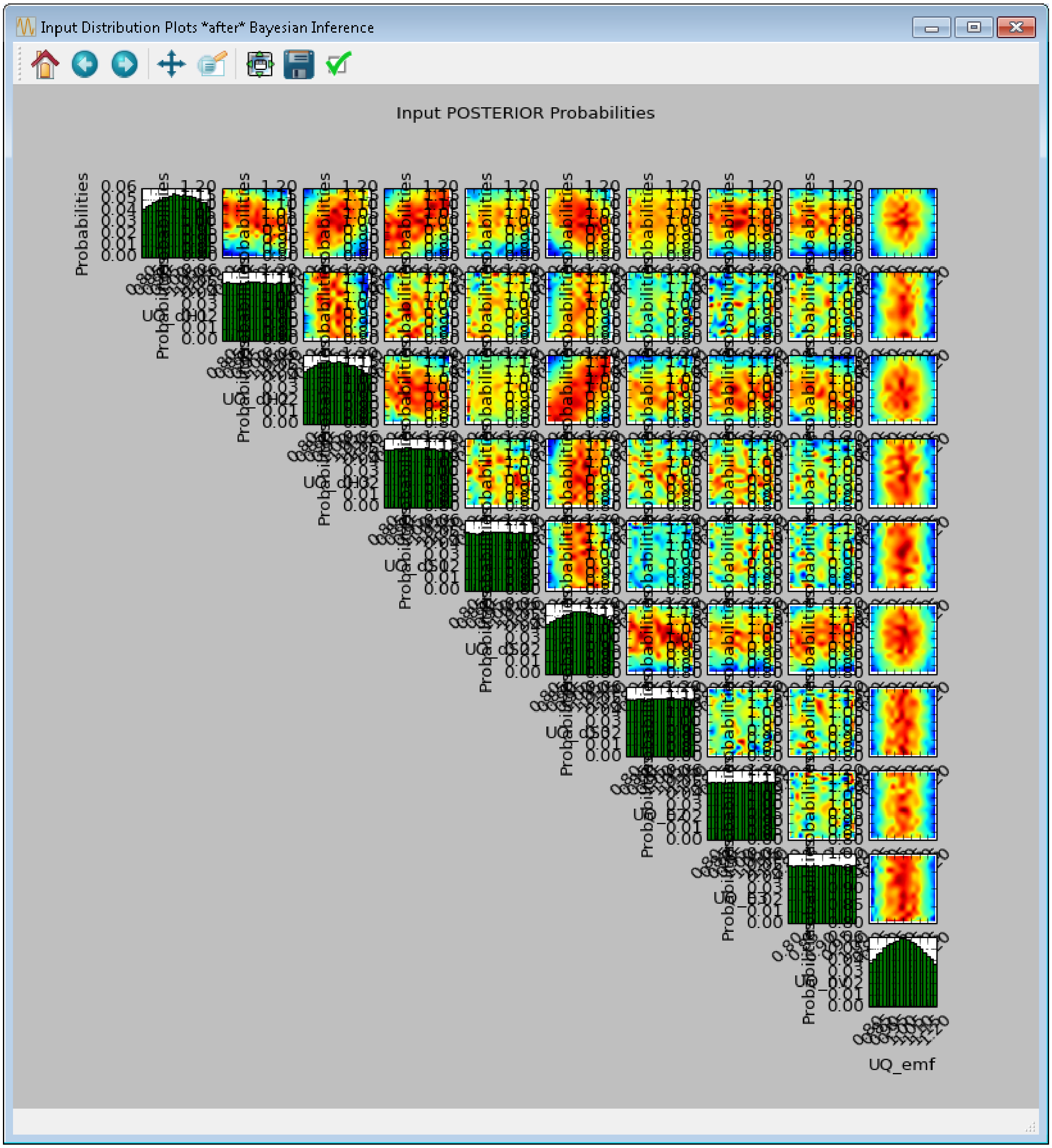


Fig. 43: Bayesian Inference Dialog for Standard Inference


Input Distribution Plots *before* Bayesian Inference
Input PRIOR Probabilities
Probabilities
UQ_emf

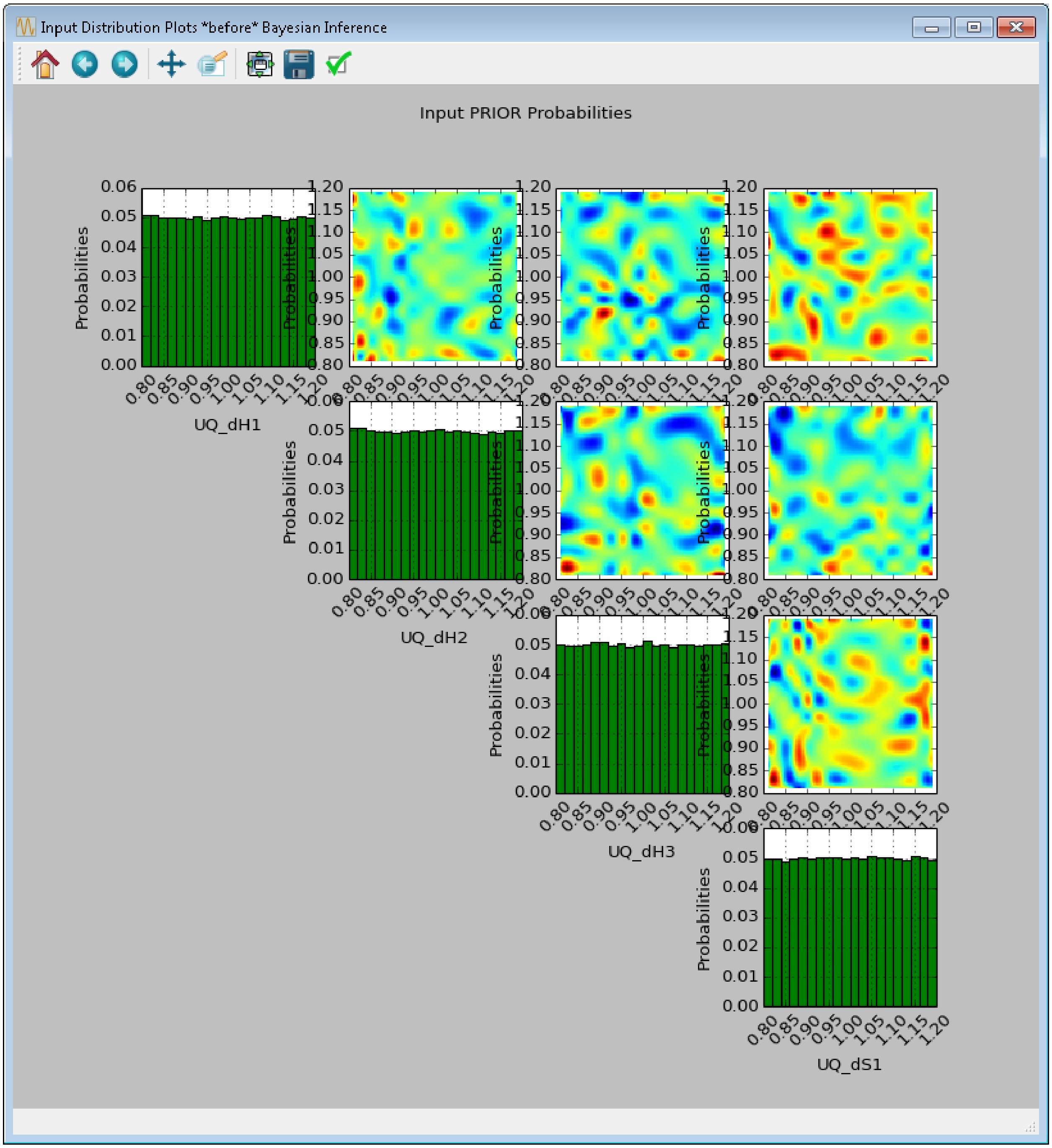


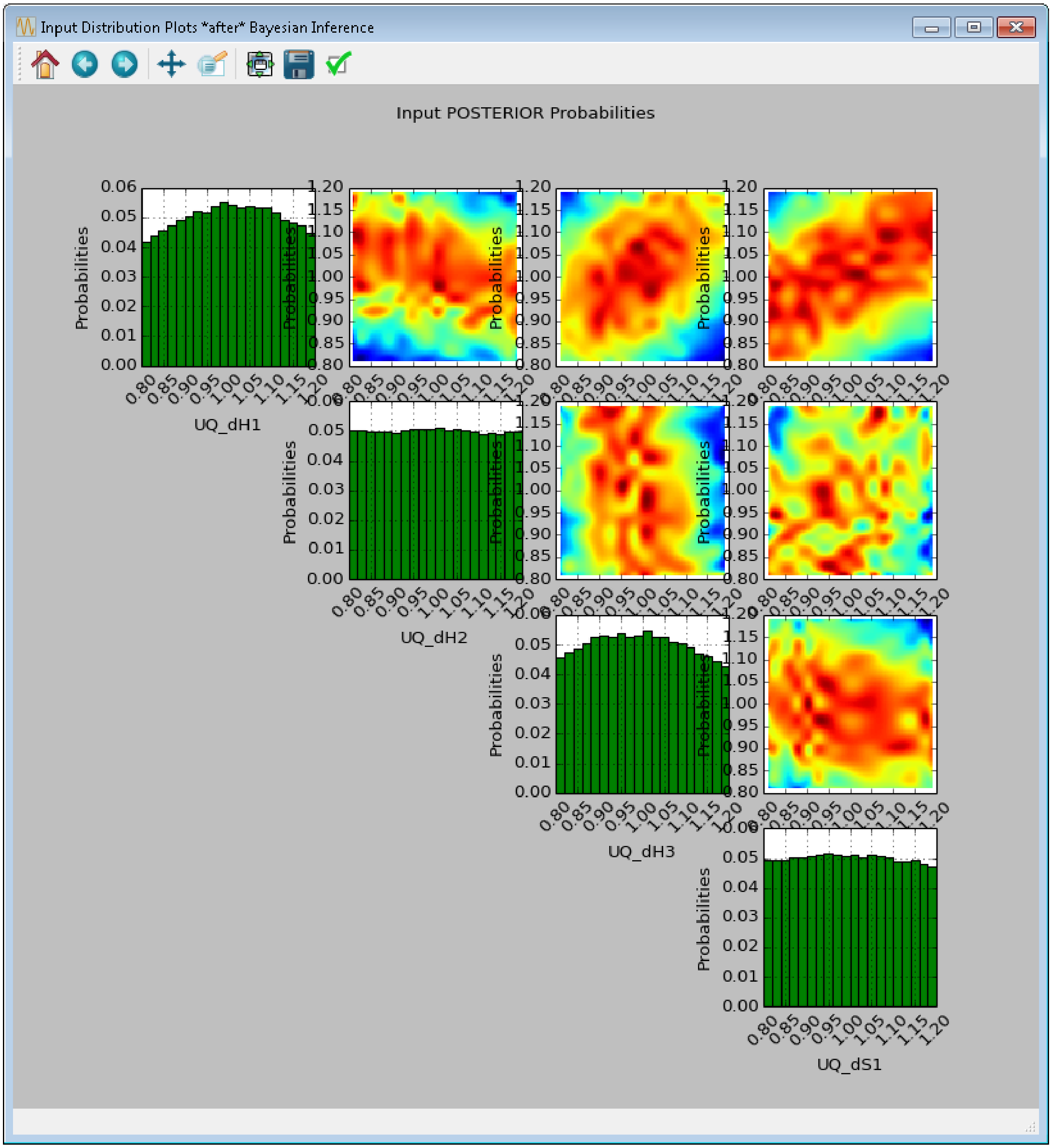
[fig:uqt_infer_results]

Once the inference and interpolation steps are complete, two windows will be displayed: a multi-plot figure of the prior distributions and another multi-plot figure of the posterior distributions. If the user has selected the **Save Posterior Input Samples to File** checkbox, then a sample file will also be written to the designated file location.

In the resulting prior and posterior plots (Figure *[fig:uqt_infer_results]*), the univariate input distributions are displayed as histograms on the diagonal. The bivariate input distributions (between pairs of inputs) are displayed as heat maps in the off-diagonal subplots. On these heat maps, the regions in red reflect the input space with higher probability. In the posterior plots, the red regions represent inputs that are more likely to have generated the specified observations on the outputs. By comparing the prior and the posterior figures, the user can see the ”before” and ”after” impact of inference on our knowledge of the input uncertainty.

To zoom in on any one of the subplots, left-click; to zoom out, right-click. To display a subset of these subplots, clear the checkbox for the inputs to be omitted (from the first column of the Input Prior Table) and click **Replot** (Figure *[fig:uqt_infer_replot_results]*).





[fig:uqt_infer_replot_results]

CHAPTER 6

Optimization Under Uncertainty

6.1 Contents

[sec:ouu_overview]

6.1.1 Reference

The FOQUS OUU module supports several variants of optimization under uncertainty. This chapter first presents the mathematical formulations of these variants. Subsequently, details of the OUU graphical user interface will be discussed.

OUU Variables

Suppose a simulation model is available for an OUU study. Let this simulation model be represented by the following function:

$$Y = F(Z_1, Z_2, Z_3, Z_4),$$
$$which is characterized by four types of variables:$$

1. **Design/Decision/Optimization variables**
   - Notation: Z_1 with dimension n_1
   - Definition: Design variables are continuous variables that may be bounded or unbounded. They are generally the set of optimization variables in a single-stage optimization or the set of outer optimization variables in the two-stage optimization.
2. **Recourse/Operating variables**
   - Notation: Z_2 with dimension n_2
   - Definition: Operating variables are optimization variables in the inner optimization for a given scenario (or realization) of the uncertain variables in a two-stage optimization.

3. **Discrete uncertain variables**
    - Notation: Z_3 with dimension n_3
    - Definition: Discrete variables are uncertain variables that have an enumerable set of states (called scenarios) such that each state is associated with a finite probability and the sum of probabilities for all the scenarios is equal to 1.
4. **Continuous uncertain variables**
    - Notation: Z_4 with dimension n_4
    - Definition: Continuous uncertain variables are associated with a joint probability distribution function from which a sample can be drawn to compute the basic statistics.

OUU Objective Functions

In the presence of uncertainties, OUU seeks to find the optimal solution in some statistical sense. For example, an optimization goal may to be find the design settings that minimizes the statistical mean of the system response. Other popular objective functions are:

1. a linear combination of statistical mean and standard deviation of some selected output,
2. probability of exceeding the best value is smaller than some percentage at any point in the design space (this is analogous to conditional value at risk).

Note that these metrics are defined in the design variable space - that is, at each iteration of an OUU algorithm, the selected metric will be computed for the decision point under consideration. Since the calculation of these statistical metrics requires a sample (possibly large), OUU can benefit from parallel computing capabilities (e.g., the Turbine gateway).

Mathematical Formulations

FOQUS supports two types of OUU methods: single-stage OUU and two-stage OUU. The main difference between single-stage and two-stage OUU is the presence of the recourse (or operational) variables. Strictly speaking, since recourse variables are generally hidden (they are only needed in the inner stage and their values are not used in the outer stage of two-stage OUU), the distinction between single-stage and two-stage OUU is not clear. Nevertheless, for the sake of clarify, we will describe details of each formulation separately. The current OUU does not support linearly or nonlinearly-constrained optimization.

Single-Stage Formulation

In this formulation, there is no recourse variable:

$$Y = F(Z_1, Z_3, Z_4)$$

$$and the optimization problem becomes:$$

$$\min_{Z_1} \mathbf{\Phi}_{Z_3,Z_4}\left[F(Z_1, Z_3, Z_4)\right]$$

where $\Phi_{Z_3,Z_4}[F(Z_1, Z_3, Z_4)]$ is the statistical metric (one of the three options given above).

For example, if the objective function is the statistical mean, then the formulation becomes:

$$\min_{Z_1} \mathbf{E}_{Z_3,Z_4}[F(Z_1, Z_3, Z_4)] \approx \min_{Z_1} \sum_{j=1}^{n_3} \pi_j \left(\int F(Z_1, Z_3, Z_4) P(Z_4) dZ_4 \right)$$

where, again, n_3 is the number of scenarios for the discrete uncertain variables, π_j is the probability of the j-th scenario, and $P(Z_4)$ is the joint probability of the continuous uncertain variables.

Two-Stage Formulation

In this formulation all four types of variables are present. The objective function is given by:

$$\min_{Z_3,Z_4} \mathbf{\Phi}_{Z_3,Z_4} \left[\min_{Z_2} F(Z_1, Z_2, Z_3, Z_4) \right].$$

If the objective function is the statistical mean, the formulation becomes:

$$\begin{aligned} & \min_{Z_1} \mathbf{E}_{Z_3,Z_4} \left[\min_{Z_2} F(Z_1, Z_2, Z_3, Z_4) \right] \\ \approx \quad & \min_{Z_1} \sum_{j=1}^{n_3} \pi_j \left(\int \left[\min_{Z_2} F(Z_1, Z_2, Z_3, Z_4) \right] P(Z_4) dZ_4 \right) \\ & Let \end{aligned}$$

$$G(\mathbf{Z_1}, \mathbf{Z_3}, \mathbf{Z_4}) = \min_{Z_2} F(Z_1, Z_2, Z_3, Z_4).$$

$$Thenthetwo - stageequationcanberewrittenas:$$

$$\begin{aligned} & \min_{Z_1} \mathbf{E}_{Z_3,Z_4} \left[G(Z_1, Z_3, Z_4) \right] \\ \approx \quad & \min_{Z_1} \sum_{j=1}^{n_3} \pi_j \left(\int G(Z_1, Z_3, Z_4) P(Z_4) dZ_4 \right) \end{aligned}$$

$$whichisasingle - stageOUUwithrespecttothe : math : `G`function.$$

Windows Users

Before using the OUU module, Windows users may need to update the following registry keys:

1. HKEY_CLASSES_ROOT\Applications\python.exe\shell\open\command
2. HKEY_CLASSES_ROOT\py_auto_file\shell\open\command

To update these registry keys:

1. Open the Registry Editor by going to the Windows Start menu, typing "regedit" (without the quotes), and selecting "regedit" (Figure *regedit in the Windows Start menu*).
2. After the Registry Editor is opened, locate "HKEY_CLASSES_ROOT" (Figure *HKEY_CLASSES_ROOT in the Registry Editor*).
3. Under "HKEY_CLASSES_ROOT", locate "Applications" (Figure *Applications under HKEY_CLASSES_ROOT*).
4. Under "Applications", locate "python.exe\shell\open\command" (Figure *python under Applications*).
5. In the table on the right, double-click "(Default)" under "Name" (Figure *python under Applications*).
6. In the input box (Figure *python under Applications*), type (including the quotations): "the location of the Anaconda 3 version of python.exe" "%1" %*
7. After clicking "OK", the information you typed in the input box should appear under "Data" in the table on the right (Figure *python under Applications*).
8. Under "HKEY_CLASSES_ROOT", locate "py_auto_file\shell\open\command" (Figure *py_auto_file under HKEY_CLASSES_ROOT*).

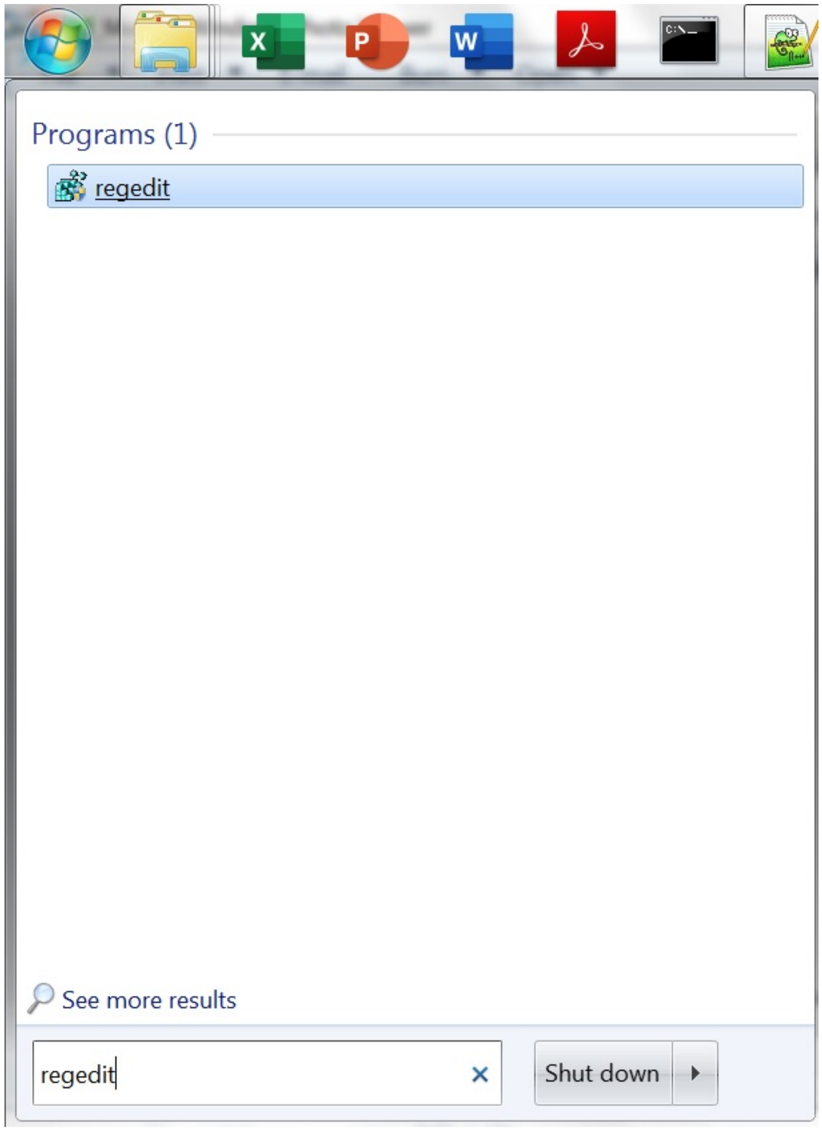


Fig. 1: regedit in the Windows Start menu

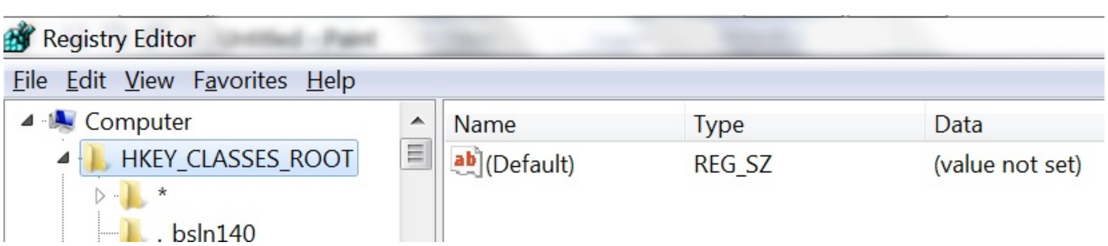


Fig. 2: HKEY_CLASSES_ROOT in the Registry Editor

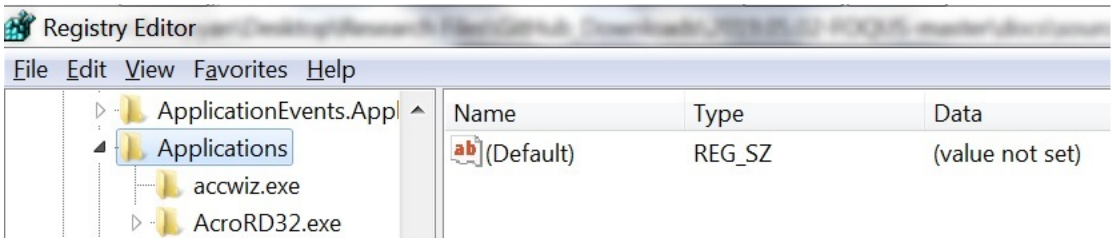


Fig. 3: Applications under HKEY_CLASSES_ROOT

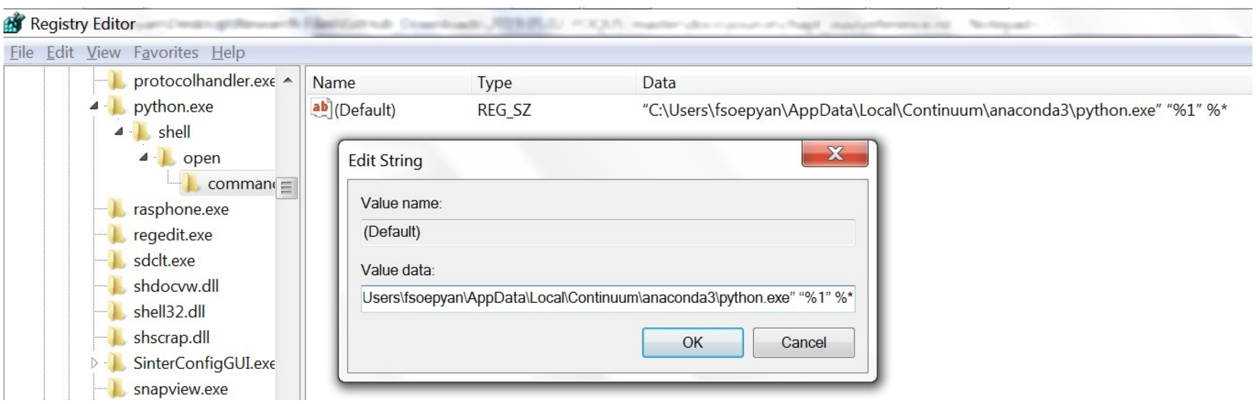


Fig. 4: python under Applications

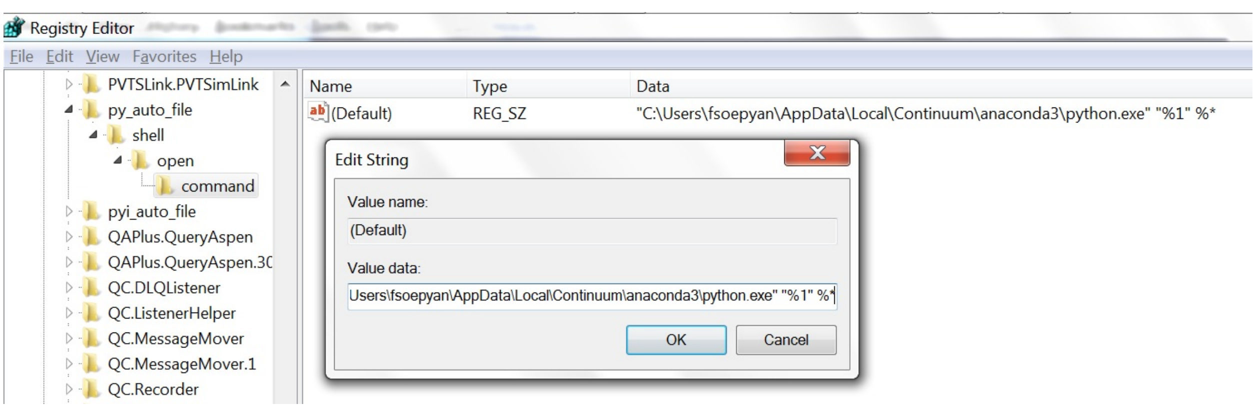


Fig. 5: py_auto_file under HKEY_CLASSES_ROOT

9. In the table on the right, double-click "(Default)" under "Name" (Figure *py_auto_file under HKEY_CLASSES_ROOT*).
10. In the input box (Figure *py_auto_file under HKEY_CLASSES_ROOT*), type (including the quotations): "the location of the Anaconda 3 version of python.exe" "%1" %*
11. Note that the code in Step 10 and Step 6 are the same (Figure *python under Applications*).
12. After clicking "OK", the information you typed in the input box should appear under "Data" in the table on the right (Figure *py_auto_file under HKEY_CLASSES_ROOT*).

OUU User Interface

The OUU module enables the user to perform optimization under uncertainty studies on a flowsheet. From the OUU tab, the user can set up the different types of optimization parameters, select from the different OUU options, and run the optimization. This screen is shown in Figure [fig:ouu_screen].

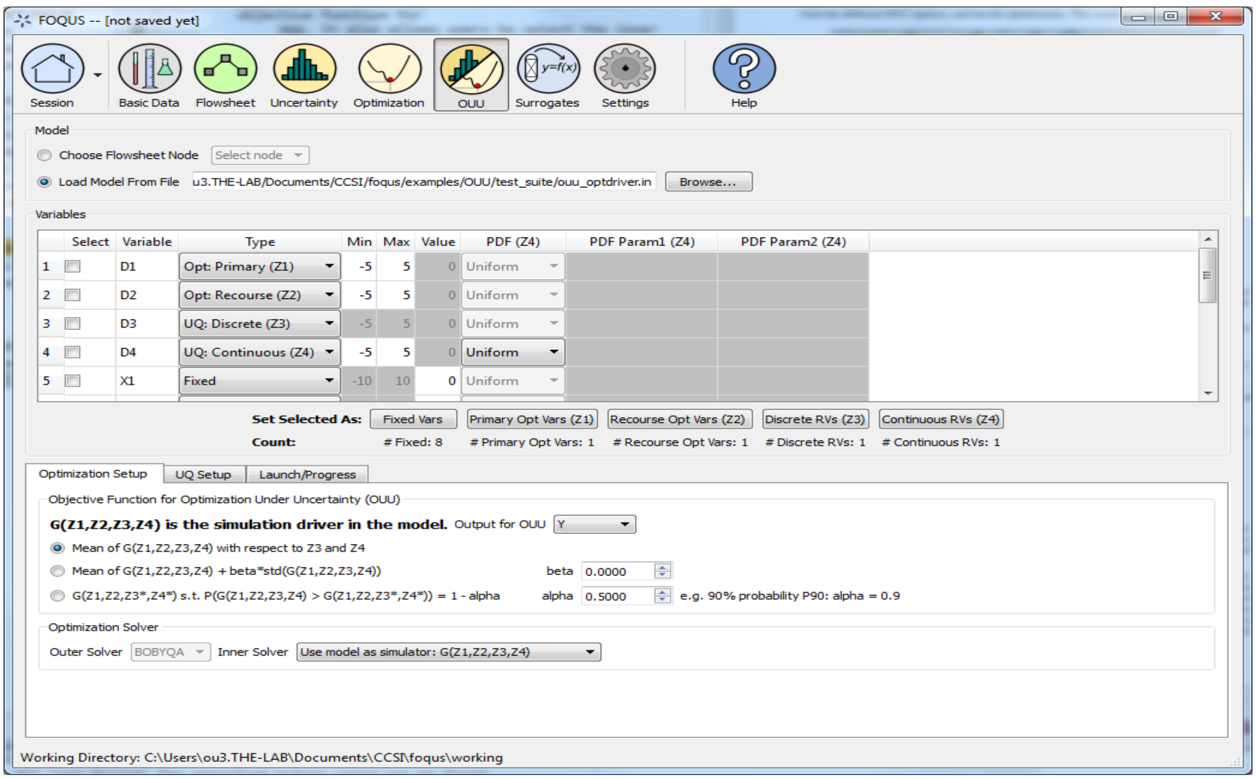


Fig. 6: Optimization Under Uncertainty Screen

1. **Model** provides two options for setting up the model: (1) select a node from the flowsheet that has already been instantiated; or (2) load the model from a file in the PSUADE full file format (with the opt_driver variable set to the simulation executable.)
2. **Variables** displays all variables defined in the model that can be used in this context. Each available variable can be set to either one of the 6 types:
   - "Fixed": The parameter's value is fixed throughout the optimization process.
   - "Opt: Primary Continuous (Z1)": Continuous parameter for the outer optimization.
   - "Opt: Primary Discrete (Z1d)": Discrete parameter for the outer optimization.

   - "Opt: Recourse (Z2)": Recourse parameter for the inner optimization.
   - "UQ: Discrete (Z3)": Discrete or categorical uncertain parameter that contributes to scenarios.
   - "UQ: Continuous (Z4)": Continuous uncertain parameter with a given probability distribution.

3. **Optimization Setup** allows users to select the objective function for OUU. It also allows users to select the inner optimization solver. There are two options for the inner solver: (1) the simulation model provided by users is an optimizer itself, and (2) the simulation provided by users needs to be wrapped around by another optimizer in FOQUS.
4. **UQ Setup** allows users to set up the continuous uncertain parameters. There are two options: (1) FOQUS can generate a sample internally, or (2) a user-generated sample can be loaded into FOQUS. The sample size should be larger than the number of continuous uncertain parameters. Optionally, response surface can be turned on to enable the statistical moments to be computed more accurately even with small samples. Users can also select a smaller subset of the sample for building response surfaces and evaluate the response surfaces with the larger samples.
5. **Launch/Progress** has the 'Run OUU' button to launch OUU runs.

6.1.2 Tutorial

This section walks through a few examples of running OUU.

Example 1: OUU with Discrete Uncertain Parameters Only

This example has only discrete uncertain parameters and the objective function is computed from the mean estimation with the scenarios from a sample file.

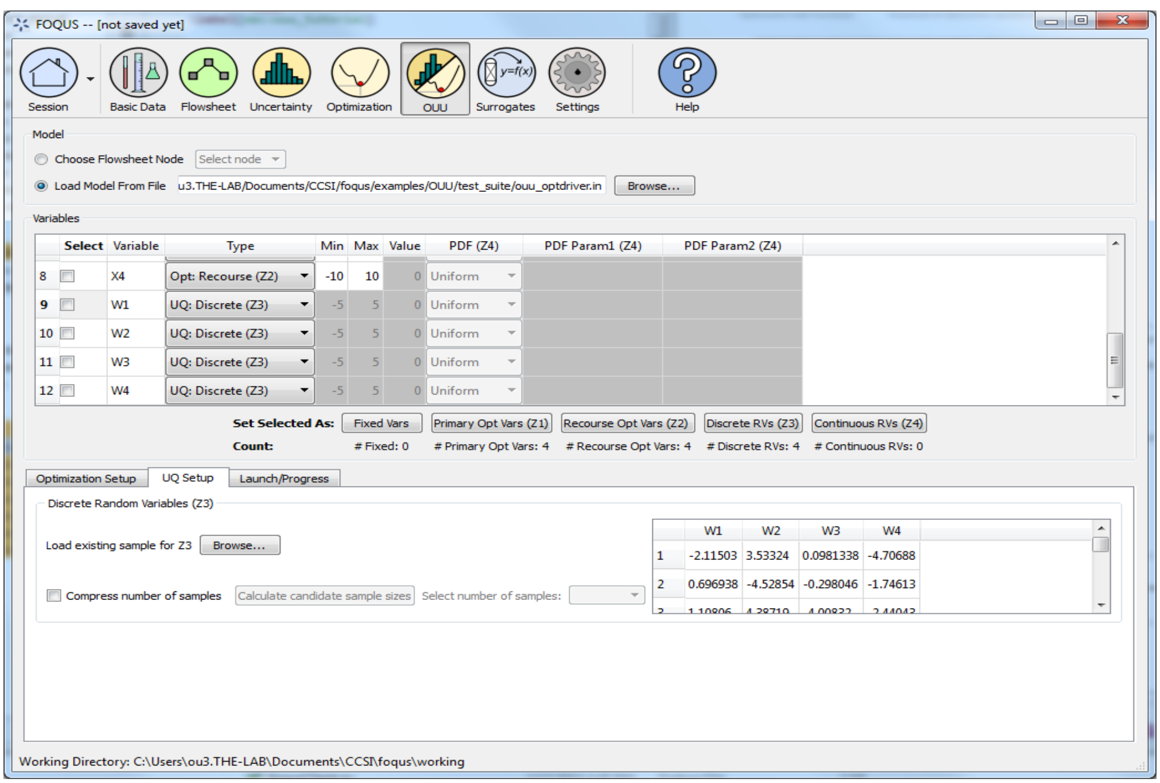


Fig. 7: OUU Example with Discrete Uncertain Parameters

1. Start FOQUS and click the 'OUU' icon.
2. Under 'Model', browse and load examples/OUU/test_suite/ouu_optdriver.in.
3. Under 'Variables', set variable $1-4$ as Z_1, variable $5-8$ as Z_2, and variable $9-12$ as Z_3.
4. Under 'Optimization Setup', select the first objection function (default) and select 'use model as optimizer' as the 'Inner Solver'.
5. Under 'UQ Setup' and 'Discrete Random Variables', browse the examples/OUU/test_suite directory and load the x3sample.smp sample file (see Figure [fig:ouu_ex1]).
6. Go to 'Launch/Progress' page, click 'Run OUU' and see OUU in action.

Example 2: OUU with Continuous Uncertain Parameters Only

This example has only continuous uncertain parameters and the objective function is computed from the mean estimation with a Latin hypercube sample of size 200 for Z_4.

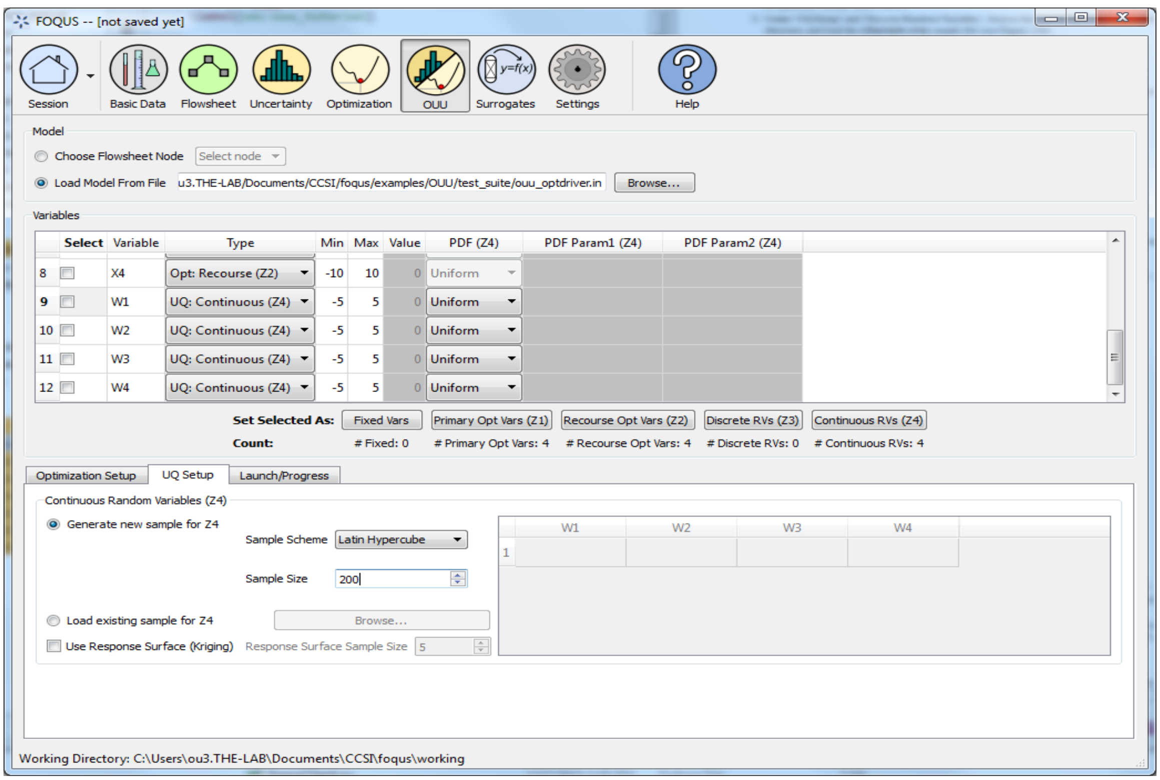


Fig. 8: OUU Example with Continuous Uncertain Parameters

1. Start FOQUS and click the 'OUU' icon.
2. Under 'Model', browse and load examples/OUU/test_suite/ouu_optdriver.in.
3. Under 'Variables', set variable $1-4$ as Z_1, variable $5-8$ as Z_2, and variable $9-12$ as Z_4.
4. Under 'Optimization Setup', select the first objection function (default) and select 'use model as optimizer' as the 'Inner Solver'.
5. Under 'UQ Setup' and 'Continuous Random Variables', select 'Generate new sample for Z_4', set 'Sample Scheme' to 'Latin Hypercube' and set sample size to 200 (see Figure [fig:ouu_ex2]).

