Thermal Reacting Gasifier Training Problem
Part 2: Project

August 2020

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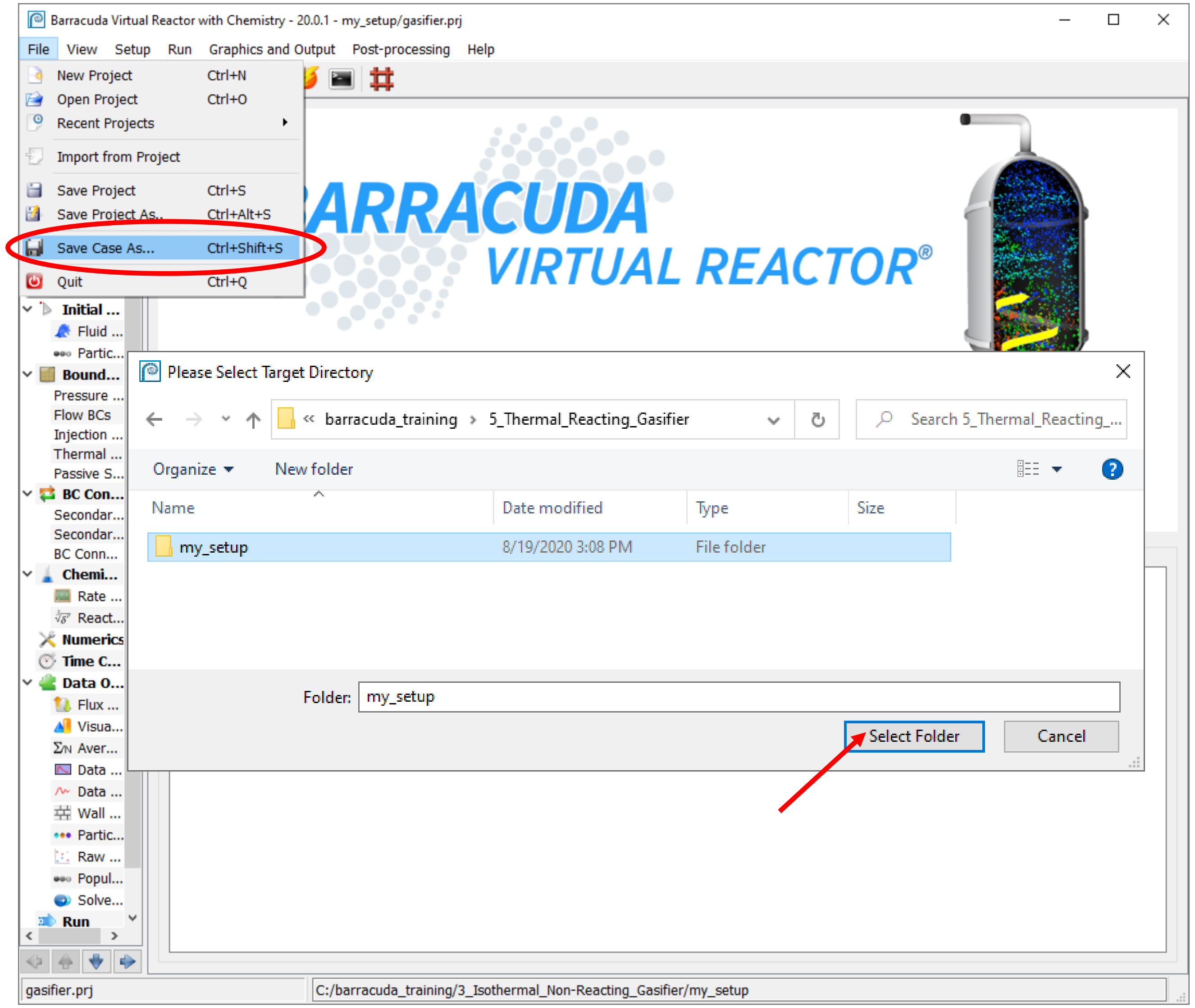
Save Case As…

Copy Gasifier project using "Save Case As…"

Open the isothermal non-reacting gasifier project with Barracuda Virtual Reactor.

- Use the Barracuda GUI menu File →Save Case As…
- Select: `5_Thermal_Reacting_Gasifier/my_setup` as the target directory



Selecting Files in the Save Case As… Dialog

A full Barracuda VR project setup includes the base project file (*prj), the geometry (*stl), transient boundary condition files (*sff), particle size distribution files (*sff, *i), and potentially other files as well.

The Save Case As… dialog allows you to select exactly which files you want to include or exclude during the copy operation.

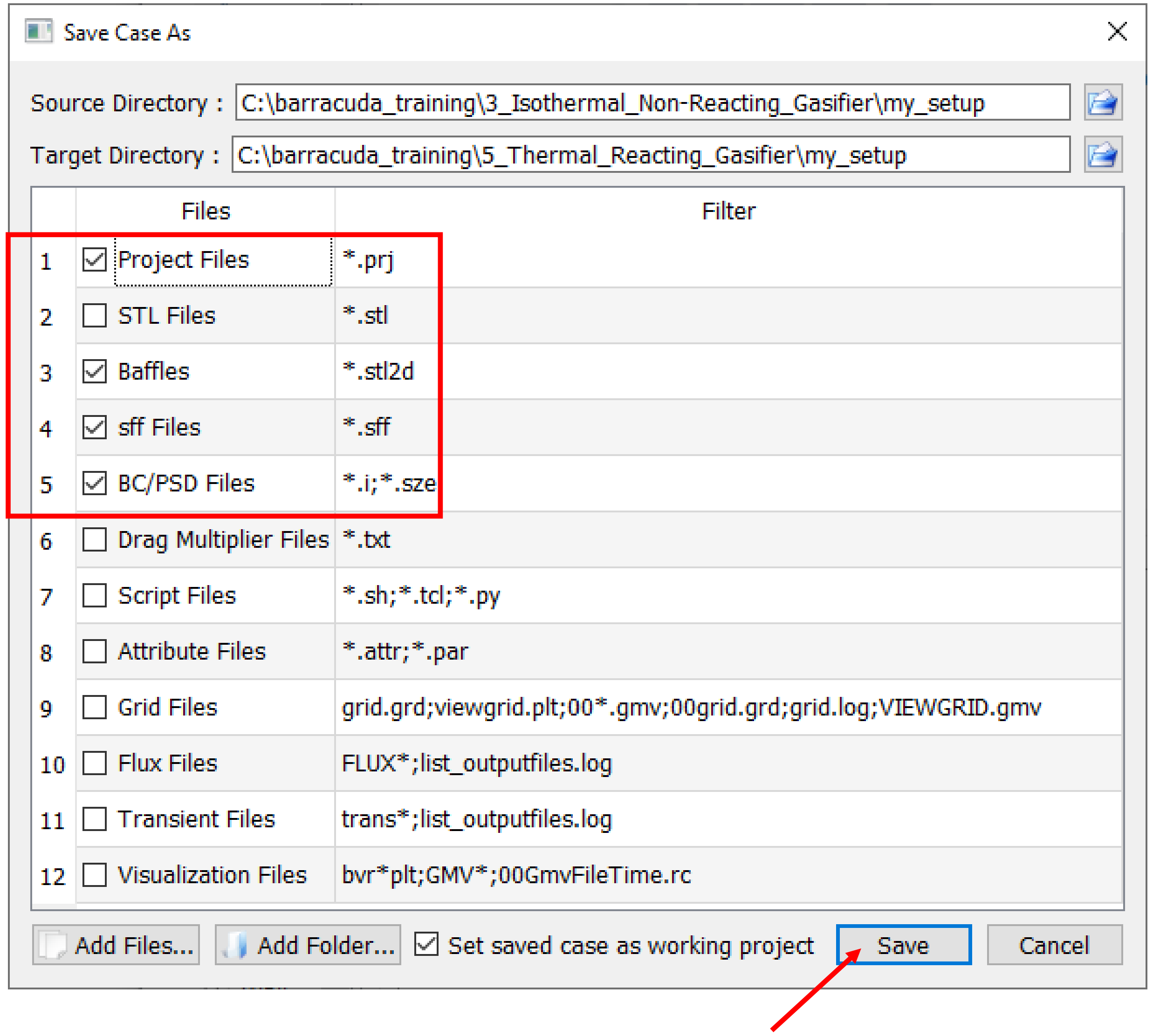
For the current case, keep:

- Project Files
- .sff, .i Files

Because this Gasifier geometry is more complex, do not keep:

- STL Files
- Grid Files

Also, we don't want to copy over any results files (Flux, Transient, or Tecplot).



Gridding

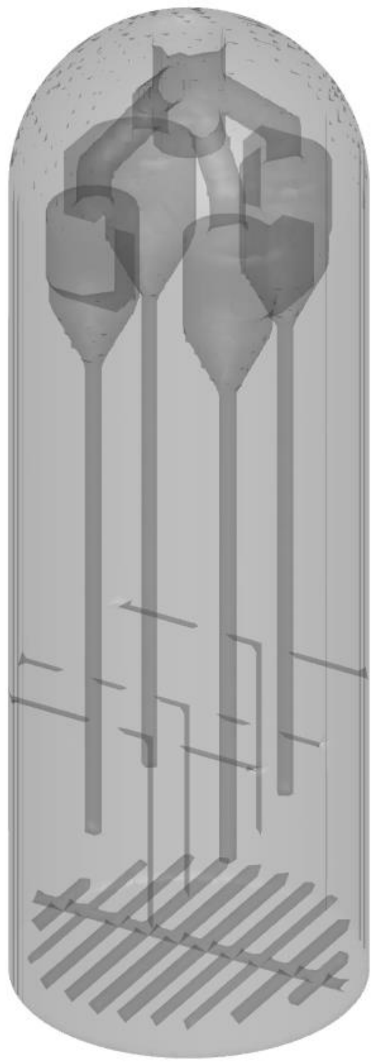
Gridding: Add the New STL File and set new Grid cells

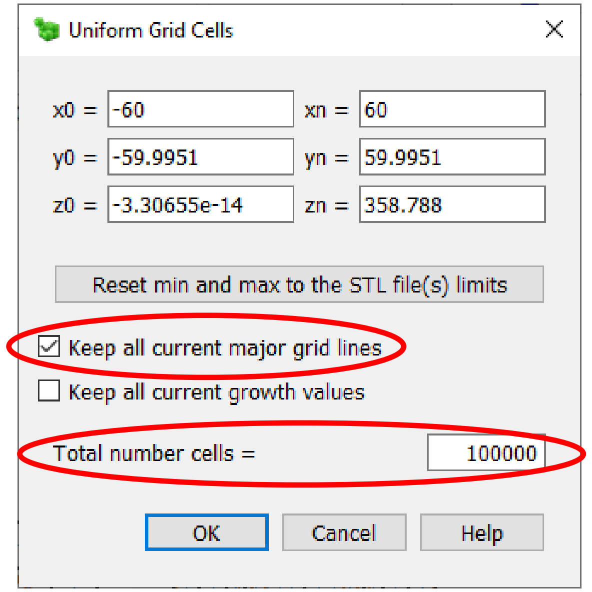
In the Setup Grid section:

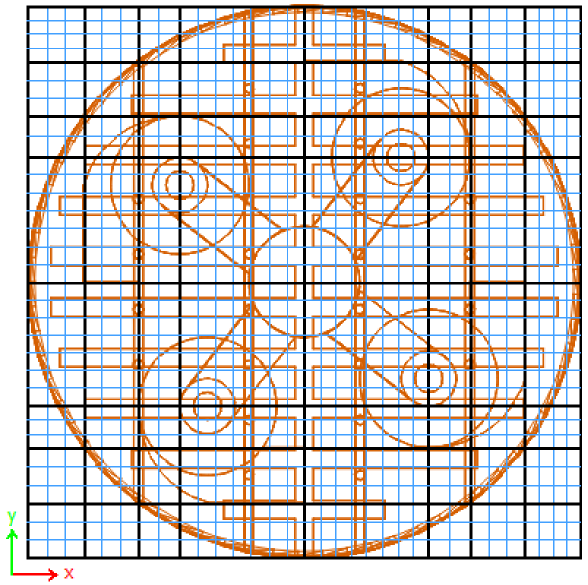
- Navigate to Geometry tab
- Highlight gasifier_isothermal_non-reacting.stl and click Remove Geometry
- Click Add Geometry and select gasifier_thermal_reacting.stl

There are more complex internals in this STL than the previous gasifier:

- Navigate to Grid Controls
- Click on Set uniform grid
- Select Keep all current major grid lines
- Change the total number of cells to 100,000
- Generate the grid
- View Output → View Transparent Model to see the areas that need more grid lines to capture all the geometry







Modify the Grid to Capture Internal Structures

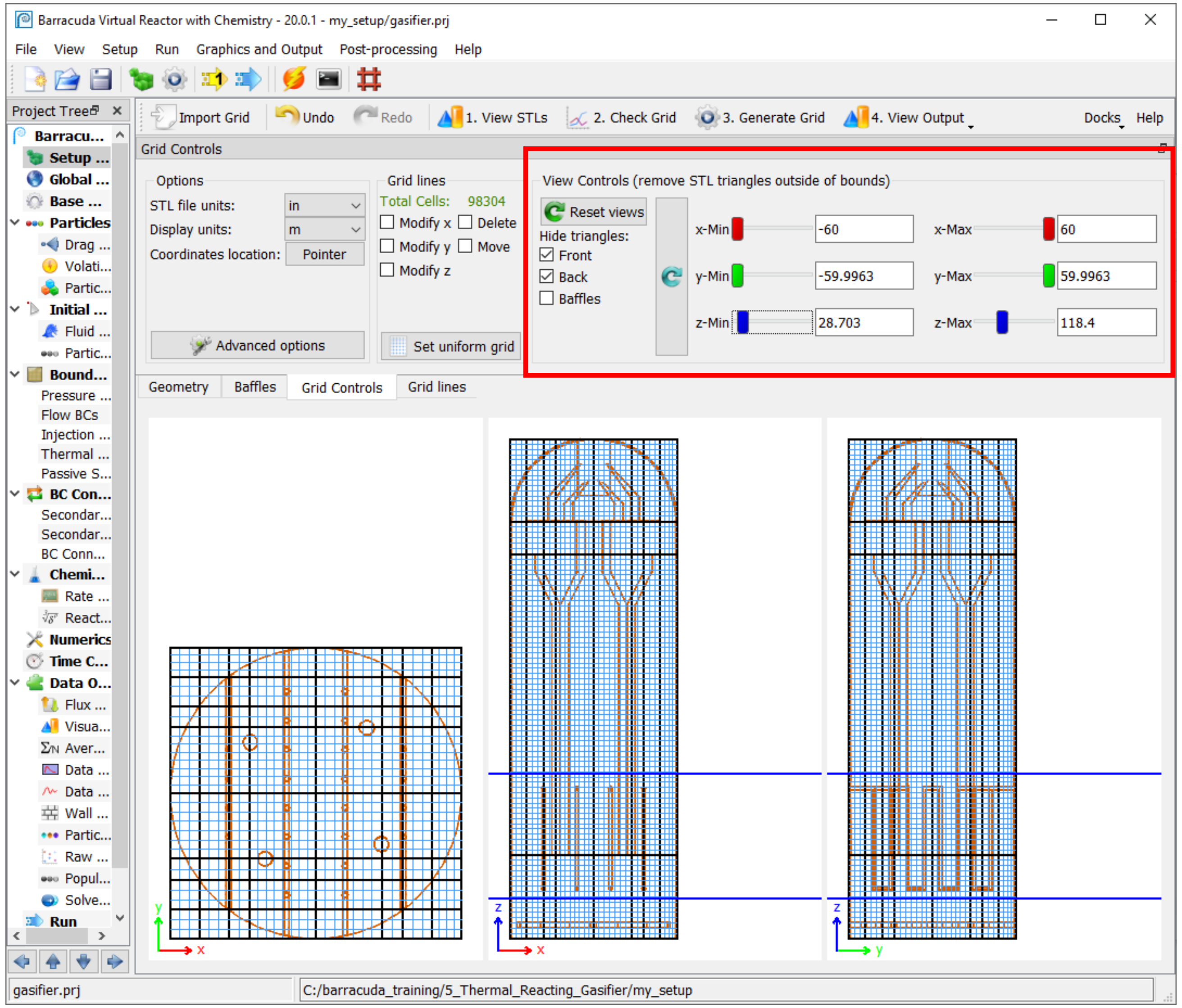
With this geometry, and with most real systems, you will not be able to capture everything perfectly.

Instead, try to capture everything fairly well, without completely missing any structures.

The heating coils are too small to capture using grid lines on all sides. Instead, use the "cross" strategy of intersecting grid lines inside the heating coils.

The sparger arms are big enough that you should be able to hit most of them with grid lines on all sides.

Using the subset sliders in the Grid Controls tab can be very useful to "hide" sections of the geometry while gridding more complex features.

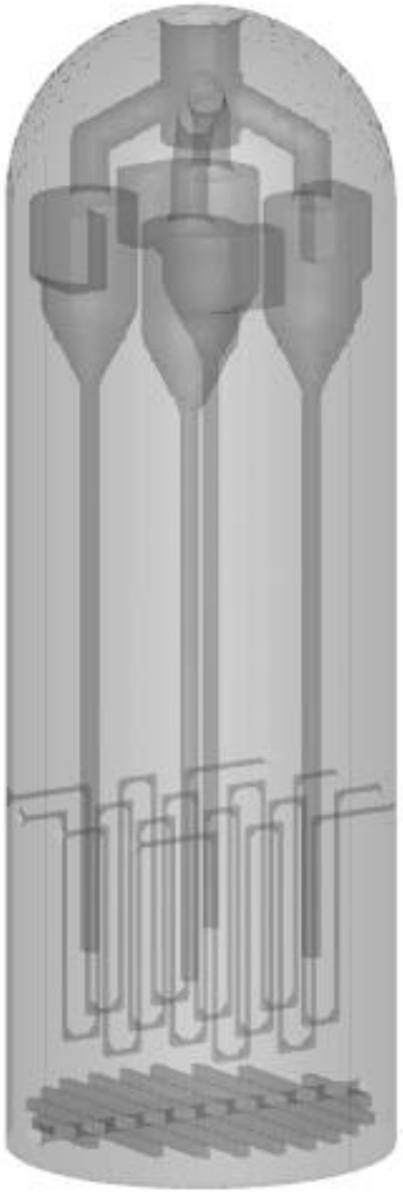


The Final Grid

As guidelines, here are the number of real and null cells in the grids for the pre-setup versions of the gasifiers:

Isothermal, Non-Reacting: 28,556
Thermal, Reacting: 119,658

Show your final grid to the instructor before proceeding to further project setup.



