

**CCSI**<sup>TM</sup>  
Carbon Capture Simulation Initiative

# **CCSI Integrated Capture Systems Model (IntCap)**

## **User Manual**

**Version 2.0.0**

**March 2018**



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To obtain support for the products within this package, please send an e-mail to [ccsi-support@acceleratecarboncapture.org](mailto:ccsi-support@acceleratecarboncapture.org).

## 1.0 REPORTING ISSUES

To report an issue, please send an e-mail to [ccsi-support@acceleratecarboncapture.org](mailto:ccsi-support@acceleratecarboncapture.org).

## 2.0 VERSION LOG

Product	Version Number	Release Date	Description
Integrated Solid Sorbent CO <sub>2</sub> Capture Process	2.0.0	3/31/2018	Open Source Release
Integrated Solid Sorbent CO <sub>2</sub> Capture Process	2015.10.0	10/31/2015	Initial release.

# Integrated Solid Sorbent CO<sub>2</sub> Capture System Model

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## 1.0 INTRODUCTION

This documentation introduces the dynamic integrated solid sorbent CO<sub>2</sub> capture and compression process model that utilizes the Moving Bed (MB), Bubbling Fluidized Bed (BFB), and CO<sub>2</sub> compression models that have been released as standalone models. This model can be used to predict the power requirements for the CO<sub>2</sub> compression while taking into account the transport delay and pressure flow characteristics of the CO<sub>2</sub> capture process. This document will give a brief overview of each sub-model that is used in the overall process model. More details of individual model's assumptions and properties can be found in their corresponding sections in this manual.

## 2.0 INTEGRATED MODEL STRUCTURE

There are two versions of the integrated model, one implemented in ACM, and the other is implemented in gPROMS® (Process Systems Enterprise Limited). The ACM integrated model is based on a Framework for Optimization and Quantification of Uncertainty and Sensitivity (FOQUS) optimized solid-sorbent steady-state process that is capable of 90% CO<sub>2</sub> capture from a 650 MW coal fired plant. The process is assumed to require six trains of a 3-stage absorber, nine trains of 2-stage regenerators, and two trains of CO<sub>2</sub> compressors. The model equations for the CO<sub>2</sub> compressor are written in the Custom Modeling library. To find the various models that have been developed:

1. In the "All Items" pane of the "Simulation Explorer," confirm the "Custom Modeling library" is expanded, and then expand the "Models" folder. A list of all models in the current simulation displays.
2. In the list of all developed models, click the desired model.
3. In the "Contents" pane, double-click the "equals" icon for the model.

The gPROMS version of the integrated model uses a two-stage BFB absorber, a 14-stage MB regenerator, and a single CO<sub>2</sub> compressor train. **Note:** This model is not based on an optimized steady-state design, however demonstrates the predictive ability of all developed process models in gPROMS.

### 2.1 IO Structure

The integrated models contains several input and output ports. Each port has associated variables that correspond to the material connection stream variables. In the ACM version, the BFB and MB share the same port types, however those ports are converted when the CO<sub>2</sub> stream enters the CO<sub>2</sub> compressor train, as many auxiliary models are from the Aspen dynamics library that utilize a different port type. Additionally, the component N<sub>2</sub> in the CO<sub>2</sub> compressor inlet is removed as the amount of N<sub>2</sub> should be negligible and the zero value would cause numerical problems with dynamic integration.

The gPROMS version of the model was developed with different ports for the MB and BFB models, so the project file contains a port convertor "model" that is used each time a stream connects one type of bed to another. Additionally, the CO<sub>2</sub> compressor model in gPROMS was developed with the default PML port type (gPROMS model libraries), as many of the auxiliary equipment was modeled with the default PML library models, so the ports change across the beds and CO<sub>2</sub> compressor train.

## 2.2 Component List and Physical Properties

There are three main parts of the integrated simulation, solid sorbent CO<sub>2</sub> capture, compression, and drying. The compression section requires accurate properties for CO<sub>2</sub> to predict compressor power. The drying section requires accurate vapor-liquid equilibrium calculations for the CO<sub>2</sub>-TEG-Water system. The MB/BFB needs accurate physical properties for hydrodynamics.

For the BFB and MB sections, two phase flow are modeled, gas and solid. Three components, carbon dioxide (CO<sub>2</sub>), water (H<sub>2</sub>O), and nitrogen (N<sub>2</sub>) are used in gas phase; and three ionic species, bicarbonate (Bic), carbamate (Car), and physisorbed water (H<sub>2</sub>O) are assumed for the solid phase which exists as the adsorbed state on sorbent. The mechanism of the adsorbate, CO<sub>2</sub> and H<sub>2</sub>O, onto an amine-impregnated mesoporous sorbent is shown in reference (Lee, et al., 2012).