6. Go to 'Launch/Progress' page, click 'Run OUU' and see OUU in action.

Example 3: OUU with Continuous Uncertain Parameters and Response Surface

This example is similar to Example 2 except that response surfaces will be used on the Z_4 sample (that is, the Z_4 sample will be used to construct response surfaces and the means will be estimated from a large sample evaluated on the response surfaces).

1. Start FOQUS and click the 'OUU' icon.
2. Under 'Model', browse and load examples/OUU/test_suite/ouu_optdriver.in.
3. Under 'Variables', set variable $1-4$ as Z_1, variable $5-8$ as Z_2, and variable $9-12$ as Z_4.
4. Under 'Optimization Setup', select the first objection function (default) and select 'use model as optimizer' as the 'Inner Solver'.
5. Under 'UQ Setup' and 'Continuous Random Variables', select 'Generate new sample for Z_4', set 'Sample Scheme' to 'Latin Hypercube' and set sample size to 200.
6. Under 'UQ Setup' and 'Continuous Random Variables', check the 'Use Response Surface' box (see Figure [fig:ouu_ex2]).
7. Go to 'Launch/Progress' page, click 'Run OUU' and see OUU in action.

Example 4: OUU with Discrete and Continuous Uncertain Parameters

This example has both discrete and continuous parameters. The discrete scenarios will be loaded from a sample file. A Latin hypercube sample will be generated for the continuous variables.

1. Start FOQUS and click the 'OUU' icon.
2. Under 'Model', browse and load examples/OUU/test_suite/ouu_optdriver.in.
3. Under 'Variables', set variable $1-4$ as Z_1, variable $5-8$ as Z_2, variable 9 as Z_3, and variable $10-12$ as Z_4.
4. Under 'Optimization Setup', select the first objection function (default) and select 'use model as optimizer' as the 'Inner Solver'.
5. Under 'UQ Setup' and 'Discrete Random Variables', browse the examples/OUU/test_suite directory and load the x3sample4.smp sample file.
6. Under 'UQ Setup' and 'Continuous Random Variables', select 'Generate new sample for Z_4', set 'Sample Scheme' to Latin hypercube and set 'Sample Size' to 100.
7. Go to 'Launch/Progress' page, click 'Run OUU' and see OUU in action.

Example 5: OUU with Mixed Uncertain Parameters and Response Surface

This example is similar to Example 4 except that response surfaces will be used to estimate the means for the continuous uncertain variables.

1. Start FOQUS and click the 'OUU' icon.
2. Under 'Model', browse and load examples/OUU/test_suite/ouu_optdriver.in.
3. Under 'Variables', set variable $1-4$ as Z_1, variable $5-8$ as Z_2, variable 9 as Z_3, and variable $10-12$ as Z_4.
4. Under 'Optimization Setup', select the first objection function (default) and select 'use model as optimizer' as the 'Inner Solver'.

5. Under 'UQ Setup' and 'Discrete Random Variables', browse the examples/OUU/test_suite directory and load the x3sample4.smp sample file.
6. Under 'UQ Setup' and 'Continuous Random Variables', select 'Generate new sample for Z_4', set 'Sample Scheme' to Latin hypercube and set 'Sample Size' to 100.
7. Under 'UQ Setup' and 'Continuous Random Variables', check the 'Use Response Surface' box.
8. Go to 'Launch/Progress' page, click 'Run OUU' and see OUU in action.

Example 6: OUU with User-provided Samples and Response Surface

This example is similar to Example 4 except that a sample for Z_4 will be used (instead of the Latin hypercube sample generated internally).

1. Start FOQUS and click the 'OUU' icon.
2. Under 'Model', browse and load examples/OUU/test_suite/ouu_optdriver.in.
3. Under 'Variables', set variable $1-4$ as Z_1, variable $5-8$ as Z_2, variable 9 as Z_3, and variable $10-12$ as Z_4.
4. Under 'Optimization Setup', select the first objection function (default) and select 'use model as optimizer' as the 'Inner Solver'.
5. Under 'UQ Setup' and 'Discrete Random Variables', browse the examples/OUU/test_suite directory and load the x3sample4.smp sample file.
6. Under 'UQ Setup' and 'Continuous Random Variables', check 'Load existing sample for Z_4' and load the Z_4 sample examples/OUU/test_suite/x4sample4.smp.
7. Go to 'Launch/Progress' page, click 'Run OUU' and see OUU in action.

Example 7: OUU with Large User-provided Samples and Response Surface

This example is similar to Example 5 except that a sample for Z_4 is provided (instead of generated internally).

1. Start FOQUS and click the 'OUU' icon.
2. Under 'Model', browse and load examples/OUU/test_suite/ouu_optdriver.in.
3. Under 'Variables', set variable $1-4$ as Z_1, variable $5-8$ as Z_2, and variable $9-12$ as Z_4.
4. Under 'Optimization Setup', select the first objection function (default) and select 'use model as optimizer' as the 'Inner Solver'.
5. Under 'UQ Setup' and 'Continuous Random Variables', check 'Load existing sample for Z_4' and load the Z_4 sample examples/OUU/test_suite/x4sampleLarge.smp (10000 sample points).
6. Under 'UQ Setup' and 'Continuous Random Variables', check 'Use Response Surface' and set 'Sample Size' to 100.
7. Go to 'Launch/Progress' page, click 'Run OUU' and see OUU in action.

CHAPTER 7

Surrogate Modeling

7.1 Contents

7.1.1 Surrogate Models Overview

Large-scale computational models are crucial tools to analyze complex systems. When coupled with uncertainty quantification and optimization methods, the resulting computational expense becomes intractable. In order to face the computational burden, surface approximation methods, black box models, or surrogate models are commonly used. FOQUS provides a selection of surrogate modeling tools all using a similar work-flow. This section provides an overview of the surrogate modeling features and capabilities. The details of each tool are provided in the tutorial sections.

The following surrogate modeling tools are currently available:

- ACOSSO – Adaptive COmponent Selection and Shrinkage Operator is a regularization method for simultaneous model fitting and variable selection based in nonparametric regression methods. ACCOSSO is suitable for approximating models with many inputs and no sharp changes.
- ALAMO – Automated Learning of Algebraic Models for Optimization generates algebraic models from data sets. These surrogate models are ideal for equation oriented optimization problems (which are easily differentiable), such as super structure optimization.
- BSS-ANOVA – Bayesian Smoothing Spline Analysis of Variance is a method similar to ACOSSO.
- iREVEAL – Surrogate models for CFD simulations using Kriging or Neural Networks. It contains special features specifically designed for working with CFDs.

Data Selection

The **Data** tab allows the selection of training data to be used to generate a surrogate model (*Surrogate Data Form*). If the session is associated with a flowsheet data (results from a single flowsheet run, optimization runs, or UQ samples), then the flowsheet data is available to be the training data and the table will be populated accordingly.

1. **Run** the surrogate modeling method.

Fig. 1: Surrogate Data Form

2. **Stop** the surrogate modeling method.
3. **Surrogate modeling tool** enables the user to select the desired surrogate modeling tool from the **Tool** drop-down list.
4. **Description** of the selected surrogate method.
5. **Add Samples** enables the user to generate new training data using a model specified in the flowsheet or an emulator (i.e., a basic response surface provided as part of the UQ module).
6. **Flowsheet Results** are summarized below.
7. The data table has a **Menu** drop-down list that contains display, import/export, and edit commands.
8. Select a data filter from the **Current Filter** drop-down for current data display.
9. Add or edit new data filters from **Edit Filters**. This dialog is shown in Figure *Sort1 Data Filter Results*.
10. The **Display** table displays the results of flowsheet evaluations stored in the FOQUS session file. The columns are:
    - **SetName** is a name assigned to samples. This is typically equivalent to one UQ sample run or one optimization run.
    - **ResultName** is a string representing a result name.
    - **Error** is the simulation result status; 0 indicates success, other numbers represent an error. A column for each node displays the error status of each node.
    - **Time** displays the time when the result was stored.
    - **Elapsed Time** describes how long a result took to calculate.
    - **Tags** enables a list of string labels to be applied to results. This could be used to mark results to be used for a particular purpose such as model validation.
    - The remaining columns display the input and output variables.

Filters can be used to select data. See Section *Flowsheet Result Data* for more information on creating filters to the results. The "All" and "None" filters are available by default. These can be used, for example, to assign all the data as a training set, or to split the data into a separate training set and a test set.

Variables

The **Variables** section is illustrated in Figure *Surrogate Variable Selection*. This section allows selection of input and output variables used in a surrogate model. Some surrogate methods such as ALAMO may generate and run additional samples while building surrogates. The **Min/Max** columns provide bounds on the variables. Selecting the checkbox next to the variable **Name** indicates that it should be included in the surrogate generation. Failure to select a checkbox for any variables will result in error during surrogate generation.

Fig. 2: Surrogate Variable Selection

Method Settings

The **Method Settings** table is illustrated in Figure *Surrogate Settings*. The settings available in this table depend on the surrogate tool. A description of each setting is provided in the third column of the table.

Fig. 3: Surrogate Settings

Execution

Clicking **Run** starts the surrogate model building process. The execution monitor displays after **Run** is clicked (see Figure *Surrogate Status Monitor*). The execution monitor displays the status of the surrogate build. The messages displayed depends on the surrogate tool.

Fig. 4: Surrogate Status Monitor

After a successful execution and model building, the results are displayed. Note that in this case, the surrogate modeling tool ends with an error, the errors are displayed in this window. After surrogate generation completes, one or two Python files will be generated depending on the tool. Each tool generates a file that encodes the surrogate model as a general Python script that can be used to evaluate output values for UQ analyses within the UQ module. The other file, if available, is a FOQUS flowsheet plugin model that allows the surrogate to be run in a FOQUS flowsheet. The next version of FOQUS will generate a FOQUS flowsheet plugin model (i.e., the second file) for all surrogate tools.

7.1.2 Tutorial

ALAMO

This tutorial focuses on the use of the ALAMO tool for building algebraic surrogate models. ALAMO builds simplified algebraic models, which are particularly well suited for rigorous equation oriented optimization. To keep the execution of this tutorial fast, a toy problem is used. In this case study the flowsheet calculations and sample generation are done within FOQUS, alternatively, the user can provide a simulation model such as: Excel, Aspen plus, Aspen custom modeler, etc.

Note: Before starting this tutorial the ALAMO product must be downloaded from the products page on the CCSI website. The path for the ALAMO executable file must be set in FOQUS settings (see Section *Settings*).

Flowsheet Setup

1. Open FOQUS.
2. Name the session "Surrogate_Tutorial_1" (Figure *Session Set Up*).

Fig. 5: Session Set Up

3. Navigate to the Flowsheet Editor (Figure *Flowsheet Setup*).
4. Add a Flowsheet Node named "eq."
5. Display the Node Editor by clicking the **Node Editor** toggle button.

The **Node Editor** displays (Figure *Node Variables*). Thefirst step to setting up the node for this problem is to add input and output variables to the node.

6. If the input variables table is not displayed as shown in Figure *Node Variables*, click the **Variables** tab and then click the **Input Variables** toolbox section.
7. Add the variables "x1" and "x2" by clicking the **Add** icon (+) above the input table.

Fig. 6: Flowsheet Setup

8. Edit the **Min/Max** value for both variables to be "-10.0" and "10.0."
9. Add two output variables "z1" and "z2."

Fig. 7: Node Variables

To keep the execution time short, the node will not be assigned to a simulation model and calculations are performed directly in FOQUS.

10. Click on the **Node Script** tab in the Node Editor to enter the test equation (this step replaces the use of a simulator).
11. Enter the following equations (Figure *Node Script*):

```
f["z1"] = x["x1"] + x["x2"]
f["z2"] = x["x1"]**2 + x["x2"]**2
```

The node script calculations are written in Python. The dictionary "f" stores output values while the dictionary "x" stores input values.

Fig. 8: Node Script

12. Test the model by running the flowsheet with the value "2" for "x1" and "x2." After running, the output variables should have the values "4.0" for "z1" and "8.0" for "z2."

Creating Initial Samples

There are two ways to start an ALAMO run: (1) generate a set of initial data, (2) use ALAMO's adaptive sampling with no initial data and let ALAMO generates its own samples. Adaptive sampling can be used with initial data to generate more points if needed. In this case, initial data is provided and adaptive sampling is used.

13. Select the UQ tool by clicking on the **Uncertainty** button on the Home window (Figure *Add a New Sample Ensemble*).
14. Click the **Add New** button.
15. The **Add New Ensemble - Model Selection** dialog will appear. Click **OK** to set up the sampling scheme.
16. The sample ensemble setup dialog displays (Figure *Sample Distributions*). Select **Choose sampling scheme**.
17. Click the **All Variable** button.
18. Select the **Sampling scheme** tab.
19. The **Sampling scheme** dialog should display (Figure *Sample Methods*). Select "Latin Hypercube" from the list.
20. Set the **# of samples** to "10."
21. Click **Generate Samples**.
22. Click **Done**.
23. Once the samples have been generated a new sample ensemble displays in the UQ tool window (Figure *Run Samples*). Click **Launch** to run and generate the samples.

Fig. 9: Add a New Sample Ensemble

Fig. 10: Sample Distributions

Data Selection

Initial and validation data can be specified by creating filters that specify subsets of flowsheet data. In this tutorial only initial data will be used. A filter must be created to separate the results of the single test run from the UQ samples.

24. Click on the **Surrogates** button from the Home window. The surrogate tool displays *Surrogate Data*.
25. Select "ALAMO" from the **Tool** drop-down list.
26. Click **Edit Filters** in the **Flowsheet Results** section to create a filter.
27. Figure fig.tut.sur.dataFilter displays the Data Filter Editor.
28. Add the filter for initial data.
    1. Click **New Filter**, and enter "f1" as the filter name.
    2. Type the **Filter expression**: c("set") = = "UQ_Ensemble".
29. Click **Done**.

Variable Selection

In this section, input and output variables need to be selected. Generally, any input variables that vary in the data set should be selected. However, in some cases, variables may be found to have no, or very little, effect on the outputs. Only the output variables of interest need to be selected. Note: Each output is independent from each other and for the model building, selecting one output is the same as selecting more.

30. Select the **Variables** tab (Figure *Variable Selection*).
31. Select the checkbox for both input variables.
32. Select the checkbox for both output variables.

Method Settings

The most important feature to generate "good" algebraic models is to configure the settings accordingly to the problem to be solved. Each setting has a good description in FOQUS. The JSON parser is used to read method settings values. Strings must be contained in quotes. Lists have the following format: [element 1, element 2].

33. Click on the **Method Settings** tab (see Figure *ALAMO Method Settings*).
34. Set the **FOQUS Model (for UQ)** to "ALAMO_tutorial_UQ.py."
35. Set the **FOQUS Model (for Flowsheet)** to "ALAMO_tutorial_FS.py"
36. Set **Initial Data Filter** to "Initial."

Fig. 11: Sample Methods

Fig. 12: Run Samples

Fig. 13: Surrogate Data

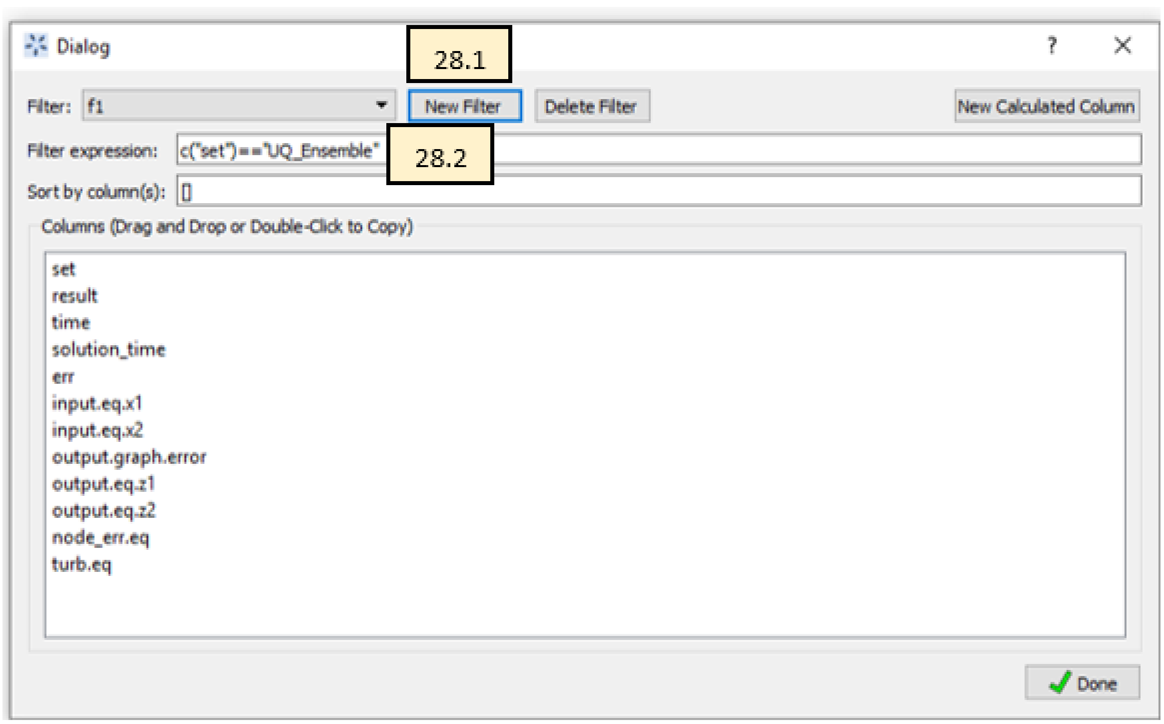


Fig. 14: Data Filter Dialog

Fig. 15: Variable Selection

37. Set **SAMPLER** to select the adaptive sampling method: "None" "Random" or "SNOBFIT." Use "None" in this tutorial.
38. Set **MONOMIALPOWER** to select the single variable term powers to [1,2,3].
39. Set **MULTI2POWER** to select the two variable term powers to [1].
40. Select functions to be considered as basis functions (**EXPFCNS**, **LOGFCNS**, **SINFCNS**, **COSFCNS**).
41. Leave the rest of settings as default (see Table *ALAMO Method Settings*).
42. Save this FOQUS session for use in the ACOSSO and BSS-ANOVA tutorials.

Fig. 16: ALAMO Method Settings

Execution

43. Click the **Run** icon at the top of the window.
44. The ALAMO **Execution** tab starts displaying execution file path, sub-directories, input files, and output files.
    1. ALAMO version.
    2. License Information.
    3. Step 0 displays the data set to be used by ALAMO.
    4. Step 1 displays the modeler used by ALAMO to generate the algebraic model.
    5. Once the surrogate model has finished, the equations are displayed in the execution window. It may be necessary to scroll up a little. The result is shown in Figure *ALAMO Execution*.
    6. Finally, the statistics display the quality metrics of the models generated.

Fig. 17: ALAMO Execution

Results

The results are exported as a PSUADE driver file that can be used perform UQ analysis of the models, and a FOQUS Python plugin model that allows it to be used in a FOQUS flowsheet. The equations can also be viewed in the results section.

See tutorial Section *Surrogates with UQ Tools* and *Surrogates with the Flowsheet* for information about analyzing the model with the UQ tools or running the model on the flowsheet.

As mentioned in section *1.5* the method settings are very important. A brief description and hints are included in Table *ALAMO Method Settings*.

Method Settings	Description
Initial Data Filter	Filter to be applied to the initial data set. Data filters help the user to generate models based on specific dat
Validation Data filter	Data set used to compute model errors at the validation phase. The number of data points in a preexisting v
SAMPLER	Adaptative sampling method to be used. Options: "None", "Random" and "SNOBFIT". Adaptive samplin
MAXTIME	Maximum execution time in seconds. This time includes all the steps on the algorithm, if simulations are n

MINPOINTS	Convergence is assessed only if the simulator is able to compute the output variables for at least MINPOIN
PRESET	Value to be used if the simulator fails. This value must be carefully chosen to be an otherwise not realizabl
MONOMIALPOWERS	Vector of monomial powers to be considered as basis functions, use empty vector for none []. Exponential
MULTI2POWER	Vector of pairwise combination of powers to be considered as basis functions. Pairwise combination of pov
MULTI3POWER	Vector of three variables combinations of powers to be considered as basis functions.
	Use or not of exp, log, sin, and cos functions as basis functions in the model.
RATIOPOWER	Vector of ratio combinations of powers to be considered in the basis functions. Ratio combinations of pow
Radial Basis Functions	Radial basis functions centered around the data set provided by the user. These functions are Gaussian and
RBF parameter	Constant penalty used in the Gaussian radial basis functions.
Modeler	Fitness metric to be used for model building. Options: BIC (Bayesian Information Criterion), Mallow's Cp
ConvPen	Convex penalty term. Used if Convex Penalty is selected.
Regularizer	Regularization method is used to reduce the number of potential basis functions before the optimization.
Tolrelmetric	Convergence tolerance for the chosen fitness metric is needed to terminate the algorithm.
ScaleZ	If used, the variables are scaled prior to the optimization problem is solved. The problem is solved using a
GAMS	GAMS is the software used to solve the optimization problems. The executable path is expected or the use
GAMS Solver	Solver to be used by GAMS to solve the optimization problems. Mixed integer quadratic programming sol
MIPOPTCR	Relative convergence tolerance for the optimization problems solved in GAMS. The optimization problem
MIPOPTCA	Absolute convergence tolerance for mixed-integer optimization problems. This must be a nonnegative scal
Linear error	If true, a linear objective function is used when solving the mixed integer optimization problems; otherwise
	Specify whether constraint regression is used or not, if true bounds on output variables are enforced.
CRNCUSTOM	If true, Custom constraints are entered in the Variable tab.
CRNINITIAL	Number of random bounding points at which constraints are sampled initially (must be a nonnegative integ
CRNMAXITER	Maximum allowed constrained regressions iterations. Constraints are enforced on additional points during
CRNVIOL	Number of bounding points added per round per bound in each iteration (must be positive integer).
CRNTRIALS	Number of random trial bounding points per round of constrained regression (must be a positive integer).
CUSTOMBAS	A list of user-supplied custom basis functions can be provided by the user. The parser is not case sensitive

ACOSSO

This tutorial covers the ACOSSO surrogate modeling method. The Adaptive COmponent Selection and Shrinkage Operator (ACOSSO) surface approximation was developed under the Smoothing Spline Analysis of Variance (SS-ANOVA) modeling framework *(Storlie et al. 2011)*. As it is a smoothing type method, ACOSSO works best when the underlying function is somewhat smooth. For functions which are known to have sharp changes or peaks, etc., other methods may be more appropriate. Since it implicitly performs variable selection, ACOSSO can also work well when there are a large number of input variables. The ACOSSO procedure also allows for categorical inputs *(Storlie et al. 2013)*.

This tutorial uses the same flowsheet and sample setup as the ALAMO tutorial in Section *ALAMO*. The statistics software "R" is also required to use ACOSSO and BSS-ANOVA. Before starting this tutorial, you will need to install R version 3.1 or later (see https://cran.r-project.org/).

Once R is installed, you will need to install the "quadprog" package. ACOSSO requires this package for solving quadratic programming problems. You will only need to perform this step once.

1. Start R. In Windows, this must be done with administrative privileges. Either run this from an administrator account, or right-click "R x64 3.1.2" and click "Run with administrator" and type in administrator credentials.
2. Inside the R console, type:
   - install.packages('quadprog')
   - library(quadprog)
   - q()

The first line installs the package. If prompted for a CRAN mirror, select the one closest to you geographically. The second line loads the package. The last line quits R. If prompted to save workspace image, choose 'y'.

Once you have done these steps, ACOSSO is ready to be invoked inside FOQUS.

1. Set the path to the RScript executable.
   1. Click the **Settings** button in the Home window.
   2. Change the RScript path if necessary. The **Browse** button opens a file browser that can be used to set the path.
2. Complete the ALAMO tutorial in Section *ALAMO* through Step 32, or load the FOQUS session saved after completing the ALAMO tutorial.
3. Click the **Surrogates** button in the Home window (Figure *ACOSSO Session Set Up*).
4. Select "ACOSSO" in the **Tool** drop-down list.
5. Select the **Method Settings** tab.
6. Set "Data Filter" to "Initial."
7. Set "Use Flowsheet Data" to "Yes."
8. Set "FOQUS Model (for UQ)" to "ACOSSO_Tutorial_UQ.py."
9. Set "FOQUS Model (for Flowsheet)" to "ACOSSO_Tutorial_FS.py."
10. Click the **Run** icon (Figure *ACOSSO Session Set Up*).

Fig. 18: ACOSSO Session Set Up

11. The execution window will automatically display. While ACOSSO is running, the execution window may show warnings, but this is normal.
12. When the run completes, a UQ driver file is created, allowing the ACOSSO surrogate to be used as a user-defined response surface in UQ analyses. (See Section *Surrogates with UQ Tools*.)
13. ACOSSO also produces a flowsheet plugin; however.

BSS-ANOVA

This tutorial covers the BSS-ANOVA surrogate modeling method. The Bayesian Smoothing Spline ANOVA (BSS-ANOVA) is essentially a Bayesian version of ACOSSO *(Reich et al. 2009)*. It is Gaussian Process (GP) model with a non-conventional covariance function that borrows its form from SS-ANOVA. It tackles the high dimensionality (of inputs) on two fronts: (1) variable selection to eliminate uninformative variables from the model and (2) restricting the level of interactions involved among the variables in the model. This is done through a fully Bayesian approach which can also allow for categorical input variables with relative ease. Since it is closely related to ACOSSO, it generally works well in similar settings as ACOSSO. The BSS-ANOVA procedure also allows for categorical inputs *(Storlie et al. 2013)*. In this current implementation, BSS-ANOVA is more computationally intensive than ACOSSO, so ACOSSO is preferred for faster surrogate generation.

This tutorial uses the same flowsheet and sample setup as the ALAMO tutorial in Section *ALAMO*. The statistics software "R" is also required to use ACOSSO and BSS-ANOVA. Before starting this tutorial, you will need to install R version 3.1 or later (see http://cran.r-project.org/).

1. Set the path to the RScript executable.
   1. Click the **Settings** button from the Home window.

  2. Change the RScript path if necessary. The **Browse** button opens a file browser that can be used to set the path.

2. Complete the ALAMO tutorial in Section *ALAMO* through Step 32, or load the FOQUS session saved after completing the ALAMO tutorial.
3. Click the **Surrogates** button from the Home window (Figure *BSS-ANOVA Session Set Up*).
4. Select "BSS-ANOVA" in the **Tool** drop-down list.
5. Select the **Method Settings** tab.
6. Set "Data Filter" to "Initial."
7. Set "Use Flowsheet Data" to "Yes."
8. Set "FOQUS Model (for UQ)" to "bssanova_tutorial_uq.py."
9. Set "FOQUS Model (for Flowsheet)" to "bssanova_tutorial_fs.py."
10. Click the **Run** icon (Figure *BSS-ANOVA Session Set Up*).

Fig. 19: BSS-ANOVA Session Set Up

11. The execution window will automatically display. While BSS-ANOVA is running, the execution window may show warnings, but this is normal.
12. When the run completes, a UQ driver file is created, allowing the BSS-ANOVA surrogate to be used as a user-defined response surface in UQ analyses. (See Section *Surrogates with UQ Tools*.)
13. BSS-ANOVA also produces a flowsheet plugin.

Surrogates with UQ Tools

For the purpose of this tutorial, we will use ACOSSO to demonstrate the use of a surrogate within the UQ module. The steps are the same regardless of the surrogate tool chosen.

To perform the UQ analysis, Python is required for use the "User Regression" response surface that will be used. Before starting this tutorial, you will need to install Python 2.7.x (not Python 3). (See https://www.python.org/downloads/). In addition, if *.py files have been re-associated with other executables (e.g. editors), please change the association back to python.exe.

1. Load a fresh session by clicking the Session button from the Home window. Select Open Session and then navigate to the "examples/UQ" directory. Select "Rosenbrock_no_vectors.foqus." This will load a session with a simple flowsheet containing a single node.
2. Click Settings and ensure that (1) FOQUS Flowsheet Run Method is set to "Local", and that (2) proper paths are set for PSUADE and RScript.
3. Train an ACOSSO surrogate of this node by clicking the **Surrogates** button from the Home window.
   1. Click Add Samples and select "Use Flowsheet". This will display the Simulation Ensemble Setup dialog.
   2. Within this dialog, ensure all variables are set to "Variable" type in the Distributions tab. In the Sampling scheme tab, select "Monte Carlo" as your sampling scheme, set the number of samples to 100, and then click Generate Samples to generate the set of input values. Click Done to return to the Surrogates screen.
   3. Once sample generation completes, click the Uncertainty button from the Home window.
   4. Click the Launch button to generate the samples.

5. Click the Surrogates button from the Home window. The Data tab of the Surrogates screen should now displays a Flowsheet Results table that is populated with the values of the new input samples.
6. From the Variables tab, select all of the checkboxes. (There should be six checkboxes for input variables and one checkbox for output variable.) Here, you are defining the inputs and outputs for your surrogate function.
7. From the Method Settings tab, note the name of the file next to "FOQUS Model (for UQ)". This will be the name of the UQ driver file that contains the Python code that implements the surrogate function.
8. On top of this screen, select "ACOSSO" as your surrogate tool from the Tool drop-down list and then click on the green arrow to start training the surrogate.
9. Once complete, a popup window will display, reminding you of the location of the drive file. Note the location as you will need this information later inside the UQ module.

4. Perform a response-surface-based uncertainty analysis by clicking the **Uncertainty** button from the Home window.
   1. In the Uncertainty Quantification Simulation Ensembles table. A row corresponding to the ensemble that was just generated for surrogate training should be displayed. This same ensemble can be used or a new one can be created to be used as the test data set for analysis. In the row corresponding to the ensemble to be analyzed, click the Analyze button to proceed. This action will bring up an analysis dialog.
   2. Within this analysis dialog, navigate to "Analysis" section. For Step 1, select "Response Surface". For Step 3, select "User Regression" in the first drop-down list. Lastly, for "User Regression File", browse to the same location as the UQ driver file that was generated within the Surrogates module. (This is the same location that was previously noted from the popup message.) At this point, your surrogate function is now set up as a user-defined response surface and all response-surface-based UQ analyses are accessible.
   3. Click Validate (Step 4) to perform response surface validation. Once complete, a figure with cross-validation results will be displayed: a histogram of errors to the left and a plot of predicted values versus actual values to the right. For more information, refer to the UQ Tutorial in Section*[tutorial.uq.rs]*.
   4. Once a "Response Surface" has been validated, other UQ analysis options are available. Choose "Uncertainty Analysis" in Step 5 and click Analyze to perform uncertainty analysis using your ACOSSO surrogate.

During validation, if the error, "RSAnalyzer: RSTest_hs.m does not exist." displays, this is likely caused by incompatibility with the surrogate and the test data. An example scenario might be your test data has six inputs, but your surrogate assumes five inputs. This is easily fixed by returning to the Surrogates screen, clicking on the **Variables** tab, and making sure the appropriate selections are made (i.e., check off six inputs instead of just five).

Surrogates with the Flowsheet

This section provides a brief tutorial for using the flowsheet plugin models generated by surrogate modeling methods. In the next FOQUS release all surrogate modeling methods will produce a model that can be run in a FOQUS flowsheet. **Currently iREVEAL does not produce a flowsheet model.**

Before doing this tutorial complete the ALAMO tutorial in Section :ref:'sec.surrogate.alamo'.

1. Open FOQUS. If FOQUS has not been closed since completing the ALAMO tutorial, close it and reopen it. There is a known issue where existing flowsheet model plugins may not update until FOQUS is restarted.
2. Enter "FS_Plugin_Tutorial" as the Session Name.
3. Click the **Flowsheet** button from the Home window.
4. Click the **Add Node** icon in the left toolbar (see Figure *Plugin Flowsheet*).
5. Click a location for the node in the Flowsheet area.

6. Enter "model" for the node name (without quotes).
7. Click the **Node Editor** icon in the left toolbar (see Figure *Plugin Flowsheet*).
8. In the **Node Editor**, select "Plugin" from the Model **Type** drop-down list.
9. Select "ALAMO_Tutorial_FS" from the **Model** drop-down list.
10. Set the **Value** of the **Input Variables** "eq.x1" to 2.
11. Set the **Value** of the **Input Variables** "eq.x2" to 3.
12. Click the **Run** icon in the left toolbar (see Figure *Plugin Flowsheet*).
13. Wait for the Flowsheet evaluation to complete. It should finish successfully.
14. Check the value of the **Output Variables**; the approximate values should be z1 = 5 and z2 = 13.

Fig. 20: Plugin Flowsheet

CHAPTER 8

Sequential Design of Experiments (SDOE)

A sequential design of experiments strategy allows for adaptive learning based on incoming results as the experiment is being run. The SDoE module in FOQUS allows the experimenter to flexibly incorporate this strategy into their designed experimental planning to allow for maximal relevant information to be collected. Statistical design of experiments is an important strategy to improve the amount of information that can be gleaned from the overall experiment. It leverages principles of putting experimental runs where they are of maximum value, the interdependence of the runs to estimate model parameters, and robustness to the variability of results that can be obtained when the same experimental conditions are repeated. There are two major categories of designed experiments: those for which a physical experiment is being run, and designs for a computer experiment where the output from a theoretical model is explored. While the methods available were initially focused on experiments for physical experiments, opportunities also exist for accelerated learning through strategic selection and updating of experimental runs for computer experiments.

The overall process for Sequential Design of Experiments (SDoE) is detailed below:

1. Identify one or more criteria over which to optimize. Common choices are (a) refining the region of interest, (b) improving the precision (or reducing the uncertainty) in the estimation of model parameters, (c) improving the precision of prediction for new observations in the design region, (d) quantifying the discrepancy between the model and data, or (e) optimizing the value of responses of interest. If more than one criterion is going to be used, then identify how they will be combined into a utility function.
2. Develop a working model of the process that can be used to calculate the criteria values based on currently available knowledge and data.
3. Define the inputs that will be manipulated during the experiment, and the ranges of interest for these factors.
4. Identify candidate input factor locations that are being considered for new experiments. This can be a grid of input combinations or continuous regions in the design space. If there are combinations of the factors that will not yield results or that are not of interest, these regions of the design space should be excluded from consideration.
5. Develop a working model of the process that is able to receive new data and incorporate them to update the calculated criteria values.
6. Develop a plan for the size of the sequential design batches, based on the time required to set-up and run the experiments as well as the computational time required to process new data and update the working model.

7. Identify the initial batch of experiments to be run at the beginning of the experiments based on the model developed in step 2 and conditional on any already available data. This involves examining the utility of new data at each candidate location, and comparing which locations have the highest anticipated utility.
8. Run the first batch of experimental runs, update the model developed in step 5 with the new results. Based on the updated model, generate the next batch of experimental runs.
9. For the duration of the experiment, repeat steps 7 and 8 for subsequent batches based on the updated model after incorporating the newly obtained data.

The first version of the SDoE module has functionality that can produce flexible space-filling designs to be created. Later versions will allow for additional design criteria to be utilized, but the first version already had considerable flexibility to construct helpful design based on several different strategies. Key features of the approach that we use in this module are: a) designs will be constructed by selecting from a user-provided candidate set of input combinations, and b) historical data, which has already been collected can be integrated into the design construction to ensure that new data are collected with a view to disperse from where data are already available.

We begin with some basic terminology that will help provide structure to the process and instructions below.

- Input factors – these are the controllable experimental settings that are manipulated during the experiment. It is important to carefully define the ranges of interest for the inputs (eg. Temperature in [200°C,400°C]) as well as any logistical or operational constraints on these input factors (eg. Flue Gas Rate < 1000 kg/hr when Temperature > 350°C)
- Input combinations (or design runs) – these are the choices of settings for each of the input factors for a particular run of the experiment. It is assumed that the implementers of the experiment are able to set the input factors to the desired operating conditions to match the prescribed choice of settings.
- Input space (or design space) – the region of interest for the input factors in which the experiment will be run. This is typically constructed by combining the individual input factor ranges, and then adapting the region to take into account any constraints. Any suggested runs of the experiment will be located in this region.
- Responses (or outputs) – these are the measured results obtained from each experimental run. These are most desirably quantitative summaries of a characteristic of interest from running the process at the prescribed set of operating conditions (eg. CO_2 capture efficiency is a typical response of interest for CCSI).
- Design criterion / Utility function – this is a mathematical expression of the goal (or goals) of the experiment that is used to guide the selection of new input combinations, based on the prior information before the start of the experiment and during the running of the experiment. The design criterion can be based on a single goal or multiple competing goals, and can be either static throughout the experiment or evolve as goals change in importance over the course of the experiment. Common choices of goals for the experiment are:

1. exploring the region of interest,
2. improving the precision (or reducing the uncertainty) in the estimation of model parameters,
3. improving the precision of prediction for new observations in the design region,
4. quantifying the discrepancy between the model and data, or
5. optimizing the value of responses of interest.

An optimal design of experiment strategy uses the design criterion to evaluate potential choices of input combinations to maximize the improvement in the criterion over the available candidates. If the optimal design strategy is sequential, then the goal is to use early results from the beginning of the experiment to guide the choice of new input combinations based on what has been learned about the responses.

8.1 Why Space-Filling Designs?

Space-filling designs are a design of experiments strategy that is well suited to both physical experiments with an accompanying model to describe the process and to computer experiments. The idea behind a space-filling design is that the design points are spread throughout the input space of interest. If the goal is to predict values of the response for a new set of input combinations within the ranges of the inputs, then having data spread throughout the space means that there should be an observed data point relatively close to where the new prediction is sought.

In addition, if there is a model for the process, then having data spread throughout the input space means that the consistency of the model to the observed data can be evaluated at multiple locations to look for possible discrepancies and to quantify the magnitude of those differences throughout the input space.

Hence, for a variety of criteria, a space-filling design can serve as good choice for exploration and for understanding the relationship between the inputs and the response without making a large number of assumptions about the nature of that relationship. As we will see in subsequent examples, the sequential approach allows for great flexibility to leverage what has been learned in early stages to influence the later choices of designs. In addition, the candidate-based approach that is supported in this module has the advantage that it can make the space-filling approach easier to adapt to design space constraints and specialized design objectives that may evolve through the stages of the sequential design.