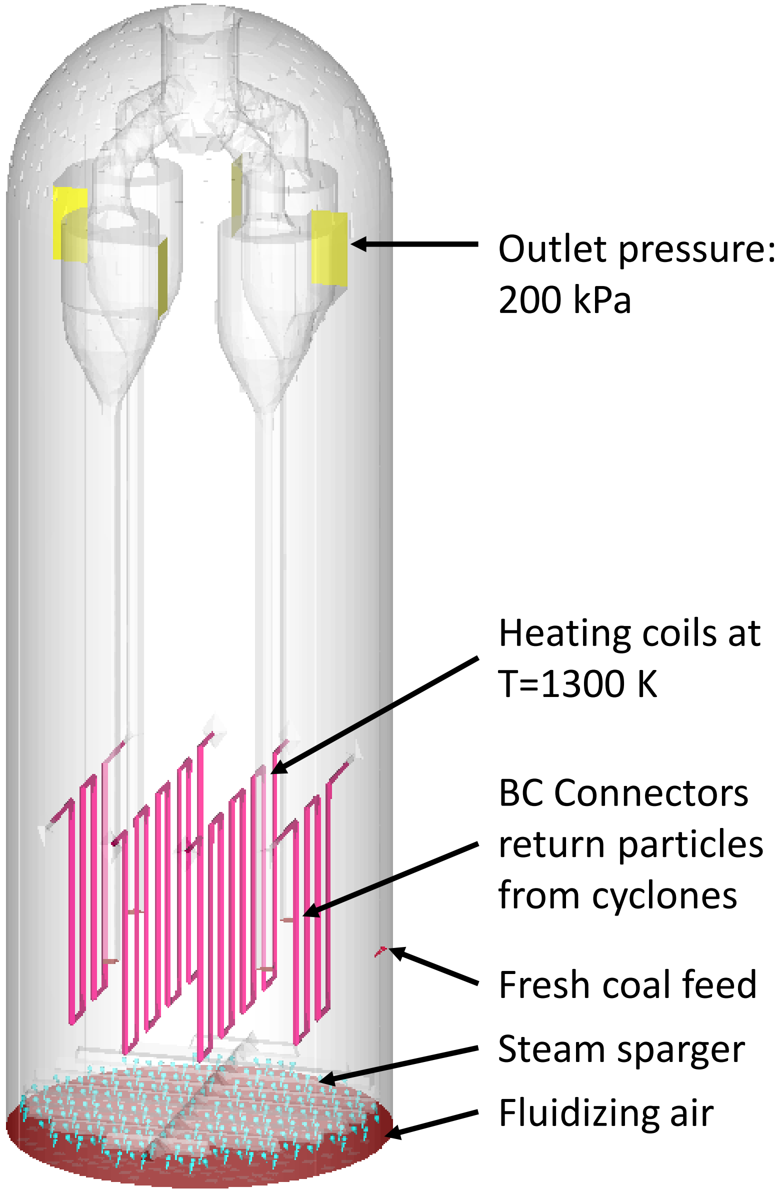
Setup

Process Sheet

Thermal calculations are enabled, initial temperature of particles and gas in bed set to 1300 K.

Chemical reactions are included.

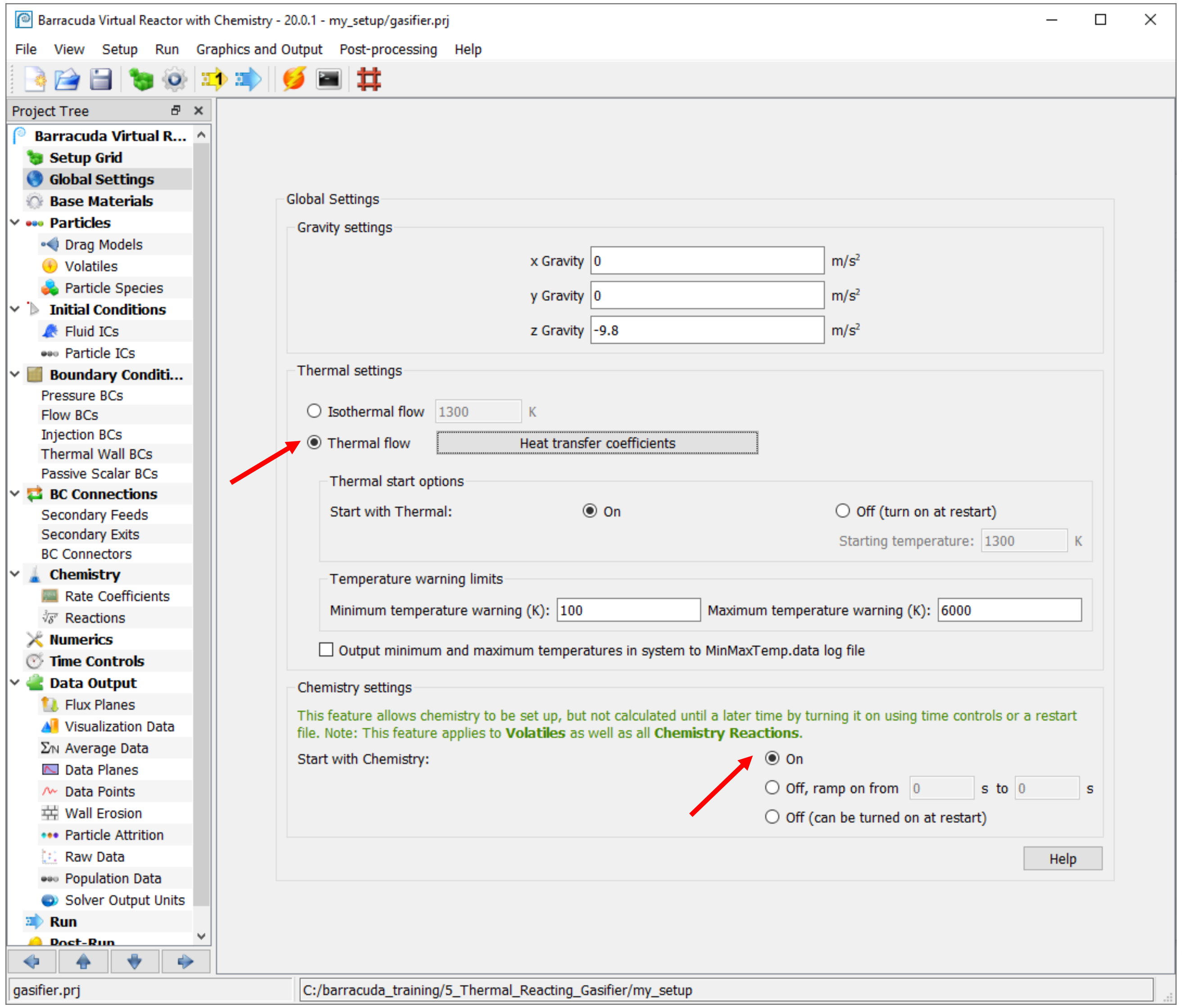
Boundary	Fluid Flow	Particle Flow
Fluidizing Air	Mass flow rate = 0.691 kg/s Temperature = 700 K Gas (mass fractions): 0.77 N_2, 0.23 O_2	None
Steam Sparger through 204 injection nozzles	Mass flow rate = 0.296 kg/s Velocity = 10 m/s Temperature = 900 K Gas: pure H_2O	None
Fresh Coal Feed	Mass flow rate = 5e-3 kg/s Velocity = 5 m/s Temperature = 500 K Gas (mass fractions): 0.77 N_2, 0.23 O_2	Fresh coal at 1 kg/s
Cyclone Diplegs	Controlled by BC Connector	Controlled by BC Connector



Enable Thermal Flow

In the Global Settings section

- Select Thermal Flow to enable thermal calculations
- Start with Chemistry On



When enabling thermal calculations, it is important to check your Base Materials section to make sure all materials have valid thermal properties.

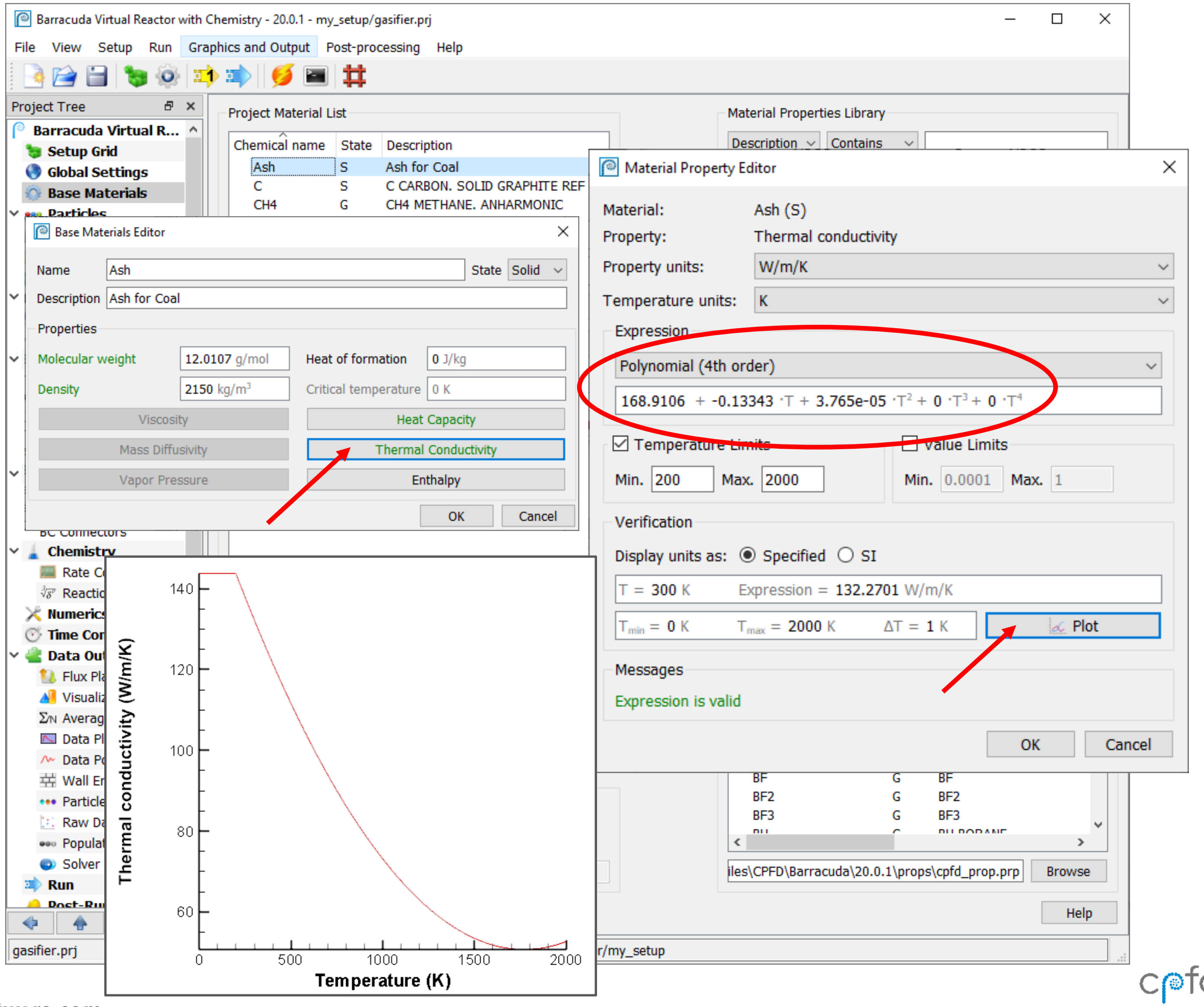
Thermal conductivity, specific heat, and viscosity are all described by various methods in Barracuda VR. It is important that these methods are valid within the temperature range expected in the simulation.

Automated Plotting of Polynomial Material Properties

This feature allows users to plot the expressions (Polynomial (4th order), Double Polynomial, Interpolated from SFF File) for property data in Base Materials.

You can visualize property data over a specified temperature range.

To view the plot for the polynomial, click on the Plot button in the GUI to launch Tecplot.

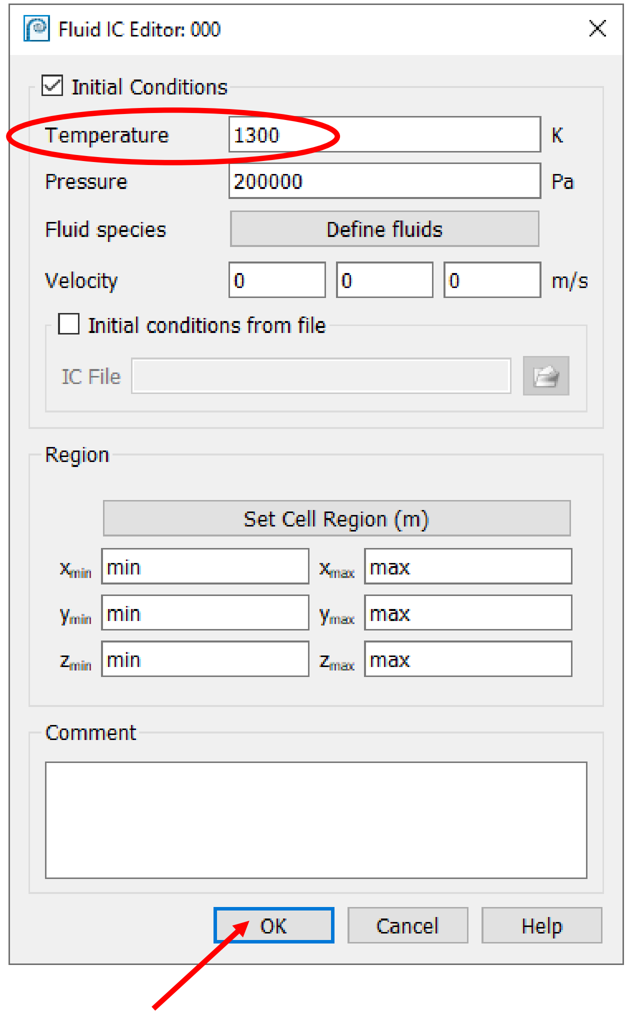


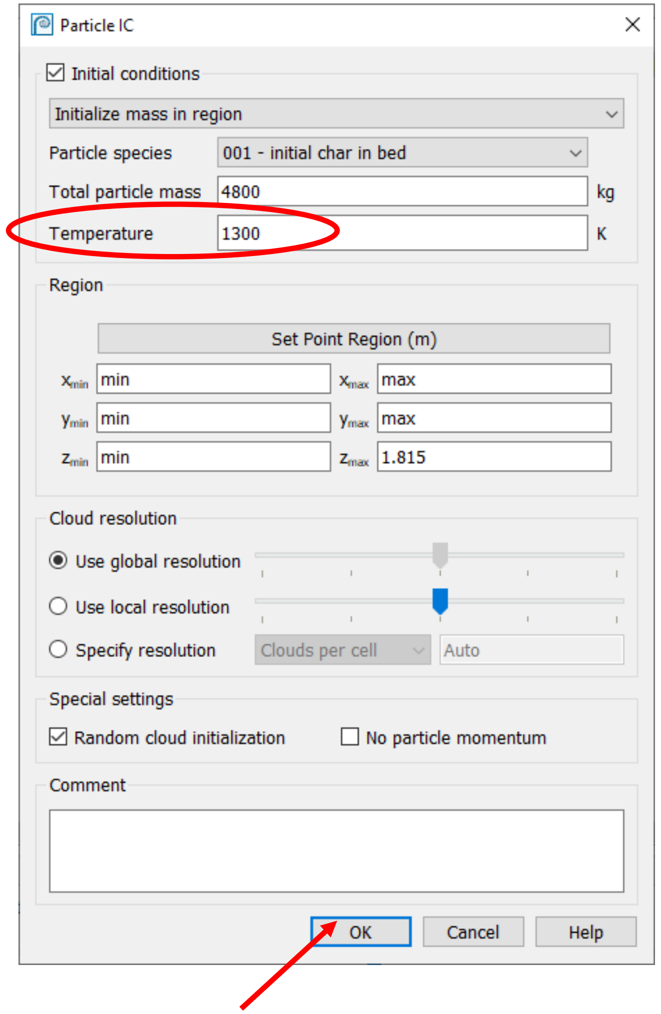
Temperatures of Initial and Boundary Conditions

When the isothermal, non-reacting gasifier was set up, it was not important to consider the temperature specifications for initial and boundary conditions.

However, when turning on thermal calculations, it is important to review the settings (some of them may have been initialized to default values by Barracuda), and apply correct temperatures to all initial and boundary conditions.

Ensure that both Fluid and Particle IC are set to 1300 K





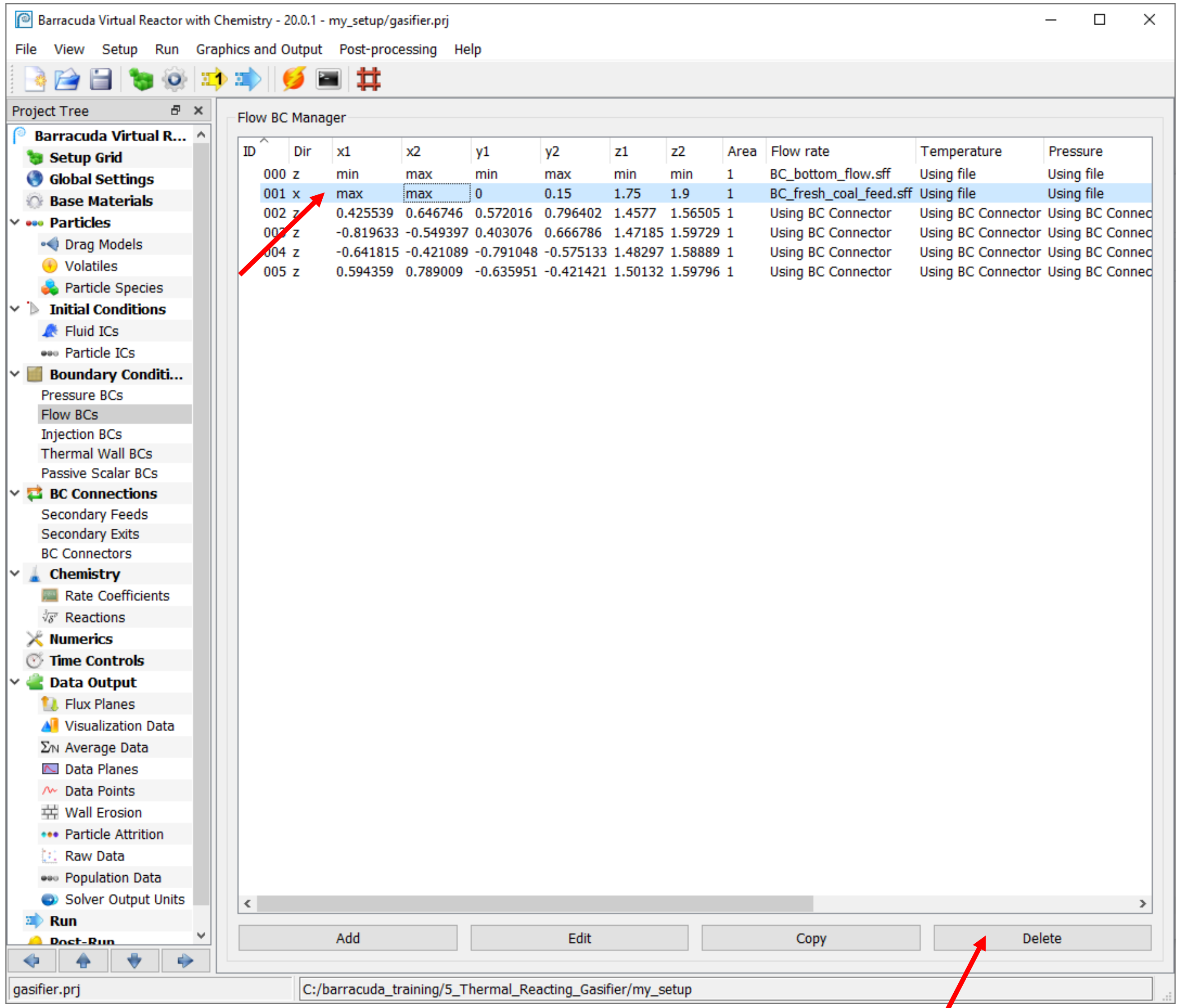
Fresh Coal Feed Injection

Instead of using a flow boundary on the wall surface to introduce fresh coal into the system, we will use an injection BC.