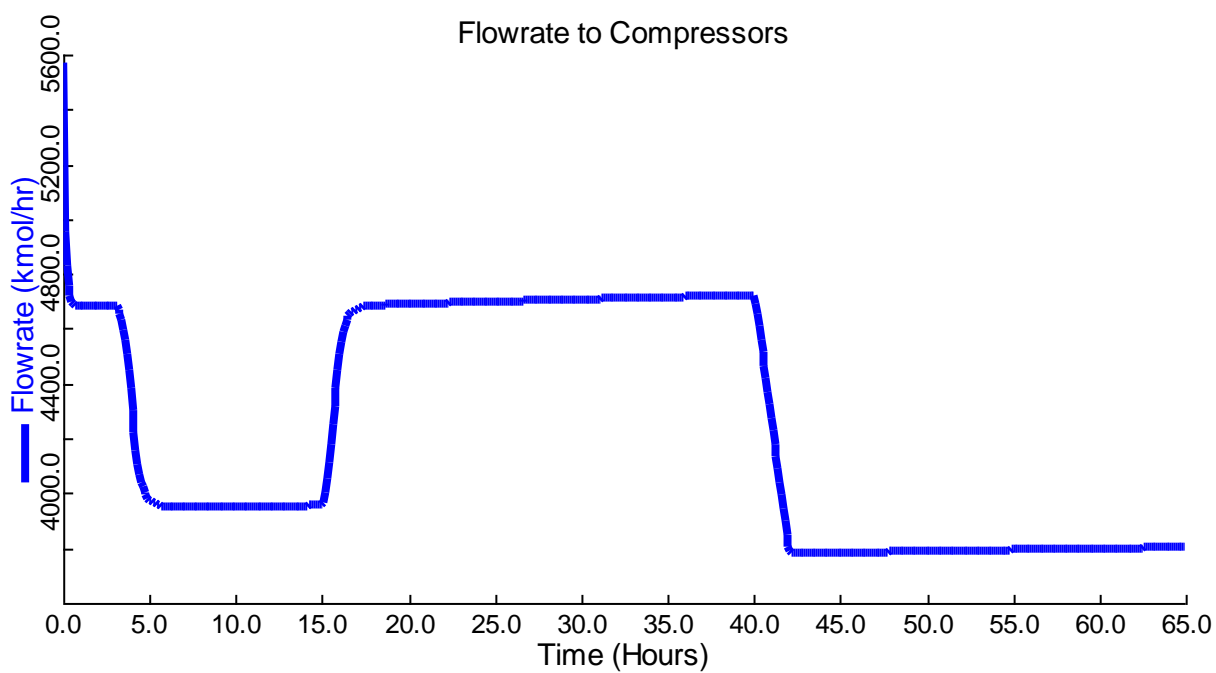
Physical properties of the fluids can be calculated using commercial property packages (Aspen Properties® in ACM and Multiflash® in gPROMS) using cubic equations of state. The sorbent properties should be specified by user, particle diameter, density, heat capacity, and heat conductivity. If the diffusion limited options to calculate the reaction rate is selected, the extra information for average pore diameter, intraparticle void fraction, and tortuosity is necessary.

The CO<sub>2</sub> compressor section uses three components, carbon dioxide (CO<sub>2</sub>), water (H<sub>2</sub>O), and TEG. The nitrogen component from the solid sorbent section of the model is removed due to numerical issues stemming from the amount of nitrogen in the CO<sub>2</sub> compressor train being near zero. The ACM version of the model uses LK-PLOCK for the compression train and the water knock-out drums, while HYSGLYCO is used for the drying section. However, the gPROMS version uses LK-PLOCK for the entire CO<sub>2</sub> compression section as HYSGLYCO is not available in Multiflash.

### 3.0 ACM INTEGRATED MODEL TUTORIAL

Example: Two ramp changes in the inlet flue gas flowrate and shutdown of one solid sorbent train.

1. Open the “ACM/Dynamic/Example\_Flowrate/Int.BFB\_CO2.acmf” file.
2. Load snapshot “int” results.
3. Run the model.
4. The flue gas ramps occur at 3hrs and 15hrs, and the shutdown of a train occurs at 40hrs. The total simulation time is 65hrs.
5. Observe the custom plot “Power,” “Flowrate,” and “CO2\_removed” as shown below (Figure 25 under “Flowsheet Explorer.”)