8.2 Using the SDoE Module - The Basics

In this section, we descibe the basic steps in for creating a design with this module. When you first click on the **SDOE** button from the main FOQUS homepage, a first window appears. To create a design, the progression of steps takes you through the **Ensemble Selection** box (top left), then a transition triggered by the **Confirm** button to the **Ensemble Aggregation** box, and finally there are optional changes that can be made in the box at the bottom of the window. The final step in this window is to click on **Analyze**.

We now consider some details for each of these steps:

1. In the **Ensemble Selection** box, click on the **Load from File..** button to select the file(s) for the construction of the design. Several files can be selected and added to the box listing the chosen files.

2. For each of the files selected using the pull-down menu, identify them as either a **Candidate** file or a **History** file. **Candidate** .csv files are comprised of possible input combinations from which the design can be constructed. The columns of the file should contain the different input factors that define the dimensions of the input space. The rows of the file each identify one combination of input values that could be selected as a run in the final design. Typically, a good candidate file will have many different candidate runs listed, and they should fill the available ranges of the inputs to be considered. Leaving gaps or holes in the input space is possible, but generally should correspond to a region where it is not possible (or desirable) to collect data. **History** .csv files should have the same number of columns for the input space as the candidate file, and represent data that have already been collected. The algorithm for creating the design aims to place points in different locations from where data have already been obtained, while filling the input space around those locations.

3. Click on the **View** button to open the **Preview Inputs** pop-up widow, to see the list of columns contained in each file. The left hand side displays the first few rows of input combinations from the file. Select the columns that you wish to see graphically in the right hand box , and then click on **Plot SDOE** to see a scatterplot matrix of the data.

The plot shows histograms of each of the inputs on the diagonals to provide a view of the distribution of values as well as the range of each input. The off-diagonals show pairwise scatterplots of each pair of inputs. This should provide the experimenter with the ability to assess if the ranges specified and any constraints for the inputs have been appropriately captured for the specified candidate set. In addition, repeating this process for any historical data will provide verification that the already observed data have been suitably characterized.

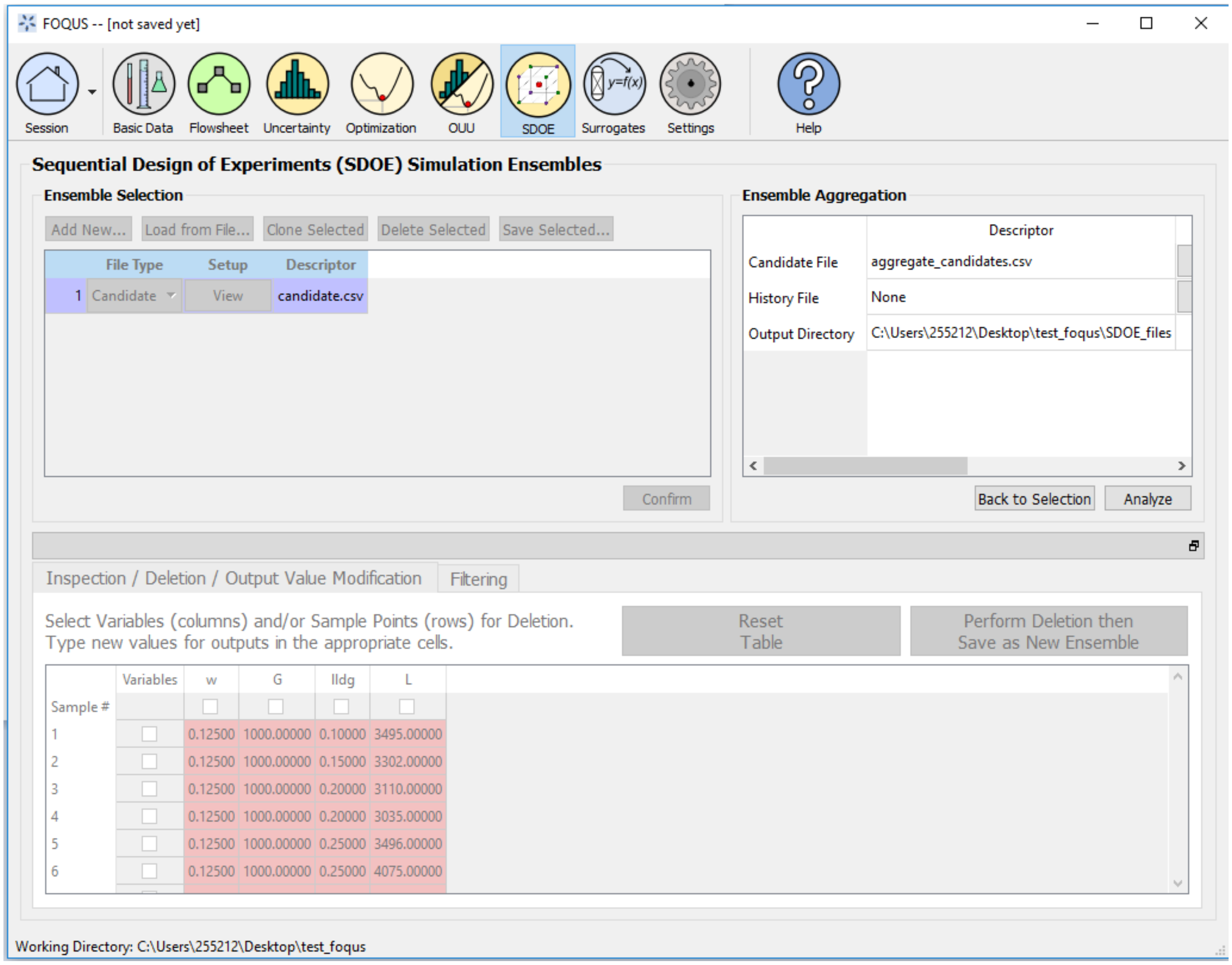


Fig. 1: SDOE Home Screen

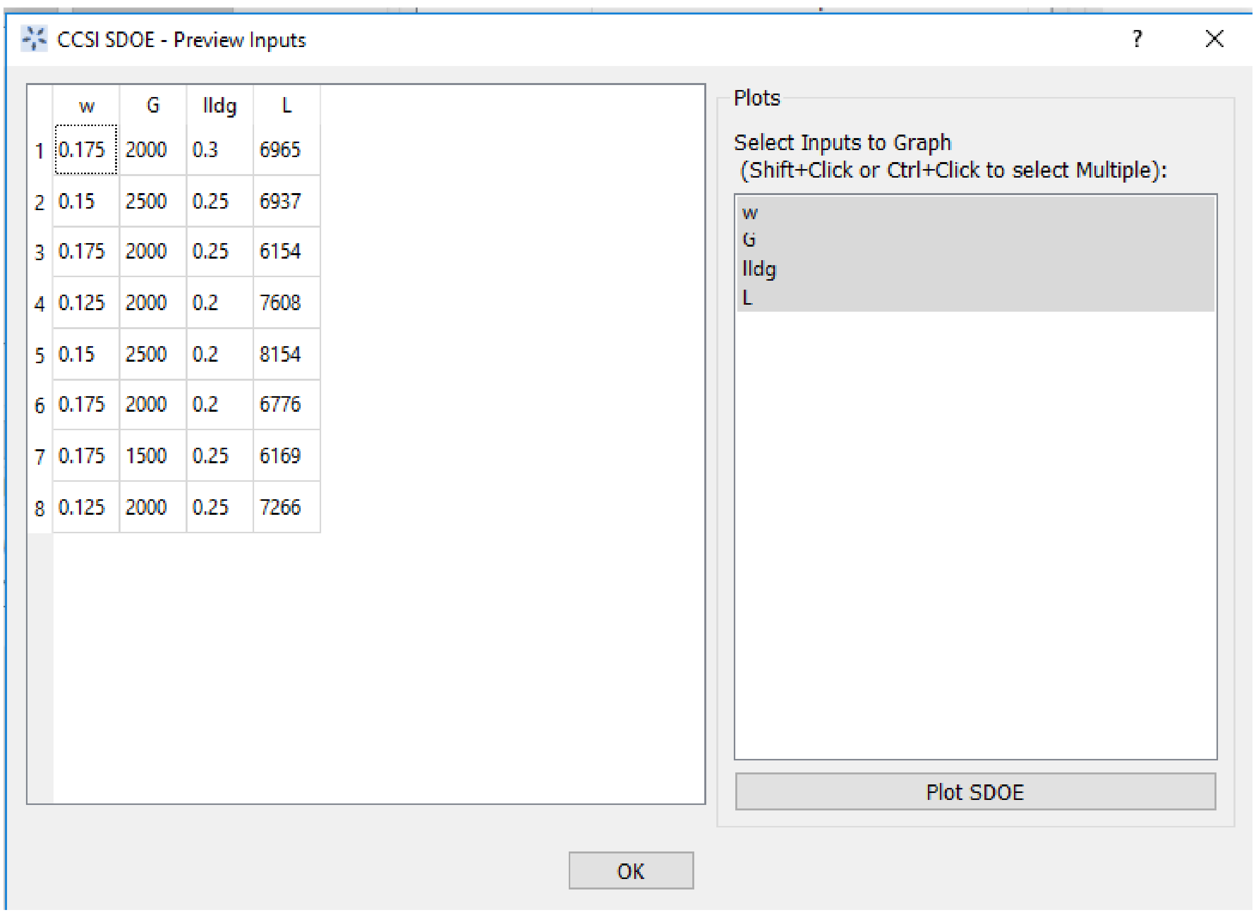


Fig. 2: SDOE preview of inputs

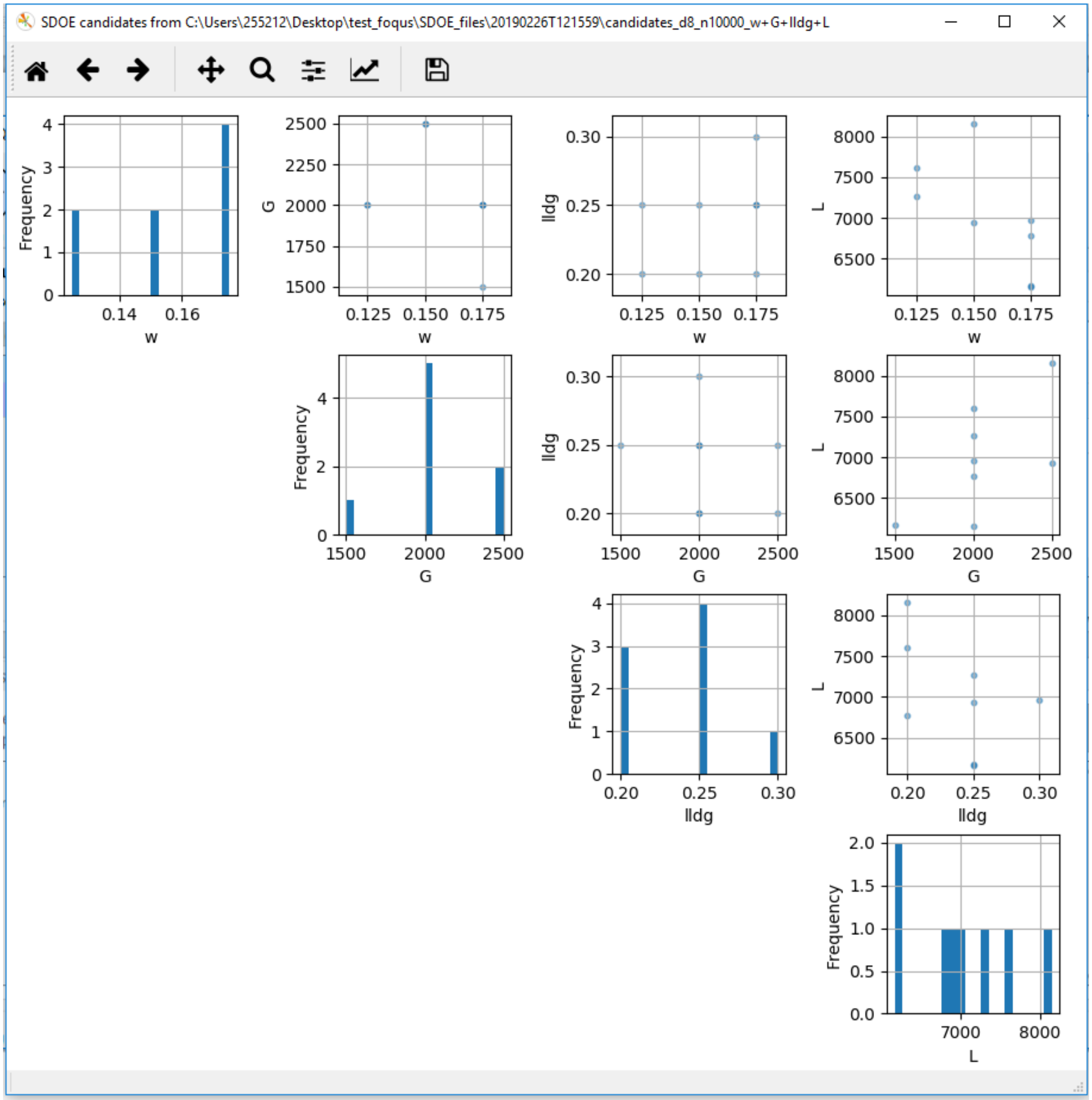


Fig. 3: SDOE plot of inputs

4. Once the data have been verified for both the **Candidate** and **History** files, click on the **Confirm** button to make the **Ensemble Aggregation** window active.
5. If more than one **Candidate** file was specified, then the **aggregate_candidates.csv** file that was created will have combined these files into a single file. Similarly if more than one **Histoy** file was specified, then the **aggregate_history.csv** file has been created with all runs from these files. If only a single file was selected for either the **Candidate** and **History** files, then their aggregated matching files will be the same as the original.
6. Once the data have been verified as the desired set to be used for the design construction, then click on the **Analyze** button at the bottom right corner of the **Ensemble Aggregation** window. This opens the second SDOE window, which allows for specific design choices to be made.

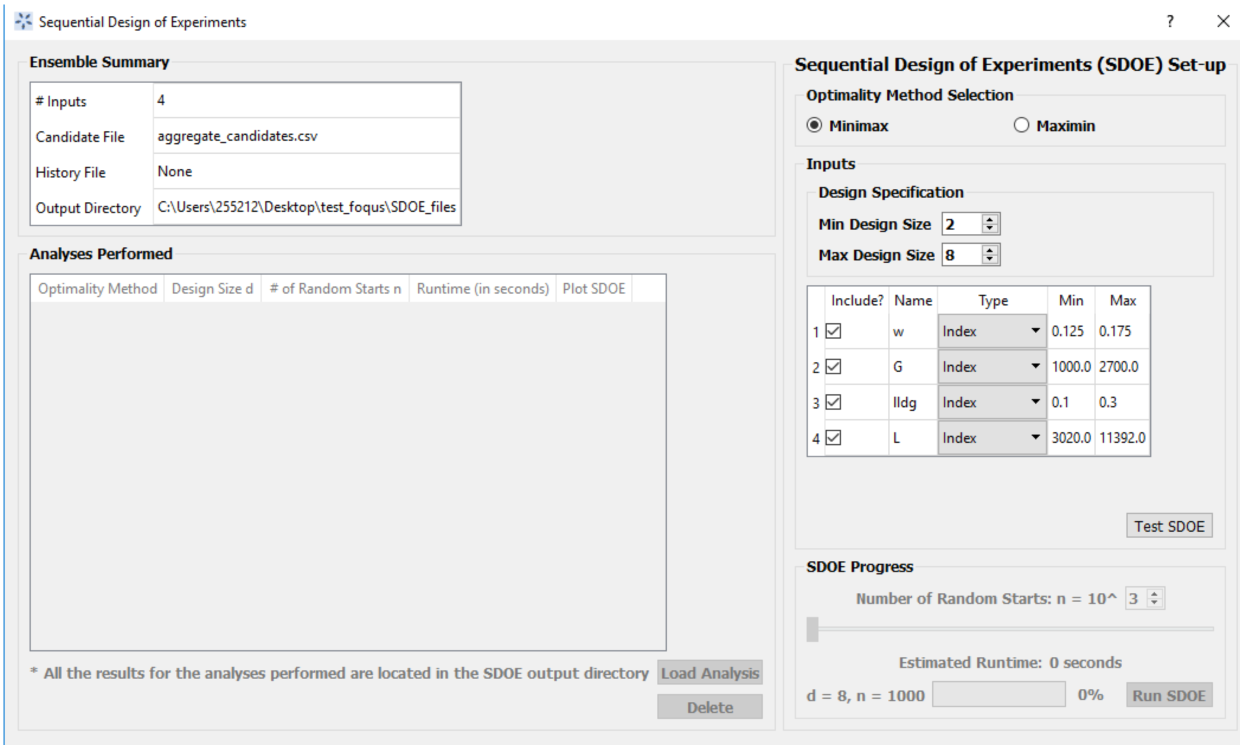


Fig. 4: SDOE second window

7. The first choice to be made for the design is whether to optimize using **minimax** or **maximin**. The first choice, **minimax**, looks to choose design points that minimize the maximum distance that any point in the input space (as characterized by the candidate set and historical data, if it is available) is away from a design point. Hence, the idea here is that if we want to use data to help predict new outcomes throughout the input space, then we never want to be too far away from an observed location. The second choice, **maximin** looks to choose a design where the design points are as far away from each other as possible. In this case, the design criterion is looking to maximize how close any two points are away from their nearest neighbor. In practice the two design criterion often give similar designs, with the **maximin** criterion tending to push the chosen design points closer to the edges of the specified regions.

Hint: If there is uncertainty about some of the edge points in the candidate set being viable options, then **minimax** would be preferred. If the goal is to place points throughout the input space with them going right to the edges, than **maximin** would be preferred. Note, that creating the designs is relatively easy, so it may be helpful to try both approaches to examine them and then choose which is preferred.

8. The next choice to be made falls under **Design Specification**, when the experimenter can select the sizes of designs to be created. The **Min Design Size** specifies the smallest design size to be created. Not that the default value is set at **2**, which would lead to choosing the best two design runs from the candidate set to fill the space (after taking

into account any historical data that have already been gathered). The **Max Design Size** specifies the largest design size to be created. The default value is set at **8**, which means that if this combination were used, designs would be created of size 2, 3, 4, 5, 6, 7 and 8. Hence, it may be prudent to select a relatively small range of values to expedite the creation of the designs, as each of these choices triggers a separate optimization search.

9. Next, there are options for the columns of the candidate set to be used for the construction of the design. Under **Include?** in the box on the right hand side, the experimenter has the option of whether particular columns should be included in the space-filling design search. Unclick a box, if a particular column should not be included in the search.

Next select the **Type** for each column. Typically most of the columns will be designated as **Inputs**, which means that they will be used to find the best design. In addition, we recommend including one **Index** column which contains a unique identifier for each run of the candidate set. This makes tracking which runs are included in the constructed designs easier. If no **Index** column is specified, a warning appears later in the process, but this column is not strictly required.

Finally, the **Min** and **Max** columns in the box allow the range of values for each input column to be specified. The default is to extract the smallest and largest values from the candidate and history data files, and use these. This approach generally works well, as it scales the inputs to be in a uniform hypercube for comparing distances between the design points.

Hint: the default values for **Min** and **Max** can generally be left at their defaults unless: (1) the range of some inputs represent very different amounts of change in the process. For example, if temperature is held nearly constant, while a flow rate changes substantially, then it may be desirable to extend the range of the temperature beyond its nominal values to make the amount of change in temperature more commensurate with the amount of change in the flow rate. (2) if changes are made in the candidate or history data files. For example, if one set of designs are created from one candidate set, and then another set of designs are created from a different candidate set. These designs and the achieved criterion value will not be comparable unless the range of each input has been fixed at matching values.

10. Once the design choices have been made, click on the **TestSDOE** button. This generates a small number of iterations of the search algorithm to calibrate the timing for constructing and evaluating the designs. The time taken to generate a design is a function of the size of the candidate set, the size of the design, as well as the dimension of the input space. The slider below **TestSDOE** now indicates an estimate of the time to construct the designs across the range of the **Min Design Size** and **Max Design Size** specified. The smallest **Number of Random Starts** is 10^3 = 1000 is generally too small to produce a good design, but this will run very quickly. Powers of 10 can be chosen with an **Estimated Runtime** provided below the slider.

Hint: The choice of **Number of Random Starts** involves a trade-off between the quality of the design generated and the time to generate the design. The larger the chosen number of random starts, the better the design is likely to be. However, there are diminishing gains for increasingly large numbers of random starts. If running the actual experiment is expensive, it is generally recommended to choose as large a number of random starts as possible for the available time frame, to maximize the chance of an ideal design being found.

11. Once the slider has been set to the desired **Number of Random Starts**, click on the **Run SDOE** button, and initate the construction of the designs. The progress bar indicates how design construction is progressing through the chosen range of designs between the **Min Design Size** and **Max Design Size** specified.

8.3 Example 1: 8-run 2-D design

For this first example, the goal is to construct a simple space-filling design with 8 runs in a 2-dimensional space using the example files provided with FOQUS.

1. From the FOQUS main screen, click the **SDOE** button. On the top left side, select **Load from File**, and select the candidate.csv file from examples folder. This identifies the possible input combinations from which the design will be constructed. The more possible candidates that can be provided to the search algorithm used to construct the design, the better the design might be for the specified criterion. *Home Screen*.

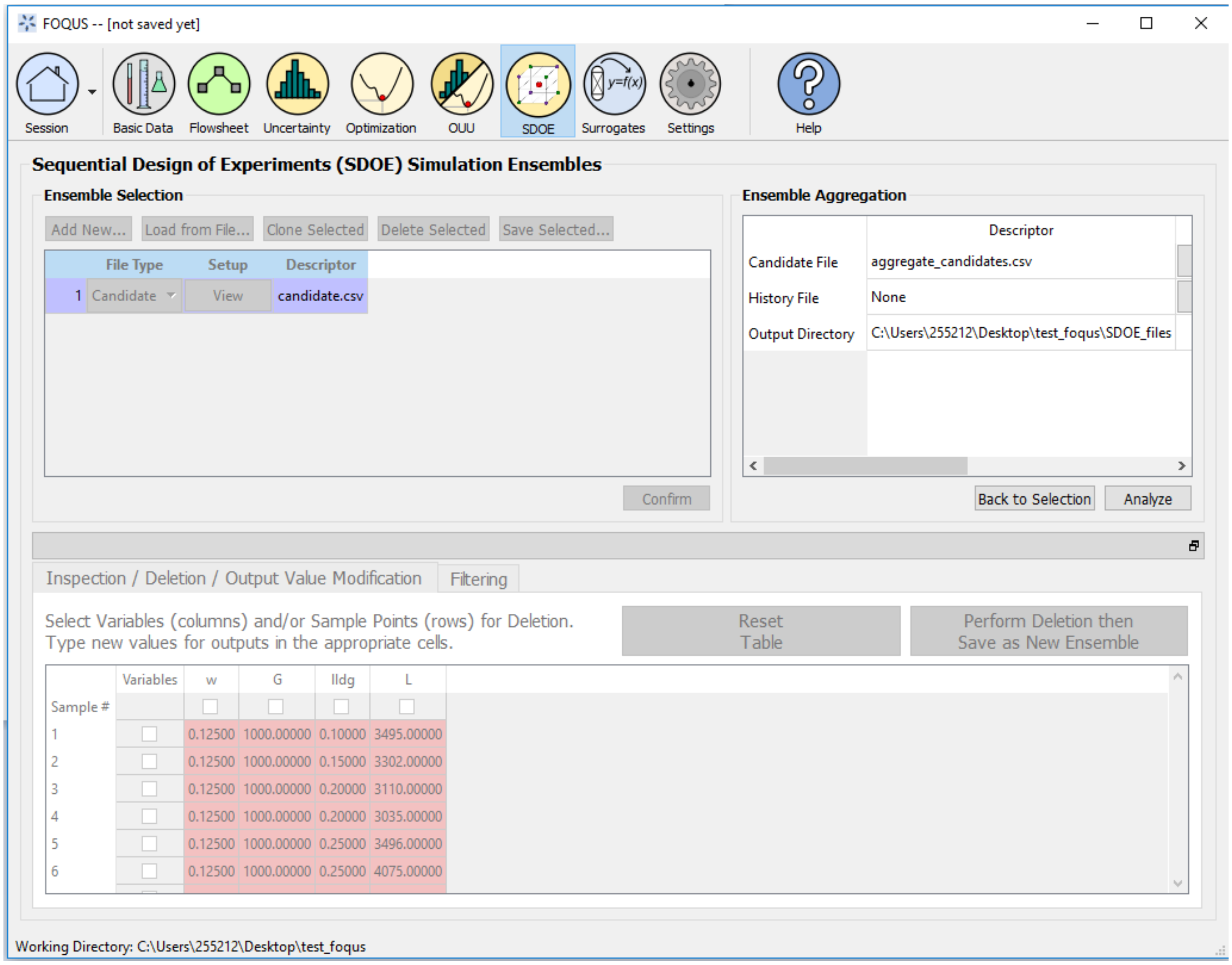


Fig. 5: Home Screen

CHAPTER 9

Solvent Fit

9.1 Contents

[sec:solvent_fit]

The SolventFit module is an uncertainty quantification tool for full Bayesian calibration of an Aspen Plus solvent process model to experimental data. SolventFit may provide improved predictions with uncertainty bounds by accounting for uncertainty in model parameters and deficiencies in the model form. The result is a posterior distribution of parameters allowing for predictions with uncertainty. uses a custom BSS-ANOVA-based response surface for the outputs. Like the Bayesian inference module, the ***SolventFit*** algorithm *(Bhat et al. 2015)* utilizes Markov Chain Monte Carlo (MCMC) to compute the posterior distributions, and uses a custom BSS-ANOVA-based response surface (emulators) that serves as a fast approximations to the actual simulation model.

9.1.1 SolventFit Instructions

To use ***SolventFit***, the user will need to install R, as well as the R packages “MCMCpack”, “abind” and “MASS”. Please refer to the installation instructions in Section [(sec.surrogate.acosso)]. Once R is installed, the user will also need to set the path to the RScript executable within FOQUS.

1. **Basic Data.** From the FOQUS main screen, click the **Basic Data** button and select **SolventFit** to enter a SolventFit session.
2. **Load Training Data** loads the file of design and variable inputs and their relevant simulation outputs (from Aspen or other computer simulation code). This file usually has extension .txt, .dat, or .csv.
3. **Output Settings** lists the available outputs for analysis. The Output Name column lists the name of each output. The user can select/deselect outputs for analysis using the checkboxes in the Observed column. The response surface in SolventFit will be prepopulated with “SolventFit Emulator” because SolventFit uses its own custom BSS-ANOVA response surface model. The simulation ensemble is used as the training data for generating the response surfaces.
4. **Input Settings** is populated with input variable information from the training data. Under the column, **Type**, the user can specify which inputs are fixed, design, or variable using the from the drop-down menu in the **Input Settings Table**. Selecting “Fixed” means that the input is fixed at its default value for all design points.

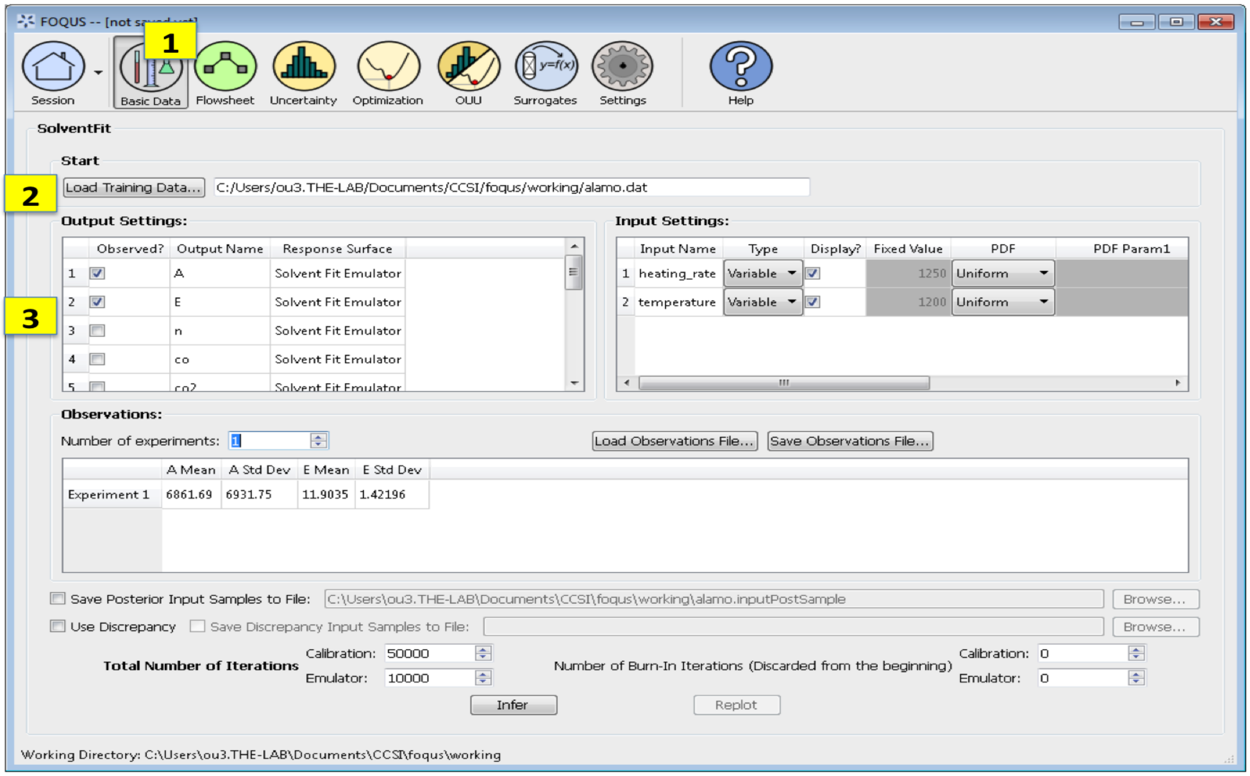


Fig. 1: SolventFit Home Screen

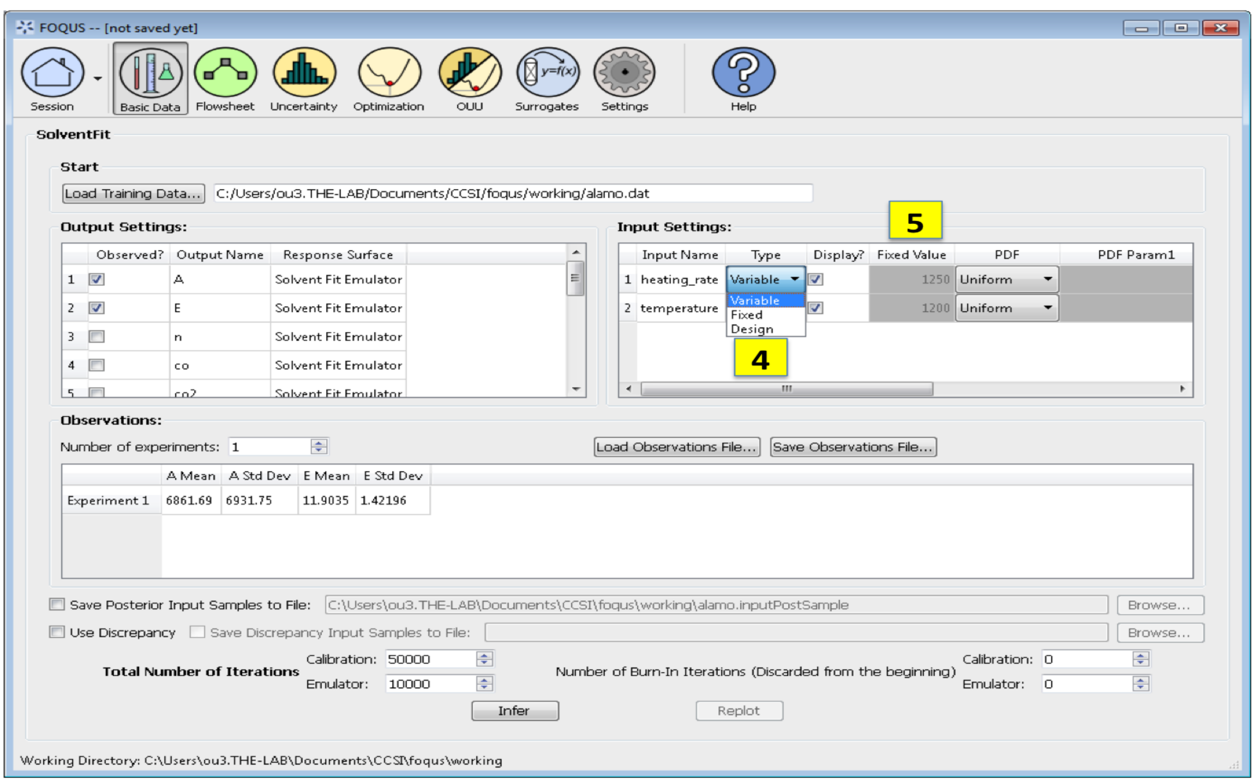


Fig. 2: SolventFit Input Settings

Changing the type to "Variable" means that the input is a calibration parameter and is uncertain; therefore, its value varies between samples. Changing the type to "Design" means that the input is an experimental input with preselected values. In addition, the user can specify which inputs are displayed in the resulting plots of the posterior distributions. To omit specific inputs, clear the checkboxes from the ***Display*** column of the table. (The default is that once inference is completed, all inputs will be displayed in the plots.)

5. **Fixed Value.** With any fixed input, the only parameter that can be changed is the default value (i.e., all samples of this input are fixed at this default value).

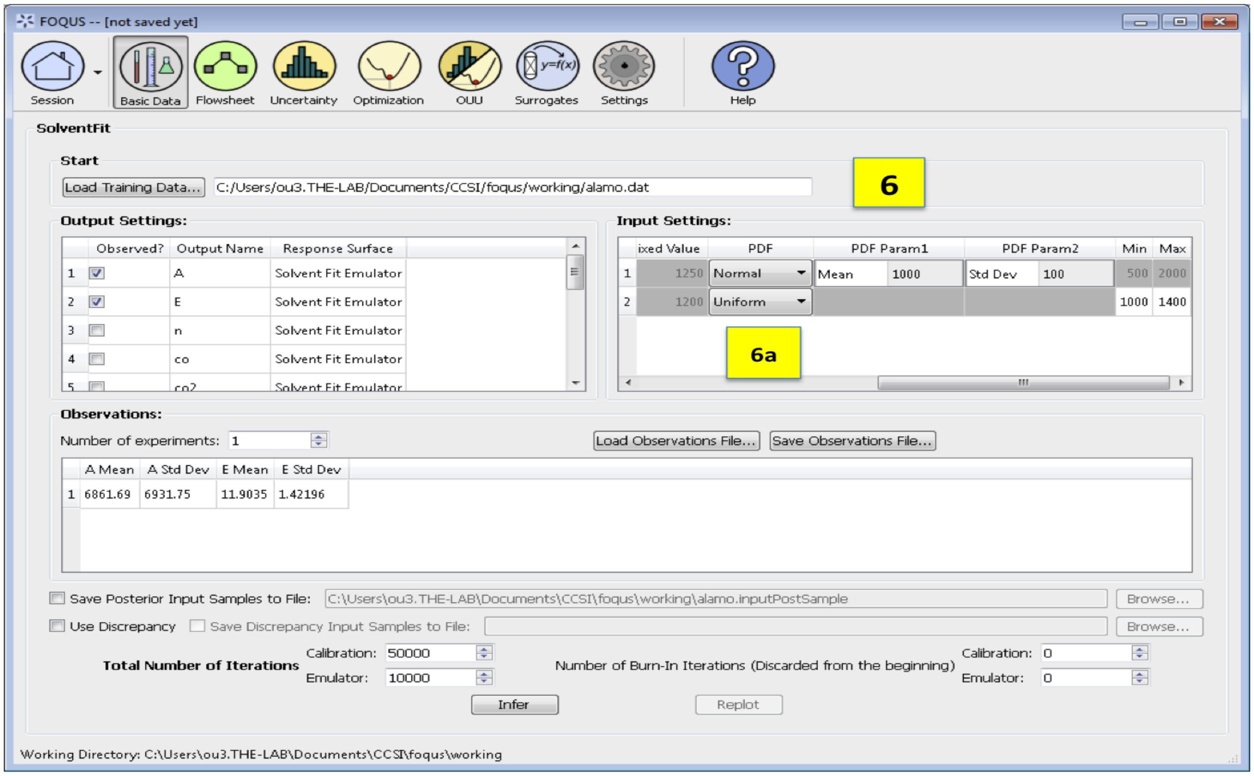


Fig. 3: SolventFit Prior PDF for Inputs

6. **PDF.** With any variable input, the minimum/maximum values, as well as the probability distribution function (PDF), for that input can be changed. The default prior is specified to be Uniform. To change the prior distribution type (e.g., Normal, Lognormal, or Gamma), use the drop-down list in the ***PDF*** column (box 6a) and enter corresponding values for the PDF parameters. To change the range of a uniform prior, scroll all the way to the right to modify ***Min/Max***.

7. **Observations** section enables the user to add experimental data in the form of observations of certain output variables. At least one observation is required; the **number of experiments** may be changed using the pull down menu. For each observation, enter the mean and standard deviation (enter zero if there is no information about the noise) for all of the outputs. If any inputs are selected as design inputs, their values will also be required here. Currently, the observation noise model is assumed to be a normal distribution. Alternatively, the user can import the file of experiments using the **Load Observation File** button (7a). The user can also export the observations using the **Save Observation File** button (7b).

8. **Number of Iterations** are the number of iterations that the Markov Chain Monte Carlo (MCMC) is run for emulation and calibration. The default number of samples is set at 10000 for emulation and 50000 for calibration. Also the number of "burn-in" samples (number of initial samples to be thrown out) for both emulation and calibration may be changed from its default of 0 using the relevant button (8a).