This allows for injection of fluid and/or particles at a specific angle and location in the system.

Before creating this injection BC, delete the fresh coal feed flow BC:

- Select the flow BC
- Click on Delete



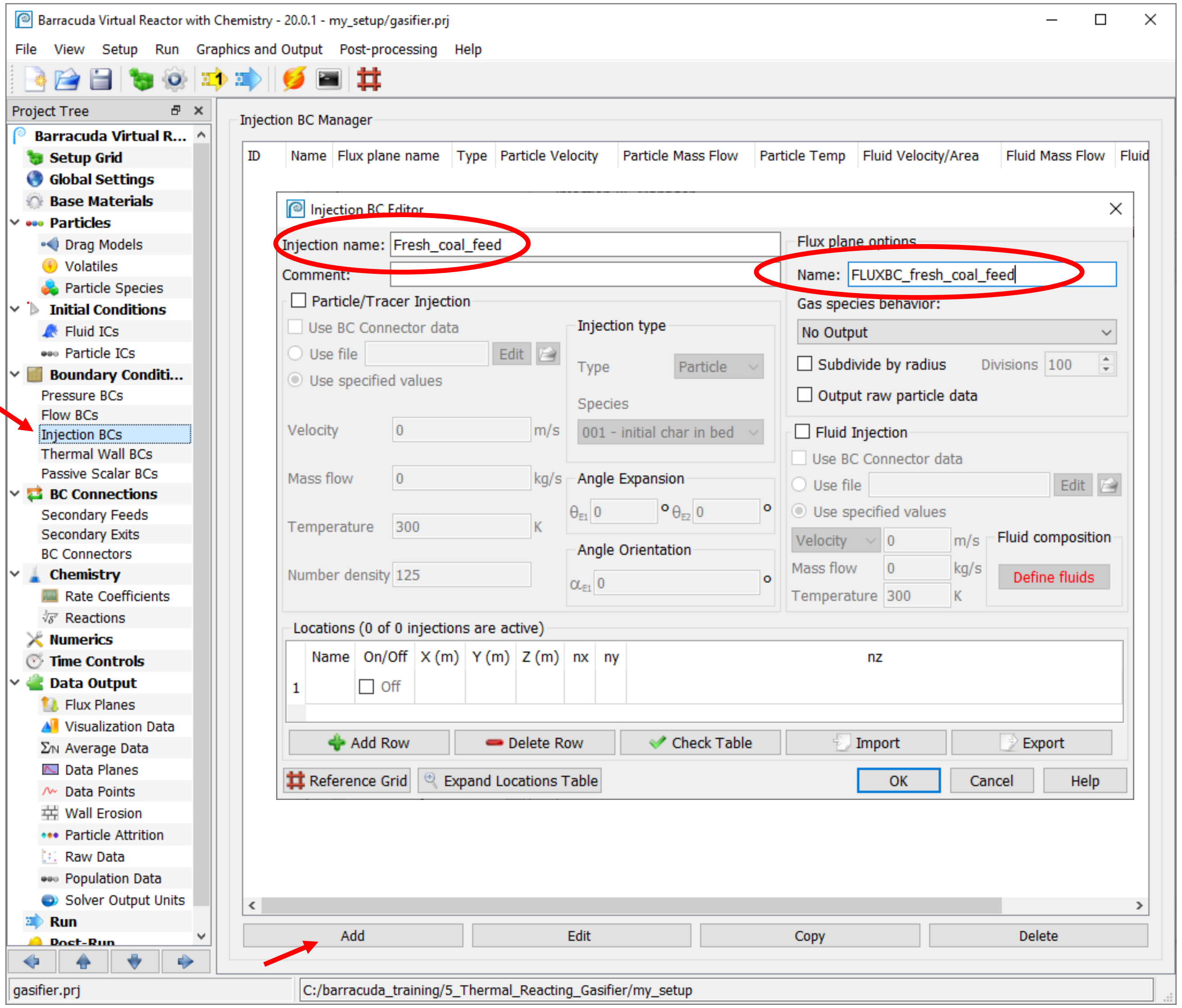
Fresh Coal Feed Injection

Click on Injection BC:

- The Injection BC page allows for the injection of fluid and/or particles to be specified at a given location, velocity, mass flow rate, and direction
- One or more injection sets may be created in a project file and each injection set may consist of one or more injection point locations
- Injection points within an injection set will have a common composition and velocity
- Each injection set can have:
  - Particle or Tracer injection alone
  - Fluid injection alone
  - Both particle/tracer and fluid injection

Click on Add

Start by entering an Injection Name and Flux Plane Name



Fresh Coal Feed Injection

Select Particle/tracer Injection

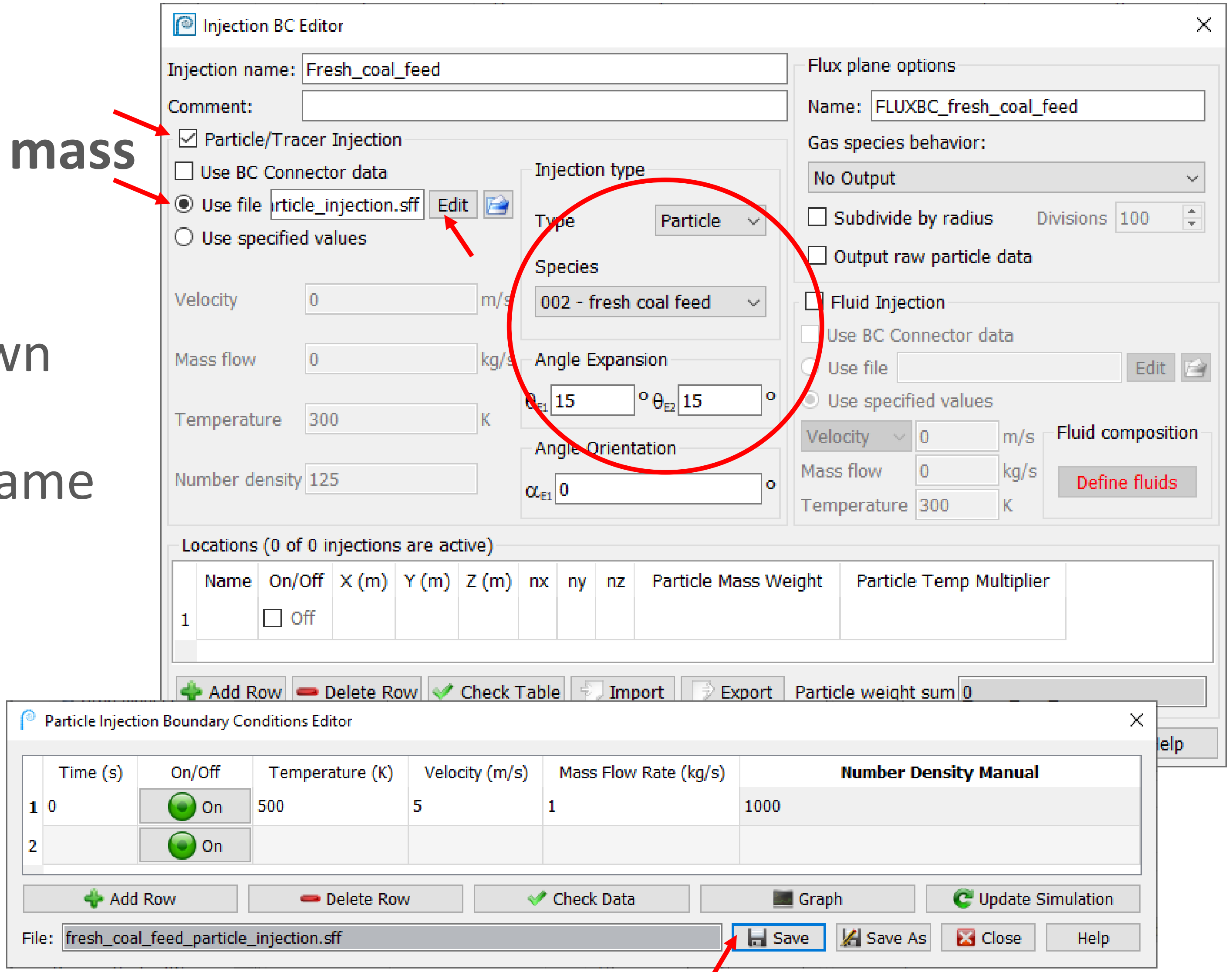
Select Use file to specify the particle mass flow rate:

- Click on Edit
- Enter the appropriate values shown below
- Save the file using a descriptive name

Select Particle for Type

Select Fresh coal feed for Species

Set the Angle Expansion to 15



Fresh Coal Feed Injection

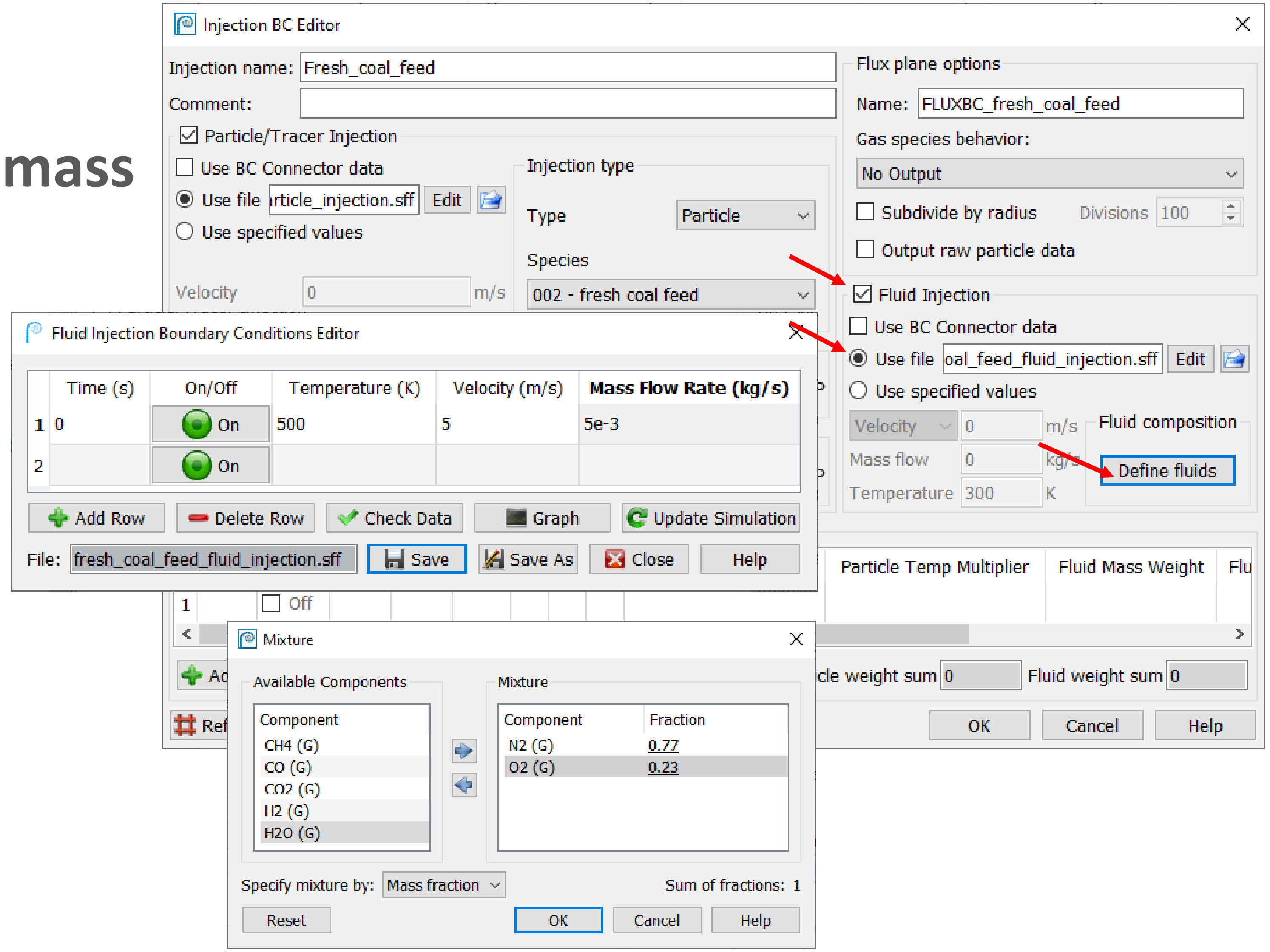
Select Fluid Injection

Select Use file to specify the fluid mass flow rate:

- Click on Edit
- Enter the appropriate values
- Save the file using a descriptive name

Specify the Fluid Composition

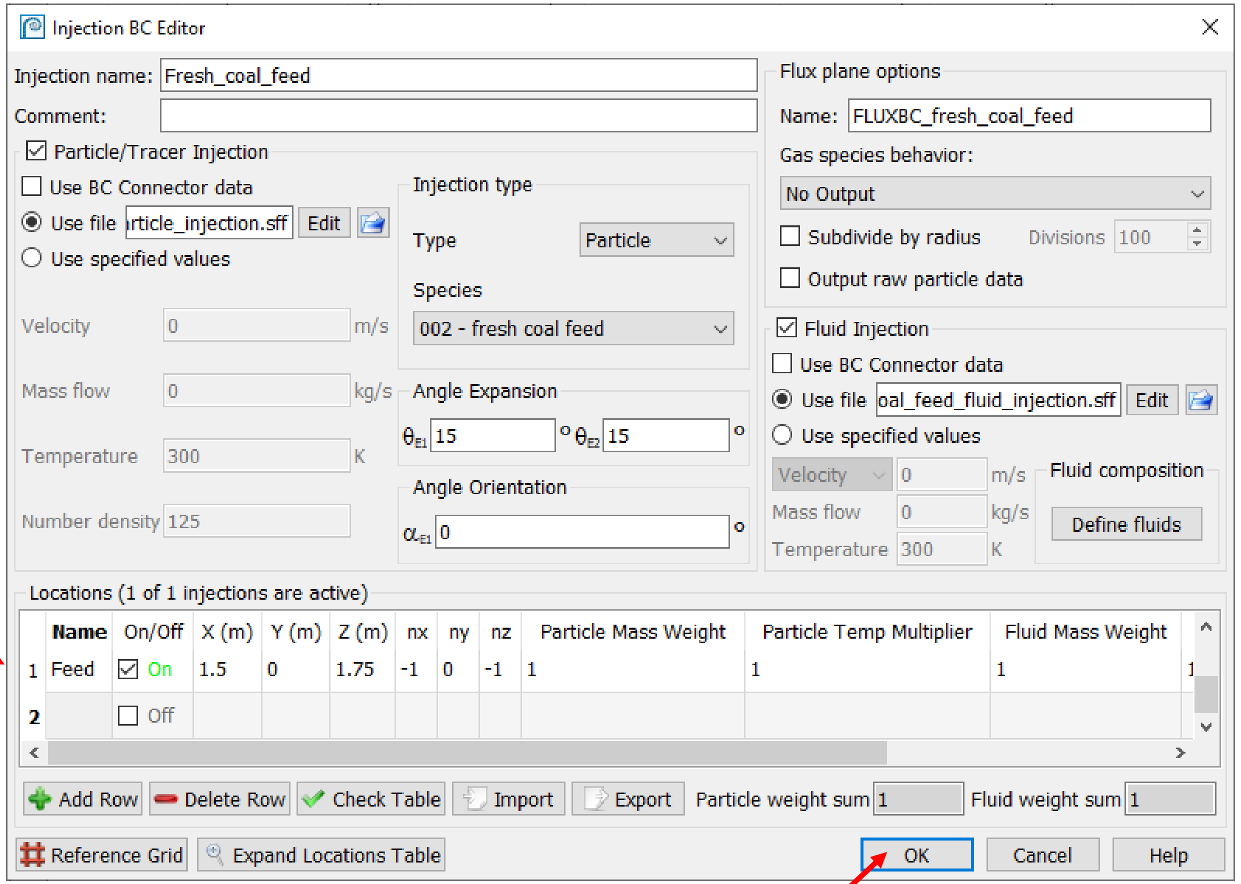
- 0.77 N2
- 0.23 O2



Fresh Coal Feed Injection

Specify the location of the fresh coal feed nozzle:

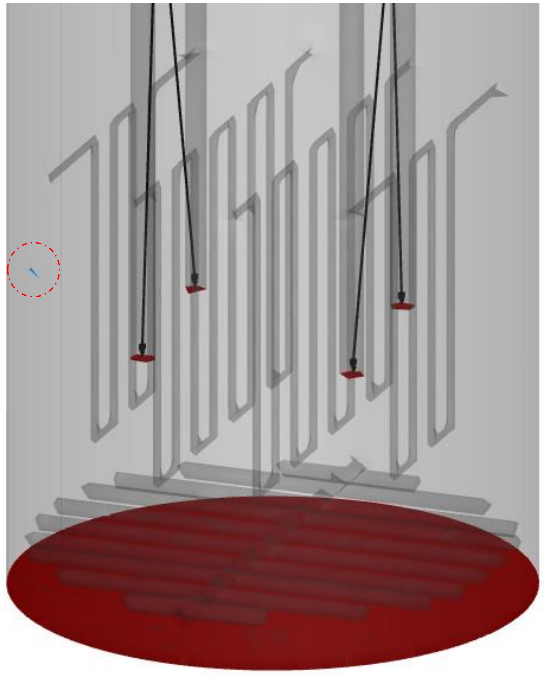
- Enter an appropriate Name for the injection point.
- Select “On”.
- Enter the x,y,z location and the directional vectors:
  - x = 1.5 m
  - y = 0 m
  - z = 1.75 m
  - nx = -1
  - ny = 0
  - nz = -1
- Enter a value of 1 for:
  - Particle Mass Weight
  - Particle Temp Multiplier
  - Fluid Mass Weight
  - Fluid Temp Multiplier
- Click OK

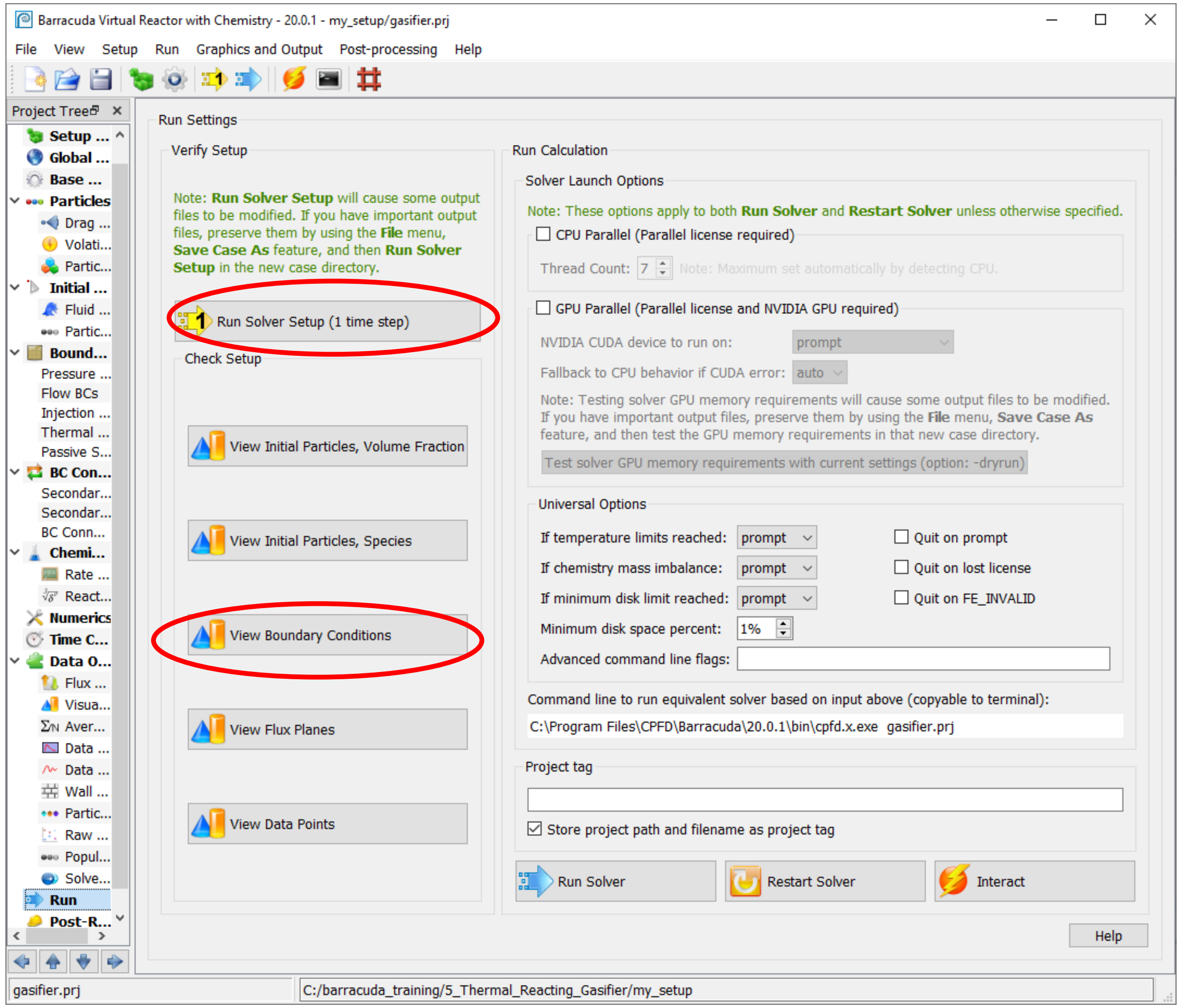


Fresh Coal Feed Injection

Before continuing with the project setup, check the location of the nozzle:

- Run Solver Setup
- View Boundary Conditions



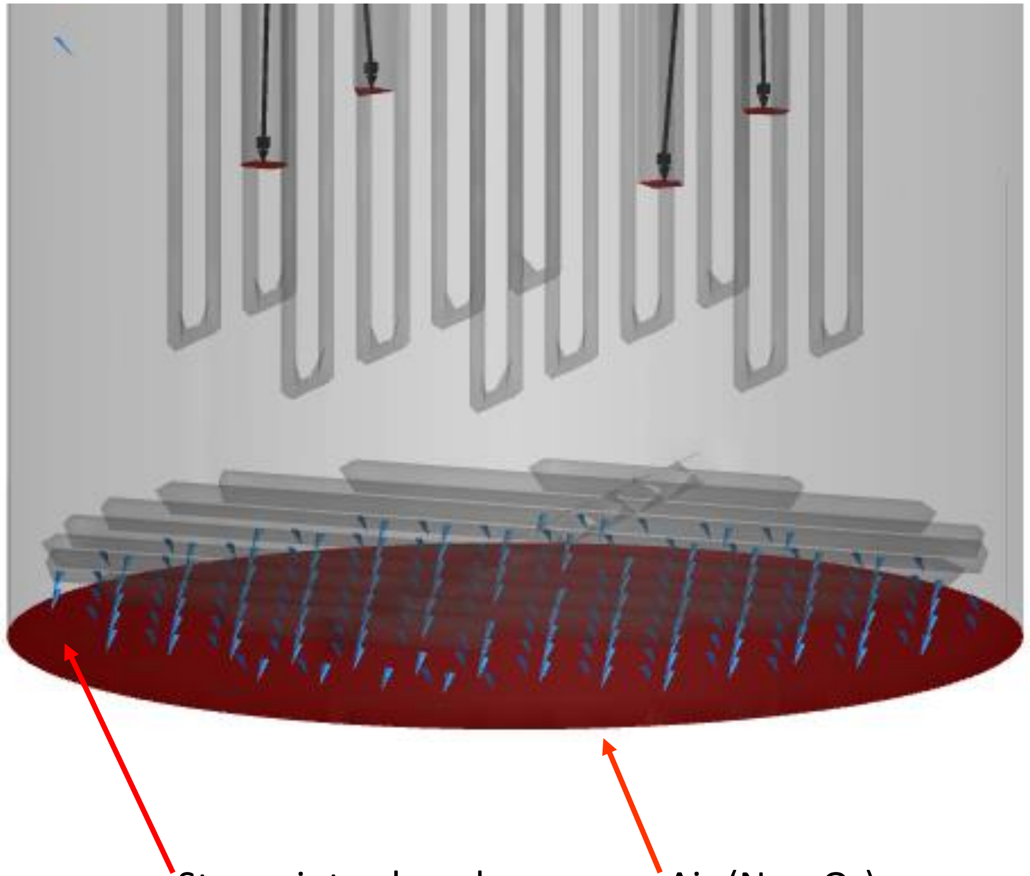


Separate the Air and Steam BCs

Exclusion of the gas sparger geometry was one simplification in the previous gasifier project.

Now that we are including the sparger, it is necessary to separate the fluidizing air (N2+O2) from the steam:

- Keep the bottom-most flow BC as a uniform air distributor.
- Create an injection BC on the bottom surface of the sparger, and introduce 100% steam at this location through 204 nozzles



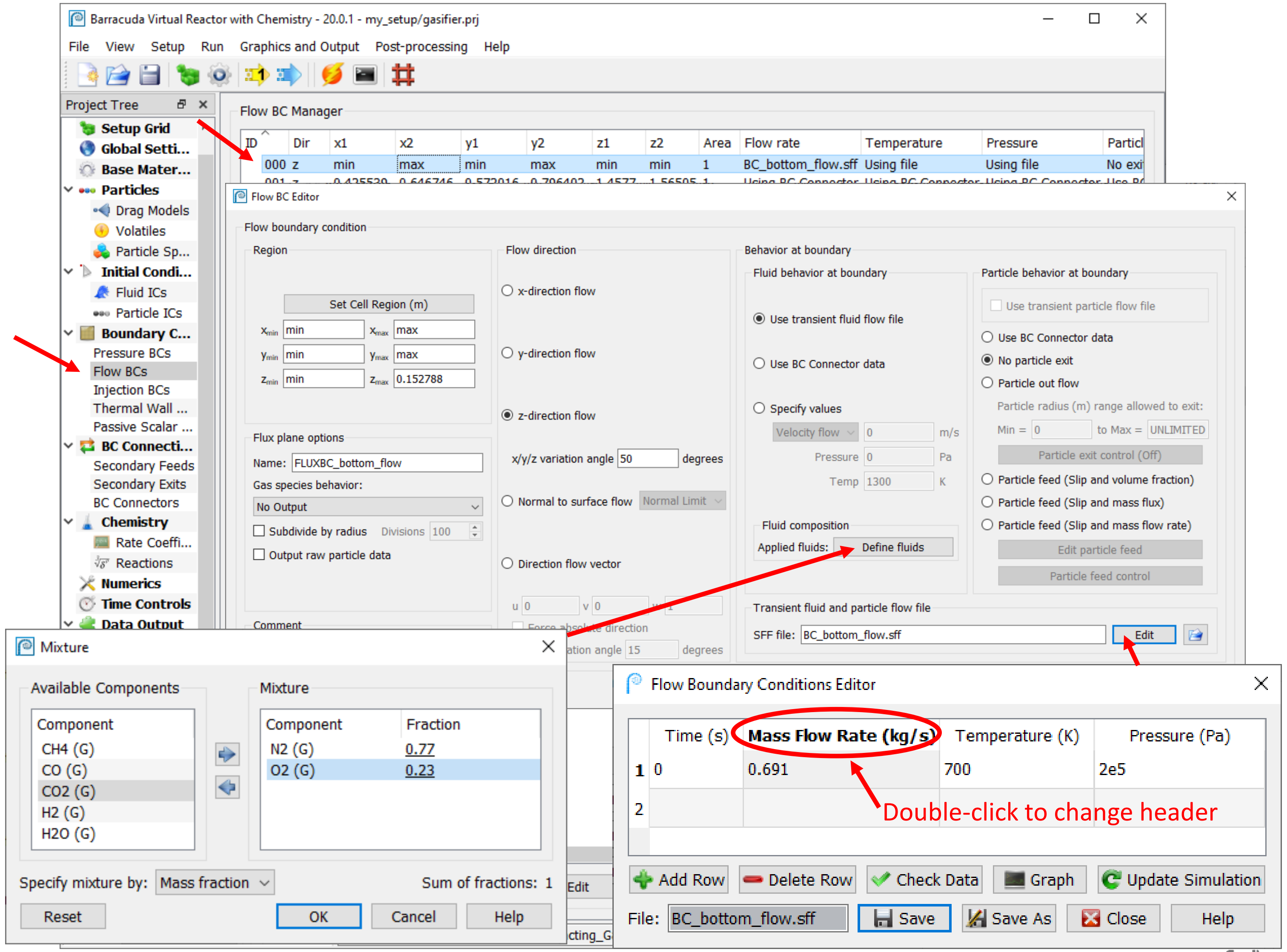
Steam introduced through 204 injection points located on the sparger

Air (N_2 + O_2) introduced through flow BC on bottom surface of vessel

Flow BC as Uniform Air Distributor

Navigate to Flow BCs window

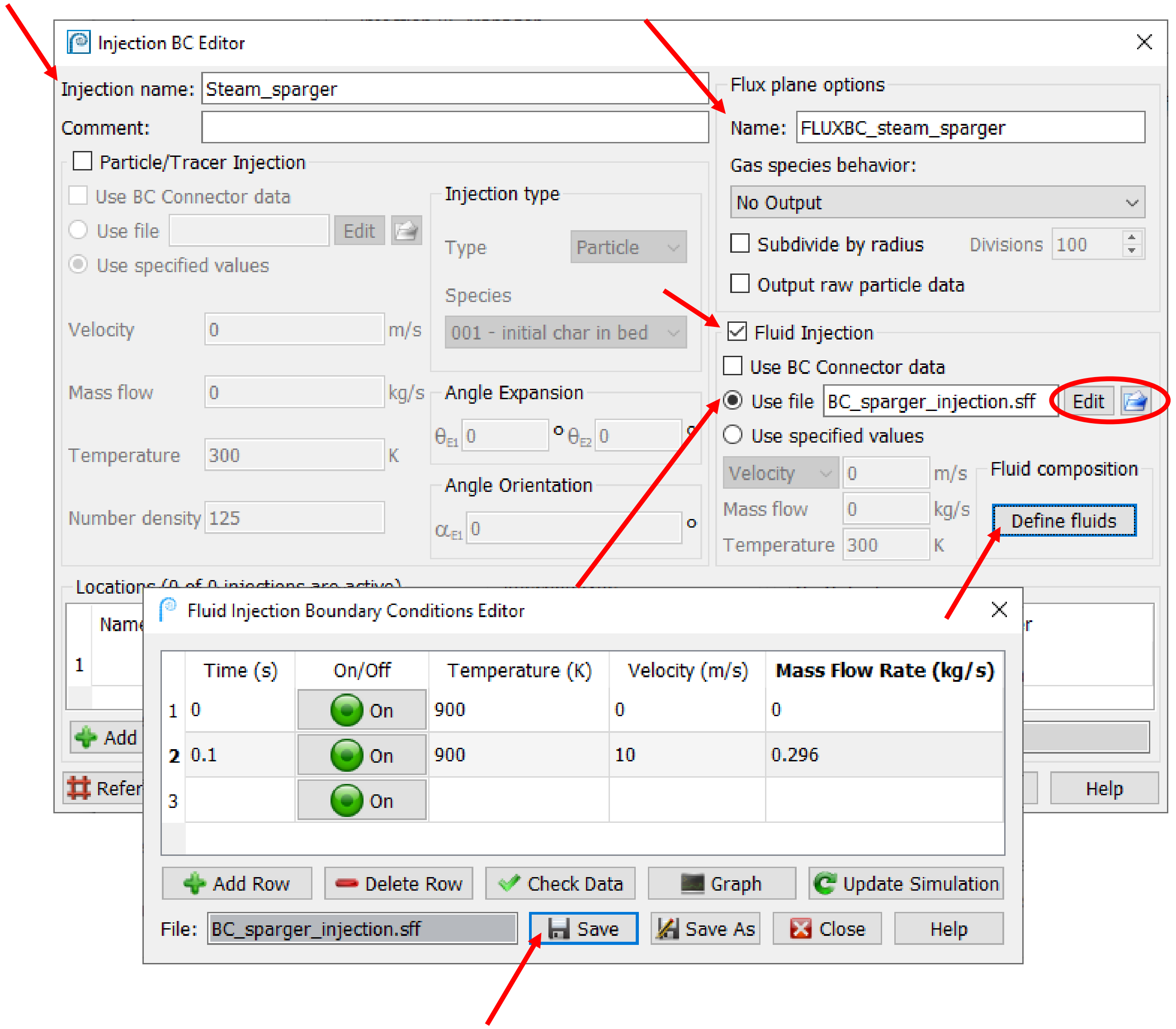
- Edit bottom flow
- Click on Define Fluid
  - 0.77 N2
  - 0.23 O2
- Edit Transient File
  - 700 K Temperature
  - 0.691 kg/s Mass flow rate (double click on header to change from Velocity to Mass flow rate)



Steam Injection BC

Create a new injection BC for the steam sparger:

- Navigate to Injection BCs window
- Click on Add
- Enter an Injection Name
- Enter a Flux Plane name
- Select Fluid Injection
- Use file to specify the fluid mass flow rate:
  - Click on Edit
  - Enter the appropriate values
  - Save the file using a descriptive name
- Click on Define fluids
  - 100% H_2O



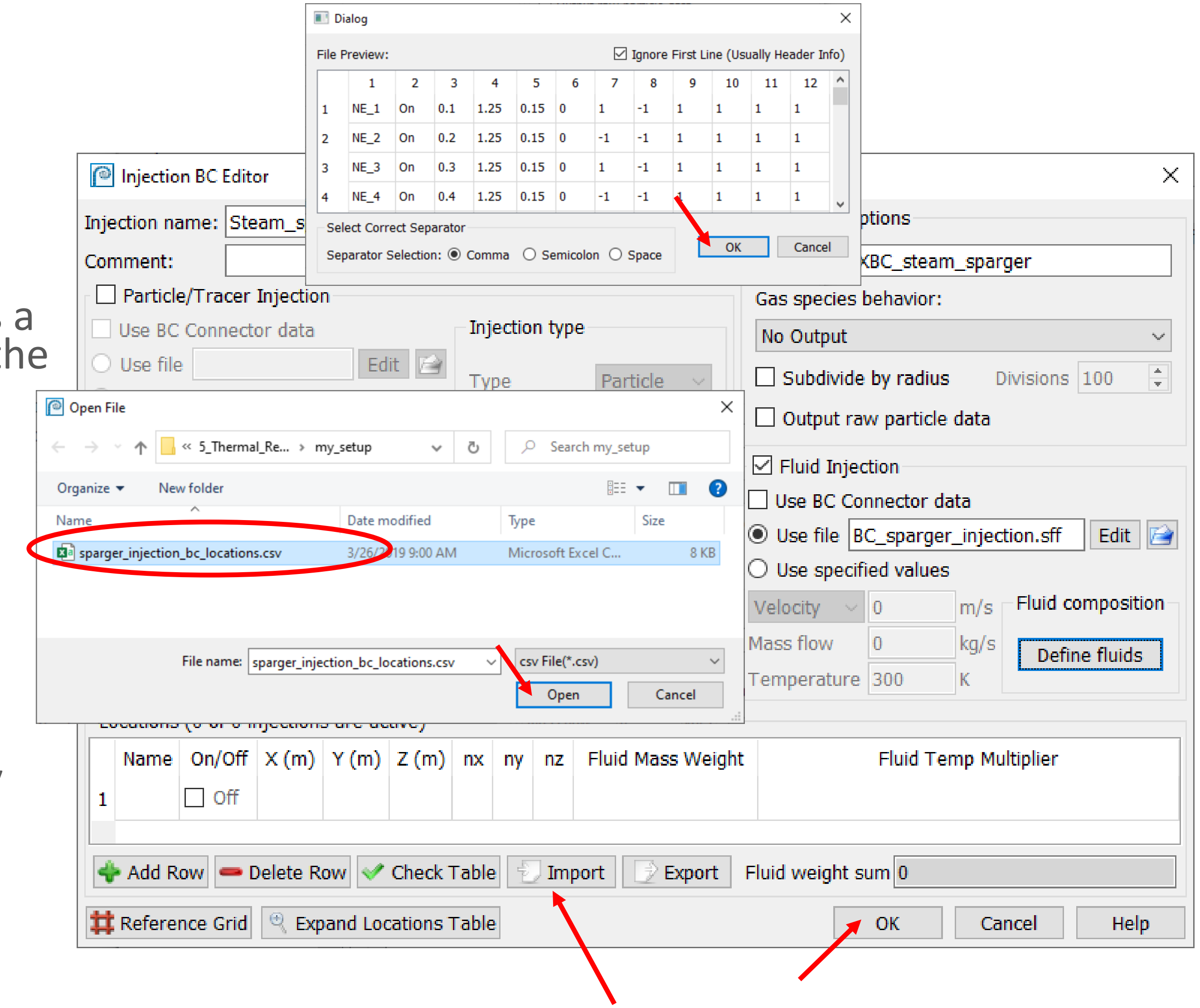
Steam Injection BC

Creating and editing large sets of location and direction data is most conveniently done in Excel, Open Office, or other spreadsheet application:

- Data from the Locations table can be exported as a comma-separated value (CSV) file by clicking on the Export button in the Barracuda VR GUI
- Once the file has been edited, it can be easily imported into the locations table

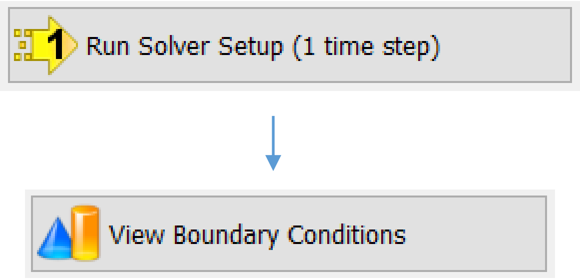
A CSV file containing the locations and directions of the 204 nozzles has already been created for this project:

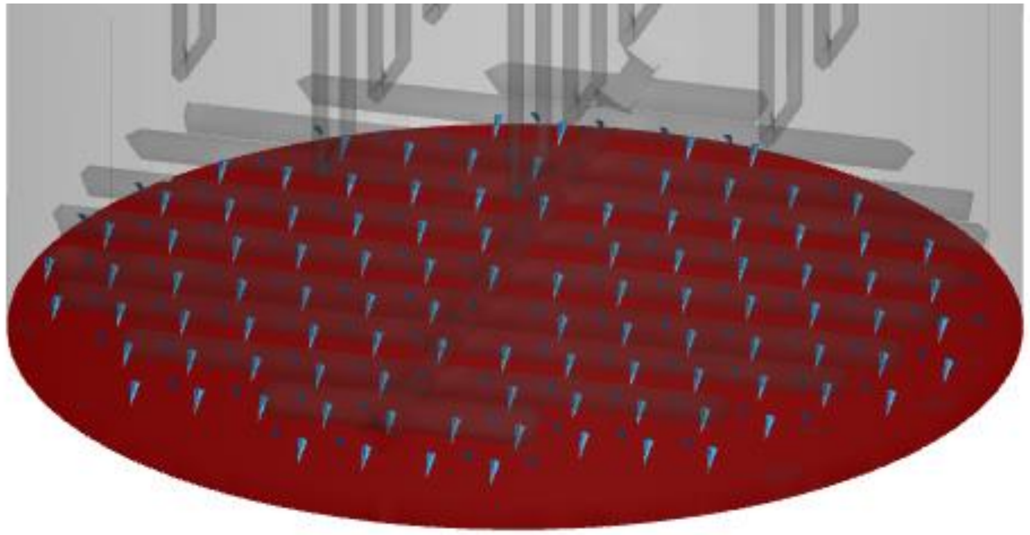
- Click on Import
- Select the file sparger_injection_bc_locations.csv
- Click on Open
- Click OK in the import dialog
- Click OK in the Injection BC Editor

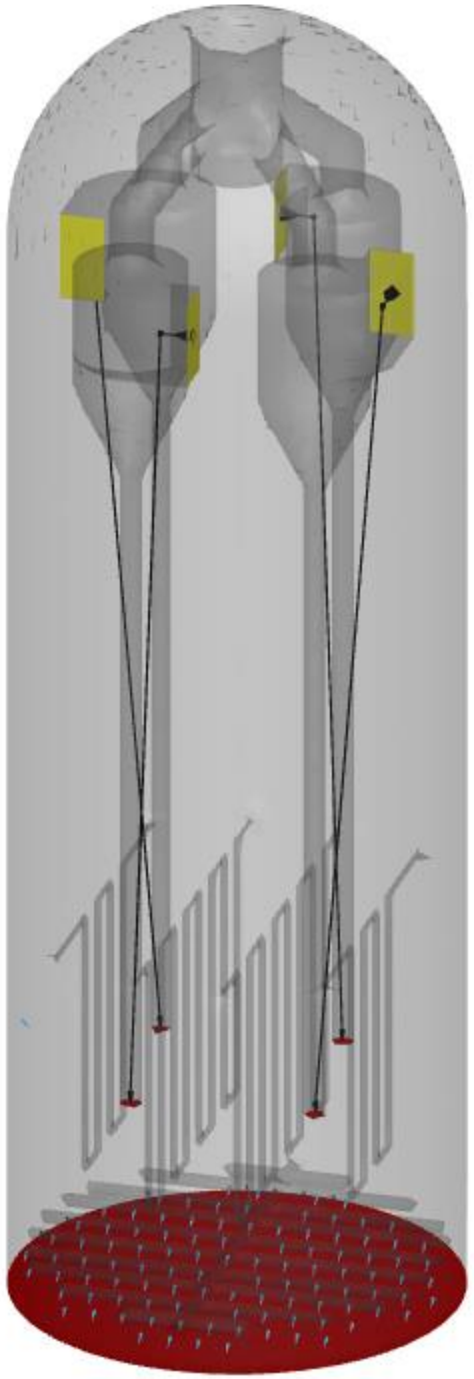


Steam Injection BC

Once the steam injections have been created, run the simulation for a single time step and check the boundary conditions.



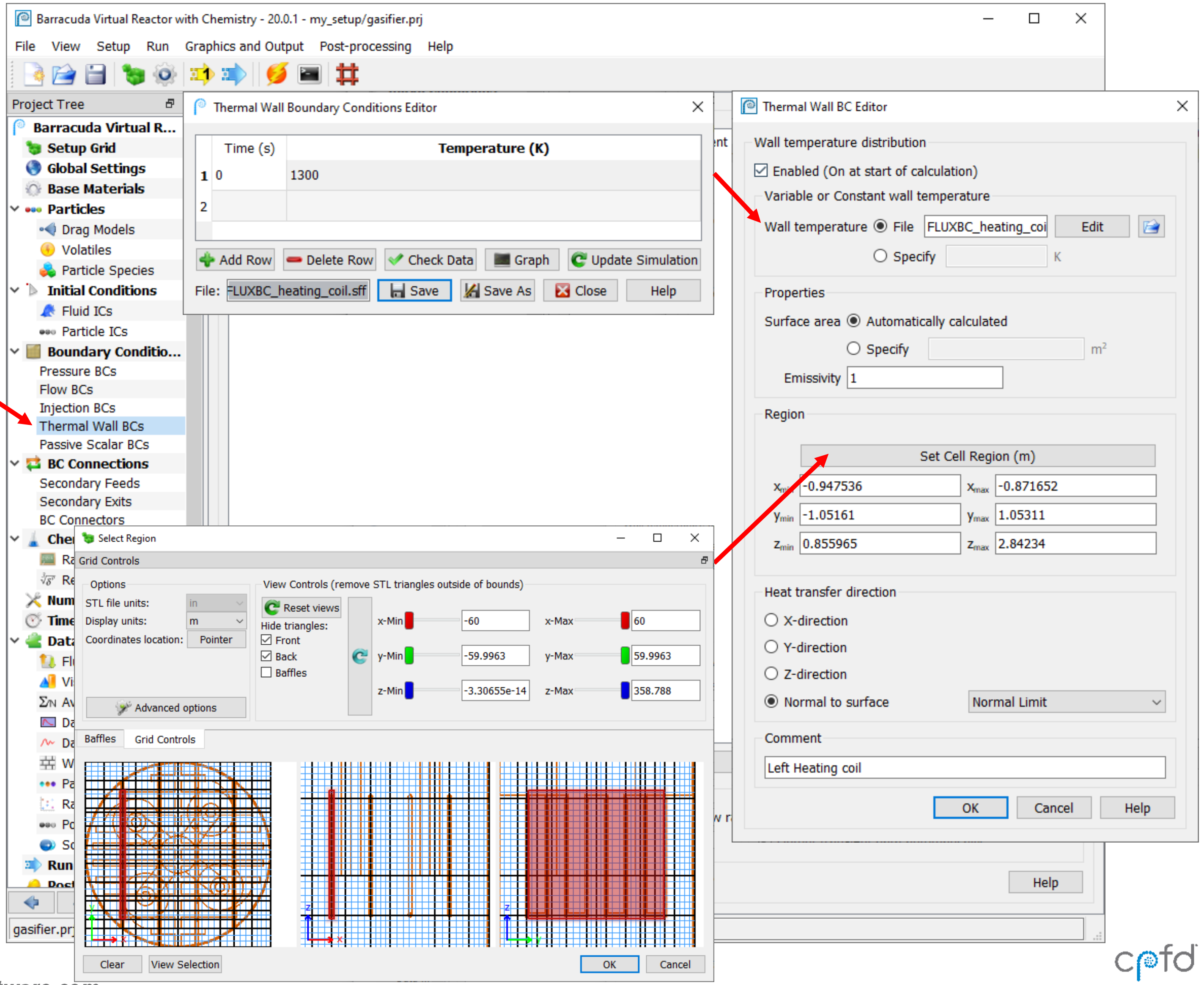




Thermal Wall BCs: Heating Coils

The gasification process requires input of heat. We will define thermal wall BCs on the heating coils:

- Navigate to Thermal Wall BCs
- Click on Add
- Select File
- Click on Edit to set Wall Temperature to 1300 K
- Set the Cell Region (you will need to create three thermal wall BCs to get all the heating coils)
- Enter a descriptive comment if desired
- Click OK
- Repeat for other two blocks of thermal wall BCs to capture all heating coils. Remember to use the same .sff file for all three blocks of thermal walls



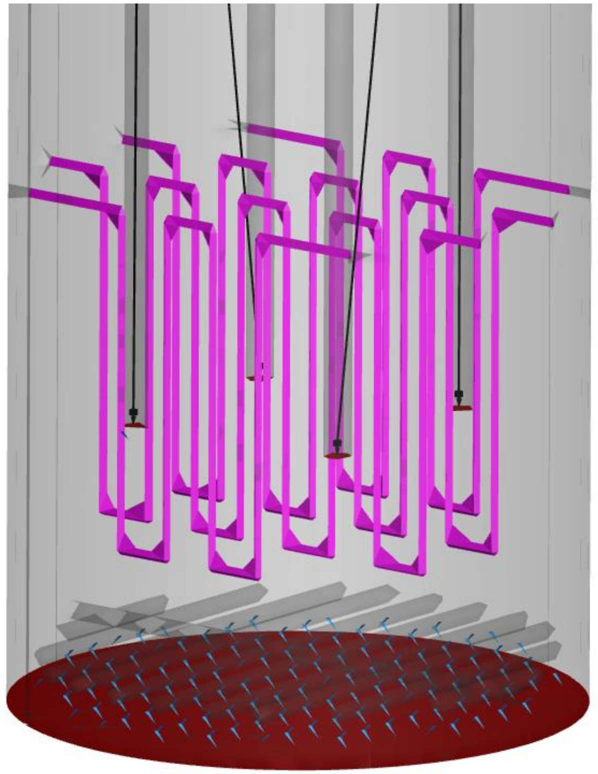
Thermal Wall BCs: Heating Coils

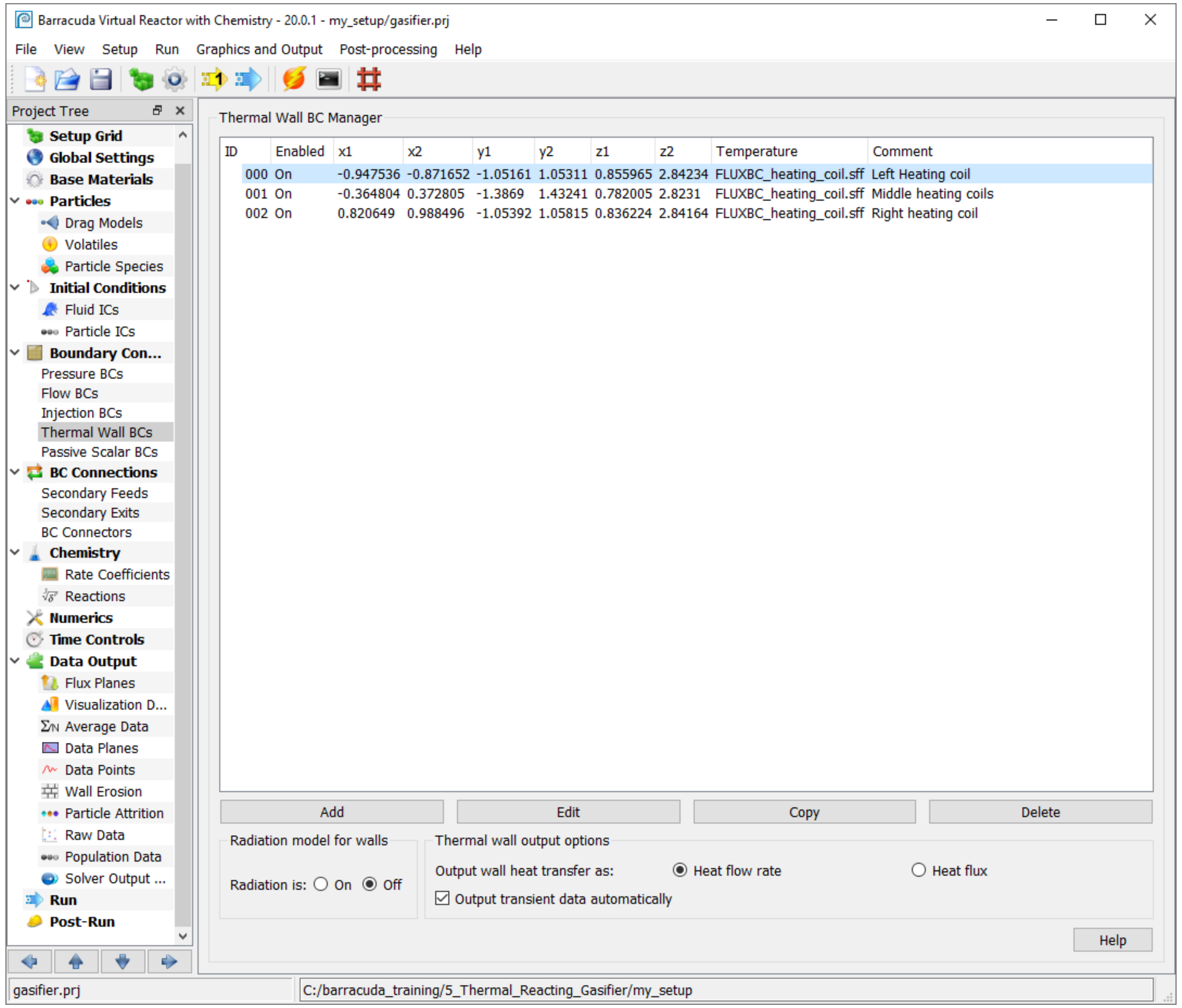
Run Solver Setup (for 1 time-step), and verify that the thermal wall BCs are applied correctly.

Run Solver Setup (1 time step)

↓

View Boundary Conditions

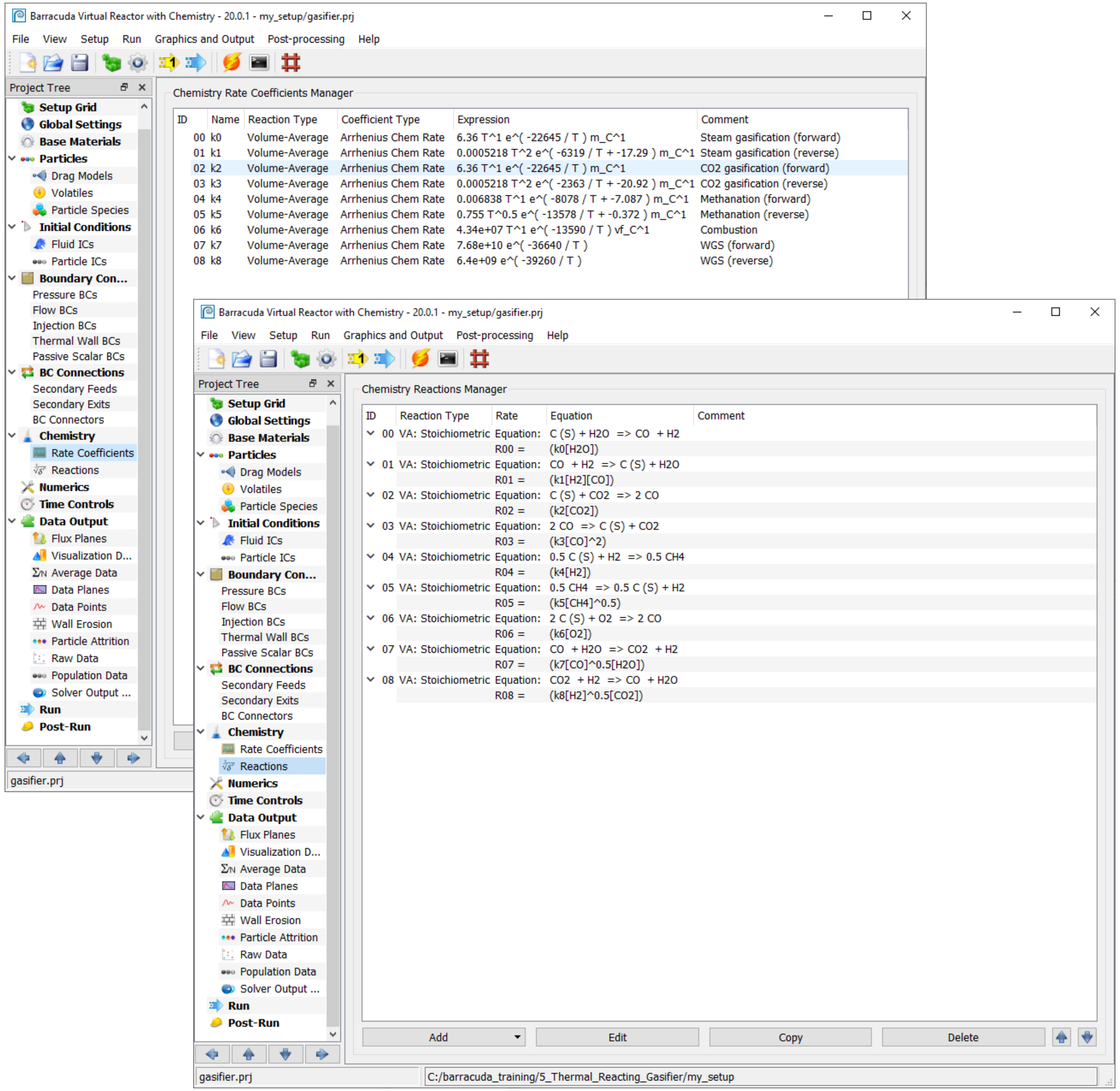




Chemistry

The gasification reactions listed on the next slide need to be input to the chemistry section.