**Figure 1: Gas flowrate to compressors.**



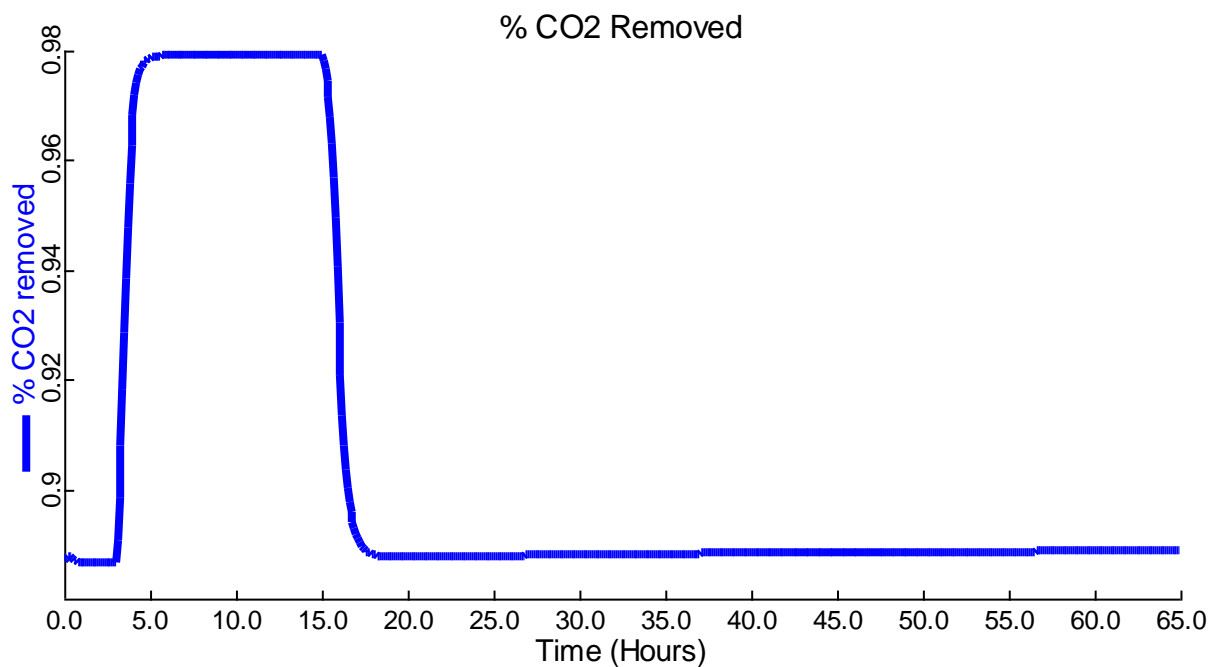


Figure 2: Percent CO<sub>2</sub> removed from the flue gas during step changes.