9. **Use Discrepancy.** Check this box if the discrepancy should be estimated in the calibration model. It is usually

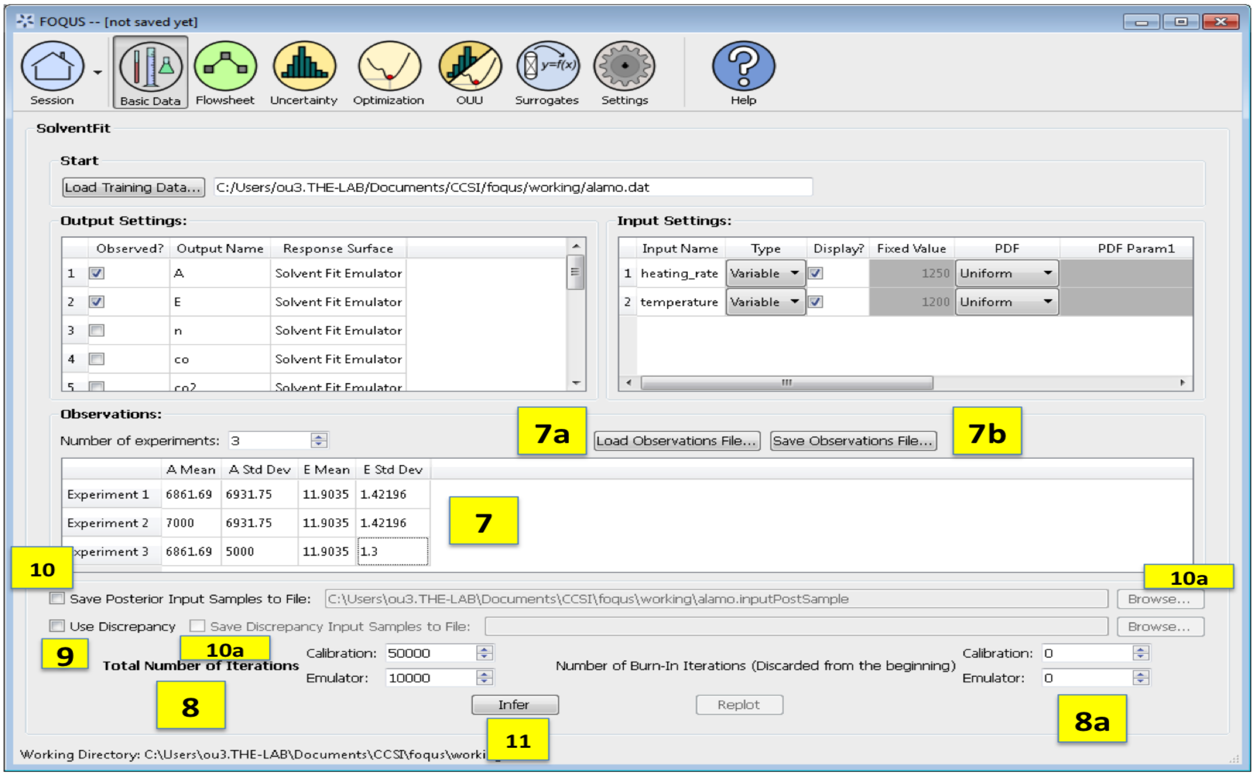


Fig. 4: SolventFit Inference Screen

good practice to include the discrepancy in the calibration analysis.

10. **Save Posterior Input Samples to File** checkbox, when selected, saves the posterior input samples as a PSUADE sample file (format described in Section [ap:psuadefiles]). This file characterizes the input uncertainty as a set of samples. In addition, the user can save the discrepancy samples to a file by selecting the checkbox **Save Discrepancy Input Samples to File** (10a). If saving posterior and/or discrepancy samples to a file, click **Browse** to set the name and location of where this file is saved (10b).

11. Click **Infer** to start the analysis. (Note: If the inference returns an invalid posterior distribution (i.e., one with no samples), it usually means the prior distributions or that the observation data are not prescribed appropriately. In this case, it is recommended that the user experiment with different priors and/or data distribution means and/or standard deviations.)

12. The plotted results for SolventFit are posterior distributions of the selected variable inputs; they are similar to the plots from the Bayesian Inference in the Uncertainty Quantification module in Figure [fig:uqt_infer_replot_results], see Section [sec:uq_tutorial] on Bayesian Inference for more details.

CHAPTER 10

Simulation Standard Interface (SimSinter)

10.1 Contents

10.1.1 SimSinter Configuration

SimSinter is the standard interface library that FOQUS and Turbine use to drive the target simulation software. SimSinter currently supports AspenPlus, Aspen Custom Modeler (ACM), gPROMS, and Microsoft Excel. SimSinter is used to: (1) open the simulator, (2) initialize the simulation, (3) set variables in the simulation, (4) run the simulation, and (5) get resulting output variables from the simulation.

To drive a particular simulation, SimSinter must be told which input variables to set and which output variables to read when the simulation is finished (there are generally far too many variables in a simulation to set and read them all). Each simulation must have a "Sinter Config File" which records this information. FOQUS keeps the simulation file and the "Sinter Config File" together and sends them to the Turbine gateway when a simulation run is requested.

The configuration is simplified by a GUI included with the SimSinter distribution called, "SinterConfigGUI." FOQUS can launch the SinterConfigGUI on simulations that have not been configured. To run the "SinterConfigGUI" the user must have:

1. SimSinter distribution installed. SimSinter is installed by the FOQUS bundle installer.
2. The simulation file the user wants to configure. For example, if the user has an Aspen Custom Modeler simulation called BFB.acmf, that file must be on the user's computer, and the user should know its location.
3. The application used to execute the simulation file. For example, if the user wants to configure an Aspen Custom Modeler simulation called BFB.acmf, Aspen Custom Modeler must be installed on the user's machine.

The rest of this section details two step-by-step tutorials on configuring a simulation with "SinterConfigGUI." The first simulation is an Aspen Custom Modeler simulation and the second, Aspen Plus. Please also see the D-RM Builder tutorials for configuring dynamic ACM models. For more details on SimSinter or a tutorial on how to configure a Microsoft Excel file, please see the "SimSinter Technical Manual," which is included in the FOQUS distribution. The default location is at C:Program Files (x86)foqusfoqusdoc. It is also available on the CCSI website.

10.1.2 Tutorial

Aspen Plus Configuration

1. The initial steps for opening a simulation and entering metadata for an Aspen Plus simulation are similar to ACM. Refer to the SimSinter ACM tutorial *Aspen Custom Modeler Configuration*. In this tutorial, a flash model “Flash_Example.bkp” installed in the “C:SimSinterFilesAspen_Plus_Install_Test” is used as an example. Open the Aspen Plus file and enter the metadata as shown in Figure *SinterConfigGUI Simulation Meta-Data with Data Completed*.

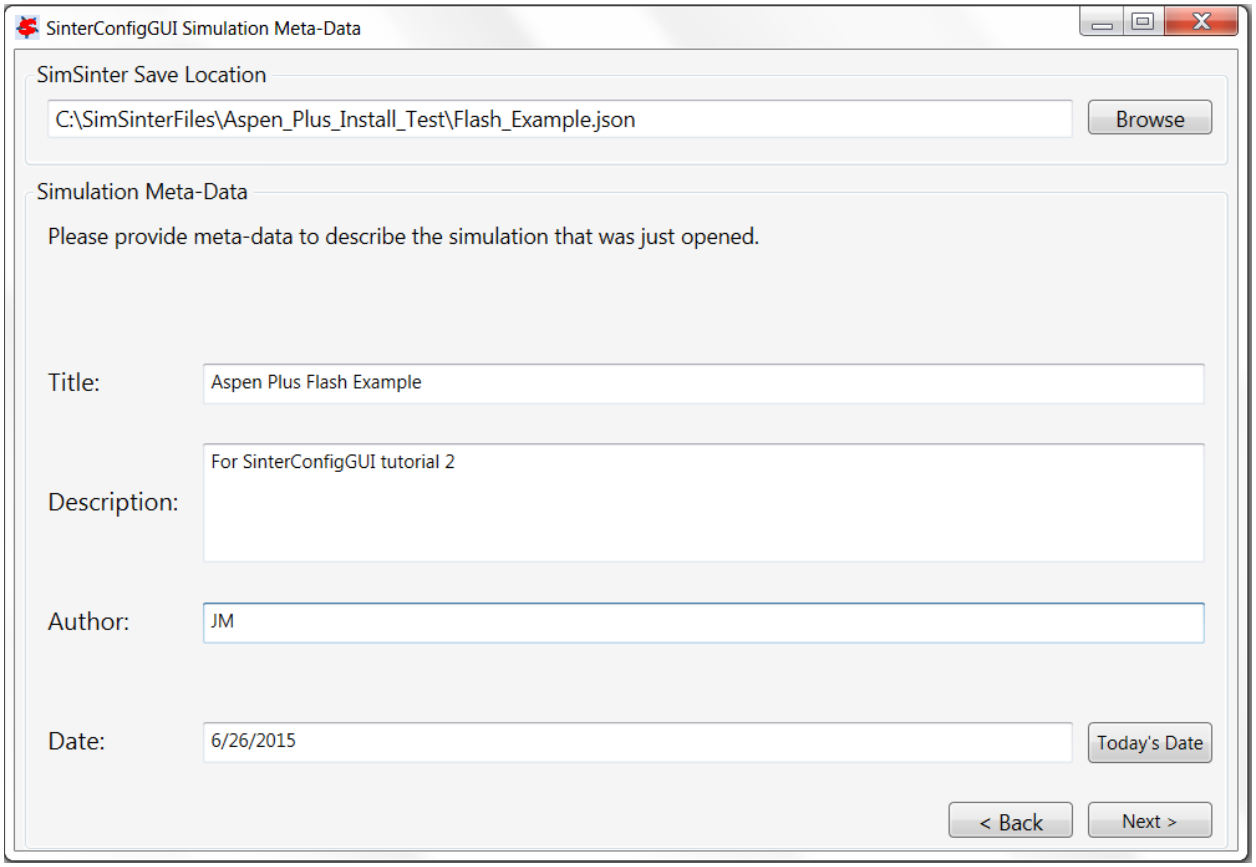


Fig. 1: SinterConfigGUI Simulation Meta-Data with Data Completed

2. The **SinterConfigGUI Variable Configuration Page** displays as illustrated in Figure *SinterConfigGUI Variable Configuration Page Empty Variables*. Aspen Plus has no settings, so there are no setting variables in the input section. Unlike ACM, AspenPlus displays the **Variable Tree** on the left side, so the user can explore the tree as is done in Aspen Plus Tools → Variable Explorer. Unfortunately, searching is not possible.

3. **Variable Tree** nodes can be expanded for searching (Figure *SinterConfigGUI Variable Configuration Page Expanded Aspen Plus Variable Tree*).

4. The user can type the node address directly into the **Selected Path** field (this is useful for copy/paste from Aspen Plus’ Variable Explorer) (Figure *SinterConfigGUI Variable Configuration Page Aspen Plus Variable Selected*). Click **Lookup** or **Preview** (which automatically causes the tree to expand and selects selected variables in the **Variable Tree**).

5. To make the temperature of the Flash chamber an **Input Variable**, click **Make Input**. Additionally, the user can **Name** the variable, fix the **Description**, and enter the **Min/Max** fields by clicking on the appropriate text and entering it.

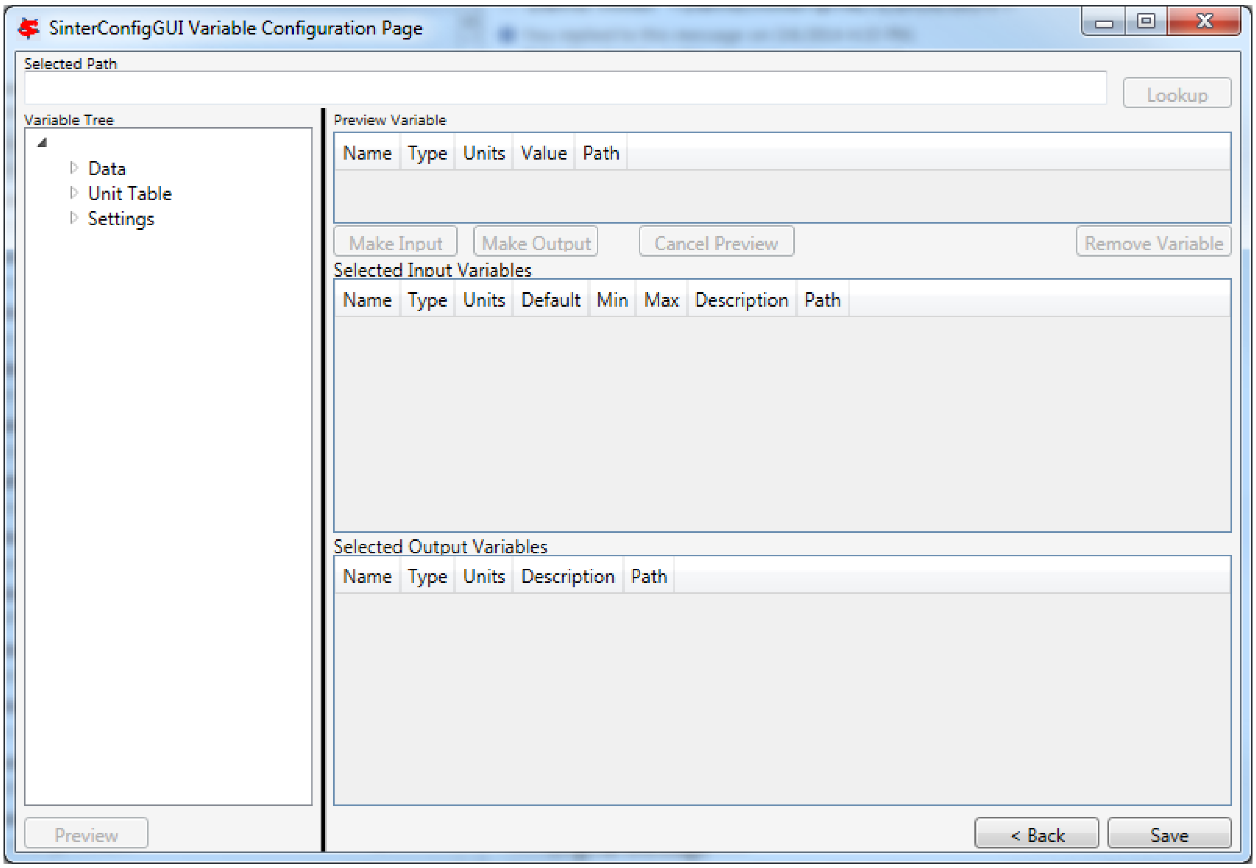


Fig. 2: SinterConfigGUI Variable Configuration Page Empty Variables

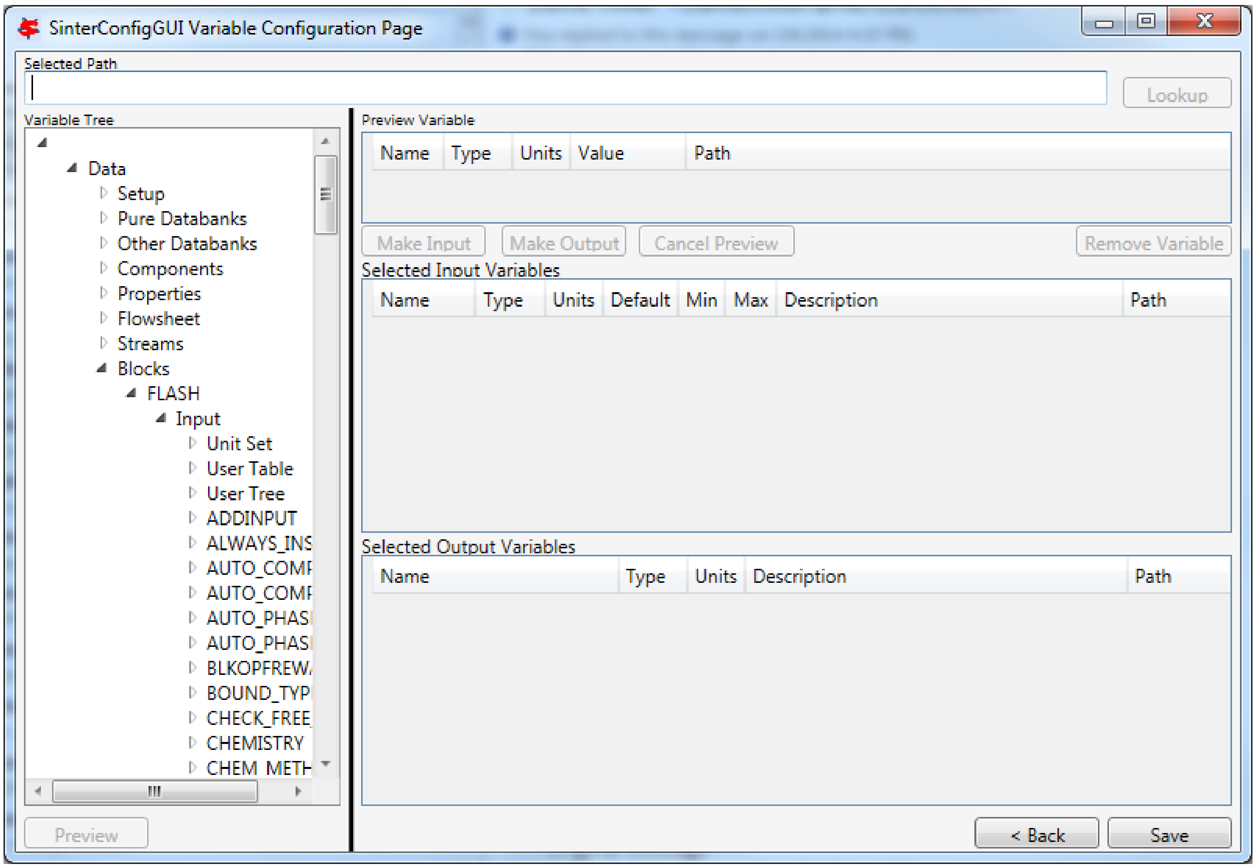


Fig. 3: SinterConfigGUI Variable Configuration Page Expanded Aspen Plus Variable Tree

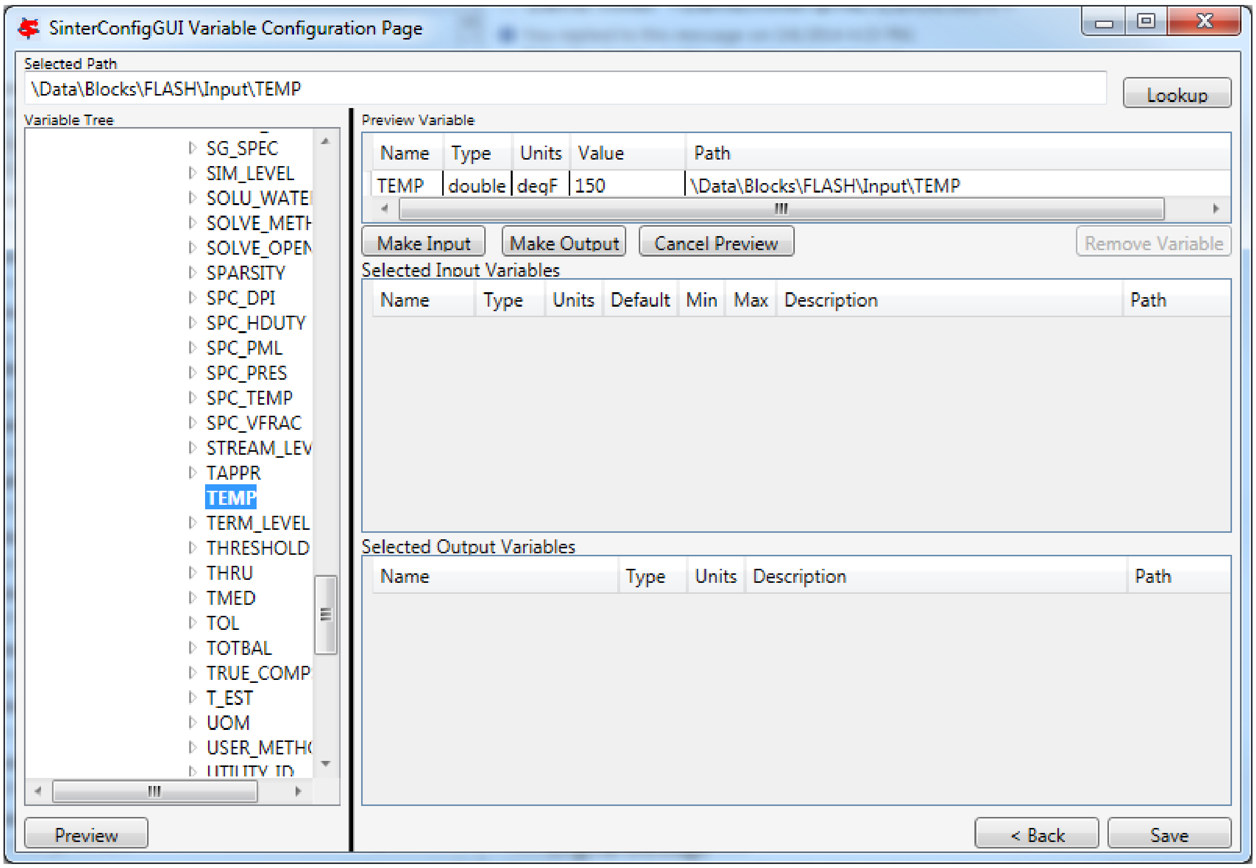


Fig. 4: SinterConfigGUI Variable Configuration Page Aspen Plus Variable Selected

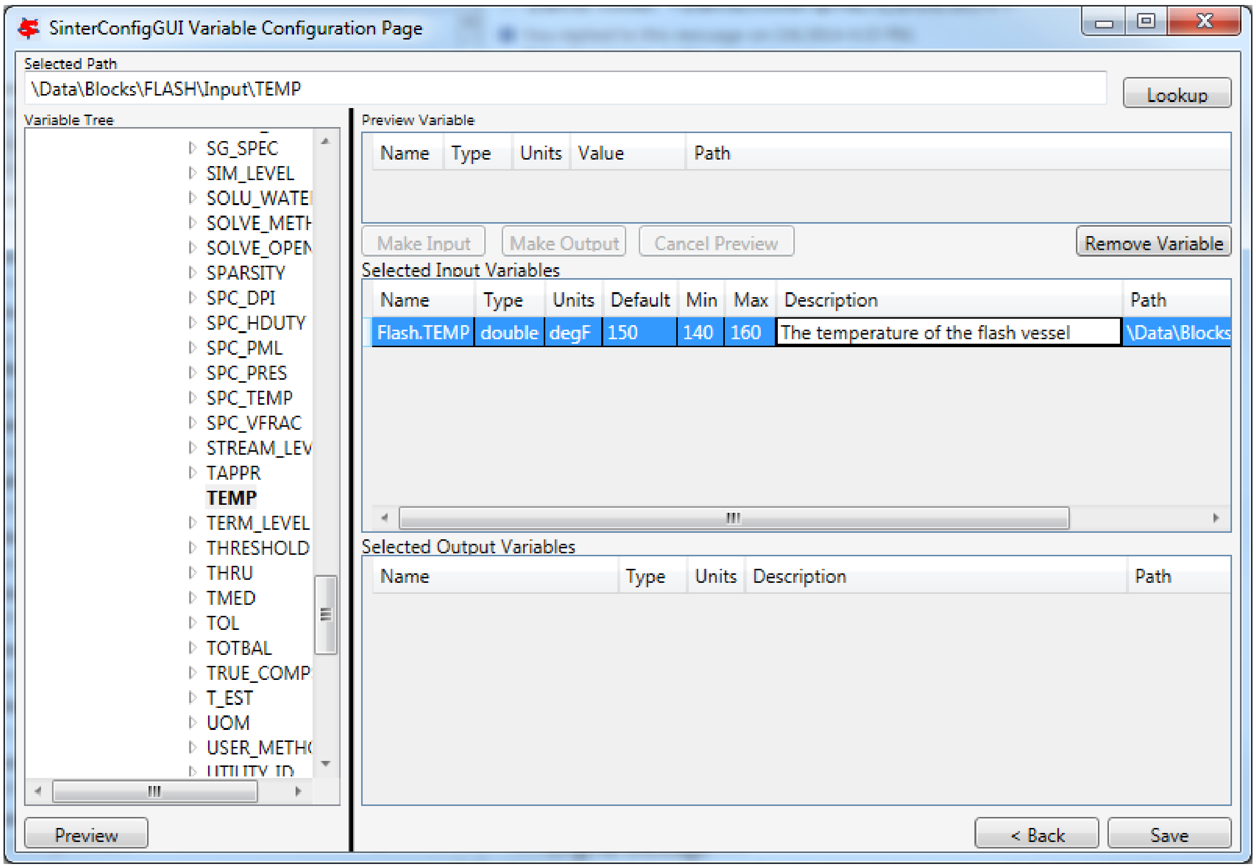


Fig. 5: SinterConfigGUI Variable Configuration Page Input Variable

6. Select an **Output Variable**, **Preview** it, and click **Make Output**. Next, update the fields as with the **Input Variable** to give a better **Name** and **Description**.

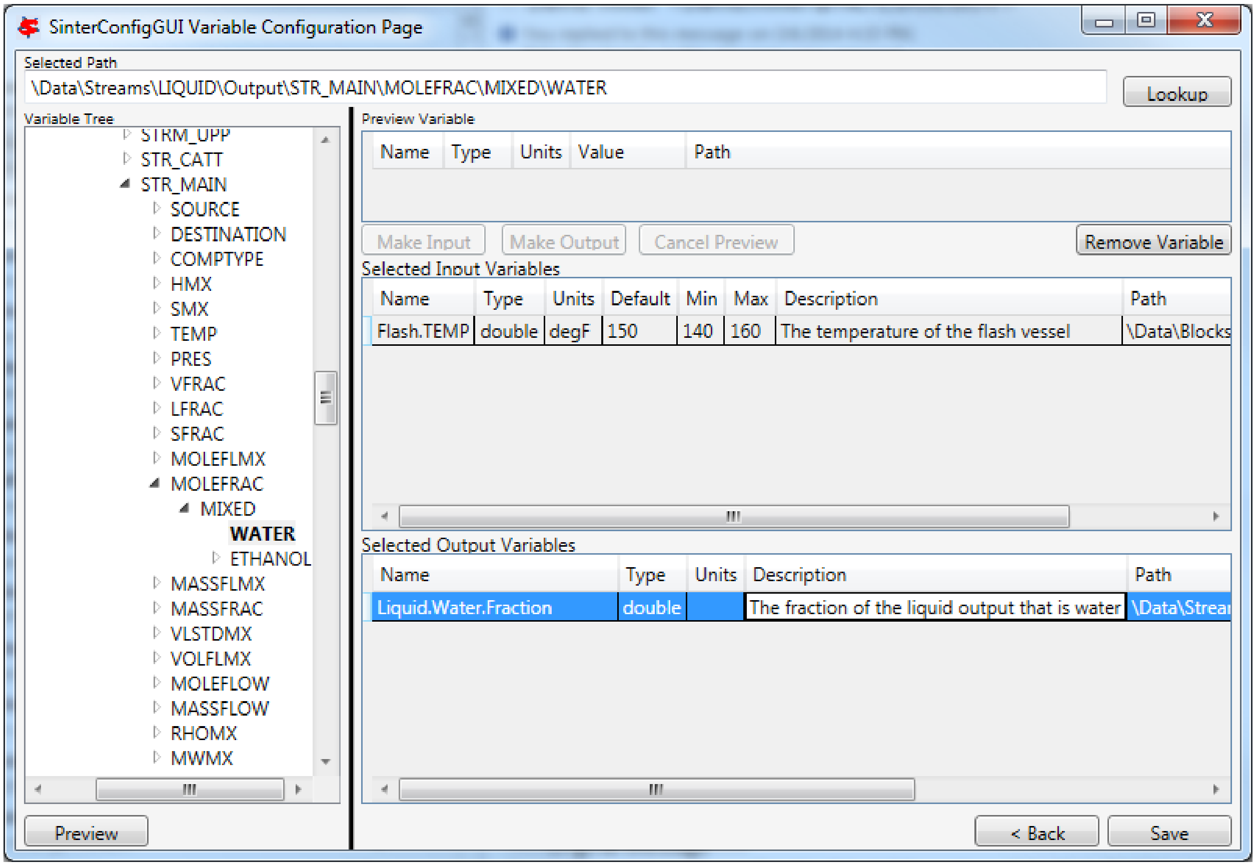


Fig. 6: SinterConfigGUI Variable Configuration Page Output Variable

7. The task is complete. Save it by clicking **Save** or CTRL+S. The file is saved to the location specified in the SinterConfigGUI Simulation Meta-Data page. If the user wishes to save a copy under a different name, navigate back to the SinterConfigGUI Simulation Meta-Data page and change the name.

Aspen Custom Modeler Configuration

1. The "SinterConfigGUI" can be launched from FOQUS, via the **Create/Edit** button found in **File**→ **Add/Update Model to Turbine** or "SinterConfigGUI" may be run on its own by selecting **SimSinter** → **SinterConfigGUI** from the Start menu.

2. The splash window displays, as shown in Figure *SinterConfigGUI Splash Screen*. The user may click the splash screen to proceed, or wait ten seconds for it to close automatically.

3. The SinterConfigGUI Open Simulation window displays (Figure *SinterConfigGUI Open Simulation Window*). If "SinterConfigGUI" was opened from FOQUS, the filename text box already contains the correct file. To proceed immediately click **Open File and Configure Variables** or click **Browse** to search for the file. For this tutorial, the ACM model for bubbling fluidized bed adsorber installed in the FOQUS examplesOUUBFB_Cap folder is selected (BFB_OUU_COE.acmf). Once the file is selected, click **Open File and Configure Variables**. The user can open a fresh ACM simulation (.acmf file) or an existing SimSinter configuration file. For this example, open a fresh simulation.

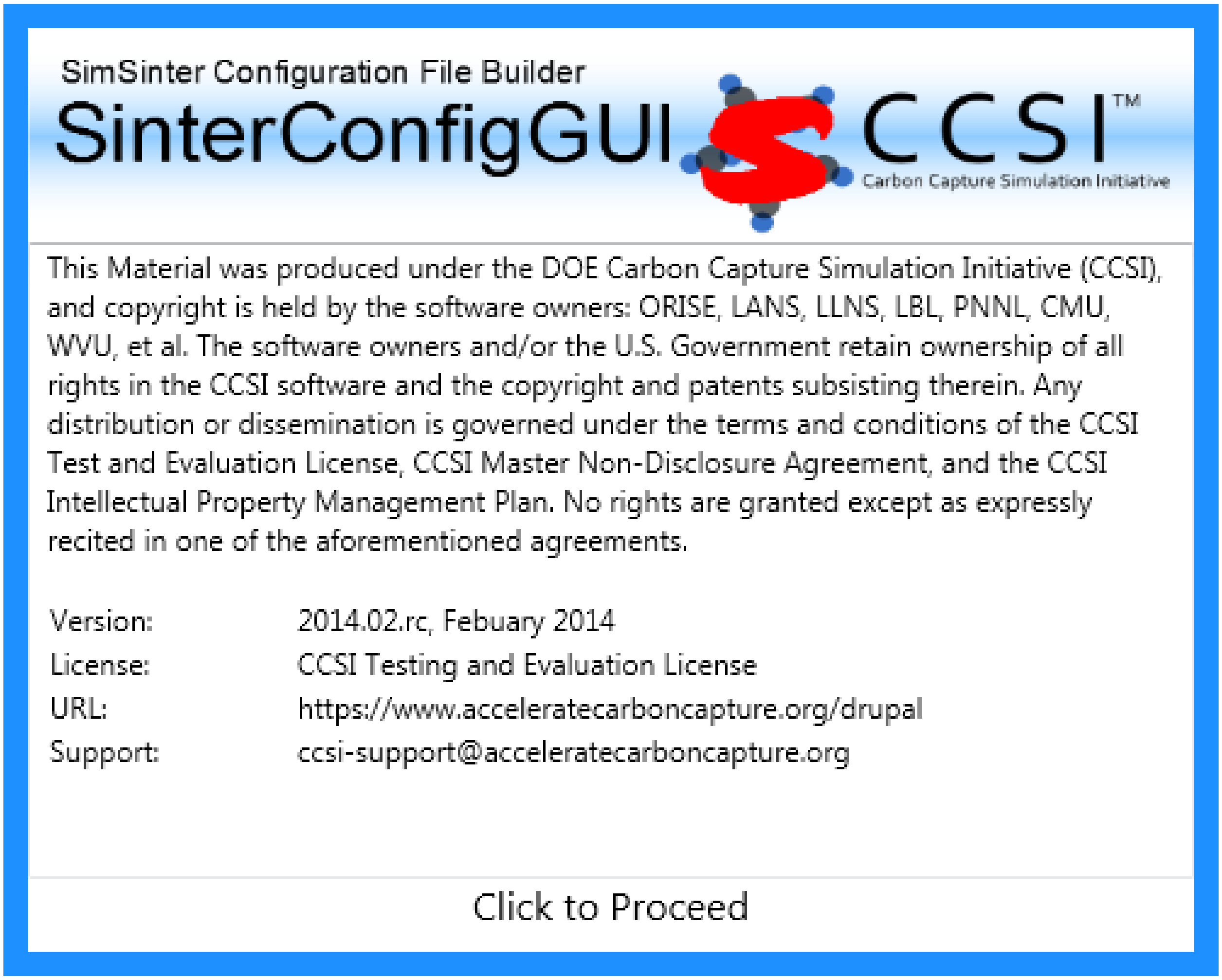


Fig. 7: SinterConfigGUI Splash Screen

Note: Opening the simulation may take a few minutes depending on how quickly Aspen Custom Modeler can be opened.

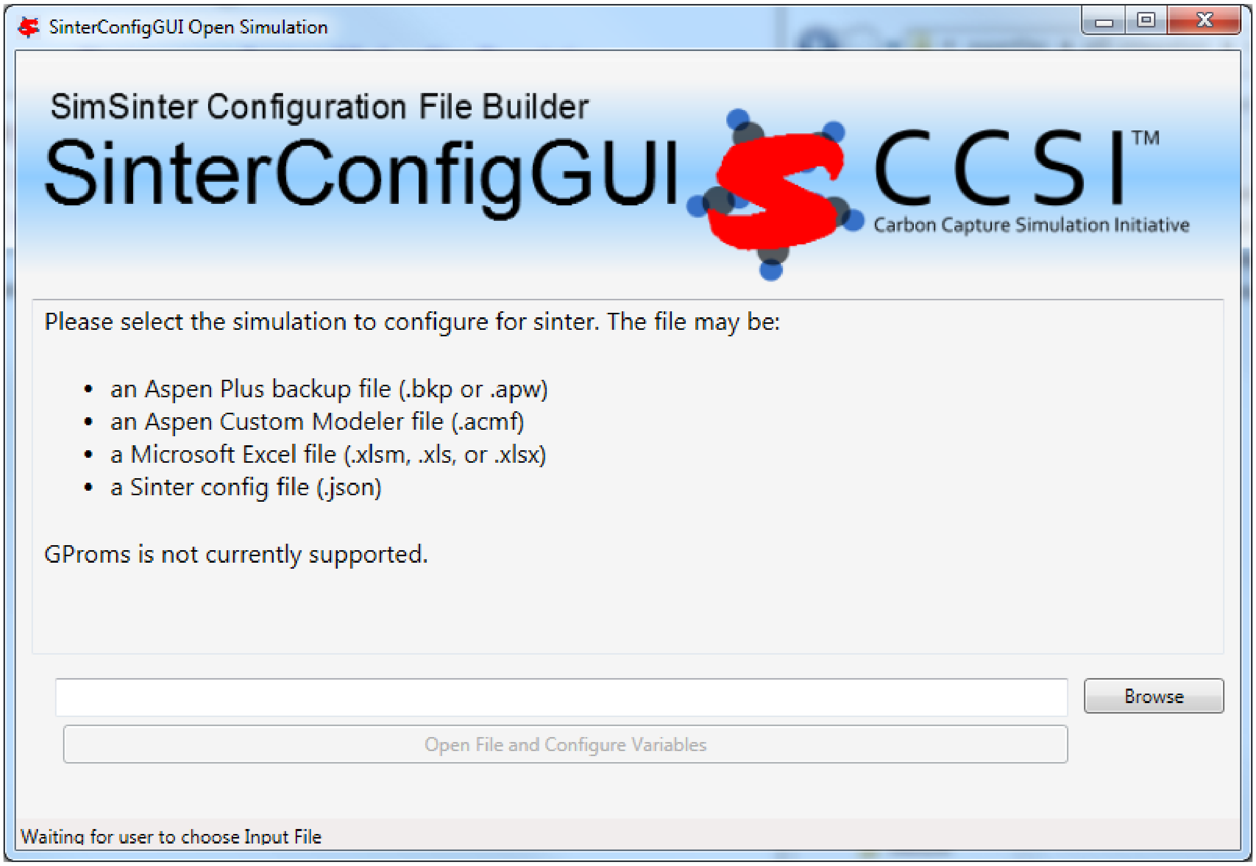


Fig. 8: SinterConfigGUI Open Simulation Window

4. Aspen Custom Modeler starts in the background. This is so the user can observe things about the simulation while working on the configuration file.
5. The SinterConfigGUI Simulation Meta-Data window displays. (Figure *SinterConfigGUI Simulation Meta-Data Page Save Name Text Box*). The first and most important piece of metadata is **SimSinter Save Location** at the top of the window. This is where the sinter configuration file is saved. The system attempts to locate a reasonable file location and file name; however, the user must confirm the correct file location, since it automatically overwrites whatever file name currently exists.
6. Continue to complete the remaining fields and then click **Next** (Figure *SinterConfigGUI Simulation Meta-Data Page with Data Completed*).
7. In the **SinterConfigGUI Variable Configuration Page**, (Figure *SinterConfigGUI Variable Configuration Page before Input*) notice that the ACM **Selected Input Variables**: **TimeSeries**, **Snapshot**, **RunMode**, **printlevel** and **homotopy** are already included in the input variables. **TimeSeries** and **Snapshot** are for dynamic simulations. **RunMode** can be either "Steady State" or "Dynamic". The Dynamic mode requires a dynamic ACM model. For this simulation, the RunMode is Steady State. The **homotopy** variable can be set to "1" so that homotopy is on by default. Notice that the **Dynamic** column (the first column) in each row contains a checkbox, enabling the user to select if the input variable in the row is a dynamic variable. Also notice that a **Variable Type** search box is on the left. This search is exactly the same as Variable Find on the Tools menu in Aspen Custom Modeler. Please refer to the ACM documentation for details on search patterns.
8. A search for everything in the "BFBAdsT" block has been selected. The following **Search in Progress** dialog