For this training problem, we will use stoichiometric, volume-average chemistry.



Chemical Reactions

Definitions and units:

- m_C = mass concentration of carbon (kg/m^3)
- T = fluid temperature (K)
- θ_C = carbon volume fraction
- [X] = mole concentration of species X (mol X / m^3 gas volume)

Reaction	Stoichiometric Equation	Reaction Rate Expression (mol m^{-3} s^{-1})	Source
Steam gasification	$C(s)+H_2O \rightarrow CO+H_2$	$r_{1,f} = 6.36 m_C T \exp\left(\frac{-22{,}645}{T}\right)[H_2O]$	Syamlal, 1992
	$CO+H_2 \rightarrow C(s)+H_2O$	$r_{1,r} = 5.218\times10^{-4} m_C T^2 \exp\left(\frac{-6{,}319}{T} - 17.29\right)[H_2][CO]$	
CO_2 gasification	$C(s)+CO_2 \rightarrow 2CO$	$r_{2,f} = 6.36 m_C T \exp\left(\frac{-22{,}645}{T}\right)[CO_2]$	Syamlal, 1992
	$2CO \rightarrow C(s)+CO_2$	$r_{2,r} = 5.218\times10^{-4} m_C T^2 \exp\left(\frac{-2{,}363}{T} - 20.92\right)[CO]^2$	
Methanation	$0.5C(s)+H_2 \rightarrow 0.5CH_4$	$r_{3,f} = 6.838\times10^{-3} m_C T \exp\left(\frac{-8{,}078}{T} - 7.087\right)[H_2]$	Syamlal, 1992
	$0.5CH_4 \rightarrow 0.5C(s)+H_2$	$r_{3,r} = 0.755 m_C T^{0.5} \exp\left(\frac{-13{,}578}{T} - 0.372\right)[CH_4]^{0.5}$	
Combustion	$2C(s)+O_2 \rightarrow 2CO$	$r_4 = 4.34\times10^{7} \theta_C T \exp\left(\frac{-13{,}590}{T}\right)[O_2]$	Yoon, 1978
Water gas- shift	$CO+H_2O \rightarrow CO_2+H_2$	$r_{5,f} = 7.68\times10^{10} \exp\left(\frac{-36{,}640}{T}\right)[CO]^{0.5}[H_2O]$	Bustamante, 2005
	$CO_2+H_2 \rightarrow CO+H_2O$	$r_{5,r} = 6.4\times10^{9} \exp\left(\frac{-39{,}260}{T}\right)[H_2]^{0.5}[CO_2]$	Bustamante, 2004

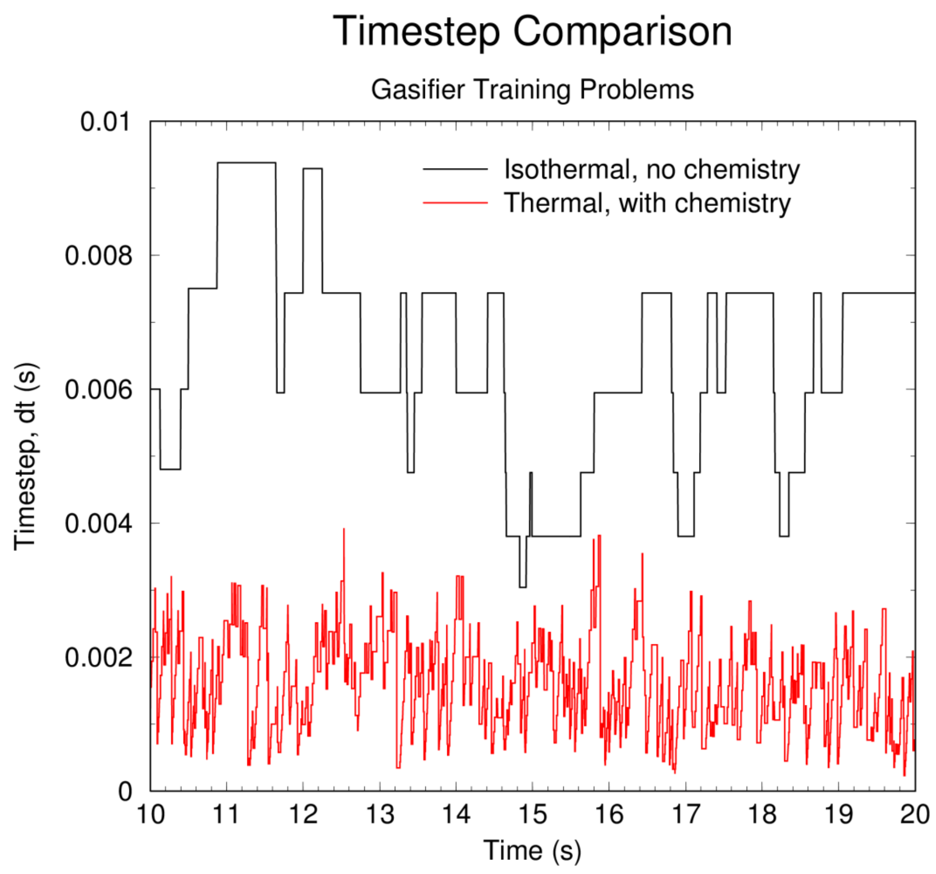
Time Controls

Leave the end-time at 100 s.

When specifying an end-time, take into consideration the various physical time-scales of the system. How long will the fluidization take to become steady? How long will thermal effects take? How long should chemical equilibrium take?

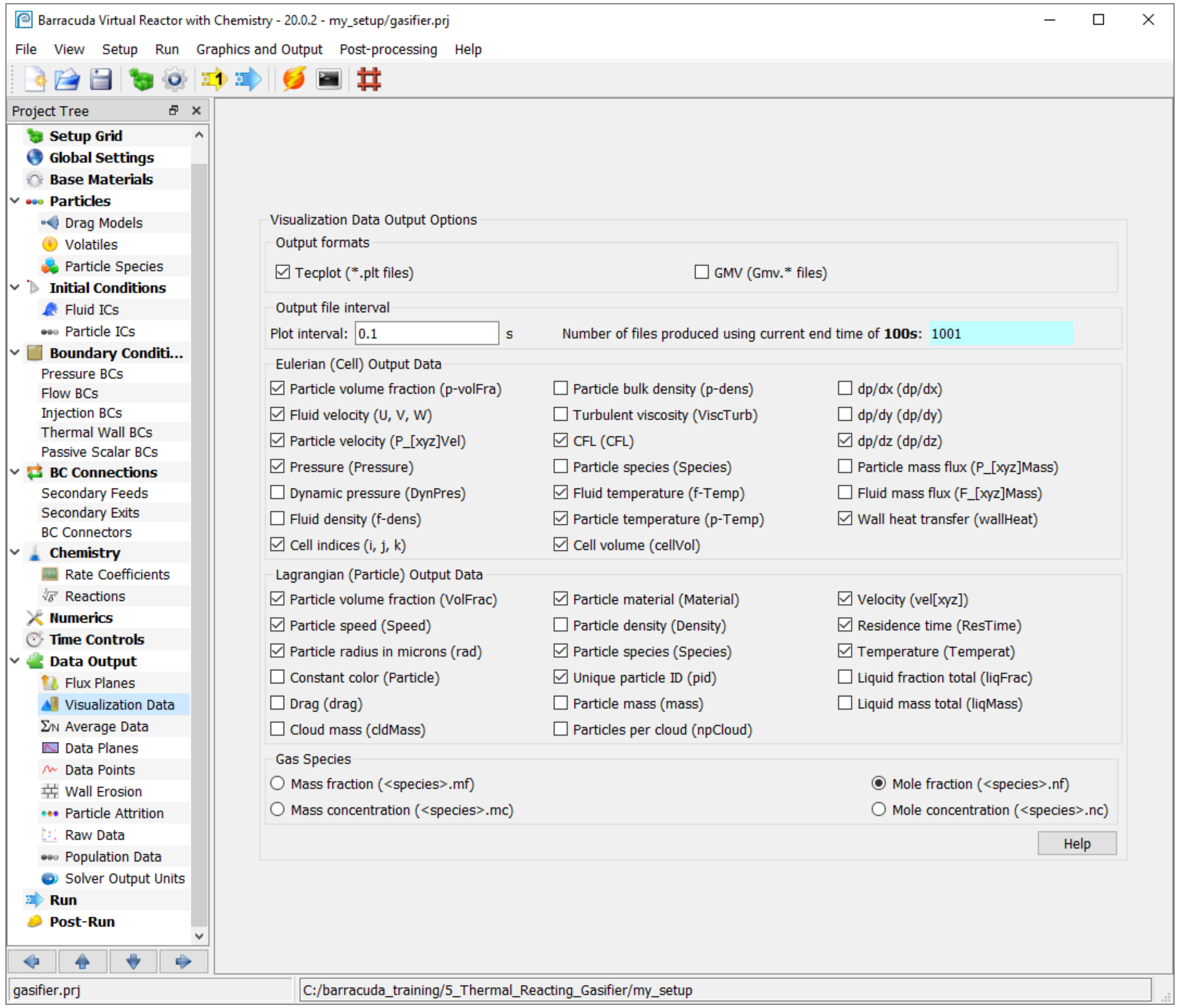
Leave the time-step at 0.01 s.

- When running this more complex case with thermal and chemistry calculations, it is likely that a smaller time-step will be required to solve these additional equations.
- Keep this initial guess of 0.01 s, but compare the time-step actually used by the solver during the run with that of the isothermal non-reacting gasifier.



Tecplot Output Options

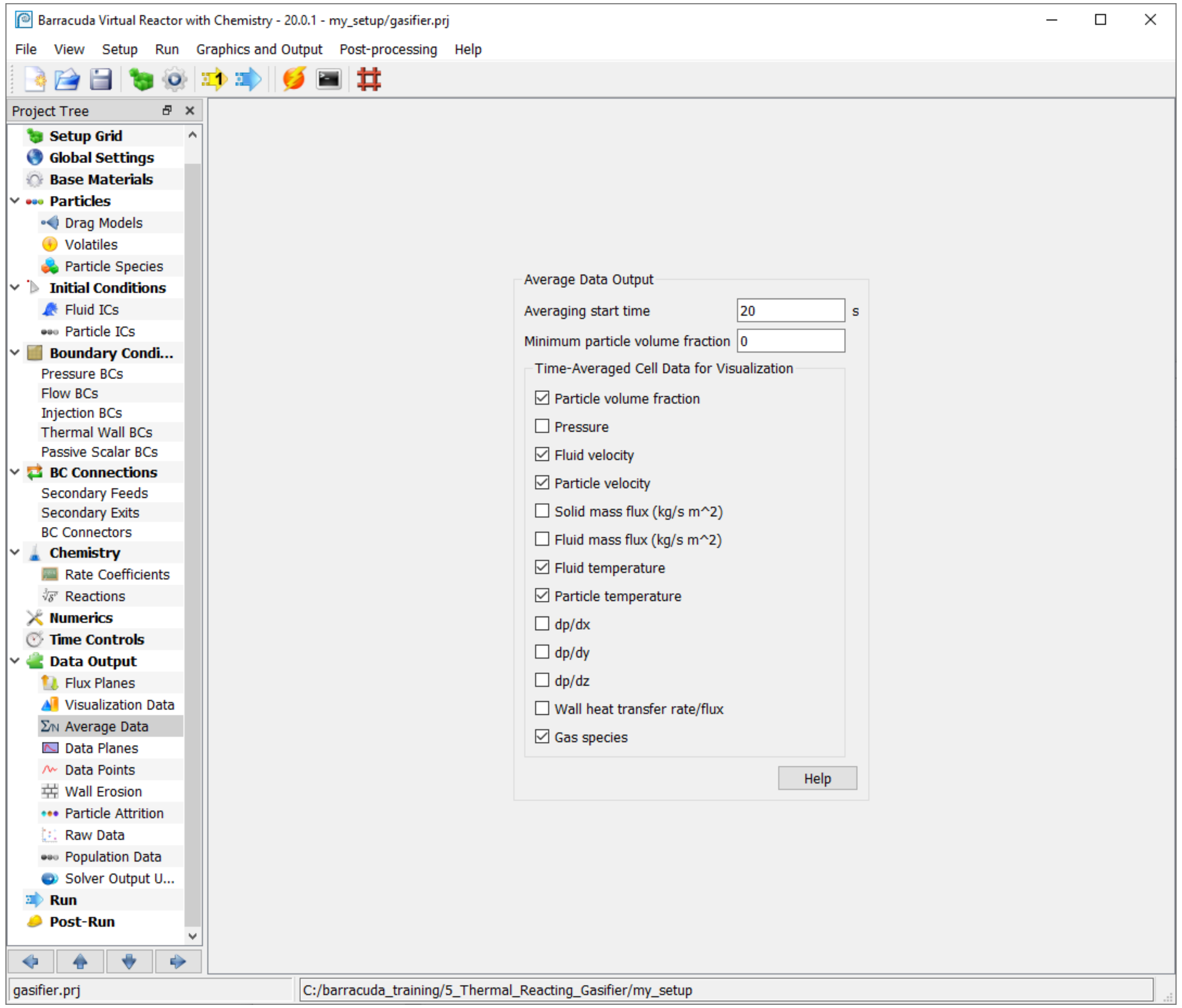
Since thermal and chemistry are now being incorporated into the model, it is important to review the data output settings. Make sure that all necessary output data is selected.



Average Data

Leave averaging start time at 20 s

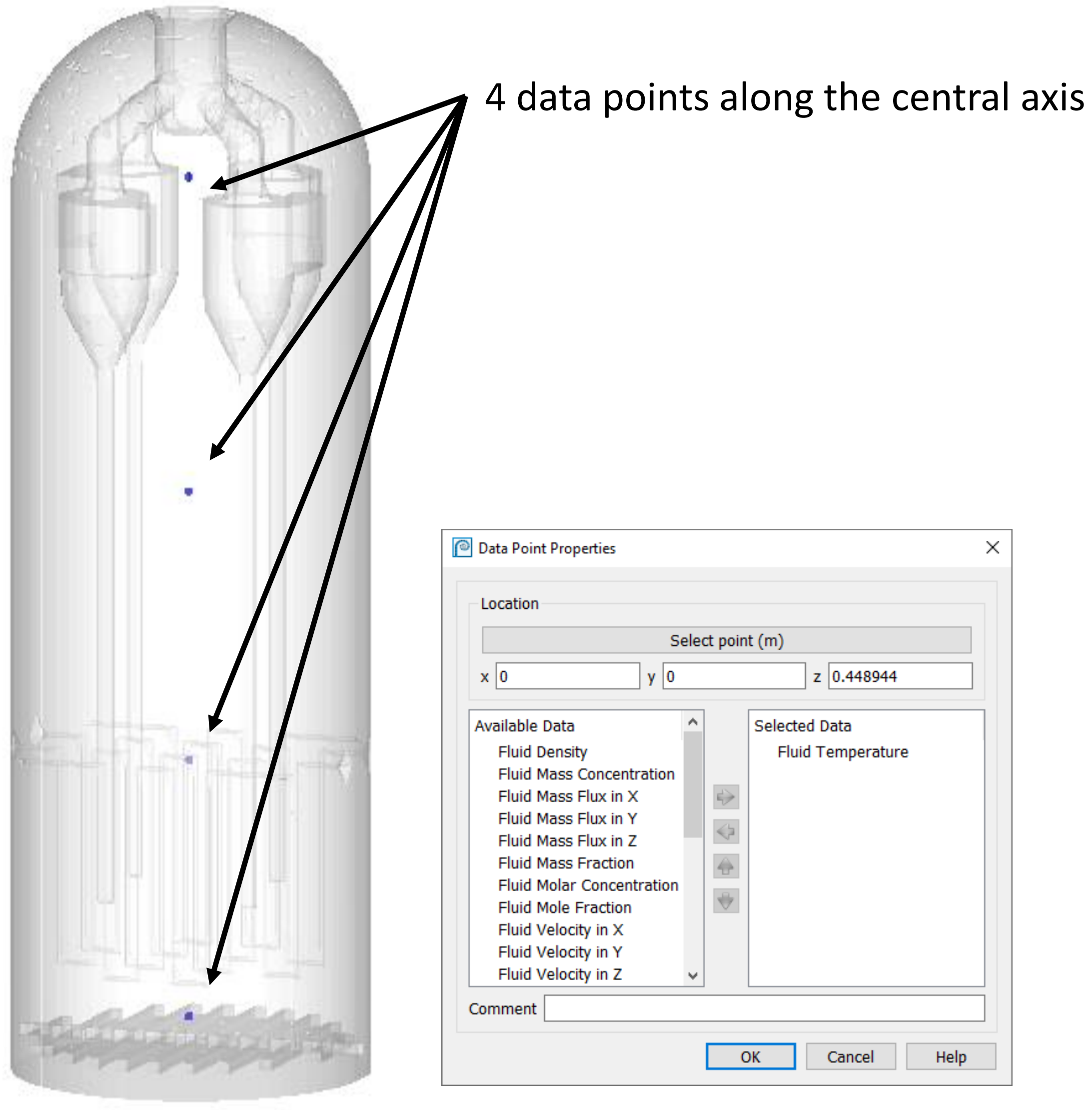
Since we have now turned on thermal and chemistry, be sure to check the boxes for Fluid and Particle temperature.