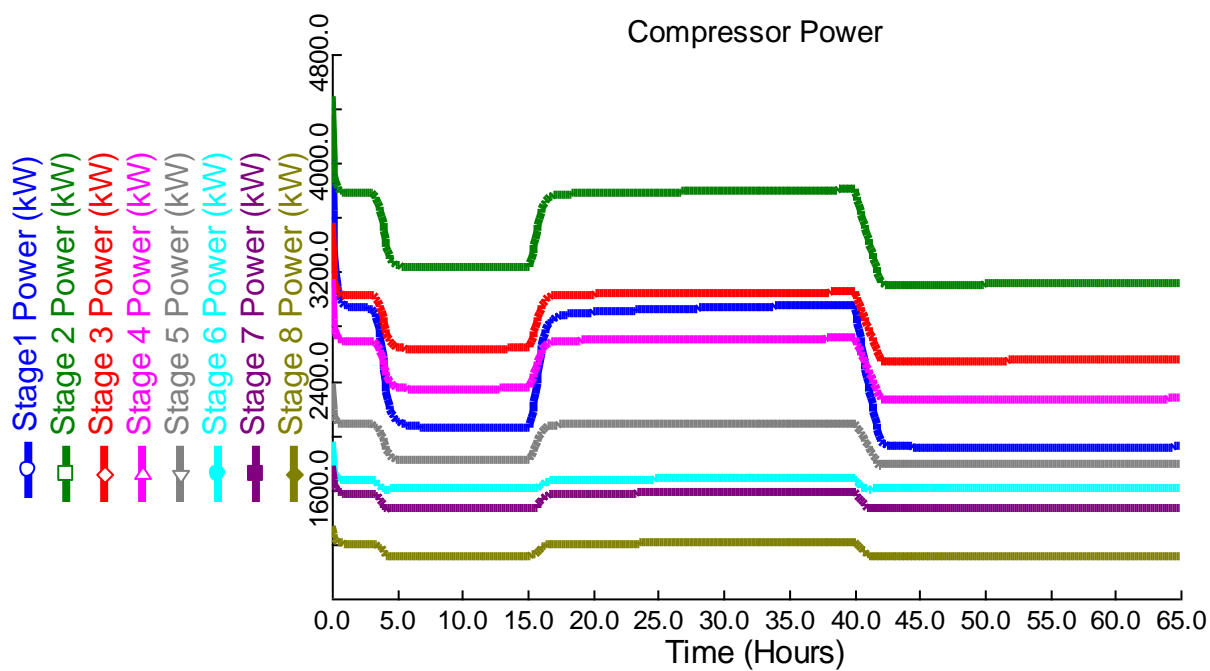
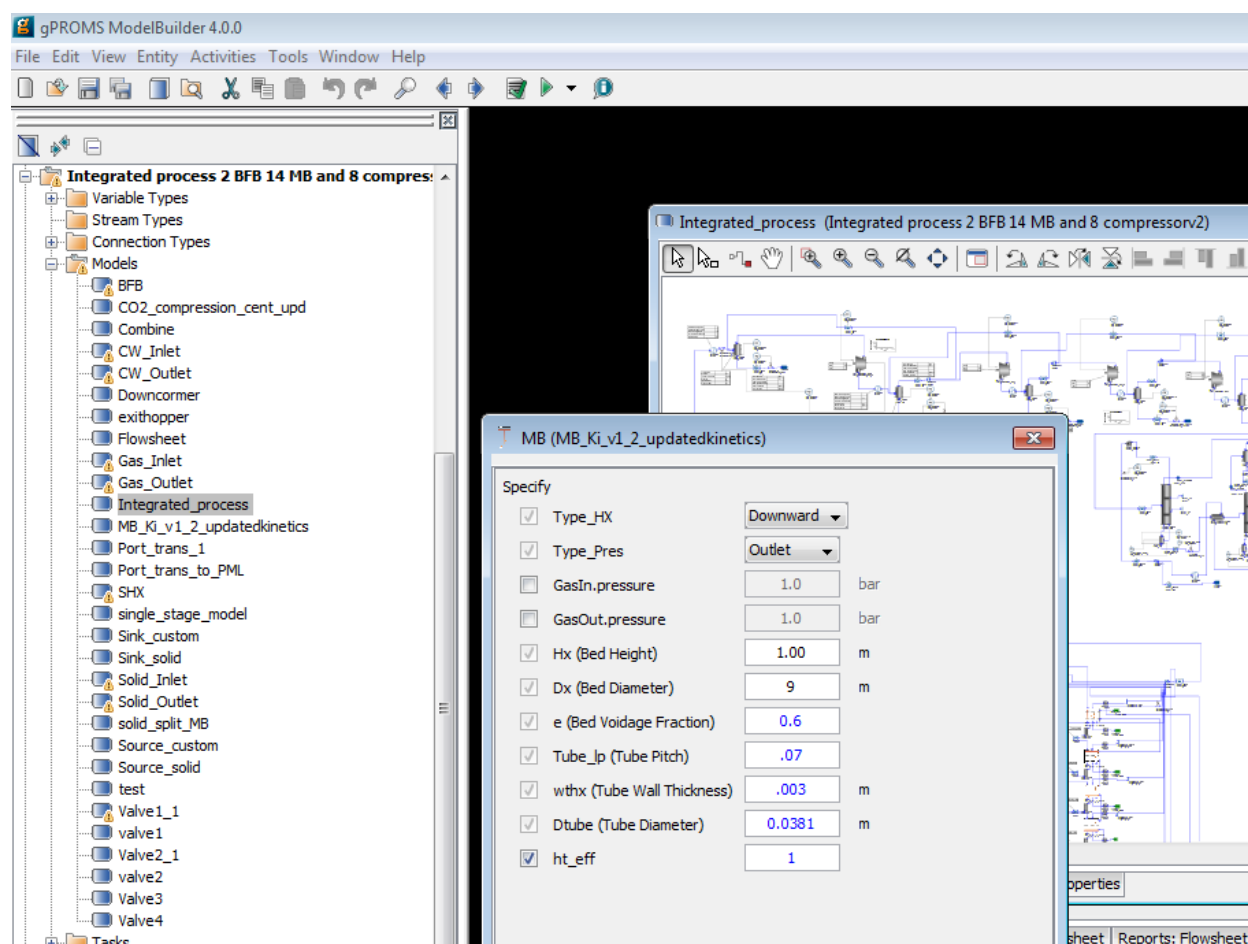


Figure 3: Power requirement of CO<sub>2</sub> compressors during step changes.