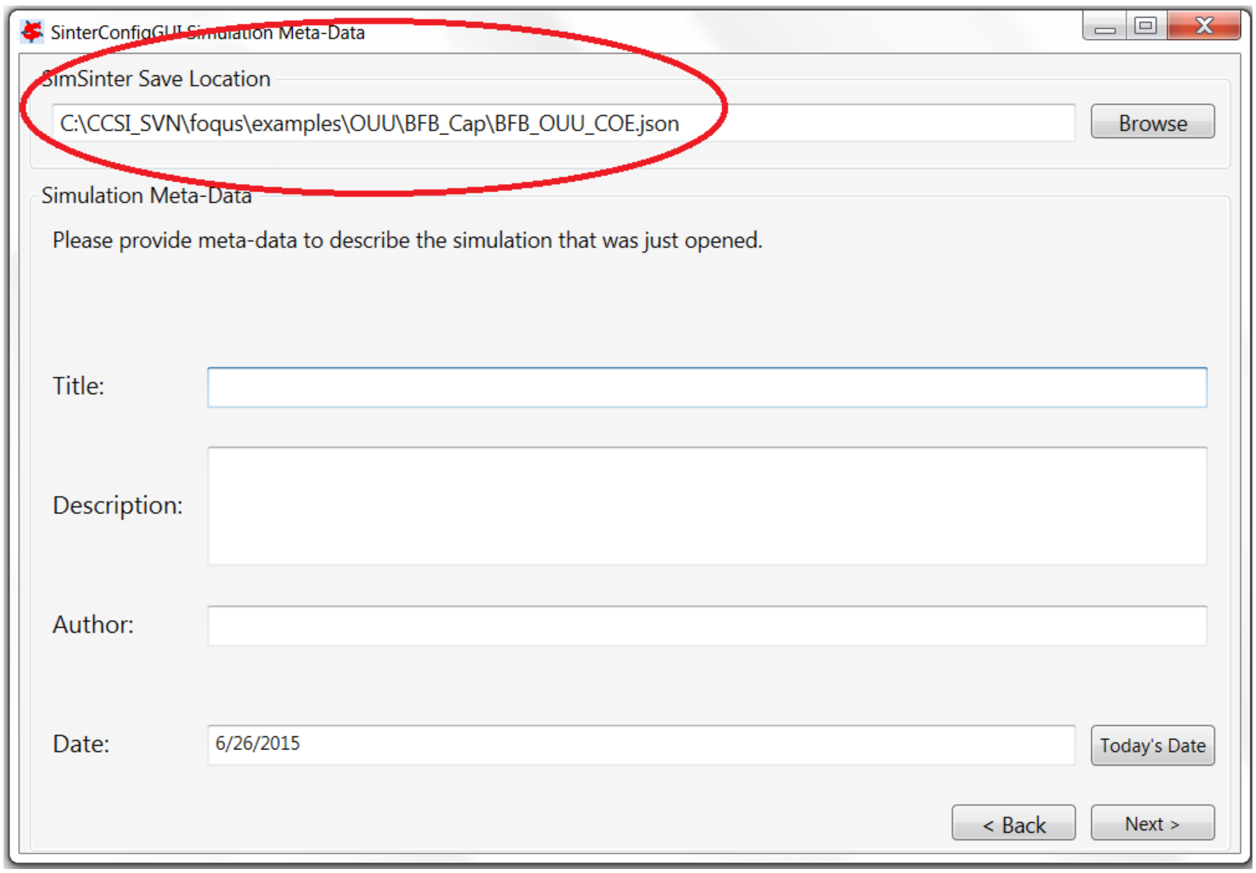


Fig. 9: SinterConfigGUI Simulation Meta-Data Page Save Name Text Box

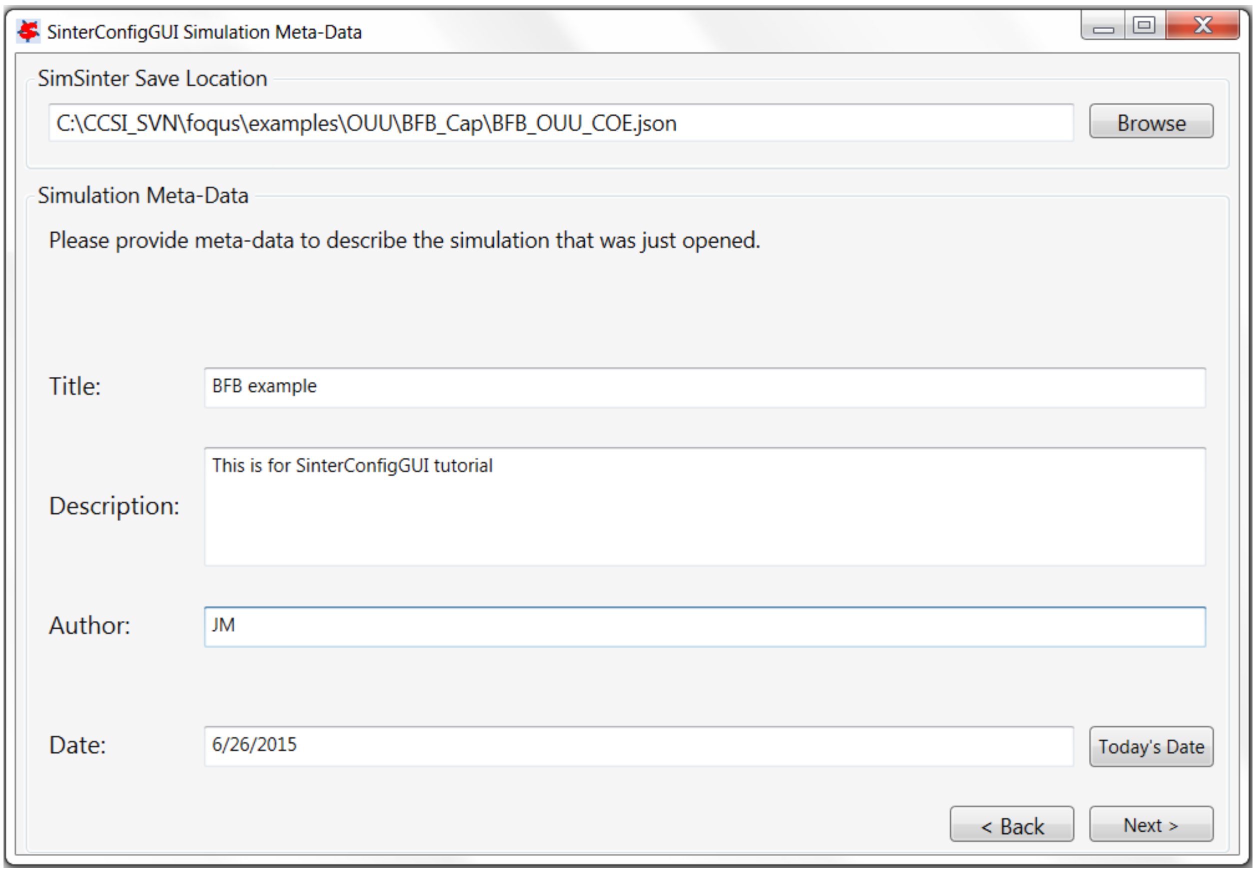


Fig. 10: SinterConfigGUI Simulation Meta-Data Page with Data Completed

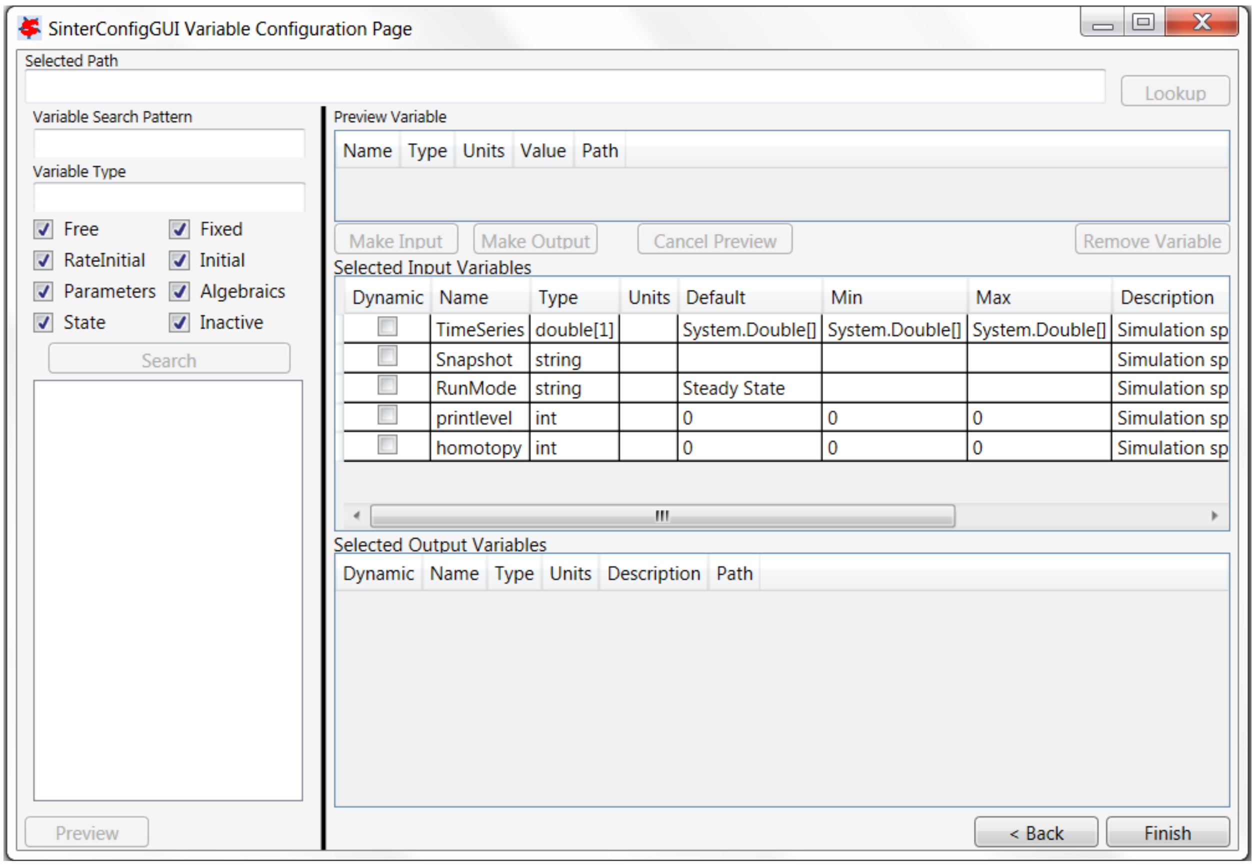


Fig. 11: SinterConfigGUI Variable Configuration Page before Input

is displayed (Figure *Search in Progress Bar Page*). Sometimes large searches take a while.

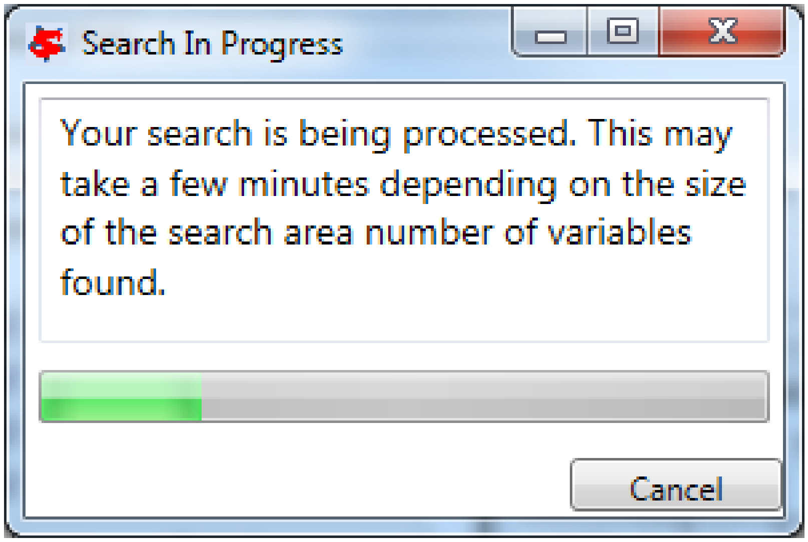


Fig. 12: Search in Progress Bar Page

9. First, select the "BFBadsT.A1" scalar variable in the **Selected Path** field (Figure *SinterConfigGUI Variable Configuration Page BFBadsT.A1 Selected*).
10. If the user double-clicks, presses Enter, or clicks **Preview** or **Lookup**, information displays in the **Preview Variable** section (Figure *SinterConfigGUI Variable Configuration Page BFBadsT.A1 Preview*). Here, the user can verify the variable choices.
11. "BFBadsT.A1" is the correct variable; therefore, click **Make Input**. Information displays in the **Selected Input Variables** section (Figure *SinterConfigGUI Variable Configuration Page BFBadsT.A1 Made Input*).
12. Change the variable name from "BFBadsT.A1" to something more descriptive (e.g., "WaterA"). Set **Name**, **Description** and **Min/Max** as shown in Figure *SinterConfigGUI Variable Configuration Page BFBadsT.A1 Change Name*.
13. One input variable is now displayed (Figure *SinterConfigGUI Variable Configuration Page Vector Preview*). At least one output variable is required. In this example, the vector of calculated bubble sizes is wanted. Scroll down under **Search** and select "BFBadsT.db.Value," "BFBadsT.db.Value(0)," "BFBadsT.db.Value(1)," etc. If a name with a number in parenthesis at the end is selected, it is a specific entry in the vector. If a basic name is selected ("BFBadsT.db.Value"), the entire vector is displayed. Select the whole vector and click **Preview**.
14. Click **Make Output** if the variable the user wants is selected. Notice that this variable has a unit "m" (Figure *SinterConfigGUI Variable Configuration Page Vector As Output*).
15. Change the **Name** of the variable to "Diameter." Bubble size is measured in meters; however, meters should be converted to millimeters (mm). Now, the output from the simulation should present bubble diameter in mm (Figure *SinterConfigGUI Variable Configuration Page Output Change Units*). Internal to the simulation, the unit remains "m."
16. To add a single item in a vector, select "BFBadsT.Ar.Value(1)" and click **Make Input** (See Figure *SinterConfigGUI Variable Configuration Page Removal Demo*). To remove item that was just added, select it and click **Remove Variable**.
17. Select the correct variable vector "BFBadsT.Ar.Value" and make it an input (Figure *SinterConfigGUI Variable Configuration Page Read Input*). Notice that a **Default** or **Min/Max** cannot be set in the GUI for a vector. The correct defaults (from the simulation) are set automatically. To change the **Min/Max** values, the user must edit the JSON file in a text editor.

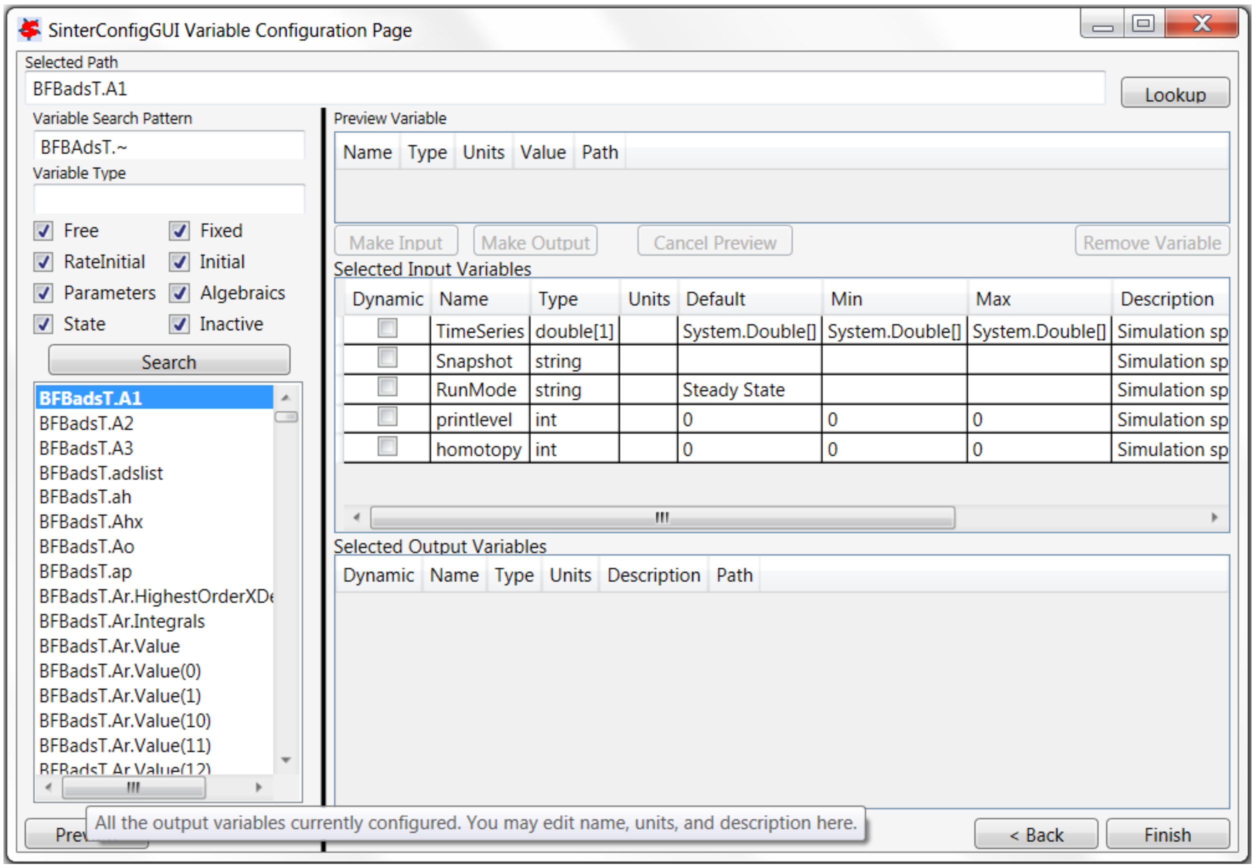


Fig. 13: SinterConfigGUI Variable Configuration Page BFBadsT.A1 Selected

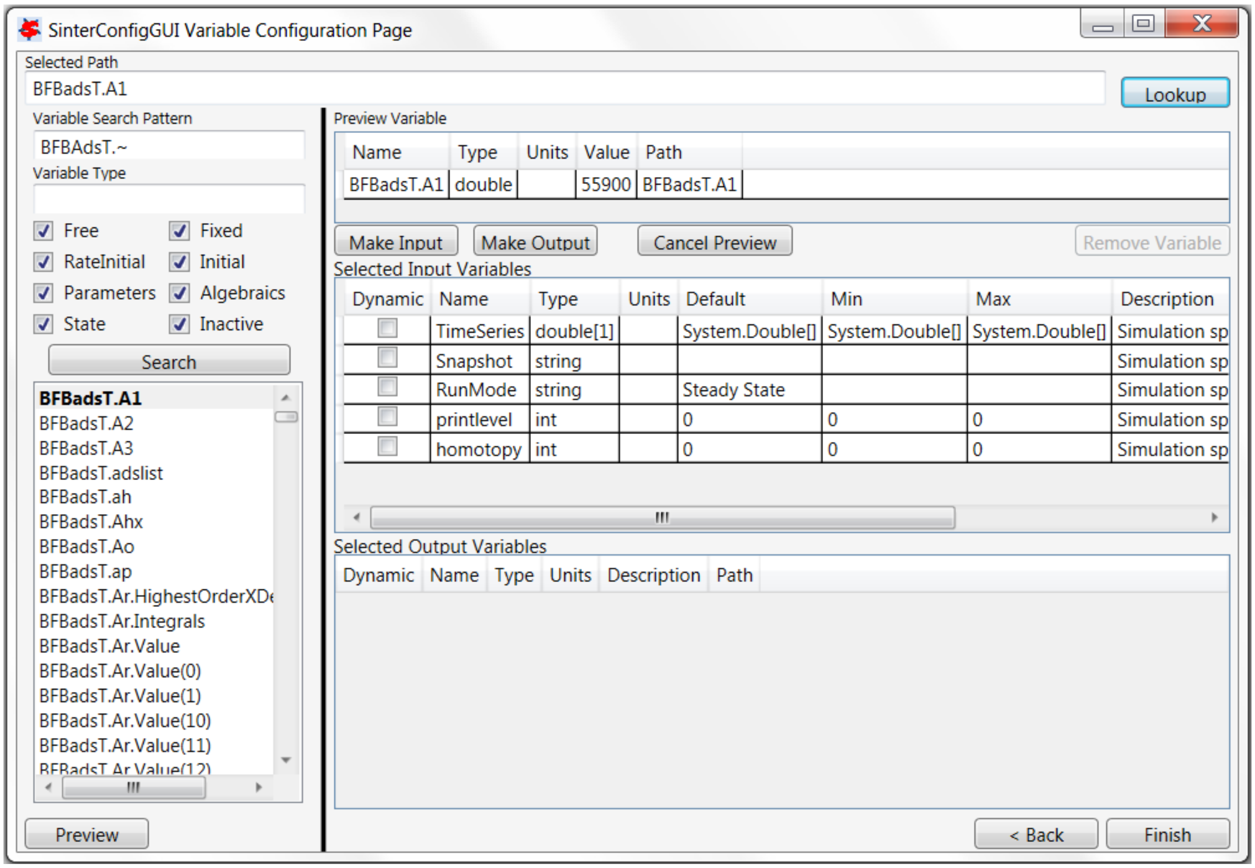


Fig. 14: SinterConfigGUI Variable Configuration Page BFBadsT.A1 Preview

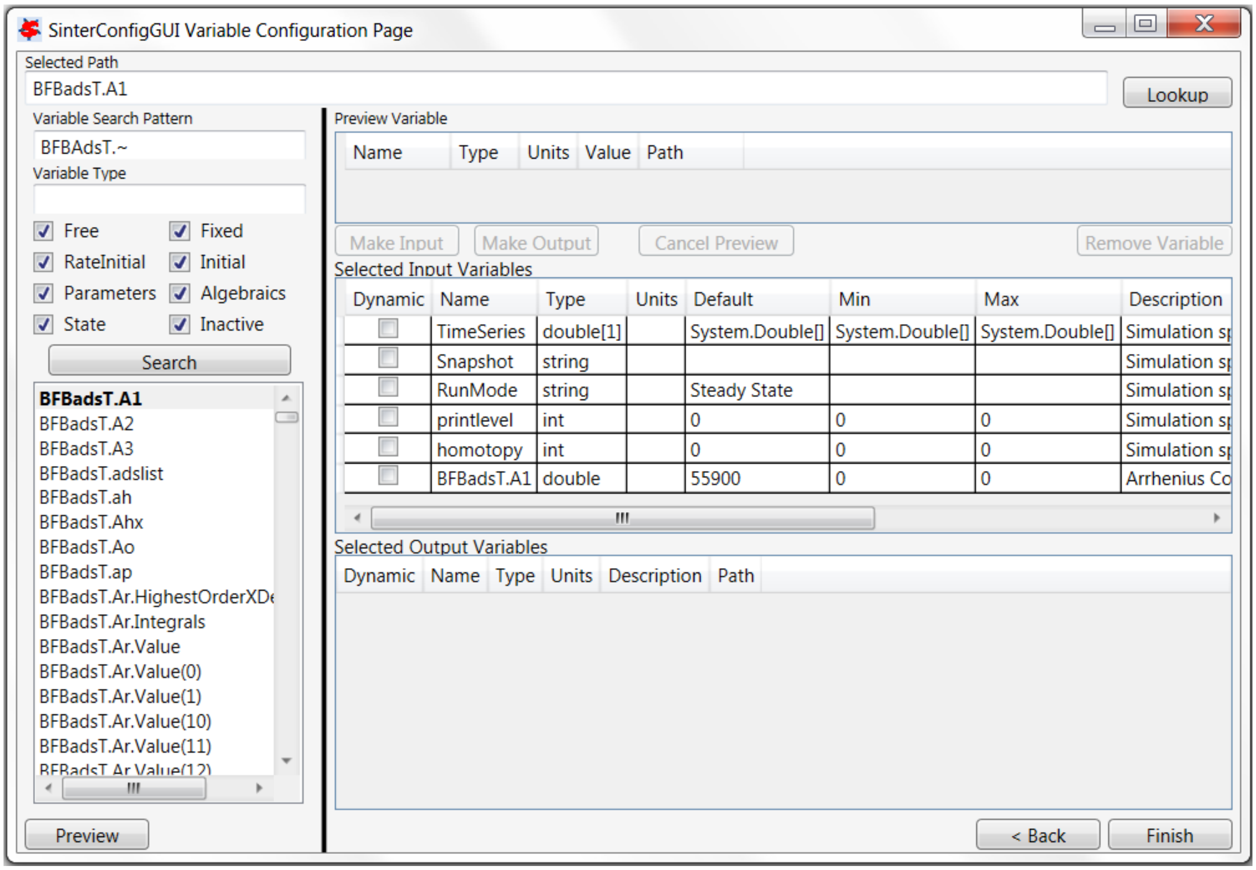


Fig. 15: SinterConfigGUI Variable Configuration Page BFBadsT.A1 Made Input

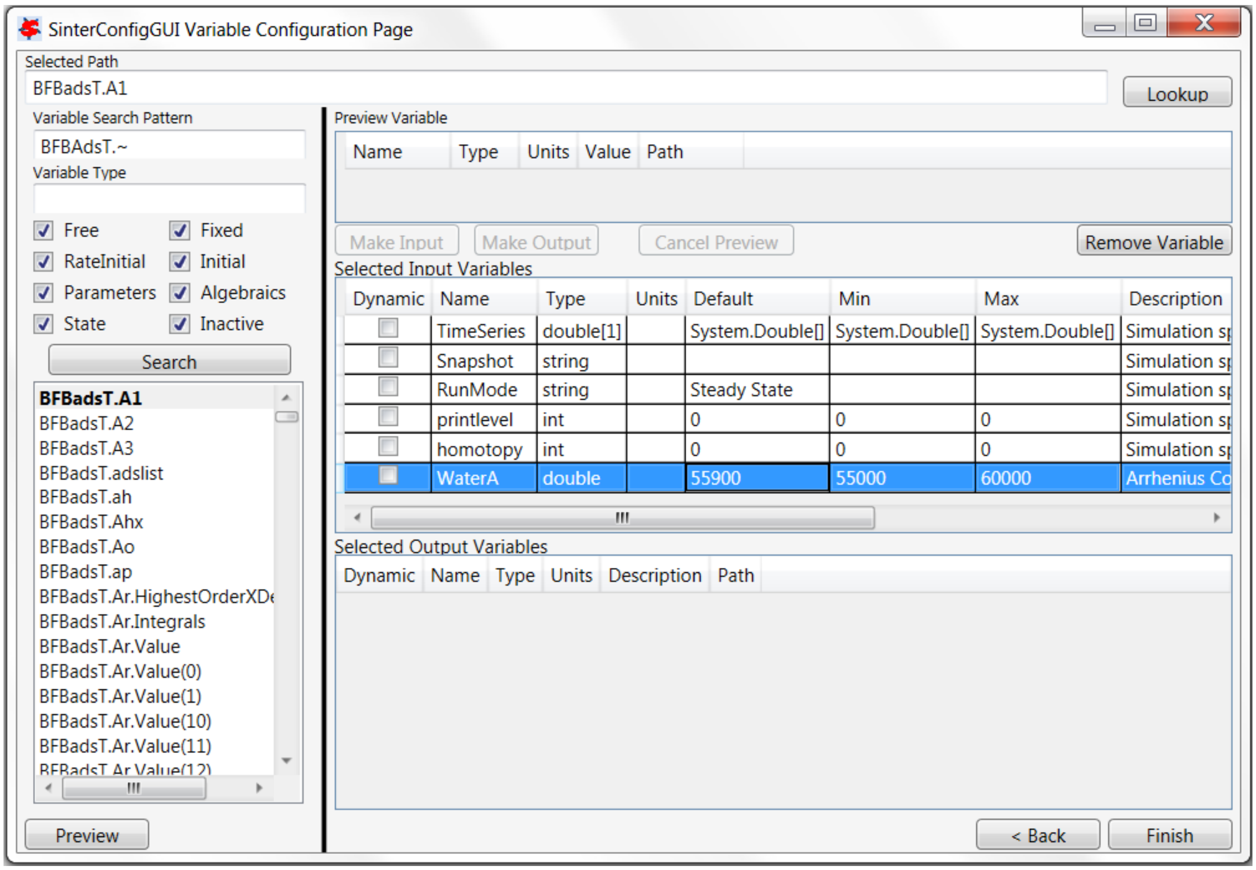


Fig. 16: SinterConfigGUI Variable Configuration Page BFBadsT.A1 Change Name

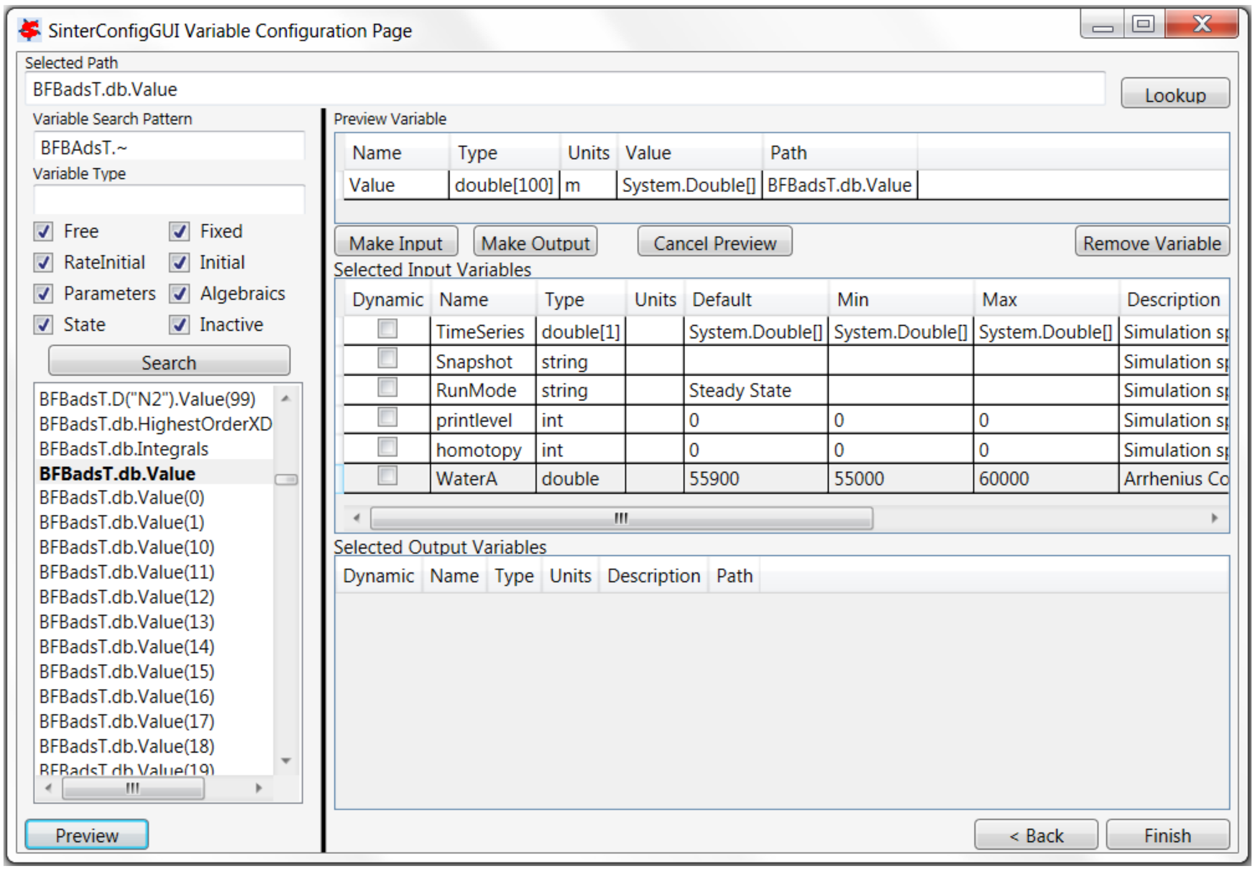


Fig. 17: SinterConfigGUI Variable Configuration Page Vector Preview

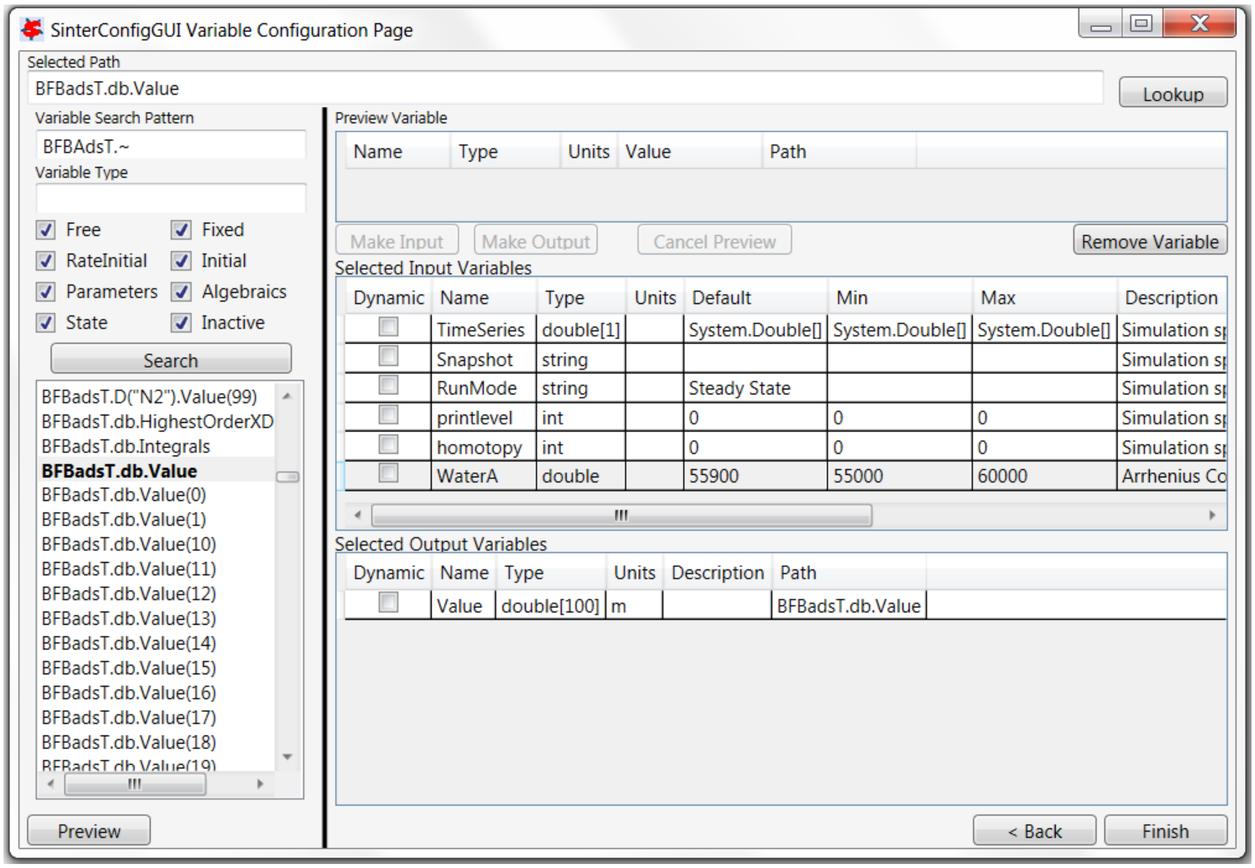


Fig. 18: SinterConfigGUI Variable Configuration Page Vector As Output

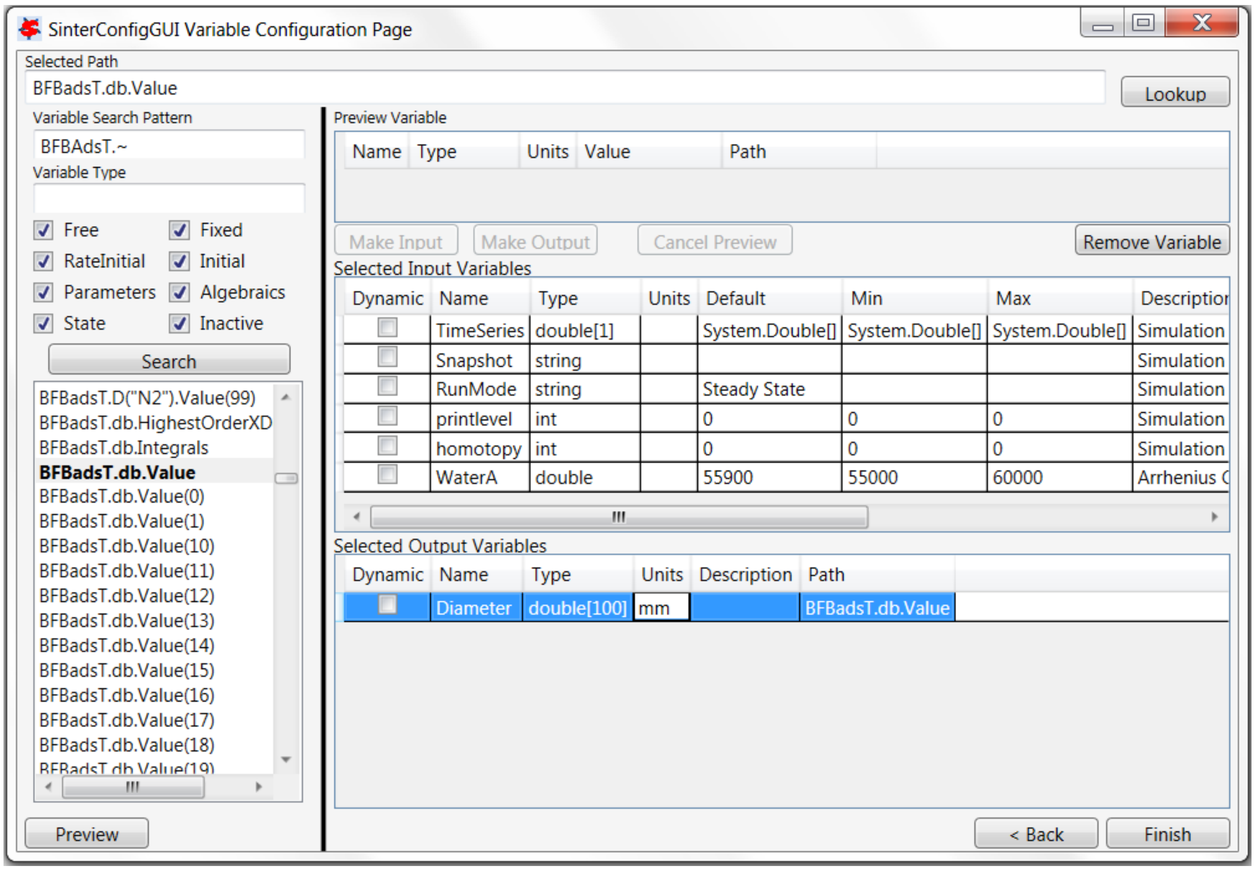


Fig. 19: SinterConfigGUI Variable Configuration Page Output Change Units

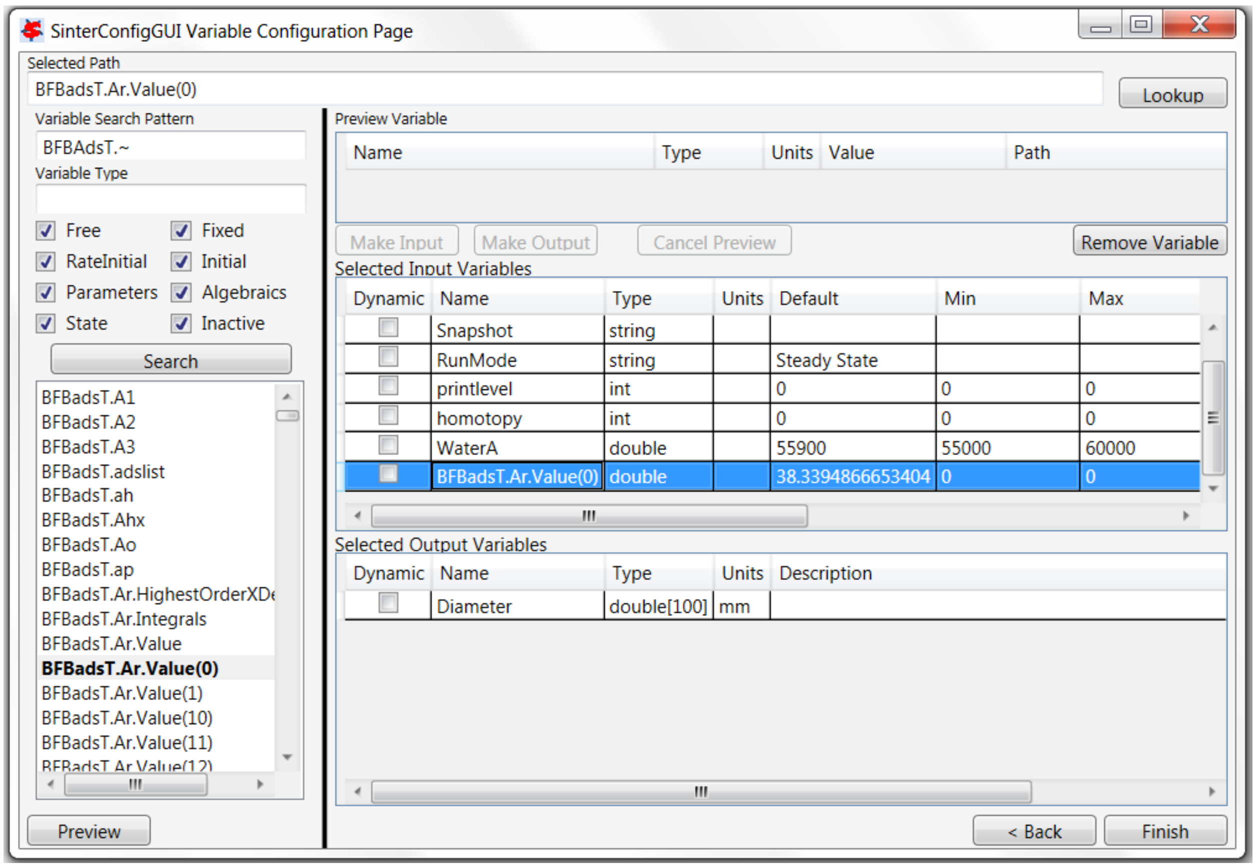


Fig. 20: SinterConfigGUI Variable Configuration Page Removal Demo

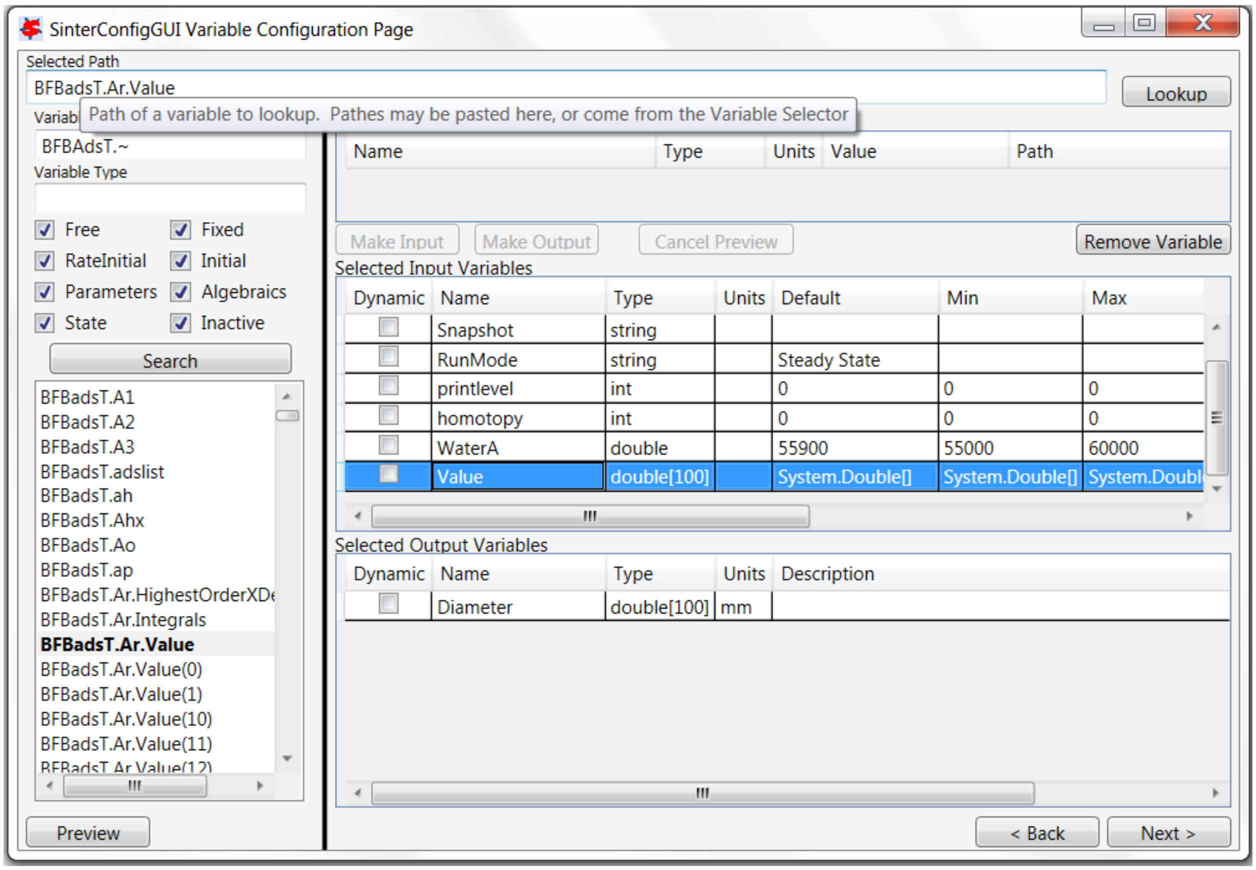


Fig. 21: SinterConfigGUI Variable Configuration Page Read Input

18. Click **Next** to display the SinterConfigGUI Vector Default Initialization window as shown in Figure *SinterConfigGUI Vector Default Initialization Input Page*. Since the input variable "Value" is a vector, its default values can be modified in the window. In this case there is no need to change the values.