Data Points

Data points can be defined to monitor many different variables during the course of a simulation.

For this model, define 4 data points at different elevations along the central axis to monitor Fluid Temperature.



Check Model Setup

Run the simulation for a single time-step.

Check the Boundary Conditions:

- Are the flow BCs applied correctly?
- Are the pressure BCs applied correctly?

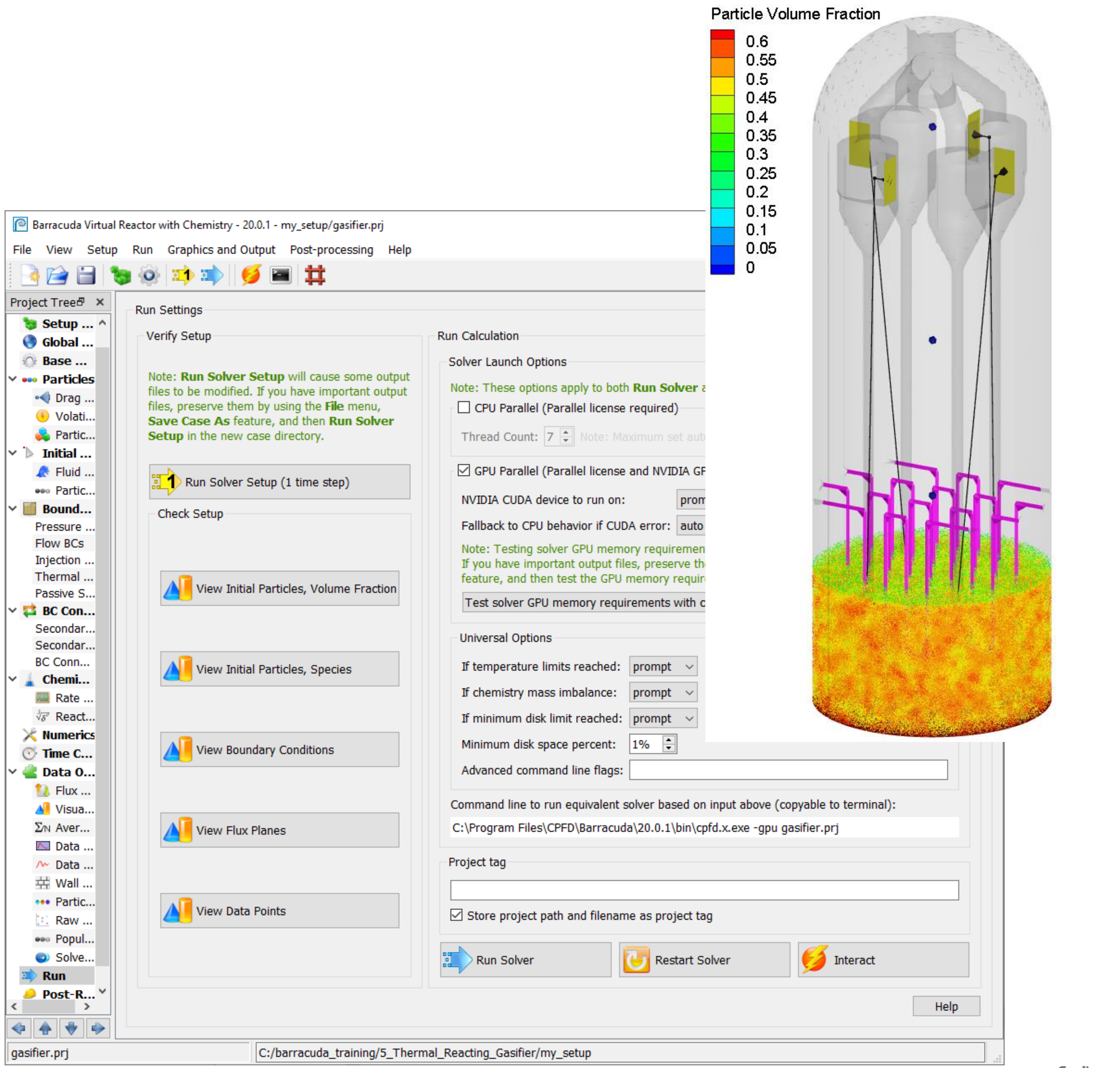
Check the Initial Conditions:

- Are particles initialized properly?
- Do you have the correct initial bed mass?

Check Data Output:

- Are all desired variables in the first Tecplot file?
- Are data points in the correct location?

Review the project setup with your instructor and then Run Solver



Post processing

Training Objectives

This post-processing training introduces several techniques that are useful in monitoring and analyzing Barracuda simulations.

- Additional XY plotting
- Combining multiple views of a simulation into a single animation
- Adding a logo to an animation

Copy Layout files

Copy and paste all layout files (.lay) from 3_Isothermal_Non-Reacting_Gasifier\my_setup to 5_Thermal_Reacting_Gasifier\my_setup

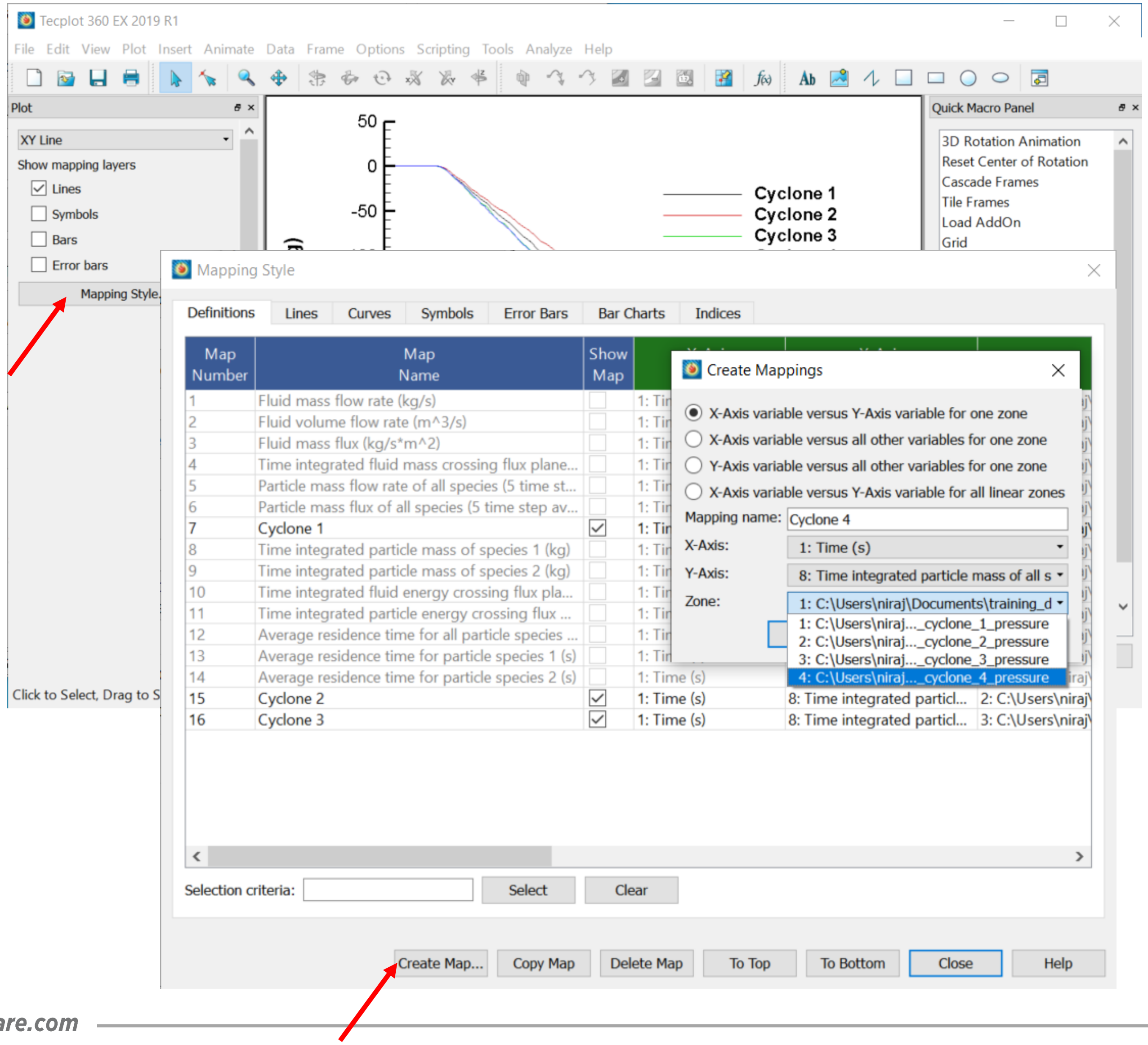
Open the layout files to compare the results between the two cases

Time-Integrated Particle Entrainment

The mass of particles entrained from a fluidized bed is often of interest. Barracuda VR records particle mass flow rate, as well as time-integrated particle mass, at flux planes.

Create a plot of the time-integrated particle mass passing through each of the four cyclones using Tecplot.

- Load all 4 Flux plane files (FLUXBC_cyclone_*_pressure) from the cyclone inlet pressure BCs using the Barracuda loader
- Create Mappings for each cyclone as shown to the right
  - Click on Mapping Style…
  - Click on Create Mapping
  - Select X Variable vs Y Variable
  - Enter a Mapping name
  - Select the file from the Zone category



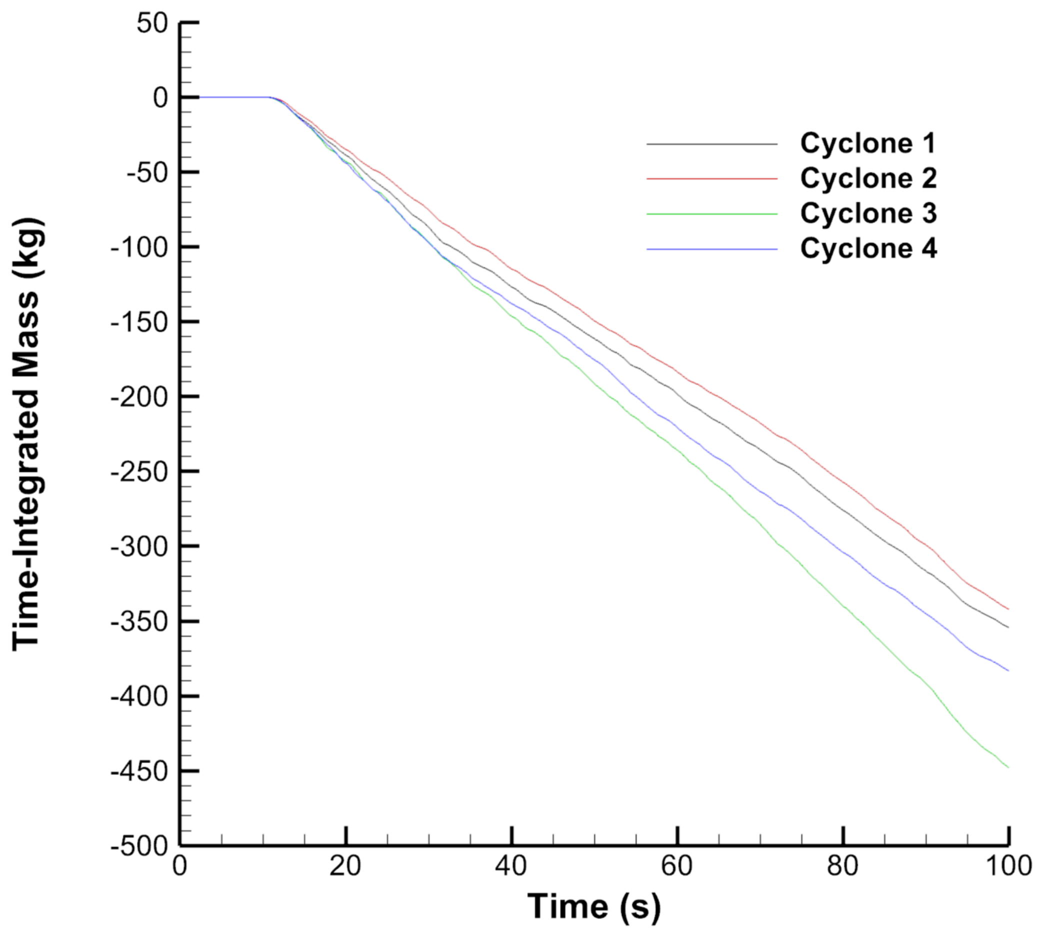
Interpreting Time-Integrated Data

It is important to have a clear understanding of time-integrated mass data, since many Barracuda files utilize this concept.

In the plot at right, we are seeing curves that represent the total particle mass that has passed through each of the four flux planes since the beginning of the simulation.

The time-integrated mass is negative due to the sign convention in Barracuda VR.

- For boundary condition flux planes (e.g., Pressure BCs and Flow BCs), flow into the system is considered positive, while flow out of the system is negative.
- For internal flux planes, the sign convention is based on axis directions. A z-direction flux plane reports positive values for flow in the positive z-direction, and negative values for negative z-direction flows.



Outlet Gas Composition

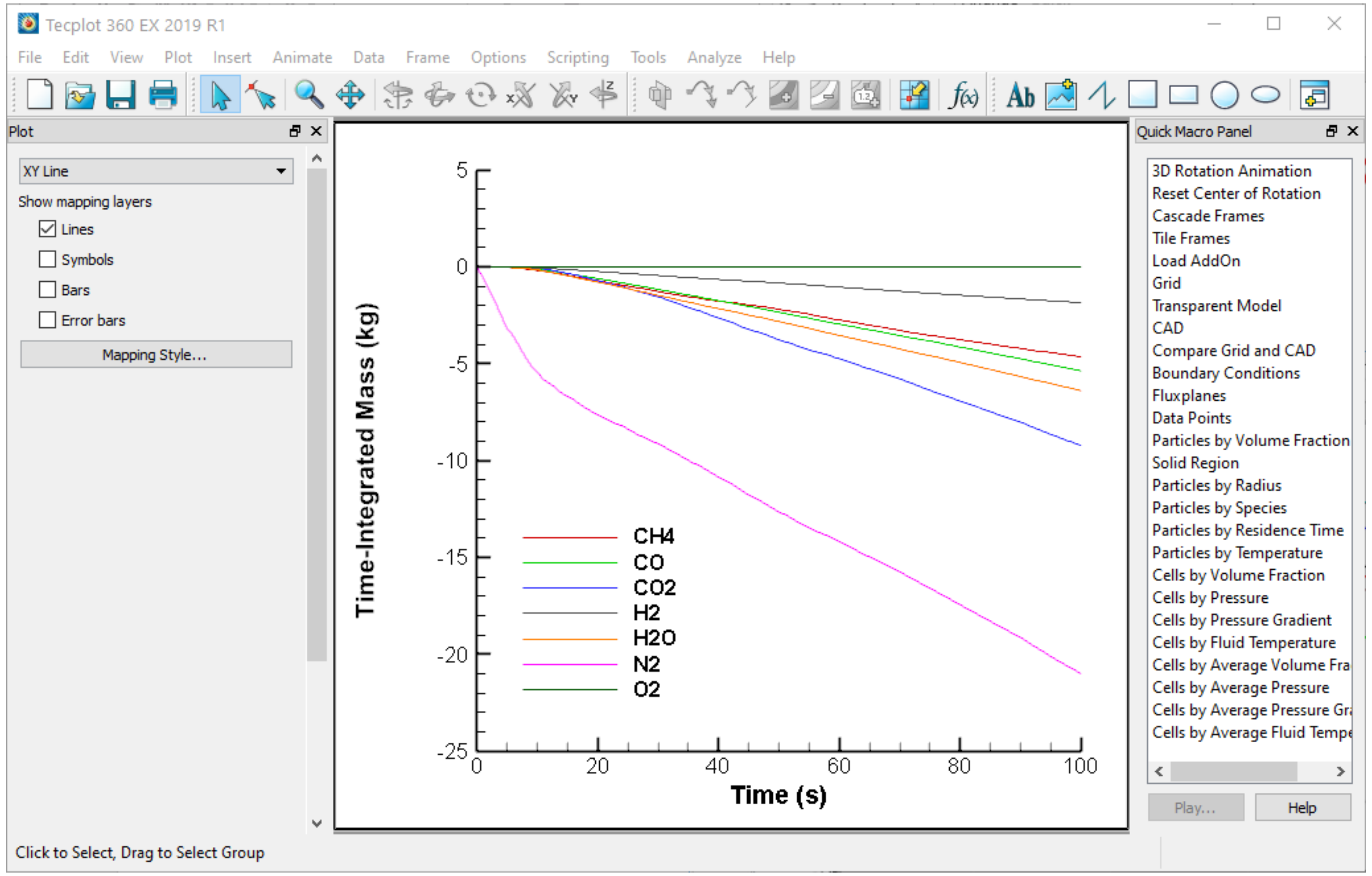
For chemically reacting systems, the gas composition at system outlets is often of interest.

In Barracuda VR, a flux plane will record gas composition information according to the option selected in the drop-down box labeled Gas species flux plane behavior.

- The gas composition flux plane file will have the same name as the normal flux plane file, with a suffix of _gasSpc000_006 (the numbers at the end are determined by the number of gas species used in the project).

For the Thermal Reacting Gasifier example, we chose Mass Time Cumulative as the gas composition format at each of the four cyclone Pressure BCs.

Create a plot of the gas composition at the Pressure BC of Cyclone 1.