## 4.0 IMPLEMENTATION OF INTEGRATED MODEL IN GPROMS

The gPROMS model is set-up and simulated using the following steps:

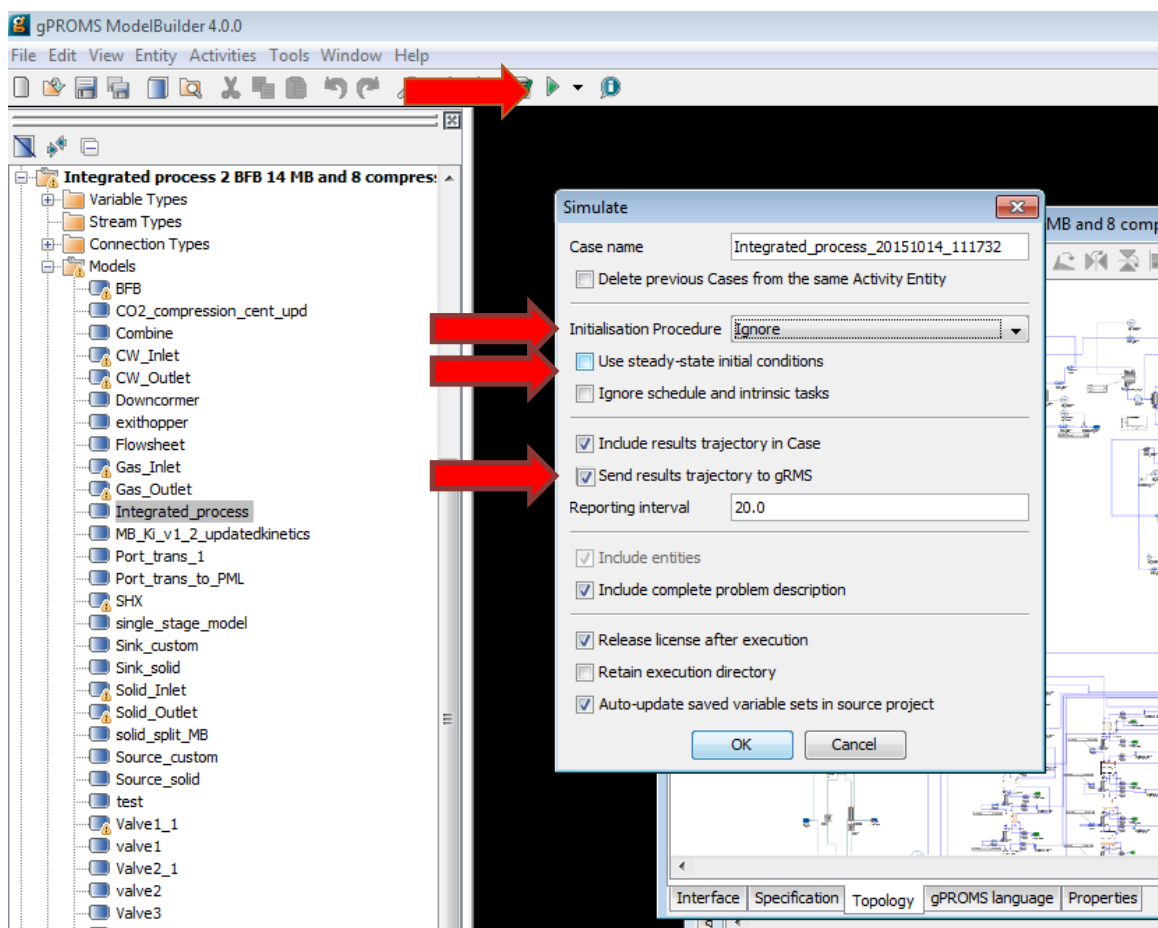
1. Open the “gPROMS/Example/Integrated\_process v1.0.gpj” file.
2. The integrated model utilizes the built in PML libraries in gPROMS. Navigate to “File” → “Open/Close Libraries.” A window opens with a list of available models. Select the “PML libraries” check box and then click “OK.”
3. In the “project tree” on the left, navigate to “Models” and then double-click “Integrated\_process” (see Figure 28).