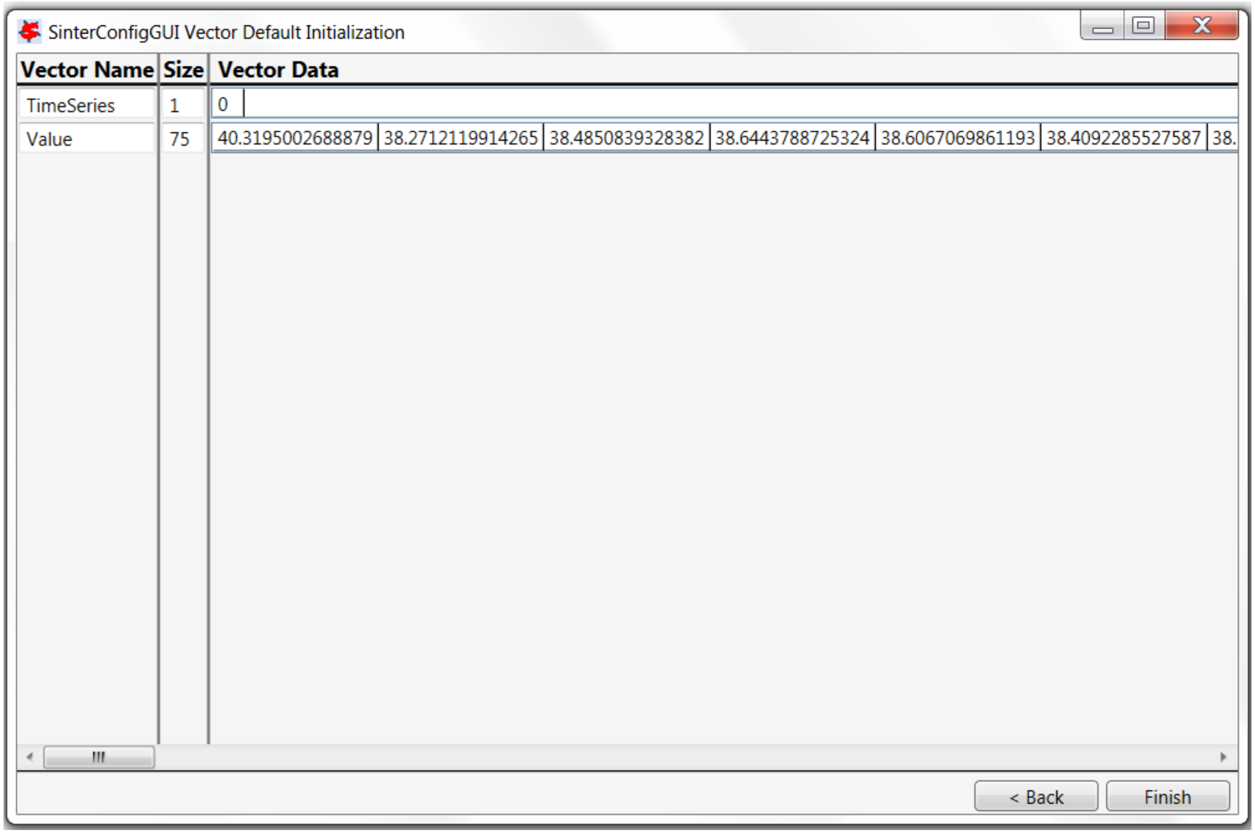


Fig. 22: SinterConfigGUI Vector Default Initialization Input Page

19. The simulation is now setup. Save the configuration file by clicking **Finish**. The file is saved to the location specified on the SinterConfigGUI Simulation Meta-Data page. Clicking **Finish** will close the SinterConfigGUI, but NOT Aspen Custom Modeler. The user must close ACM manually.

20. If "SinterConfigGUI" was launched from FOQUS, the path to the configuration file is automatically passed to FOQUS. The next step in FOQUS is to click **OK** in the Add/Update Turbine Model window. FOQUS may then be used to upload it to the Turbine gateway. If "SinterConfigGUI" was not launched from FOQUS (e.g., it was launched from the Start menu), the configuration file name must be entered in FOQUS manually.

Microsoft Excel Configuration

1. The "SinterConfigGUI" can be launched from FOQUS, via the **Create/Edit** button found in **File**→ **Add/Update Model to Turbine** or "SinterConfigGUI" may be run on its own by selecting **CCSI Tools** → **FOQUS** → **SinterConfigGUI** from the Start menu.

2. The splash window displays, as shown in Figure *SinterConfigGUI Splash Screen*. The user may click the splash screen to proceed, or wait 10 seconds for it to close automatically.

3. The SinterConfigGUI Open Simulation window displays (Figure *SinterConfigGUI Open Simulation Window*). If "SinterConfigGUI" was opened from FOQUS, the filename text box already contains the correct file. To proceed immediately click **Open File and Configure Variables** or click **Browse** to search for the file. For this tutorial, a fresh copy of the BMI test is opened. It can be found at:

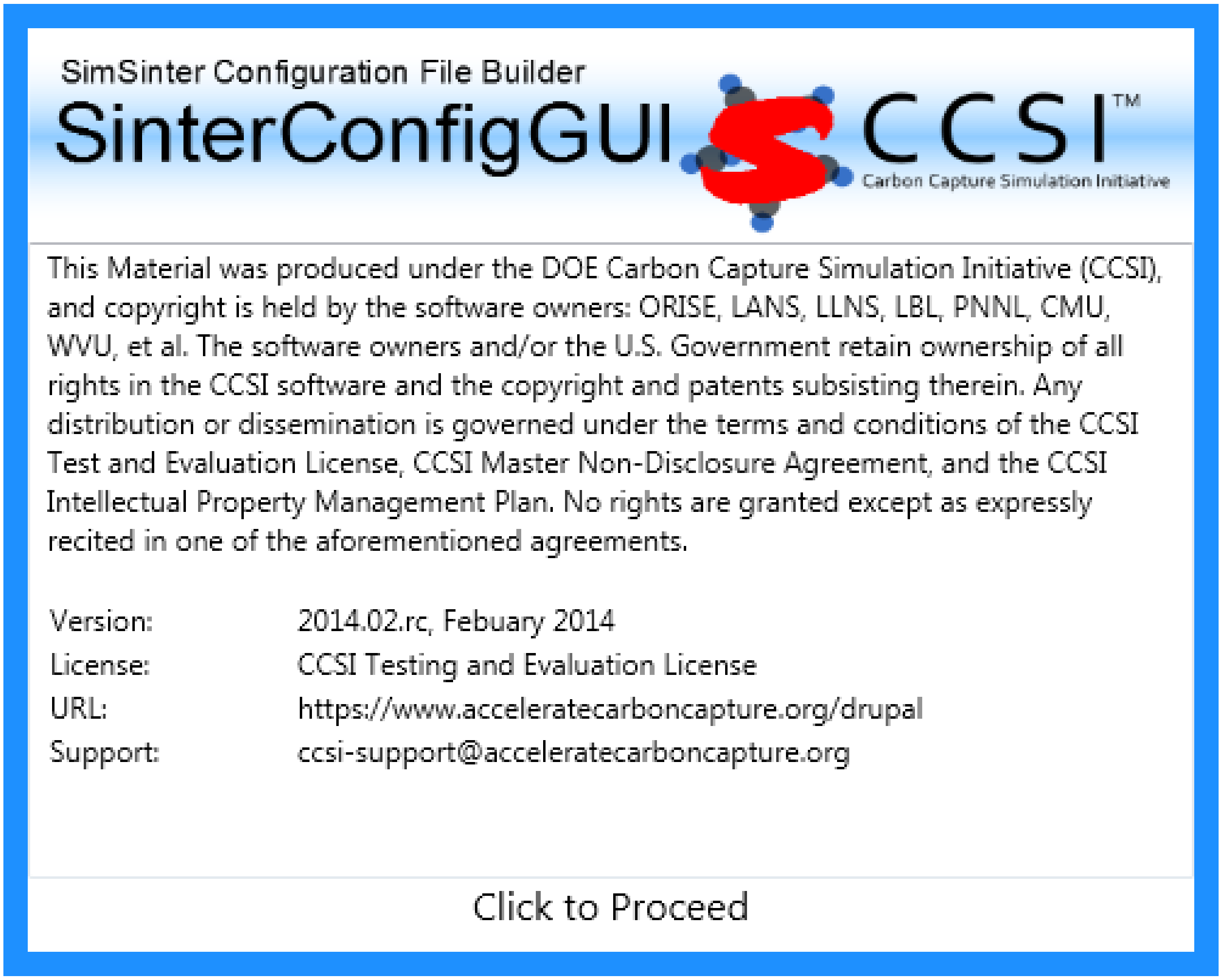


Fig. 23: SinterConfigGUI Splash Screen

C:SimSinterFiles\ Excel_Install_Testexceltest.xlsm.

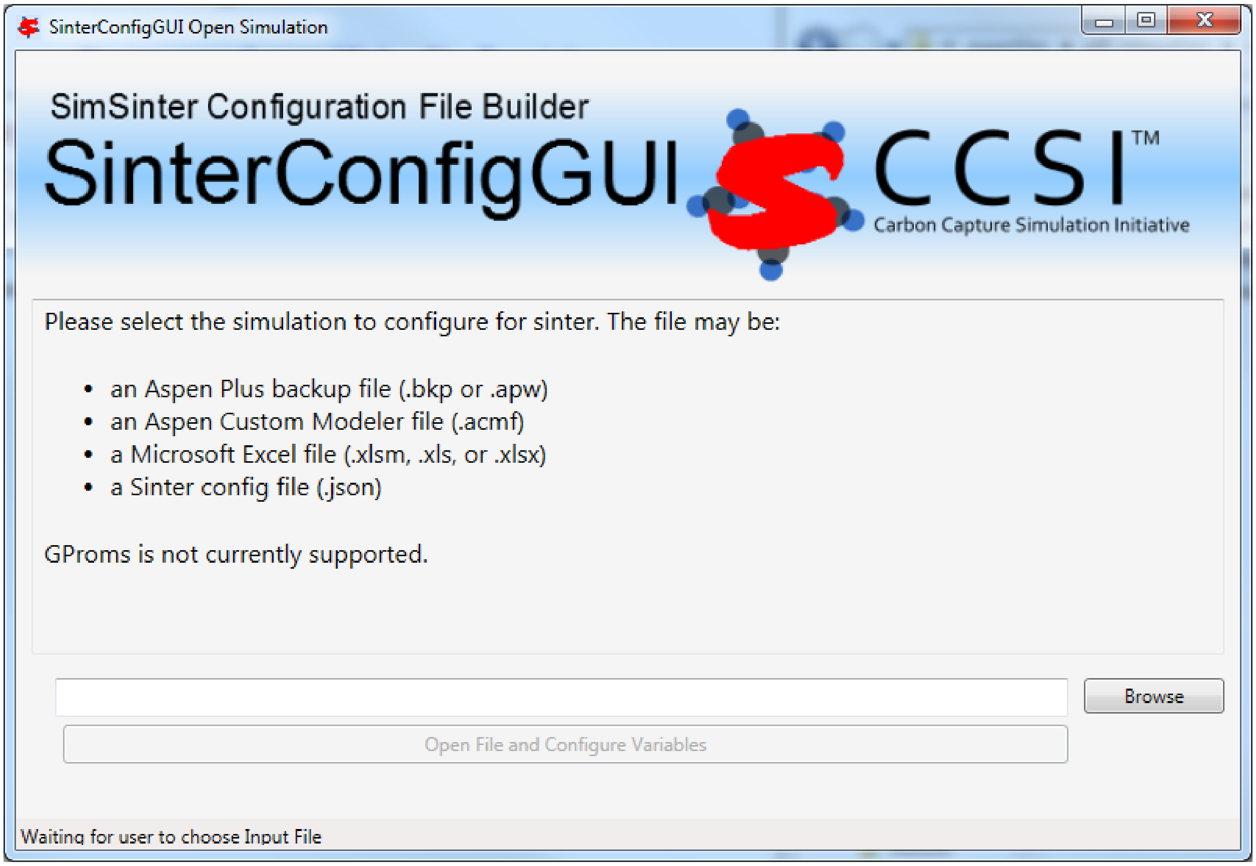


Fig. 24: SinterConfigGUI Open Simulation Screen

4. Microsoft Excel starts in the background. This is so the user can observe things about the worksheet while working on the configuration file.

5. In the "SinterConfigGUI" the SinterConfigGUI Simulation Meta-Data page is now displayed (Figure *SinterConfigGUI Simulation Meta-Data Save Text Box*). The first and most important piece of metadata is **Save Location** at the top of the window. This is where the sinter configuration file is saved. The system attempts to locate a reasonable file location and file name; however, the user must confirm the correct file location, since it automatically overwrites whatever filename currently exists.

6. Continue to complete in the remaining fields and click **Next**.

7. In the SinterConfigGUI Variable Configuration Page, (Figure *SinterConfigGUI Variable Configuration Page before Input*) notice that the Excel setting variable **macro** is already included in the **Selected Input Variables.** If the Excel spreadsheet has a macro that should be run after SimSinter sets the inputs, but before SimSinter gets the outputs, enter the macros name in the **Name** text box. If the default is left blank, no macro is run (unless a name is supplied in the input variables when running the simulation).

8. The Excel simulation has the same **Variable Tree** structure as Aspen Plus, as shown in (Figure *SinterConfigGUI Variable Configuration Page Selecting a Variable from the Excel Variable Tree*). Only the variables in the active section of the Excel spreadsheet appear in the **Variable Tree**. If, for some reason, a cell does not appear the in tree, the user may manually enter the cell into the **Selected Path** text box. In this case, select the "height$C$4" variable.

   Note: Row is first in the **Variable Tree**, yet column is first in the **Path**.

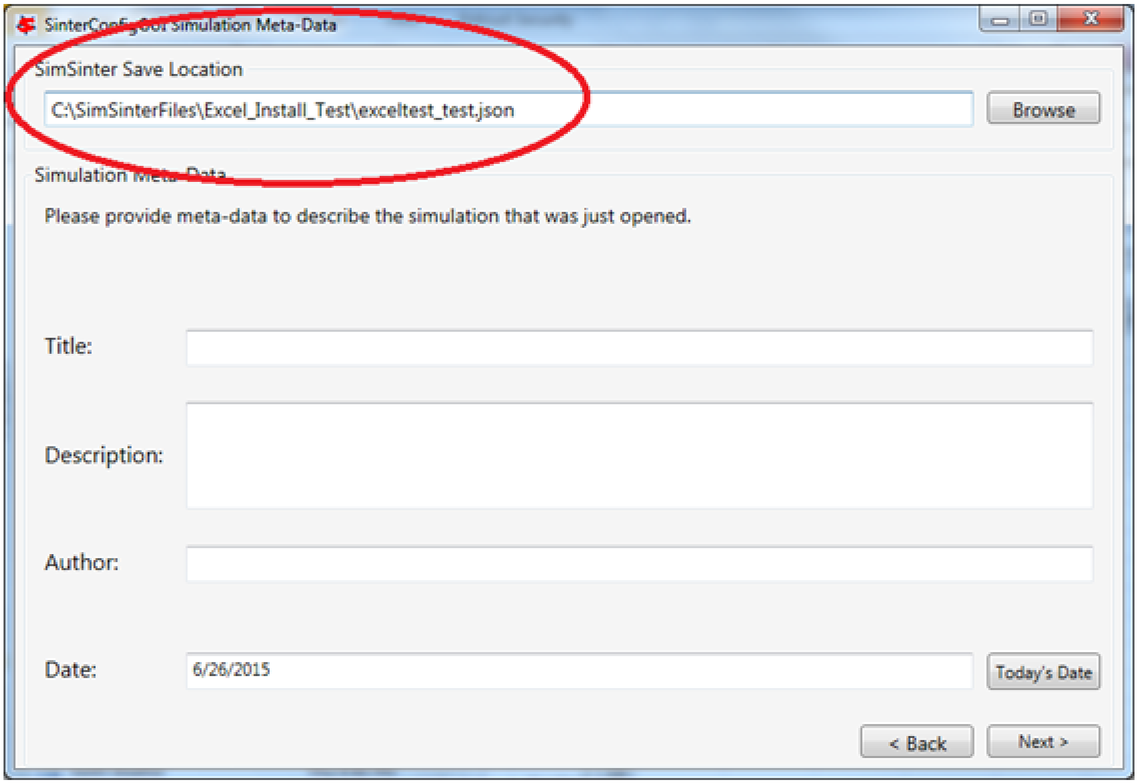


Fig. 25: SinterConfigGUI Simulation Meta-Data Save Text Box

9. If the user double-clicks, presses enter, clicks **Preview**, or clicks **Lookup**, the variable will be displayed in the **Preview Variable** frame. Click the **Make Input** button to make the variable an input variable. Now the variable is in the **Selected Input Variables** section, and its meta-data may be edited (Figure *SinterConfigGUI Variable Configuration Page Description "Joe's Height"*).
10. Enter an output variable (such as, "BMIC3"), by selecting the variables in the **Variable Tree**, clicking **Preview**, and then clicking **Make Output** (Figure *SinterConfigGUI Variable Configuration Page Selecting Excel Output Variables*).
11. The simulation is now set up. To save the configuration file, click **Finish** or press CTRL+S. The file is saved to the location that was set on the SinterConfigGUI Simulation Meta-Data window. A user can save a copy under a different name, by navigating back to the SinterConfigGUI Simulation Meta-Data window using **Back**, and then changing the name. This creates a second version of the file.

gPROMS Configuration

gPROMS is significantly different from the other simulators SimSinter supports, and the workflow is also significantly different. If you plan to use gPROMS simulations with FOQUS, the CCSI team strongly encourages you to read the "SimSinter gPROMS Technical Manual," which is included in the FOQUS distribution. The default location is at C:Program Files (x86)foqus \foqus \doc. It is also available on the CCSI website.

Unlike Aspen, changes must be made to the gPROMS simulation process in order to work with SimSinter. Therefore, this section consists of a series of tutorials for every step of configuring gPROMS and SimSinter to work together. All the tutorials are required in order to have a gPROMS simulation be runnable with SimSinter. They are divided up to make later reference easier.

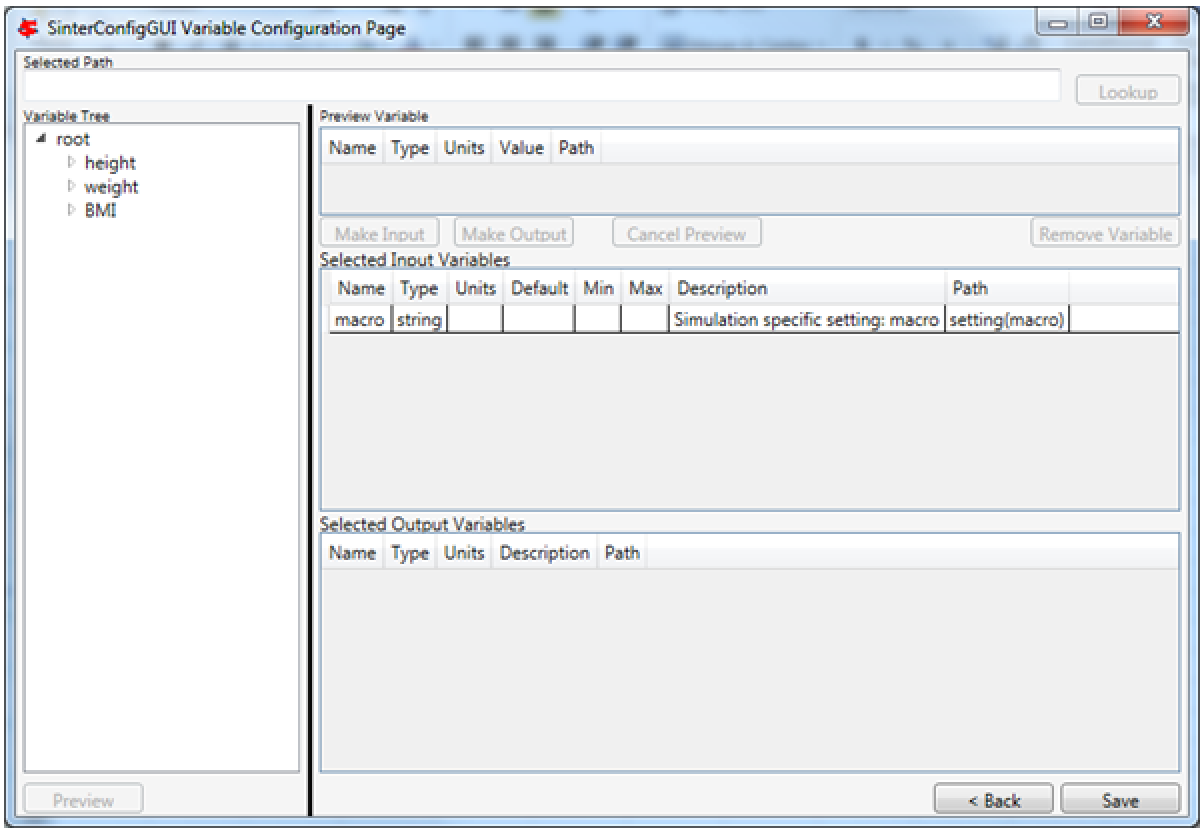


Fig. 26: SinterConfigGUI Variable Configuration Page before Input

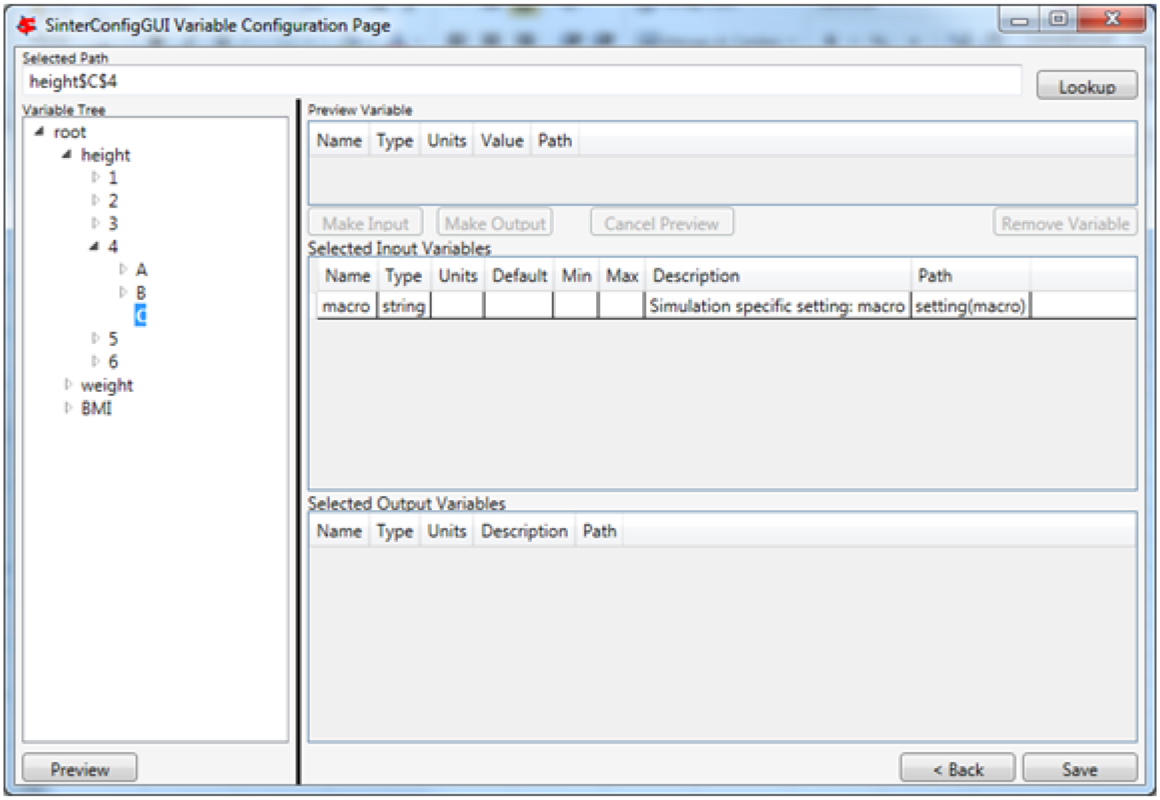


Fig. 27: SinterConfigGUI Variable Configuration Page Selecting a Variable from the Excel Variable Tree

Configuring gPROMS to Work with SimSinter

Unlike Aspen, changes have to be made to the gPROMS simulation process in order to work with SimSinter. In fact, SimSinter does not define the inputs to the simulation, gPROMS does. On the other hand, gPROMS does not determine the outputs, SimSinter does. This odd and counter-intuitive situation is the result of how gPROMS gO:Run_XML is designed.

The modification to the gPROMS simulation must be done by a developer with an intimate understanding of the simulation, usually the simulation writer. In some cases additional variables may need to be added to handle an extra step between taking the input and inserting it into the variable where gPROMS will use the data.

1. Open the gPROMS simulation file (ends in .gPJ) in ModelBuilder 4.0 or newer. For this example, use the gPROMS install test file "BufferTank_FO.gPJ", found in:

   C:\ SimSinterFilesgPROMS_Test\ BufferTank_FO.gPJ

   Double-click on the .gPJ file to open ModelBuilder, as shown in Figure *Opening BufferTank in gPROMS Model Builder*.

2. This simulation was originally a simple BufferTank simulation. However, it was modified into an example of all the different kinds of variables the user can pass into gPROMS via SimSinter. Therefore, it has a lot of extra variables that do not really do anything, with very generic names, like "SingleInt." The simulation consists of a single model, "BufferTank", that contains all the simulation logic, and most of the parameter and variable declarations. The SimSinter simulation will change some of these PARAMETERS and VARIABLES to change the output of the simulation.

3. The example file contains two Processes. SimSinter can only run gPROMS Processes, so any gPROMS simulation must be driven from a Process. "SimulateTank" is the original BufferTank example with hardcoded values,

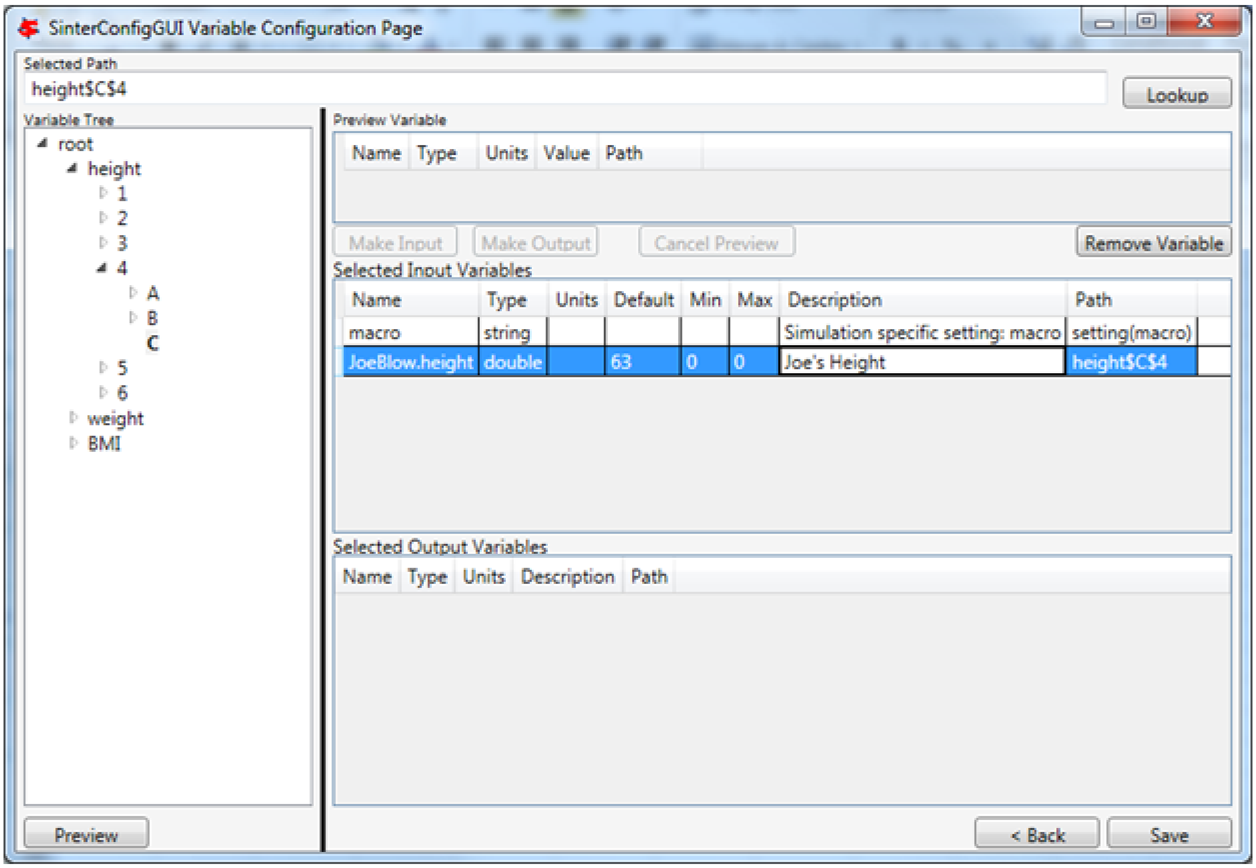


Fig. 28: SinterConfigGUI Variable Configuration Page Description "Joe's Height"

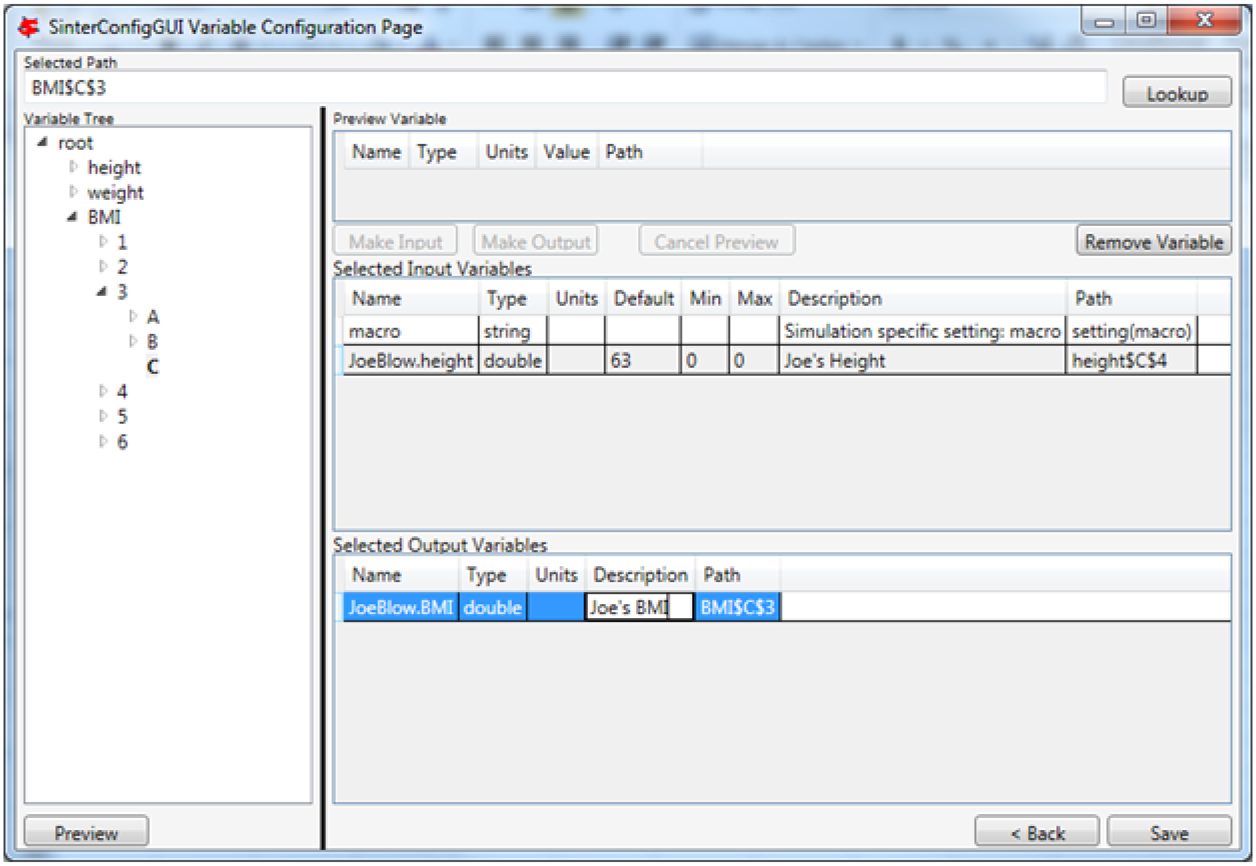


Fig. 29: SinterConfigGUI Variable Configuration Page Selecting Excel Output Variables

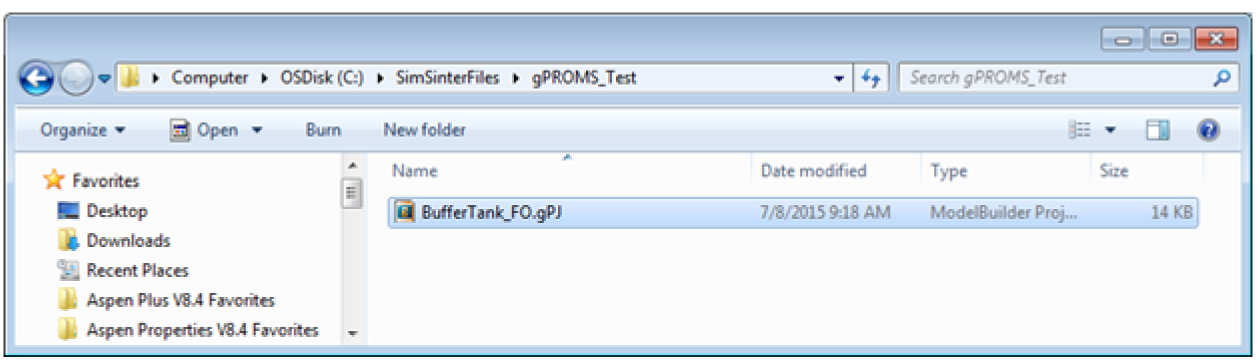


Fig. 30: Opening BufferTank in gPROMS Model Builder

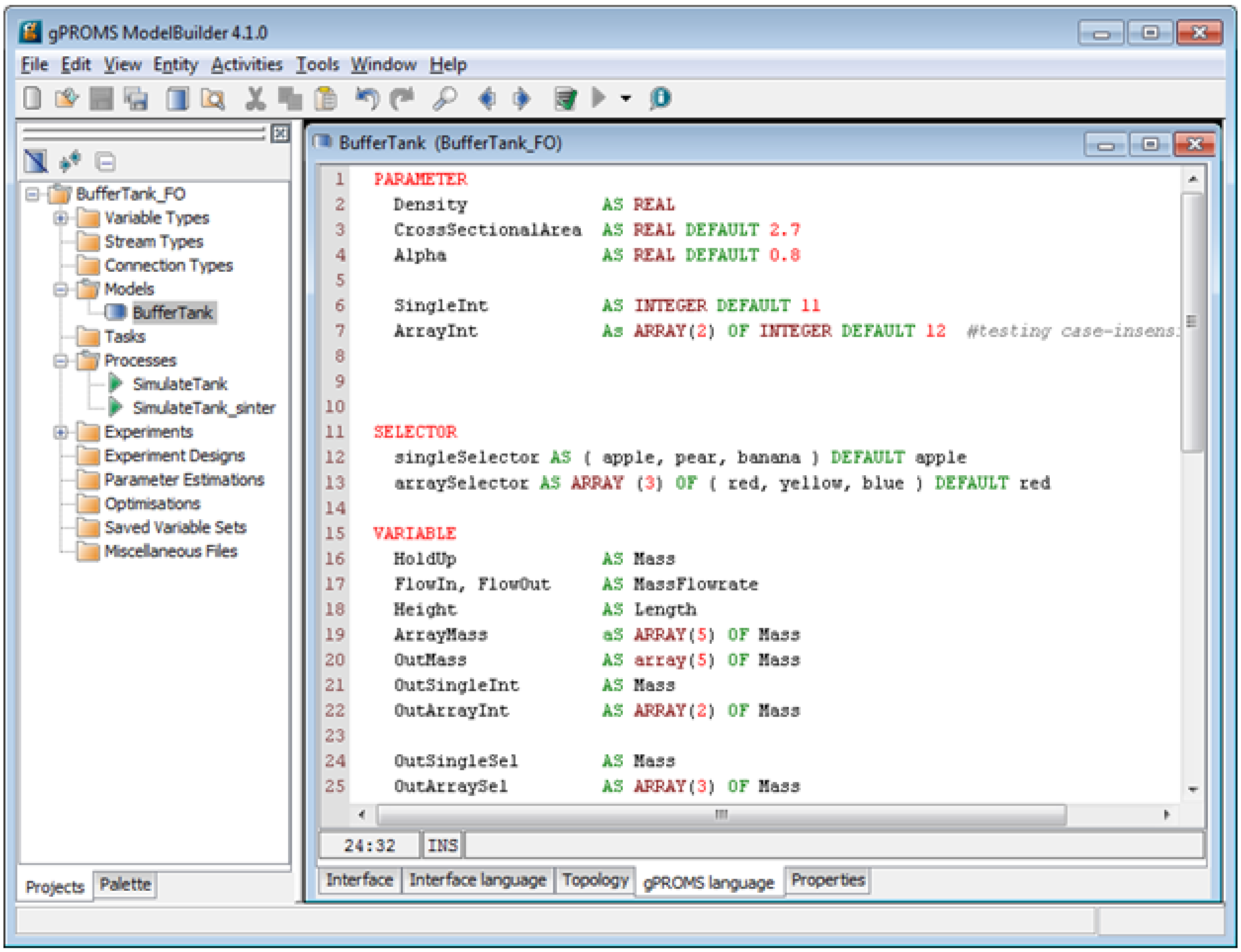


Fig. 31: Viewing BufferTank in gPROMS Model Builder

"SimulateTank_Sinter" contains the example of setting values with Sinter. The "SimulateTank_Sinter" example will be recreated in this tutorial.