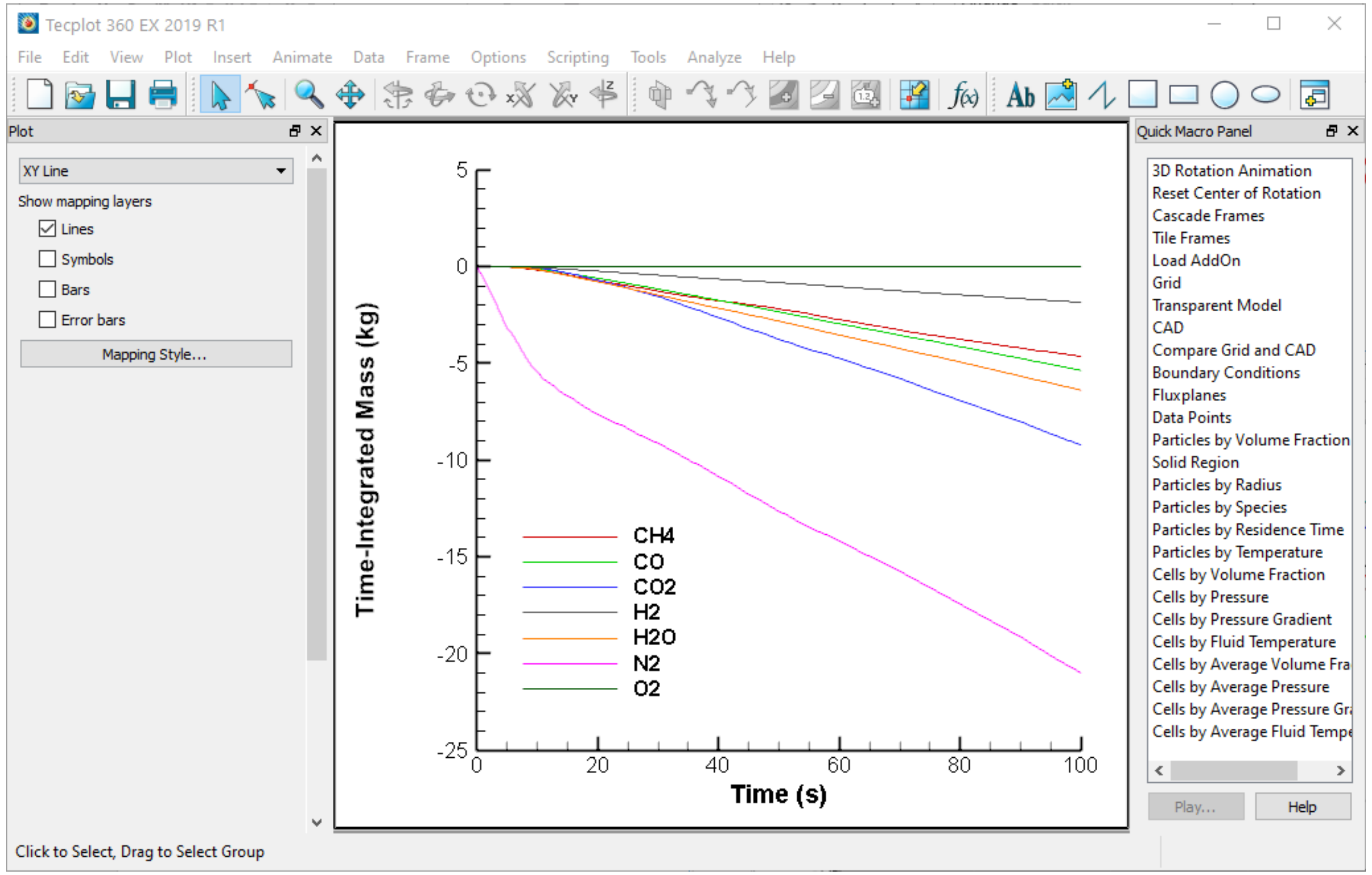
Interpretation of Gas Composition Plot

This plot is showing time-integrated data, not mass flow rate. Be careful to note the difference in meaning.

The sign convention at Boundary Condition flux planes is:

- In-flow = positive
- Out-flow = negative

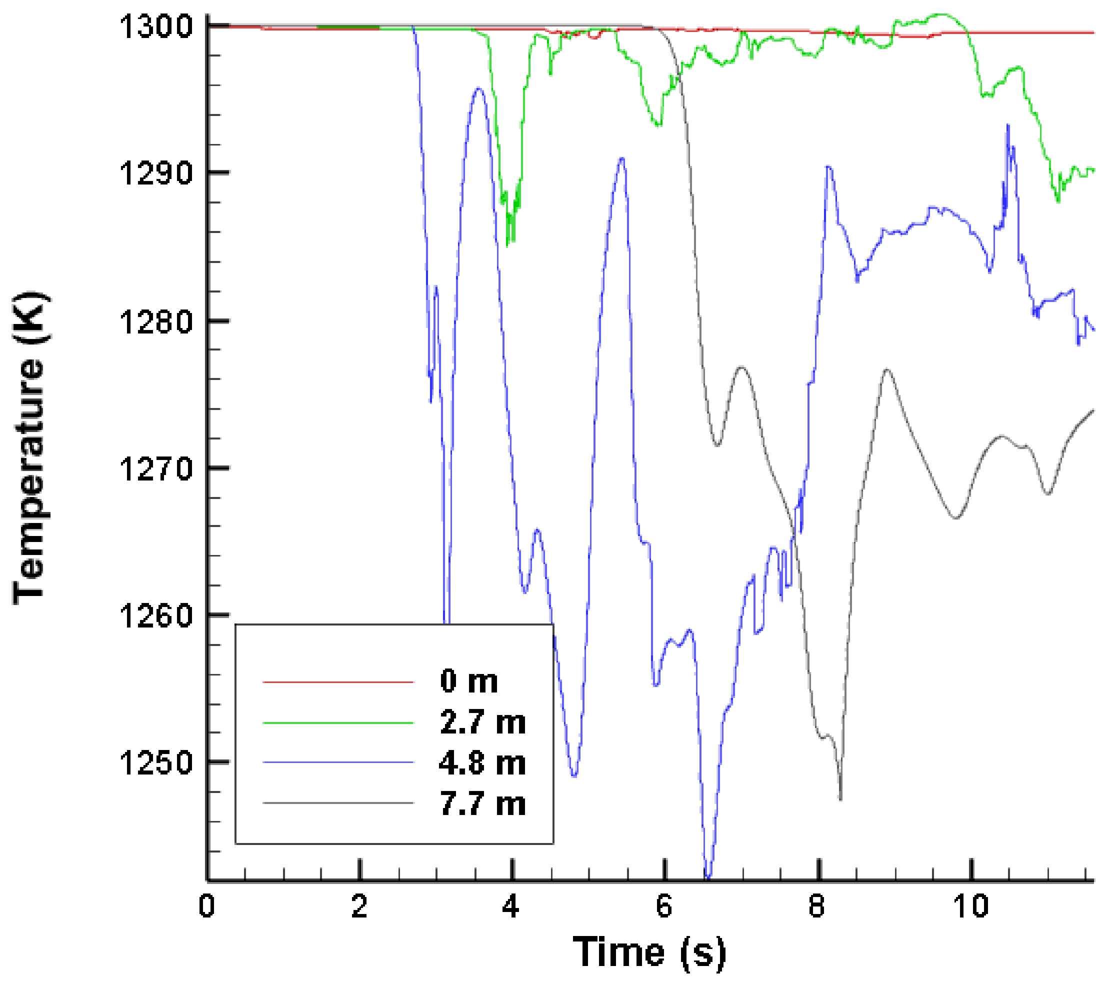
The gas composition plot can be used to help judge when the system reaches pseudo-steady state. Once the time-integrated lines achieve constant slope, the gas composition at the outlet is no longer changing.



Plotting Fluid Temperature from Data Points

Create an xy plot from trans.data00 file

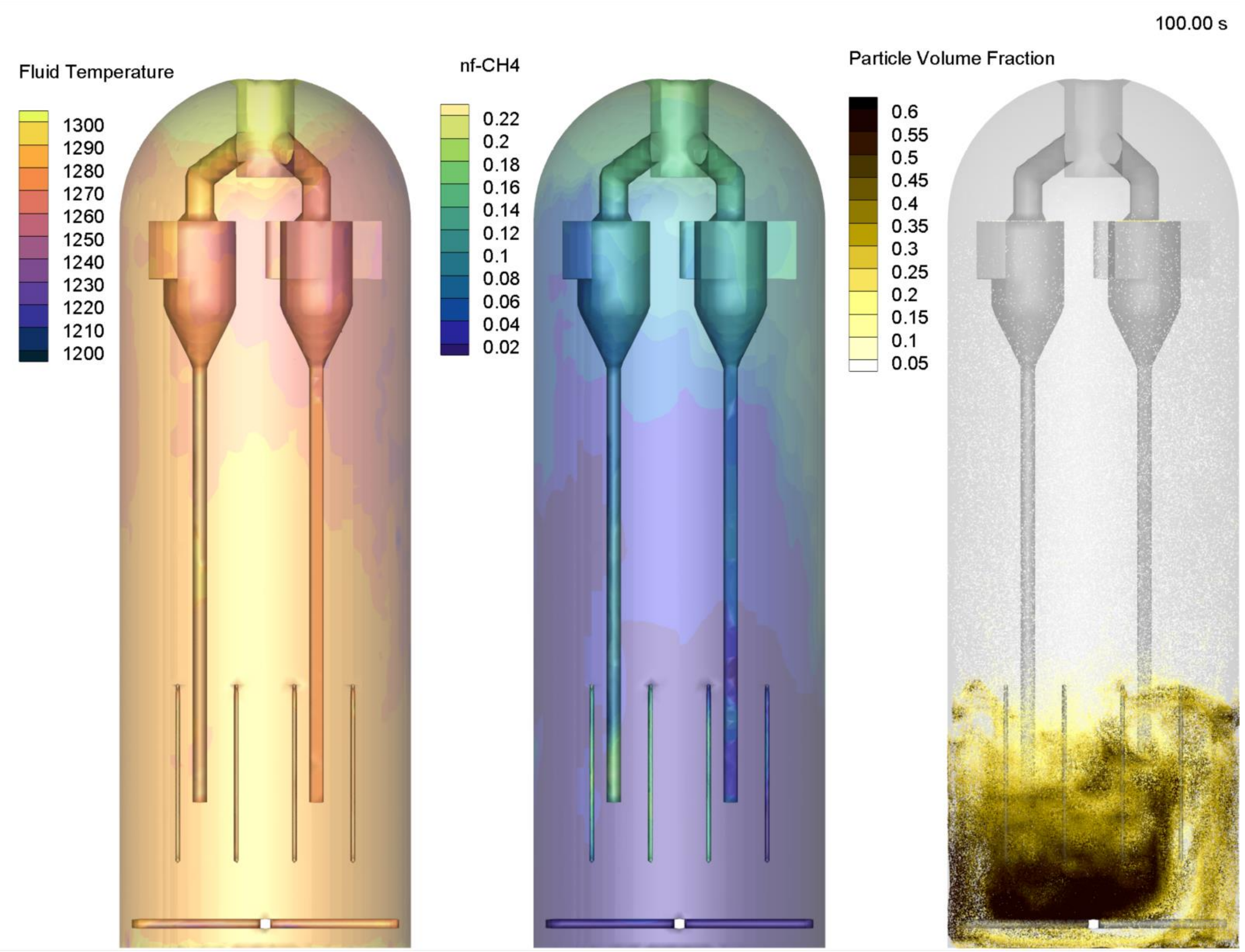
Plot data from all 4 data points



Combining Animations

Using Frames, we can combine multiple views into a single view.

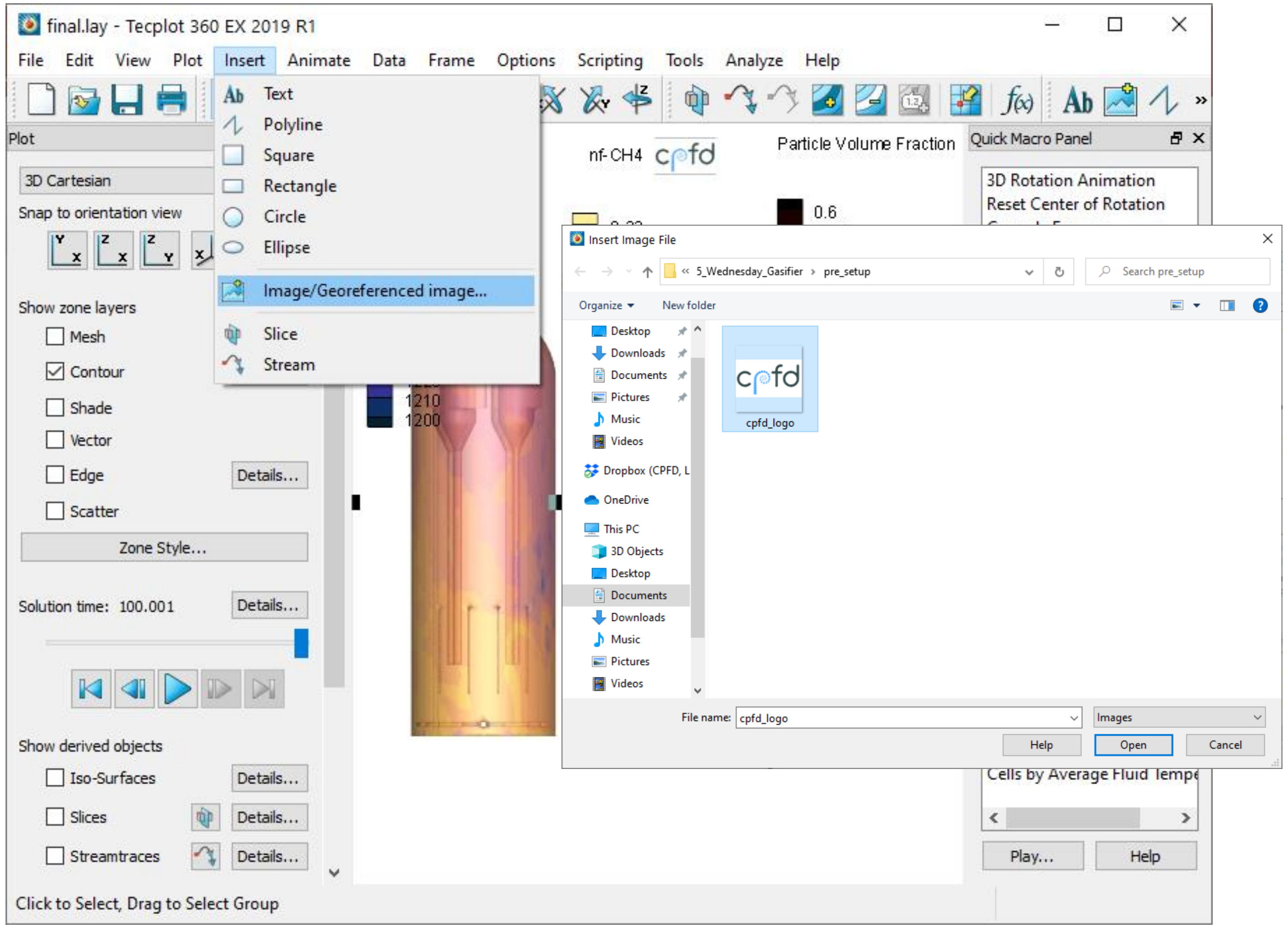
Watch this video and then create an image like the one to the right



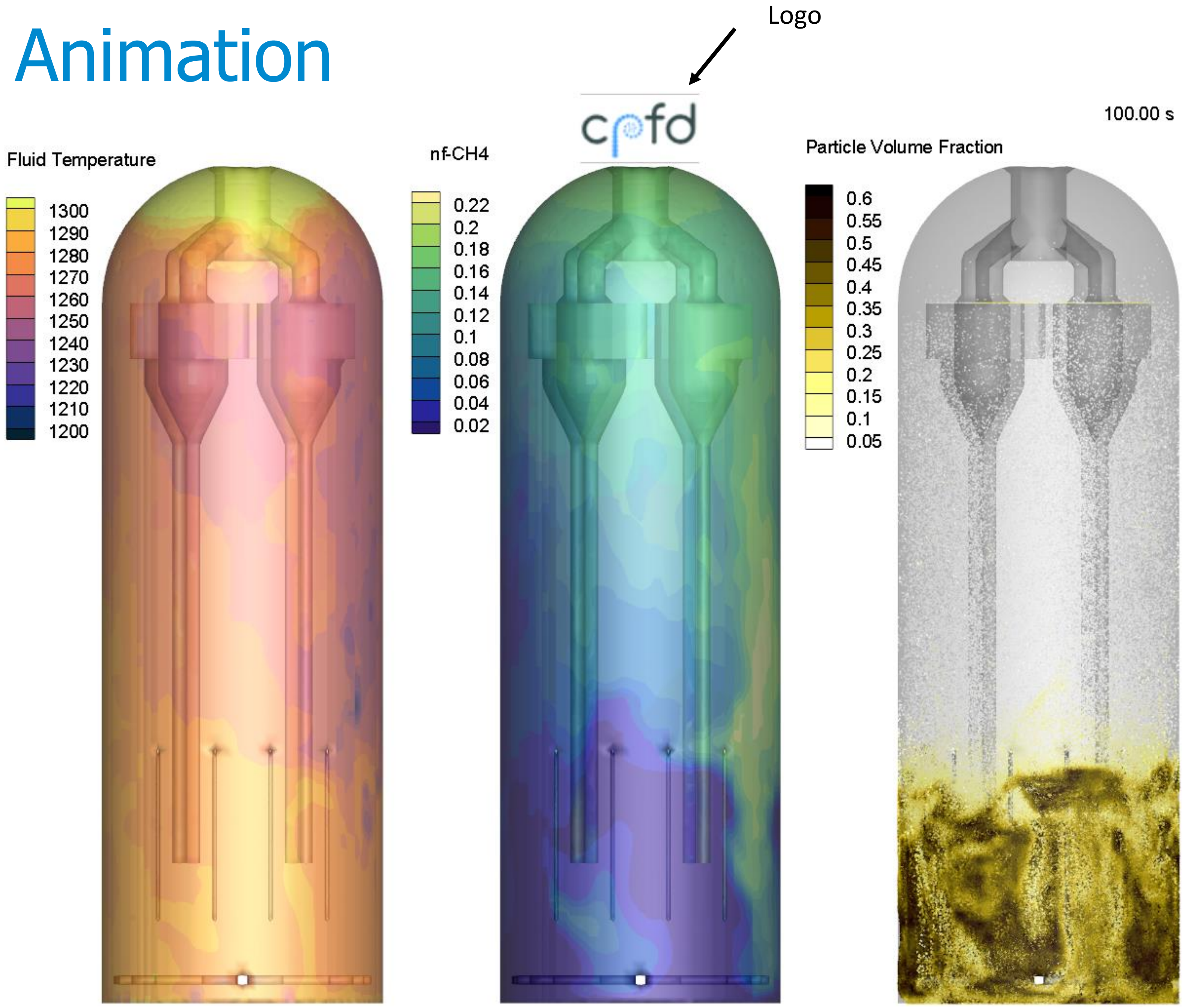
Adding Logos to Animations

Adding your company's logo to an animation can be easily done in Tecplot.

- Navigate to the **Insert → Image/Georeferenced Image...** and select the desired image from the file explorer
- Watch this video and follow along to add a logo to your frame



The Final Animation



Additional Post-Processing

Using the skills learned for plotting and making animations, answer the following questions.

- Does the addition of thermal and chemistry calculations increase the particle entrainment? Plot the entrainment from the "early entrainment flux plane" for both the isothermal and thermal + reacting gasifiers.
- Make a combined animation of all gas species mole fractions. This type of animation is often very informative about the behavior of the chemistry.