**Figure 4: Specification box for MB model. The process flowsheet model “Integrated\_process” is highlighted in the “project tree” menu on the left.**

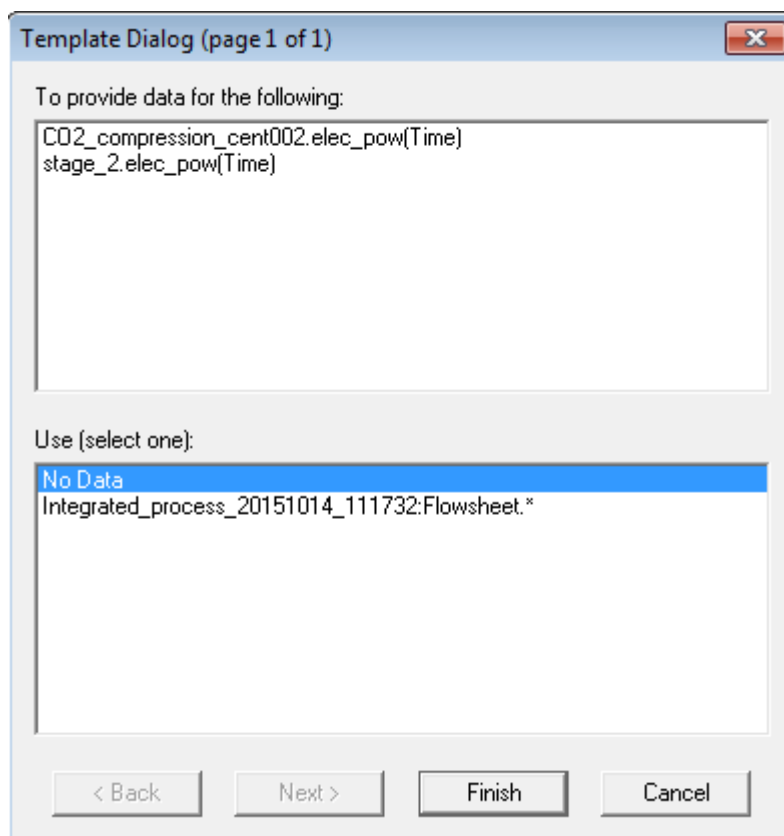
**Note:** Specifying the required variables is done by double-clicking each piece of process equipment under the “Topology” tab of the “process\_MB” window. These values are set to default values. Like the ACM model, if these variables are changed, it may require an initialization procedure. This can be turned on or off in the next step by selecting “Execute” or “Ignore.”

- Run the model by clicking “Play” (the green button on the top of the toolbar). The “Simulate” option menu displays. Be sure the check box for “Use steady-state initial conditions” is clear (see Figure 29). The model is setup to automatically select initial conditions. Additionally, be sure to select the “Send results trajectory to gRMS” check box. This sends the results of the simulation to gPROMS data management software, where templates for plotting the results have already been provided. Lastly, ensure that the “Ignore schedule and intrinsic tasks” is left cleared. This runs the schedule already set up (it introduces a disturbance) which can be viewed by opening the “Integrated\_process” under the “Processes” folder in the “project tree” and then navigating to the “Schedule” tab. Select the check box to run a steady-state simulation. The disturbance configured is a decrease of inlet flue gas by closing the valve opening.