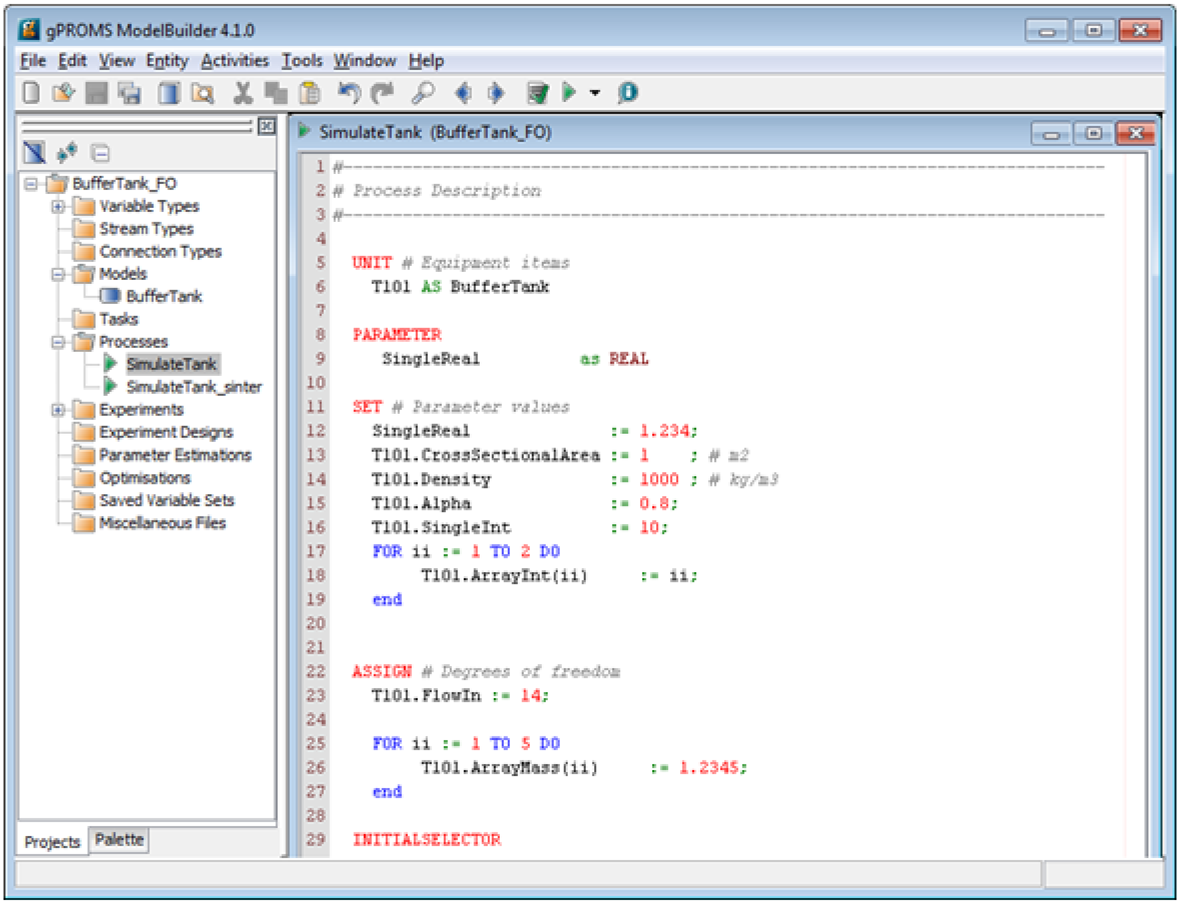


Fig. 32: Viewing SimulateTank in gPROMS Model Builder

4. First copy the existing hard-coded Process "SimulateTank".
5. Right-click on Processes and select **Paste** to make a new process.
6. The new process will be named "SimulateTank_1". Rename the process by right-clicking on it and selecting **Rename**.
7. Now open up the new "SimulateTank_tutorial" Process. It has the same hard-coded values as "SimulateTank".
8. First, the user needs to add a FOREIGN_OBJECT named "FO" in the PARAMETER section. Then the user needs to set that FOREIGN_OBJECT to "SimpleEventFOI::dummy" in the SET section. This FOREIGN_OBJECT is how inputs are received from SimSinter.
9. This particular simulation has a large number of input variables that simply demonstrate how to set different types. These are named based on their type. Any variable named similarly to "SingleInt" or "ArraySelector" can be safely ignored for this tutorial. For a full list of the methods for setting different types see the later section specifically for covering that. Any variable in the simulation can be an input, whether it is defined in the Process or one of the models referenced by the process, or in a model referenced by a model, etc. All inputs take their values from the FOREIGN_OBJECT defined, followed by the type name, two underscores, the input variable name, an open parenthesis, an optional index variable (for arrays), and closed with a close parenthesis and a semicolon. For a scalar:

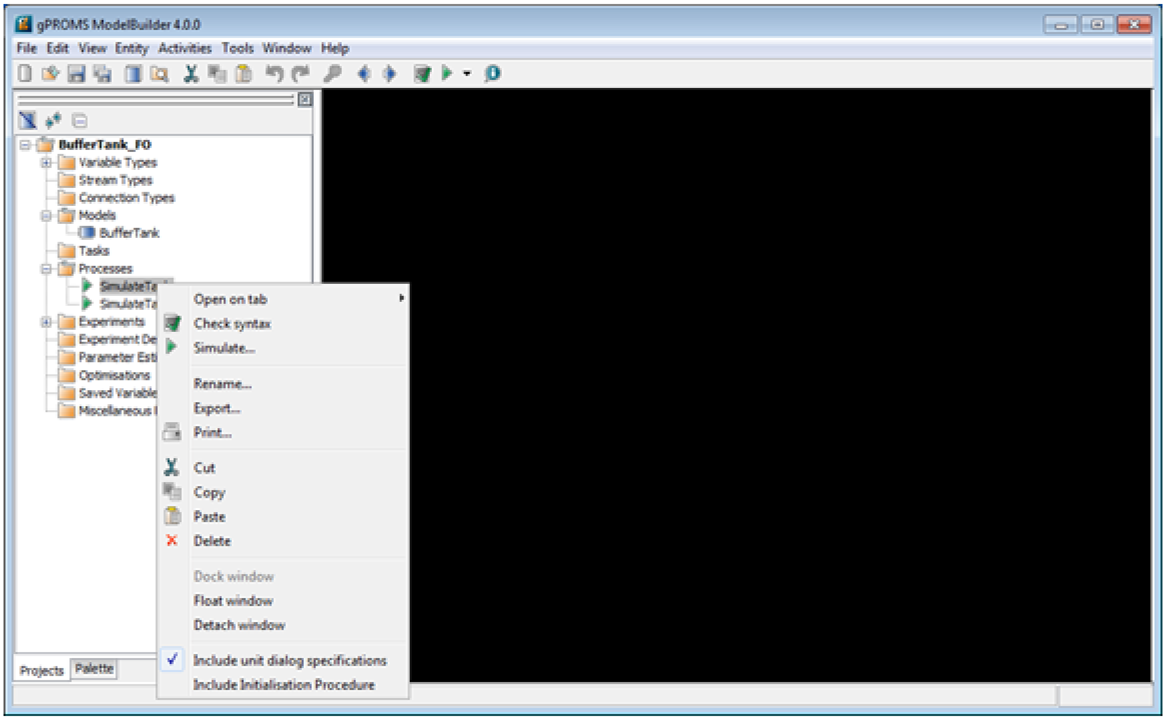


Fig. 33: Copying SimulateTank

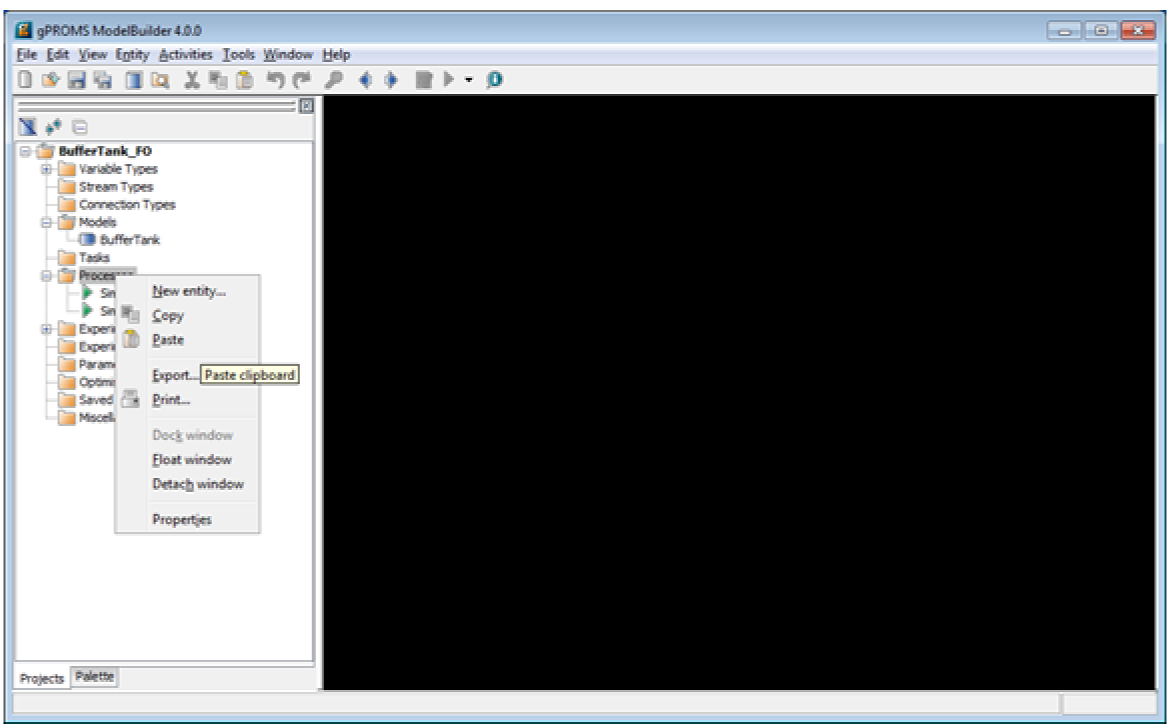


Fig. 34: Paste SimulateTank

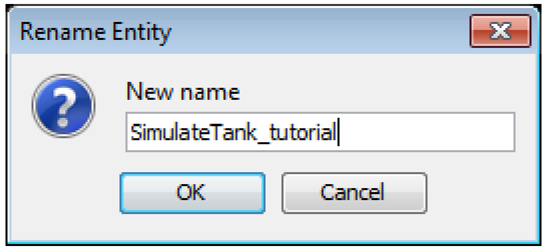


Fig. 35: Rename SimulateTank

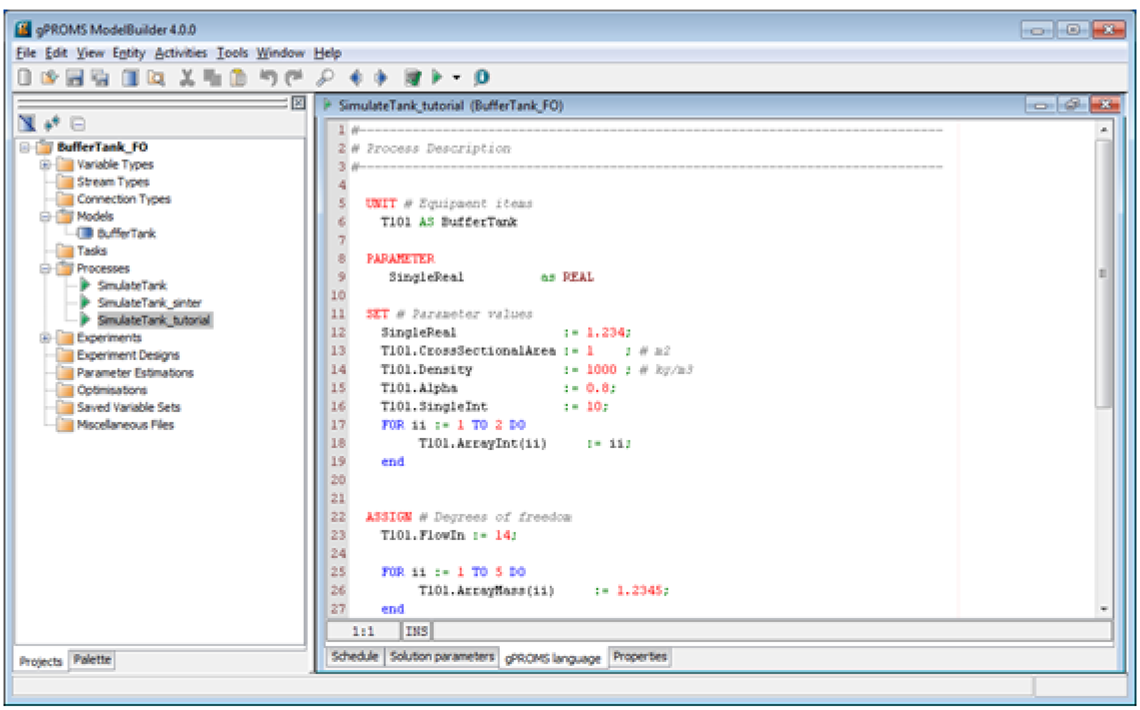


Fig. 36: Opening SimulateTank_tutorial

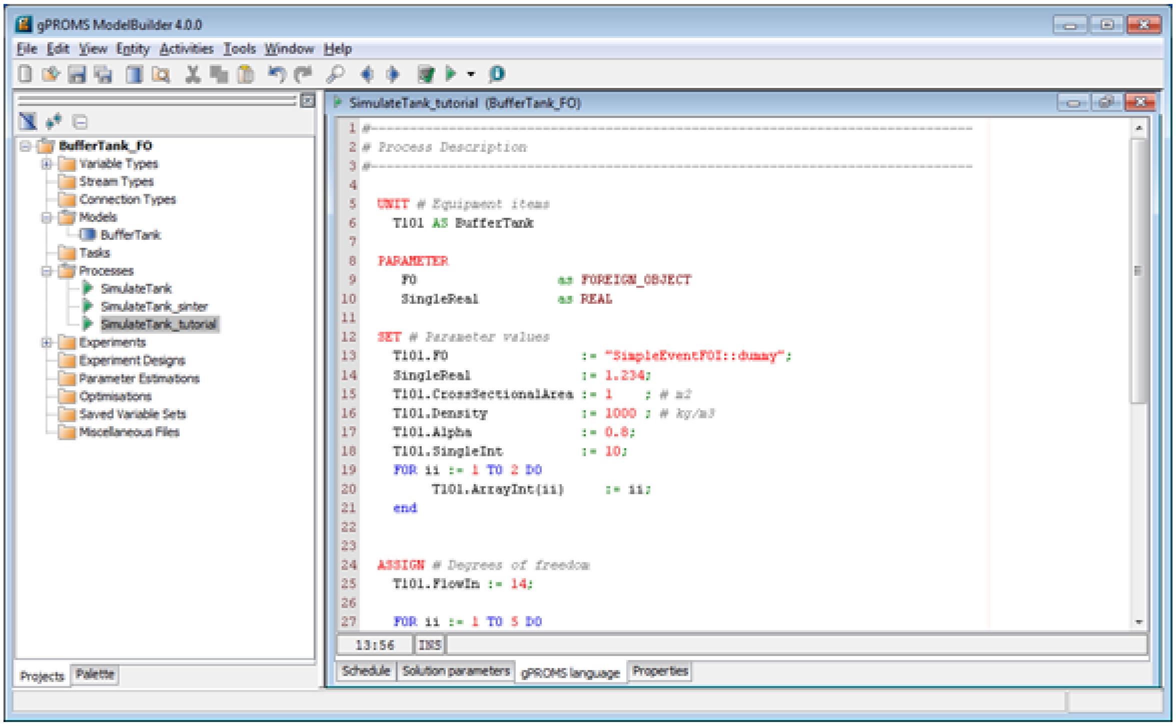


Fig. 37: Adding the FOREIGN_OBJECT

```
FO.<Type>__<InputName>();
```

SimSinter can only handle arrays inputted in FOR loops such as:

```
FOR ii := 1 TO <array size> DO
  <ArrayName>(ii) := FO.<Type>1__<InputName>(ii);
END
```

For this example the user only really needs to set "T101.Alpha" in PARAMETER, "T101.FlowIn" in ASSIGN, and "T101.Height" in INITIAL.

10. Now test "SimulateTank_tutorial" by selecting it and clicking the green **Simulate** triangle. When the simulation runs it will ask for every input variable the user has defined. For the example variables that do not effect the simulation, such as "SingleInt", any valid value will work. For the values that do effect the simulation, these values work:

```
REAL__AlphaFO = .08
REAL__FlowInFO = 14
REAL__HeightFO = 7.5
```

Exporting an Encrypted Simulation to Run with SimSinter

SimSinter can only run encrypted gPROMS simulations. These files have the .gENCRYPT extension. If the additions to the simulation for reading input variables ran correctly in the previous section, the user is ready to export that process for use by SimSinter.

1. Right-click on the Process to export ("SimulateTank_tutorial") and select **Export**.

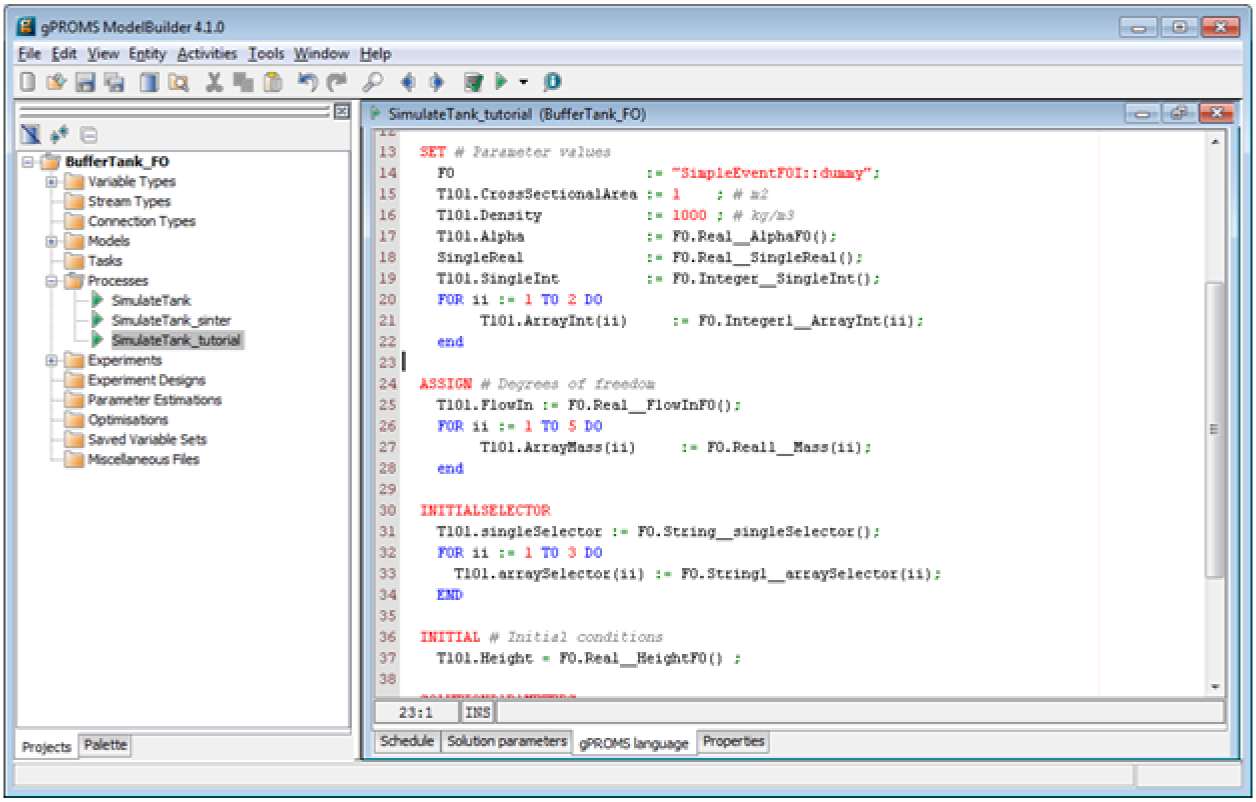


Fig. 38: Setting up Input Variables

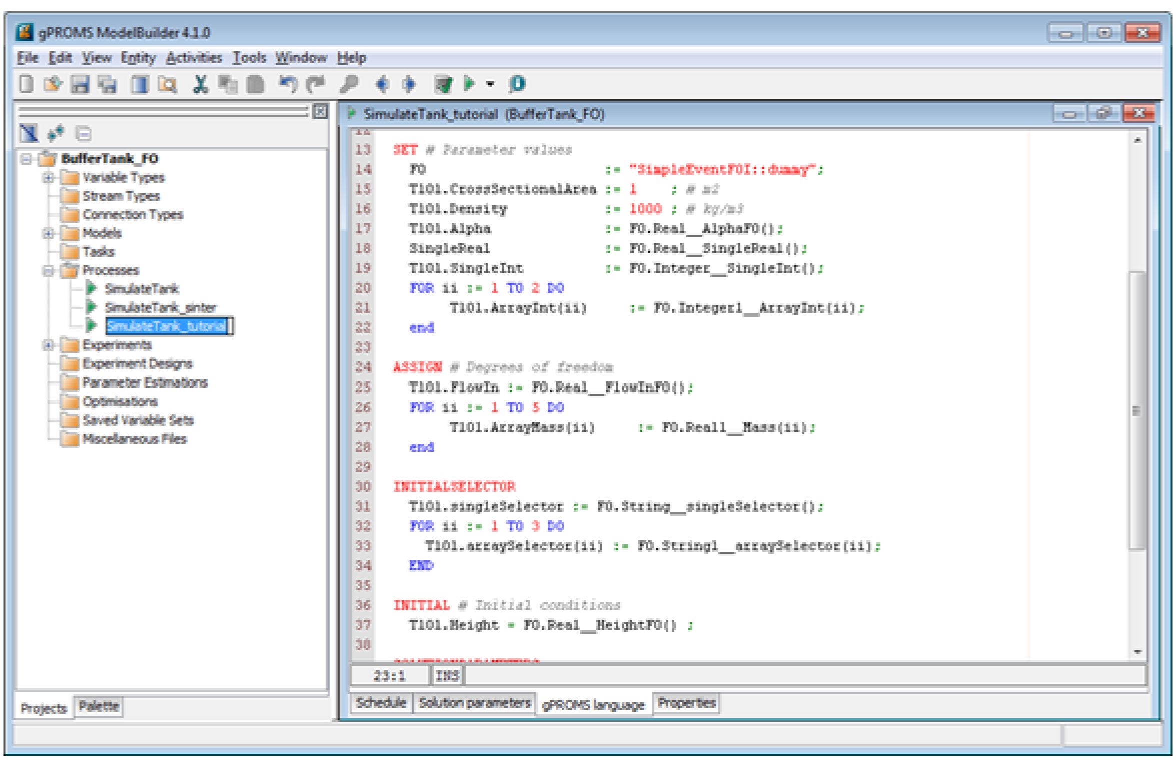


Fig. 39: Testing SimulateTank_Tutorial

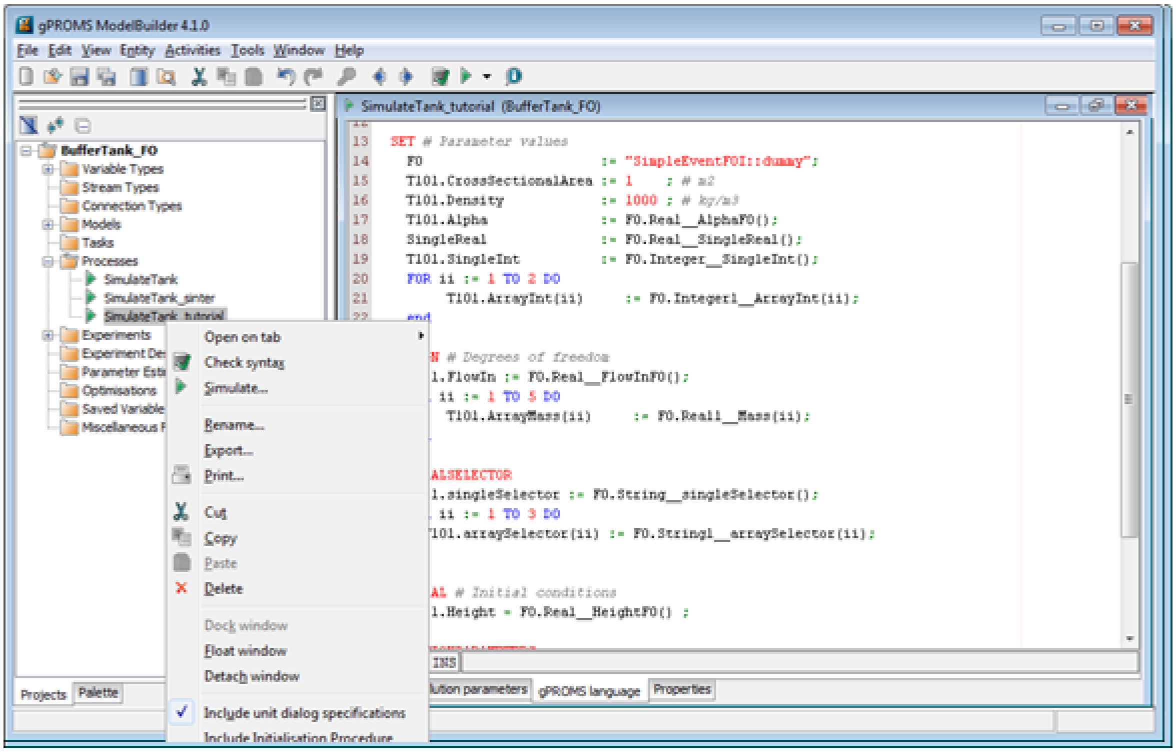


Fig. 40: Select "Export"

2. In the resulting Export window, select **Encrypted input file for simulation by gO:RUN** and click **OK**.
3. On the second page, set the **Export directory** to a directory the user can find. Preferably one without any other files in it so the user will not be confused by the output. If the filename or the **Encryption password** are not changed, SimSinter will be able to guess the password. If either of those values are changed, the user will have to set the correct password in the SinterConfigGUI password setting. A Decryption password is probably unnecessary, as the user has the original file. SimSinter does not use it. When the user has finished setting up these fields, click **Export Entity**.
4. The resulting .gENCRYPT file will be saved to a subdirectory named "Input" in the save directory specified in Step 3. The first part of the name will be identical to the .gPJ filename. The user should not rename it because the SinterConfig file will guess this name, and currently changing it requires editing the SinterConfig file.

Configuring SimSinter to Work with gPROMS

Now that the gPROMS process has been prepared, the SimSinter configuration can be done.

1. The "SinterConfigGUI" can be launched from FOQUS, via the **Create/Edit** button found in **File**→ **Add/Update Model to Turbine** or "SinterConfigGUI" may be run on its own by selecting **CCSI Tools** → **FOQUS** → **SinterConfigGUI** from the Start menu.
2. The splash window displays, as shown in Figure *SinterConfigGUI Splash Screen*. The user may click the splash screen to proceed, or wait 10 seconds for it to close automatically.
3. The SinterConfigGUI Open Simulation window displays (Figure *SinterConfigGUI Open Simulation Screen*). If "SinterConfigGUI" was opened from FOQUS, the filename text box already contains the correct file. To proceed immediately click **Open File and Configure Variables** or click **Browse** to search for the file.

   This tutorial will use the .gPJ file edited in Section *1.1*. Remember that SinterConfigGUI cannot read the

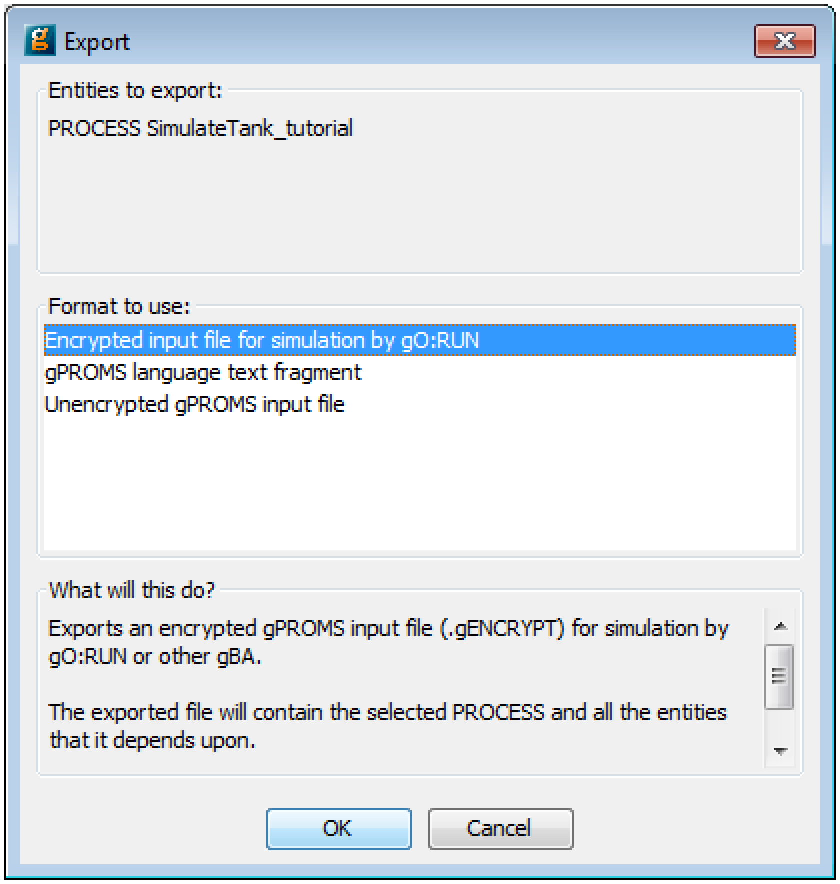


Fig. 41: Select "Encrypted Input File"

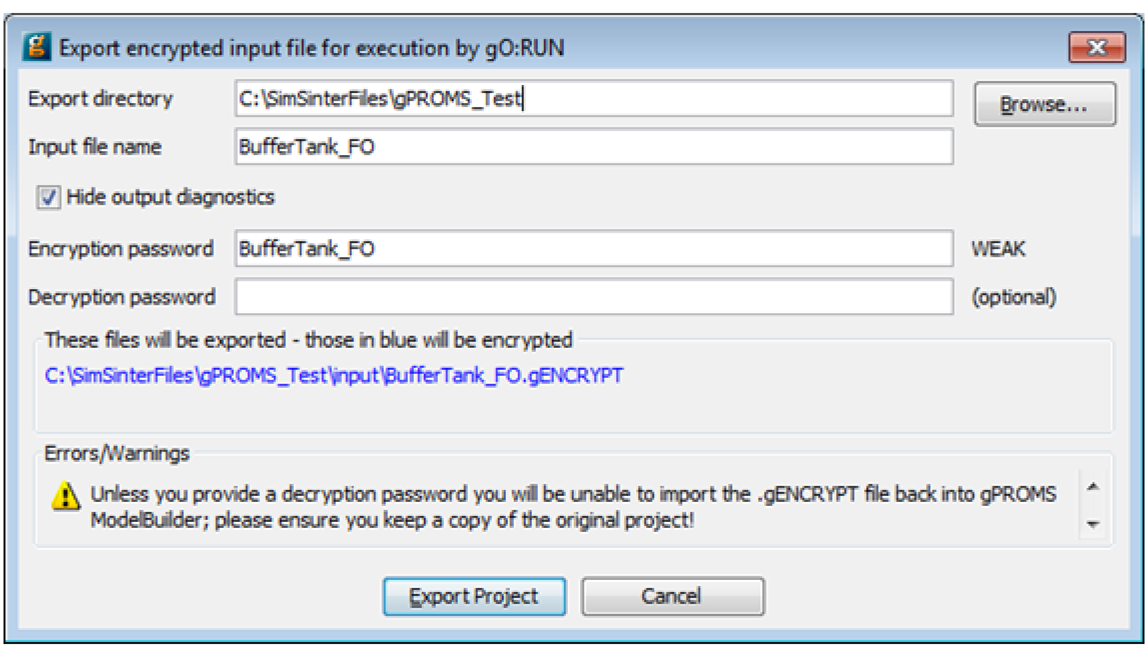


Fig. 42: Export Entity Page

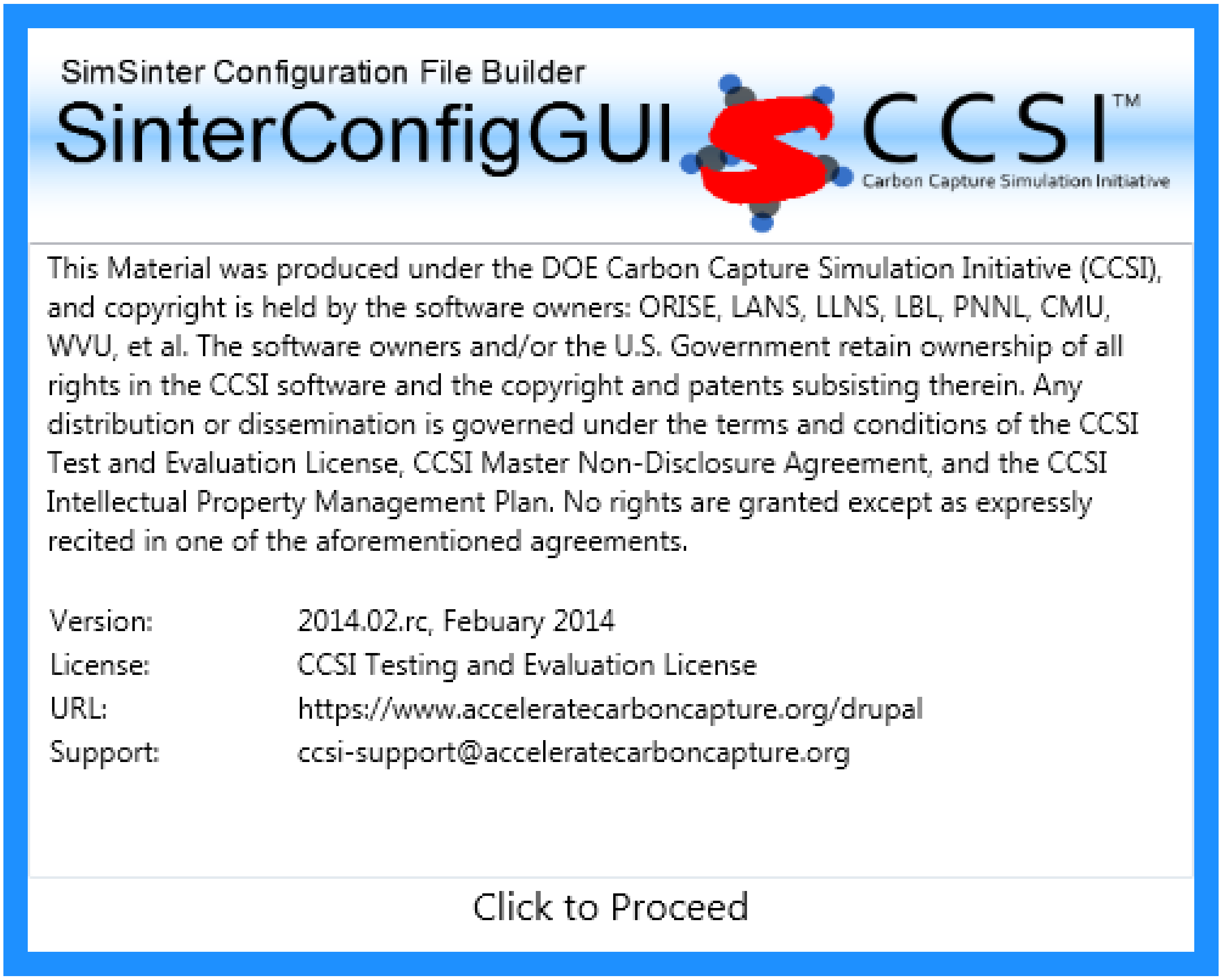


Fig. 43: SinterConfigGUI Splash Screen

.gENCRYPT file that is actually run by SimSinter. Instead, the user must open the .gPJ file the ModelBuilder uses.