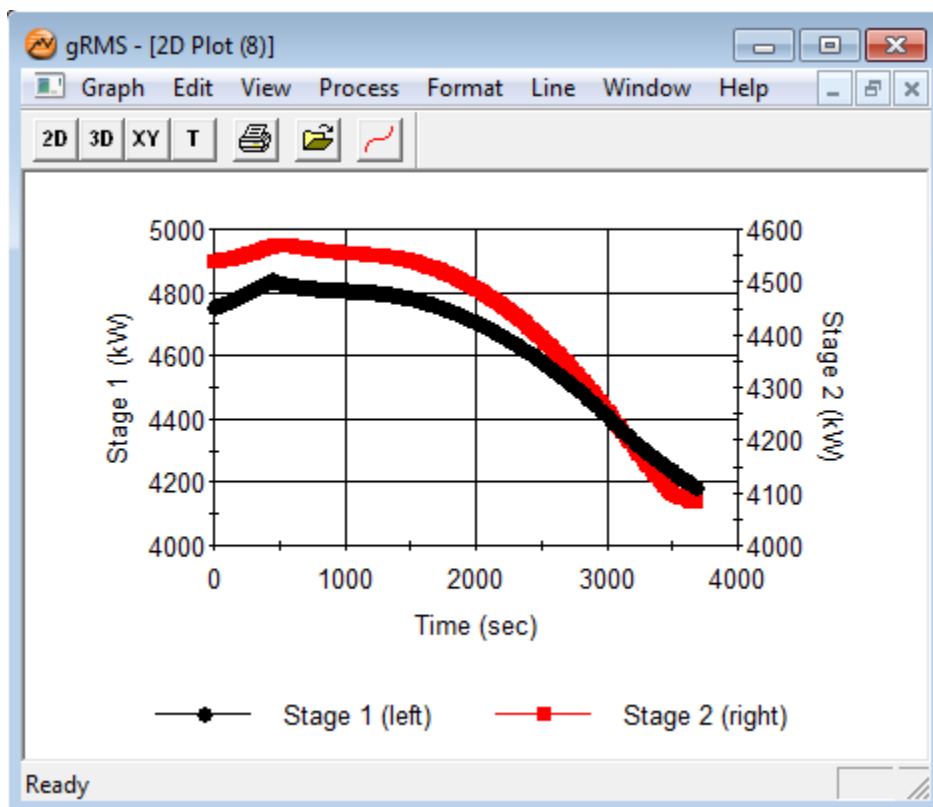


**Figure 5:** Click “Play” (the green arrow on the top toolbar) while the “process\_MB Model” window is open to open the “Simulate” window. The “Initialisation Procedure” drop-down menu enables the user the option to run the initialization procedure. Select the “Ignore” option.

5. Click “OK” on the “Simulate” options window to begin the simulation.
6. A new results window displays (listed at the bottom of the “project tree”).
7. A ramp change occurs at 1,000s and the simulation time is 20,000s.
8. To view the results, navigate to the “gRMS” window that displayed once the simulation is run. gRMS is a data management program with numerous options and the ability to save a template for the plots, allowing plots to be generated quickly for new simulation results. Six of these templates have been provided as “.gpt” files. In the “gRMS” window, navigate to “Graph” → “Open Template” and then select the desired template that has been provided. A window displays asking to specify what results the user would like to plot (see Figure 30). Select the “Integrated\_process\_XXXXXX\_XXXXX” data that is currently being generated. The results will be plotted. Assuming the simulation has not completed running yet, the plots will automatically update as the simulation is solved in gPROMS. Figure 31 shows the resulting plot that results from loading “stage12.gpt.”



**Figure 6: Data selection window for gRMS template.**



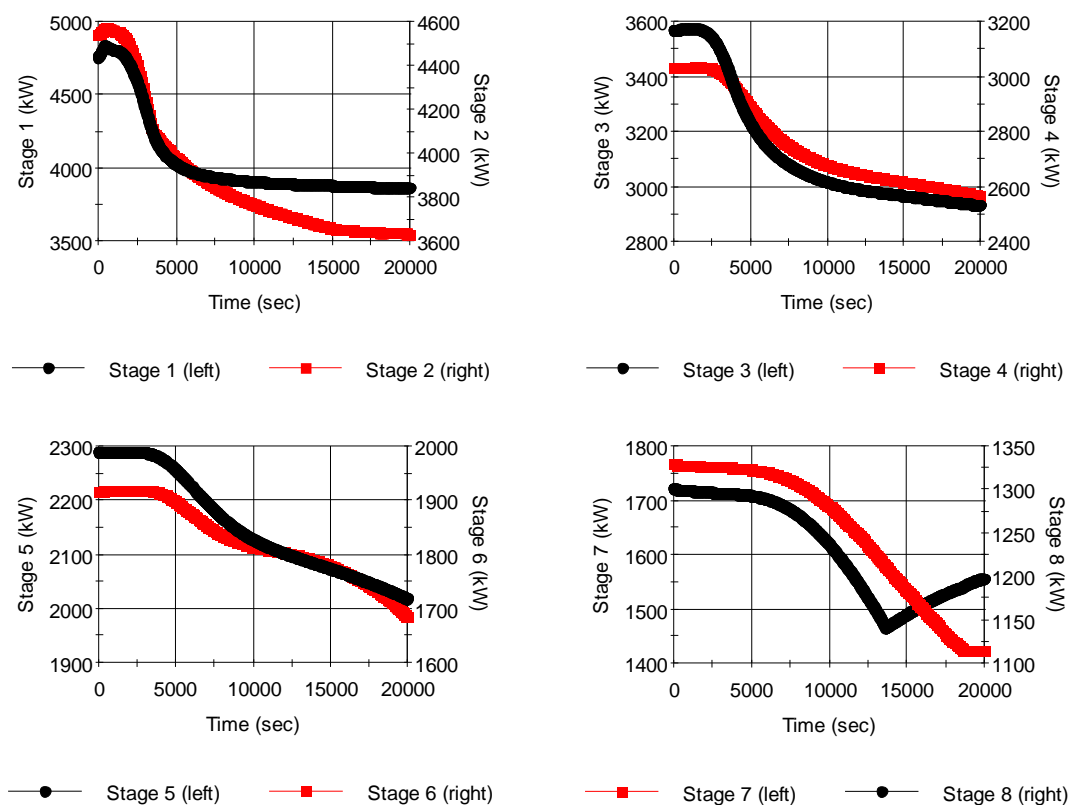
**Figure 7: A plot that results from loading template “stage12.gpt.”**