Once the file is selected, click **Open File and Configure Variables.**

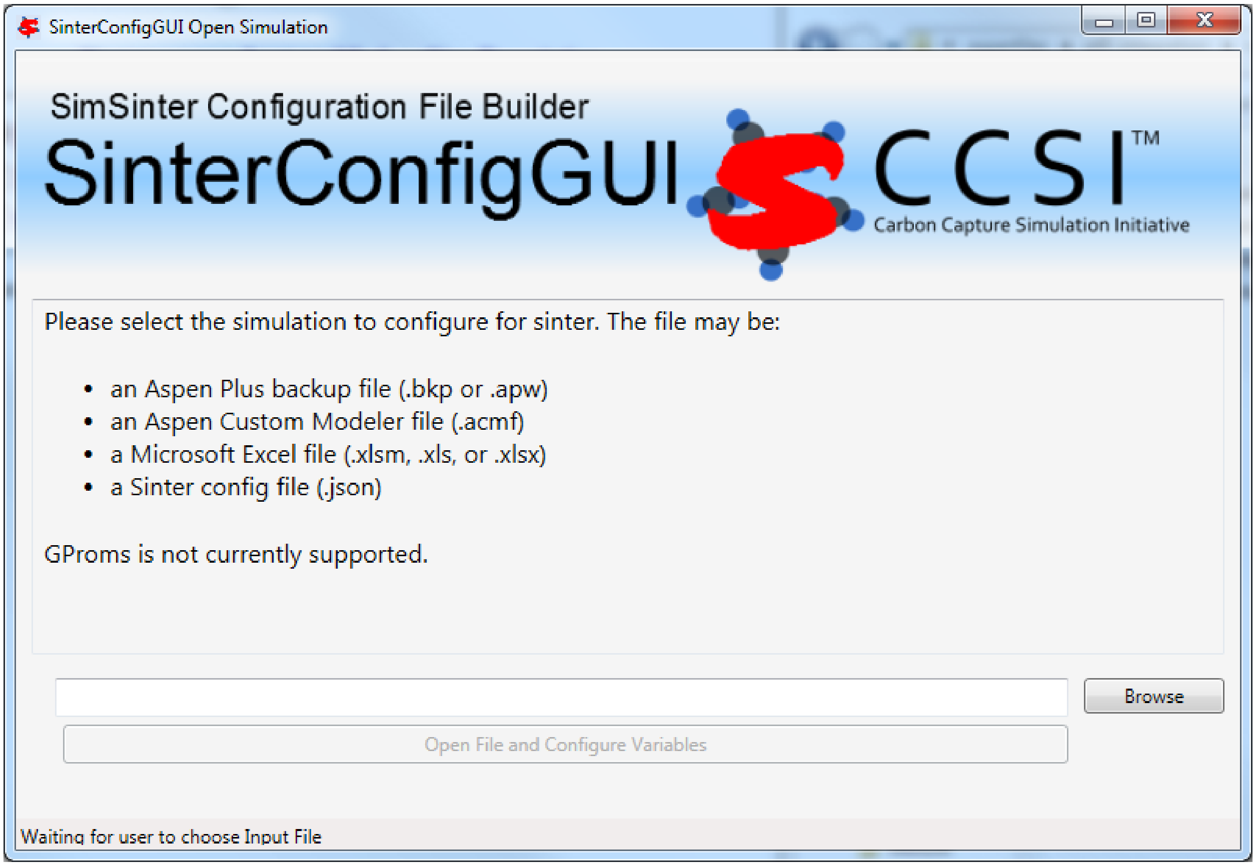


Fig. 44: SinterConfigGUI Open Simulation Screen

4. The SinterConfigGUI Simulation Meta-Data window displays as shown in (Figure *SinterConfigGUI Simulation Meta-Data Save Text Box*). Unlike the other simulations, gPROMS has not started up in any way. SinterConfigGUI does not get information from gPROMS directly, it must parse the .gPJ file instead.
5. The first and most important piece of meta-data is the **SimSinter Save Location** at the top of the window. This is where the Sinter configuration file is saved. The system suggests a file location and name. The user should confirm this is the intended location of the files to not accidently overwrite other files. Enter the remaining fields to provide the meta-data to describe the simulation that was just opened and then click **Next**.
6. The SinterConfigGUI Variable Configuration Page window displays as shown in Figure *SinterConfigGUI gPROMS Settings Configuration*. gPROMS has two settings, **ProcessName** and **password**. SimSinter has guessed at both the **ProcessName** and the **password**. For this example the **password** is correct, but the **ProcessName** is incorrect. SimulateTank is the process that isn't configured to work with SimSinter. On the left side we can see the **Variable Tree**. The root is connected to the three processes defined in this .gPJ file. First, change the **ProcessName** to "SimulateTank_tutorial".
7. After changing the **ProcessName**, click Enter (or clicks away). The **Selected Input Variables** will automatically display all of the available input variables. This is because the input variables have been configured in gPROMS, and SimSinter has parsed them out of the .gPJ file, as long as you have the **ProcessName** set correctly. This also means that the user cannot add new input variables in SinterConfigGUI, only in gPROMS. SimSinter also does its best to identify the **Default** values, **Min**, and **Max** of the variables. The default can only be calculated

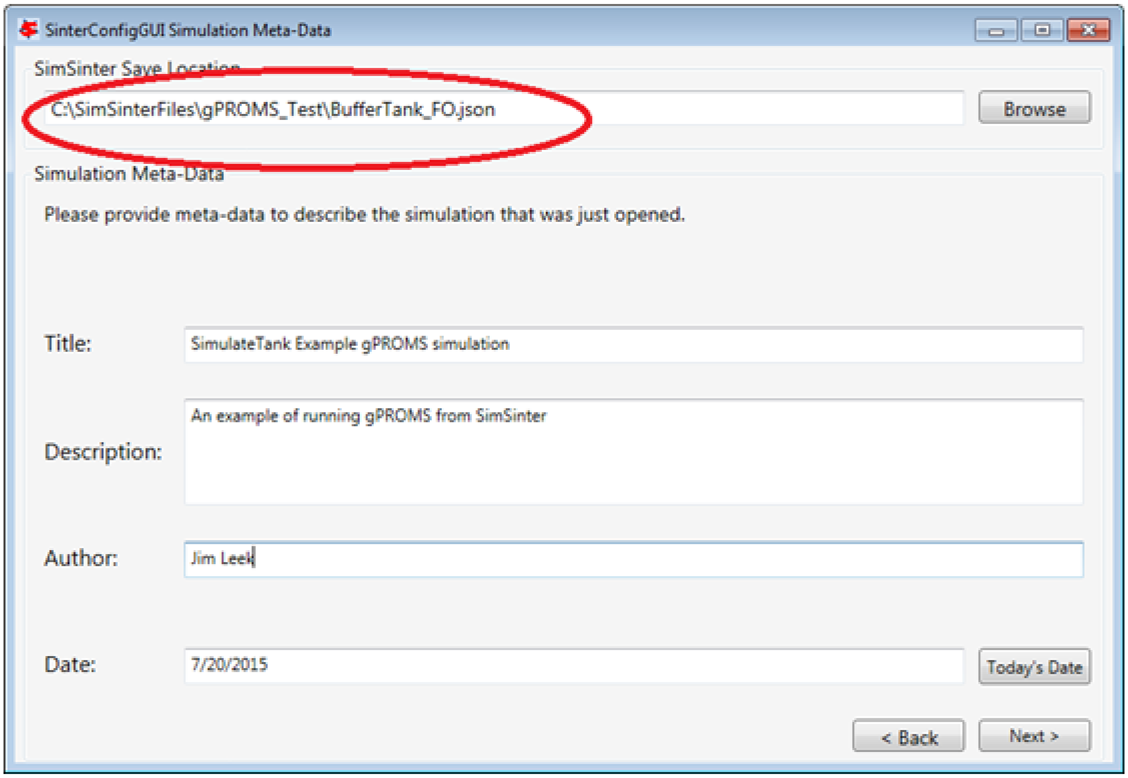


Fig. 45: SinterConfigGUI Simulation Meta-Data Save Text Box

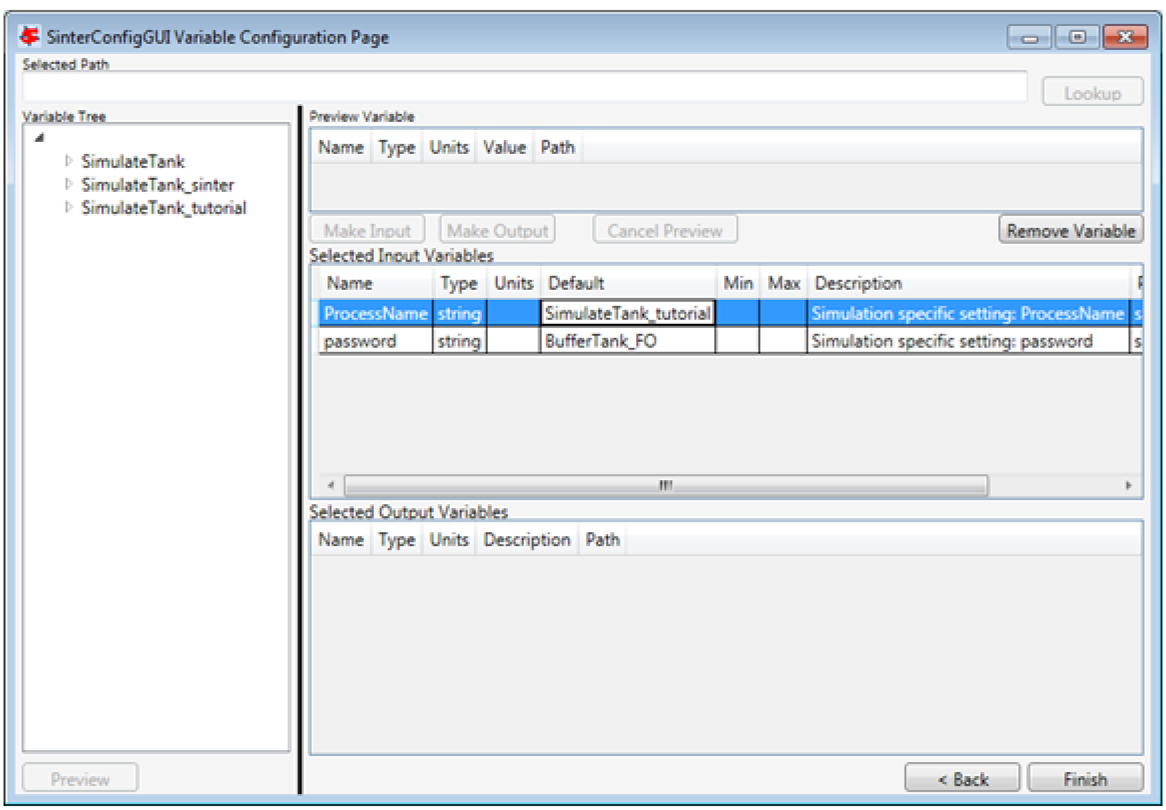


Fig. 46: SinterConfigGUI gPROMS Settings Configuration

from the file if it was defined purely in terms of actual numbers. SimSinter cannot evaluate other variables or functions. Therefore,

```
DEFAULT 2 * 3.1415 * 12
```

will work. However,

```
DEFAULT 2 * PI * radius
```

will not work, because SimSinter does not know the value of either PI or radius, and SimSinter will just set the default to 0.

Min and **Max** values are taken from the variable type, if there is one.

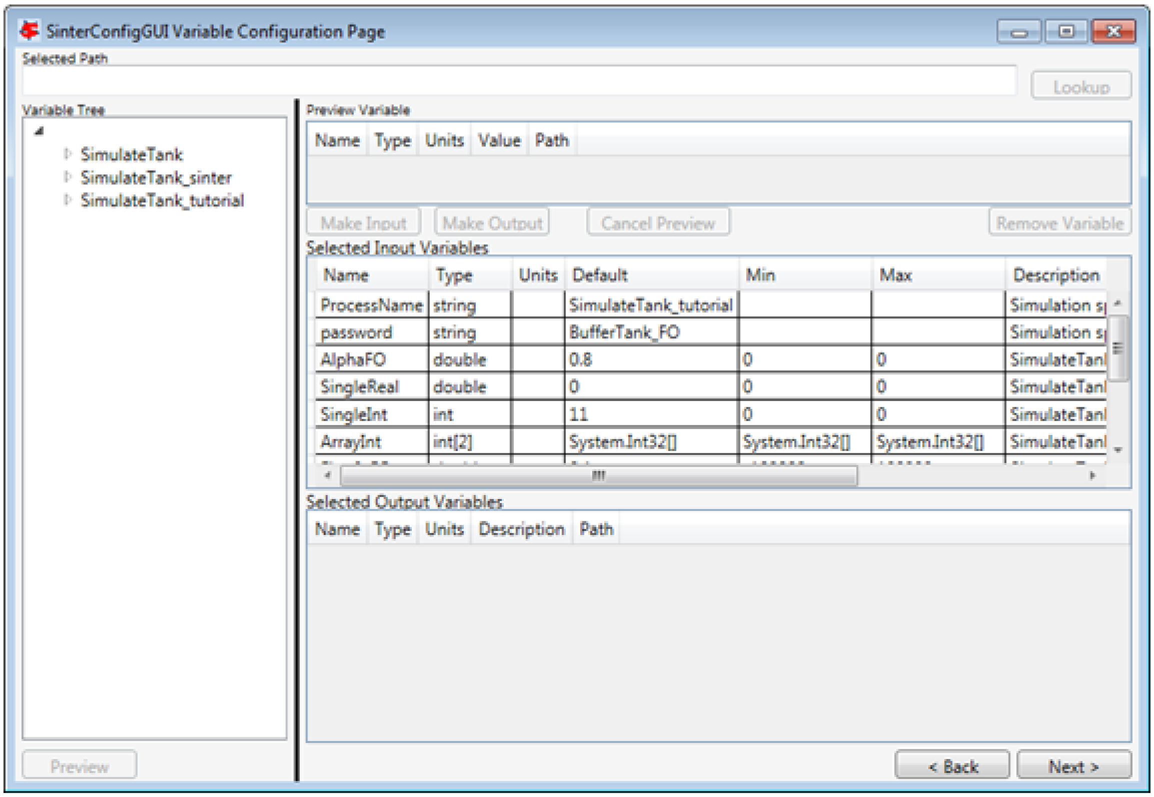


Fig. 47: SinterConfigGUI Automatically Displays Input Variables

8. Now the output values can be entered. Expand the "SimulateTank_tutorial" Process on the Variable Tree, expand the "T101" model, and then double-click on "FlowOut" to make it the Preview Variable. Notice that the **Make Input** button is disabled. As stated above, the user cannot make new Input Variables in SinterConfigGUI. Only **Make Output** is allowed.
9. If **Make Output** is clicked, "FlowOut" will be made an Output Variable as shown in Figure *FlowOut as an Input Variable*. The Description can be updated, but SimSinter made a good guess in this example; therefore, there is no need to change the description.
10. By the same method, make Output Variables "HoldUp" and "Height."
11. The variables names should be made shorter. Simply click on the **Name** column and change the name to your preferred name.
12. For future testing, make sure the defaults are good values. The only three input variables that matter have the following defaults:

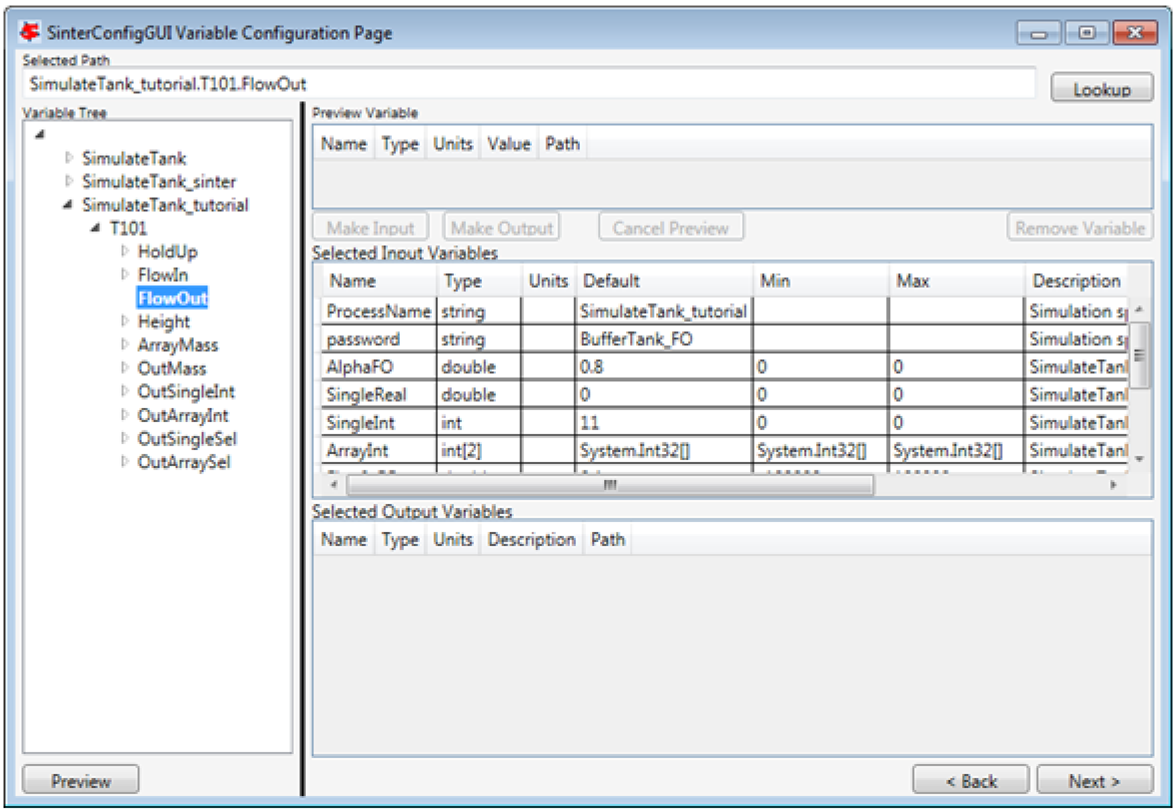


Fig. 48: Preview of the FlowOut Variable

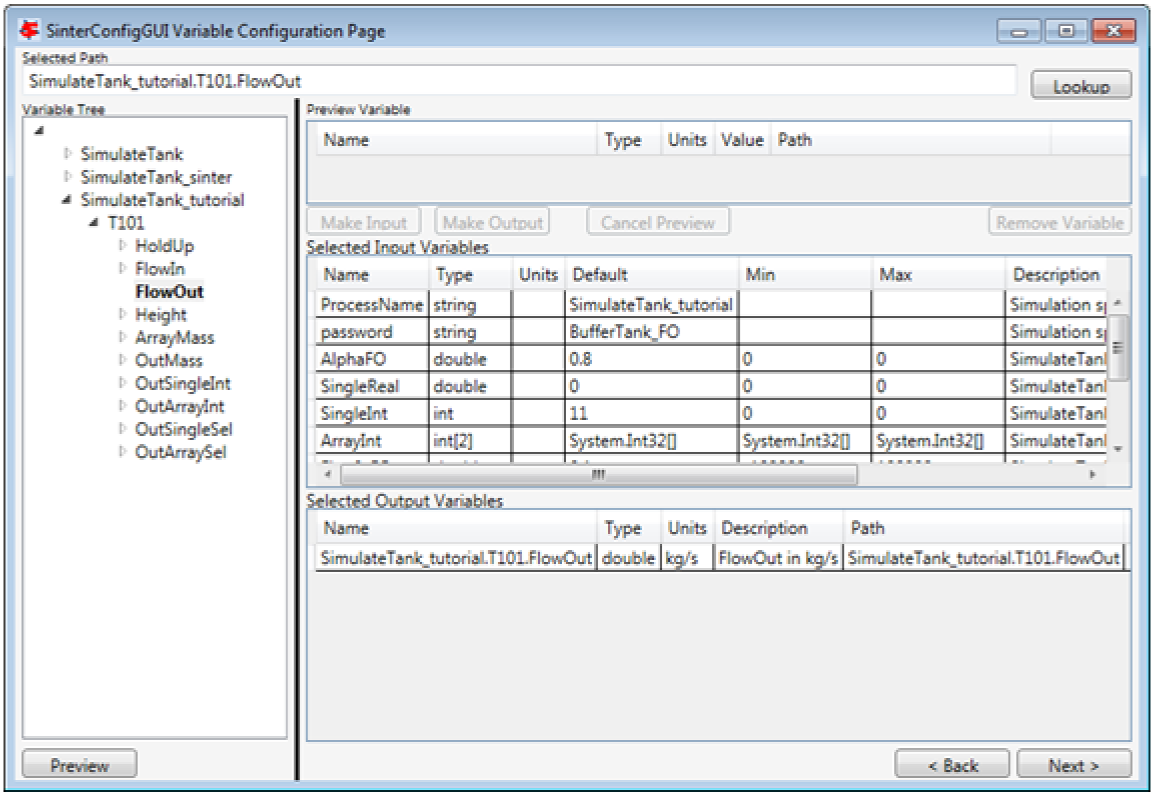


Fig. 49: FlowOut as an Input Variable

```
AlphaFO  = 0.8
FlowInFO = 14
HeightFO = 7.5
```

13. When finished making output variables, click **Next** at the bottom of the variables page. If there were any input vectors, the Vector Default Initialization page will display. Here the default values of the vectors may be edited.
14. Finally, click **Finish** and save your configuration file. Your gPROMS simulation should now be runnable from FOQUS.

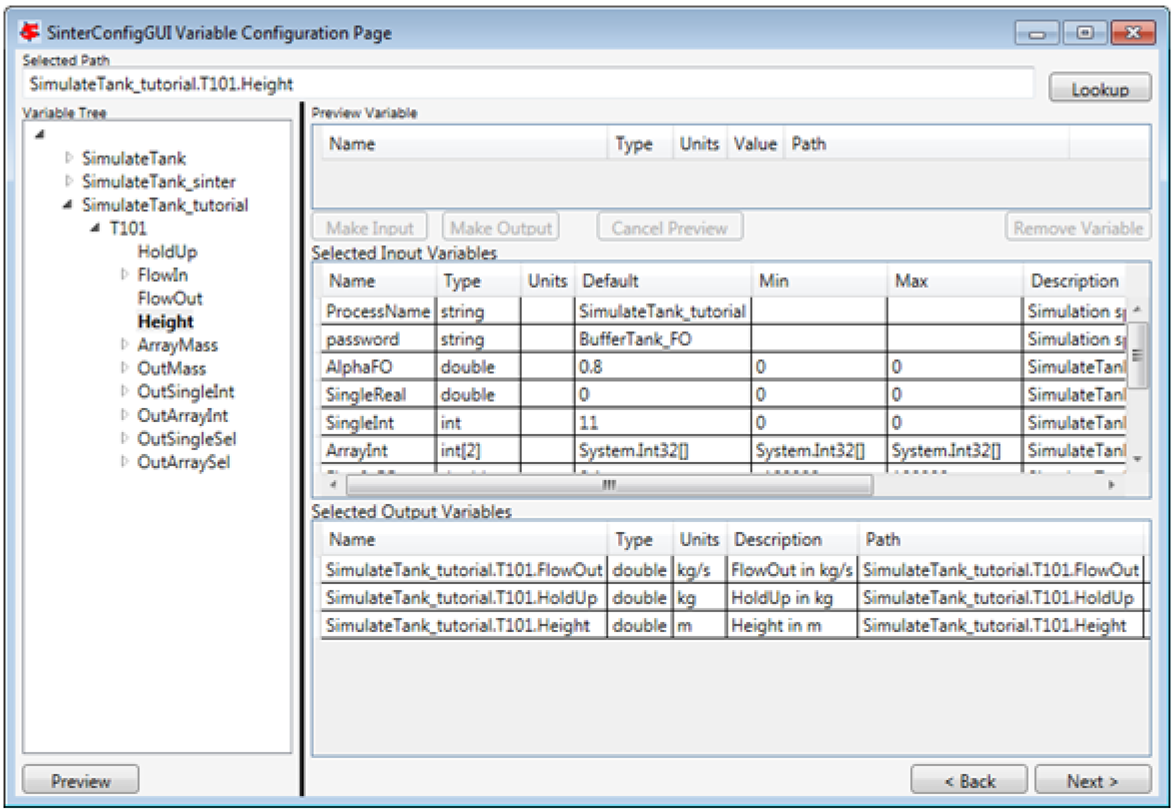


Fig. 50: HoldUp and Height Output Variables

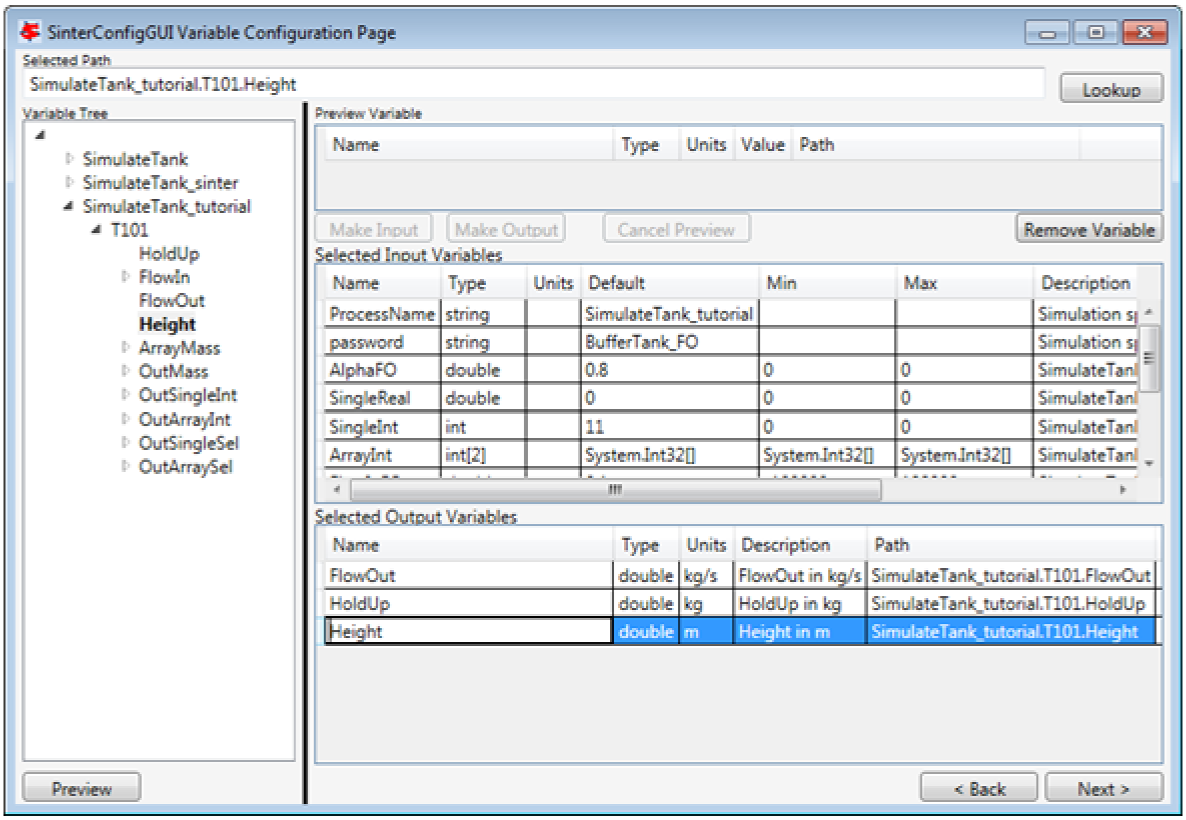


Fig. 51: Editing Variable Names

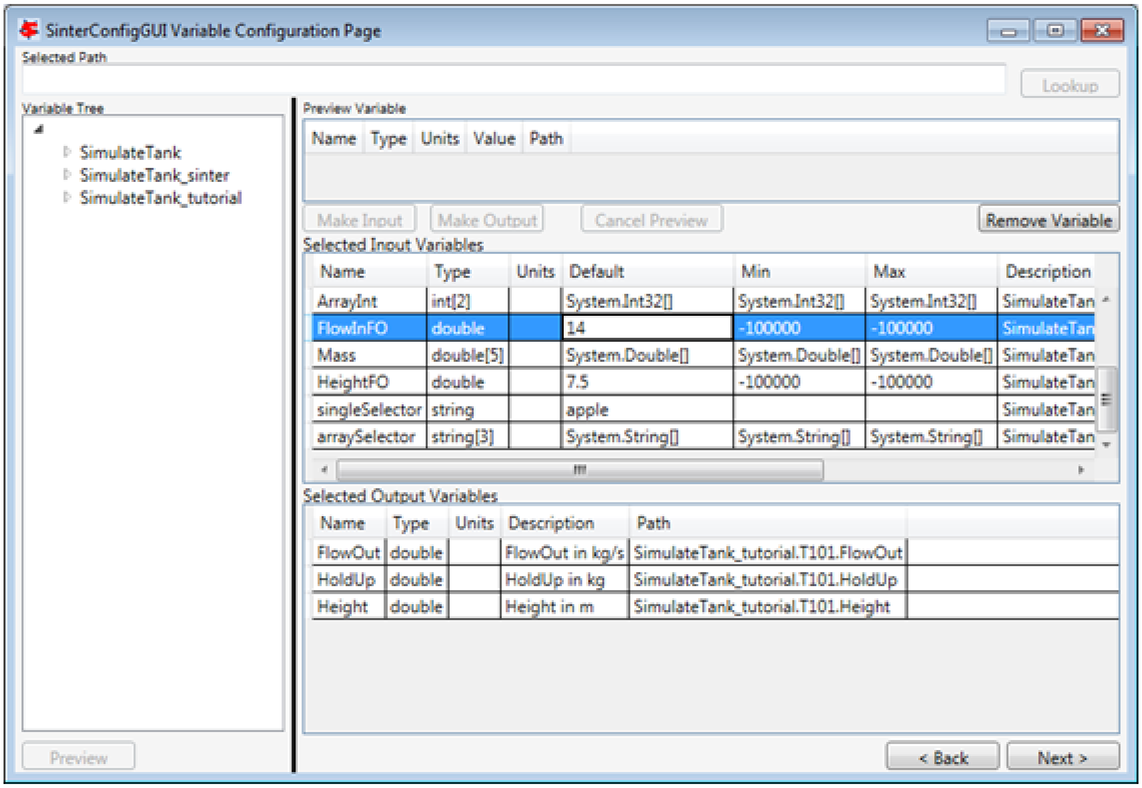


Fig. 52: Editing Defaults

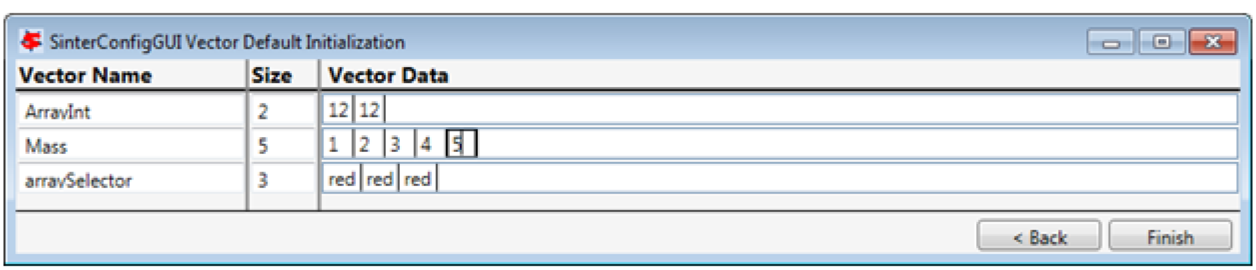


Fig. 53: Editing Vectors

CHAPTER 11

Debugging

This chapter contains information that may be helpful in resolving a problem or filing a bug report.

11.1 How to Debug

Log files may contain very useful information when reporting problems. The log files are contained in the logs sub-directory of the FOQUS working directory. To change the log message levels in FOQUS go to the FOQUS **Settings** button from the Home window. From there various log settings can be changed. The debugging log level provides the highest level of information.

Almost any error that occurs in FOQUS should be logged. Occasionally, an error may occur that is difficult to find, or causes FOQUS to crash before logging it. In that case the "FOQUS Console" application can be used. All output from FOQUS, including messages that cannot be seen otherwise will be shown in a "cmd" window which will remain open even after FOQUS closes.

When running heat integration, the debugging information can be found in
\gamsHeatIntegration.lst. This file includes detailed results and errors returned by GAMS.

Most UQ routines interact with PSUADE via Python wrappers. When PSUADE is running, the stdout is written to psuadelog in the working directory. (At present, only some PSUADE commands write to this log; however, this will be standardized in the near future so that all PSUADE commands write to this log.) Other errors that are due to the Python wrappers or PySide GUI components are written to the logs subdirectory in the working directory.

11.2 Known Issues

The following are known unresolved issues:

- The FOQUS flowsheet can be edited while a flowsheet evaluation, optimization, or UQ is running. This should not be allowed, and may cause problems.

- With the windows installer, FOQUS may produce output to standard error, especially if it immediately fails to launch. Output is usually caught and redirected to the FOQUS log and displayed in dialog boxes within FOQUS, but rare instances may occur where error messages are not caught. Output to standard error is logged in the directory with foqus.exe in the file foqus.exe.log. The user does not typically have permission to write to the FOQUS install location, so an error message such as "Cannot write to foqus.exe.log" will be displayed. If this occurs there are two solutions (1) change the permissions for the FOQUS install directory or (2) run "FOQUS Console" application, which will direct FOQUS output to the "cmd" window.
- The win32com module generates Python code, which it needs to run. This code is generated in the FOQUS install location "\distwin32comgen_py." In some cases there may be a problem writing to that directory due to permission settings. This will prevent FOQUS from running simulations locally. If this error is encountered the solution is to make the "gen_py" directory user writable. So far, in testing, this error seems to occur in Windows 8 and 10, but not 7.
- The user regression analysis features, iREVEAL and ALAMO, of the UQ tool requires a separate Python 2.7 installation. Furthermore, Python must be both in PATH variable and associated with .py files. Details on installing Python and fixing any issues encountered may be found in the iREVEAL Installation Guide and the iREVEAL User Manual, Known Issues section.
- FOQUS has trouble getting files from Turbine and saving them to the DMF when dealing with files in Turbine involving directories.
- The default port for TurbineLite is 8080. If another program is already using port 8000, there will be an error in FOQUS when connecting to TurbineLite. In the **Turbine** Tab of the Settings window, there is a tool to change the TurbineLite port. If the TurbineLite port is changed the configuration file that FOQUS uses to connect to TurbineLite, must also be changed.

11.3 Reporting Issues

To report an issue, please send an email to:

Please include detailed steps on how to reproduce the error, including screenshots and log files.

CHAPTER 12

References

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CHAPTER 13

Copyright and License

13.1 Copyright Notice

13.2 License Agreement

CHAPTER 14

FOQUS

14.1 Overview

The Framework for Optimization, Quantification of Uncertainty, and Surrogates (FOQUS) serves as the primary computational platform enabling advanced Process Systems Engineering (PSE) capabilities to be integrated with commercial process simulation software. It can be used to synthesize, design, and optimize a complete carbon capture system while considering uncertainty. FOQUS enables users to effectively screen potential capture concepts in the context of a complete industrial process so that trade-offs can be appropriately evaluated. The technical and economic performance characteristics of the capture process are highly dependent on employing an effective approach for process synthesis. Since large-scale carbon capture processes are outside of current experience, heuristic and evolutionary approaches are likely to be inadequate. Thus, a key aspect of FOQUS is that it bridges this gap by supporting a superstructure-based approach to determine the optimal process configuration and equipment interconnections.

14.2 Modules

1. SimSinter provides a wrapper to enable models created in process simulators to be linked into a FOQUS Flowsheet.
2. The FOQUS Flowsheet is used to link simulations together and connect model variables between simulations on the flowsheet. FOQUS enables linking models from different simulation packages.
3. Simulations are run through Turbine, which manages the multiple runs needed to build surrogate models, perform derivative-free optimization or conduct an Uncertainty Quantification (UQ) analysis. Turbine provides the capability for job queuing and enables these jobs to be run in parallel using cloud- or cluster-based computing platforms or a single workstation.
4. The Surrogates module can create algebraic surrogate models to support large-scale deterministic optimization, including superstructure optimization to determine process configurations. One of the available surrogate models is the Automated Learning of Algebraic Models for Optimization (ALAMO). ALAMO is an external product due to background Intellectual Property (IP) issues.

5. The Derivative-Free Optimization (DFO) module enables derivative-free (or simulation-based) optimization directly on the process models linked together on a FOQUS Flowsheet. It utilizes Excel to calculate complex objective functions, such as the cost of electricity.
6. The UQ module enables the effects of uncertainty to be propagated through the complete system model, sensitivity of the model to be assessed, and the most significant sources of uncertainty identified to enable prioritizing of experimental resources to obtain additional data.
7. The Optimization Under Uncertainty (OUU) module combines the capabilities of the DFO and the UQ modules to enable scenario-based optimization, such as optimization over a range of operating scenarios.
8. The SolventFit module is an uncertainty quantification tool for the calibration of an Aspen Plus® solvent process model. The current state of the art is a regression that yields single best fit point estimates of some parameters. This shows neither the level of uncertainty in each parameter, nor the level of uncertainty in model output, such as equivalent work. SolventFit allows for predictions with uncertainty bounds by accounting for uncertainty in model parameters and deficiencies in the model form. This yields an improved understanding of the model parameters and results in more complete predictions with uncertainty bounds. This distribution of parameters allows for predictions with uncertainty.
9. The Sequential Design of Experiments (SDOE) module currently provides a way to construct flexible space-filling designs based on a user-provided candidate set of input points. The method allows for new designs to be constructed as well as augmenting existing data to strategically select input combintions that minimizes the distance between points. Development of this module is continuing and will soon include other options for design construction.