**This plot shows the dynamic power requirements of the stage 1 and stage 2 compressor.**

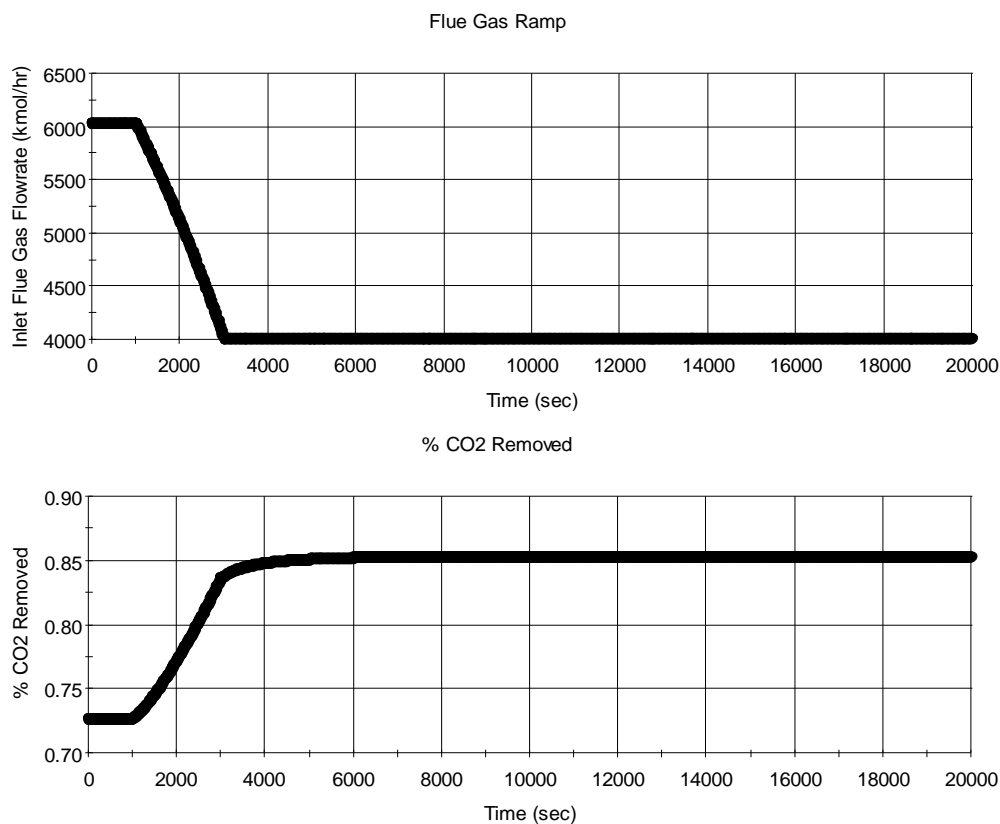
**Note: The data will be added as the simulation to continue, therefore the generated plot may contain more or less time series data than is shown here.**

**Note:** Results can also be viewed by navigating to the “Trajectories” → “Flowsheet” folder in the results file that is generated at the bottom of the “project tree.” Simply navigate to the desired variable within the flowsheet.

9. The simulation of 20,000 sec will require several hours to complete. When the simulation completes, the results of each template provided are given in Figures 32 and 33.



**Figure 8: gPROMS simulation power requirement for CO<sub>2</sub> compressors during ramped decrease in flue gas.**



**Figure 9: gPROMS simulation inlet flue gas flowrate and percent CO<sub>2</sub> removed.**

## 5.0 INSTALLATION REQUIREMENTS

The minimum suggested hardware requirement is desktop/laptop running Windows® 7 on Intel Core i-5 family 2.8 GHz or faster and 8 GB of RAM. With lower configuration, the simulation speed can be slower. The ACM and gPROMS models have been tested on Aspen V8.4 and gPROMS ModelBuilder 4.0.0, respectively.

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