Isothermal Non-Reacting Gasifier Part 2: Project

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Training Objectives

Setup and Gridding

- Barracuda gridding exercise
  - Barracuda Grid Generator
  - Using Tecplot to inspect the grid
- Set up a complete Barracuda model based on specified process conditions
- Use several new features of Barracuda
  - Multi-material particles
  - Volatile materials in particles
  - Particle feed
  - BC Connections to maintain system mass

Post processing

- Revisit basic Tecplot functionality and study common post processing techniques
  - Using blanking to display sections of the domain
  - Making animations
  - Using blanking to filter particles based on properties
  - Making isovolumes
- Revisit basic xy plotting of data with Tecplot

Creating a New Project

Create a New Barracuda Project

Launch Barracuda, and create a new project file. Name the project gasifier.prj

- Click on File → New Project
- Fill in Project Name
- Browse to Project Directory
- Click OK

Suggested Project Directory:

- Linux: ~/barracuda_training/3_Isothermal_Non-Reacting_Gasifier/my_setup/
- Windows: C:\barracuda_training\3_Isothermal_Non-reacting_Gasifier\my_setup\
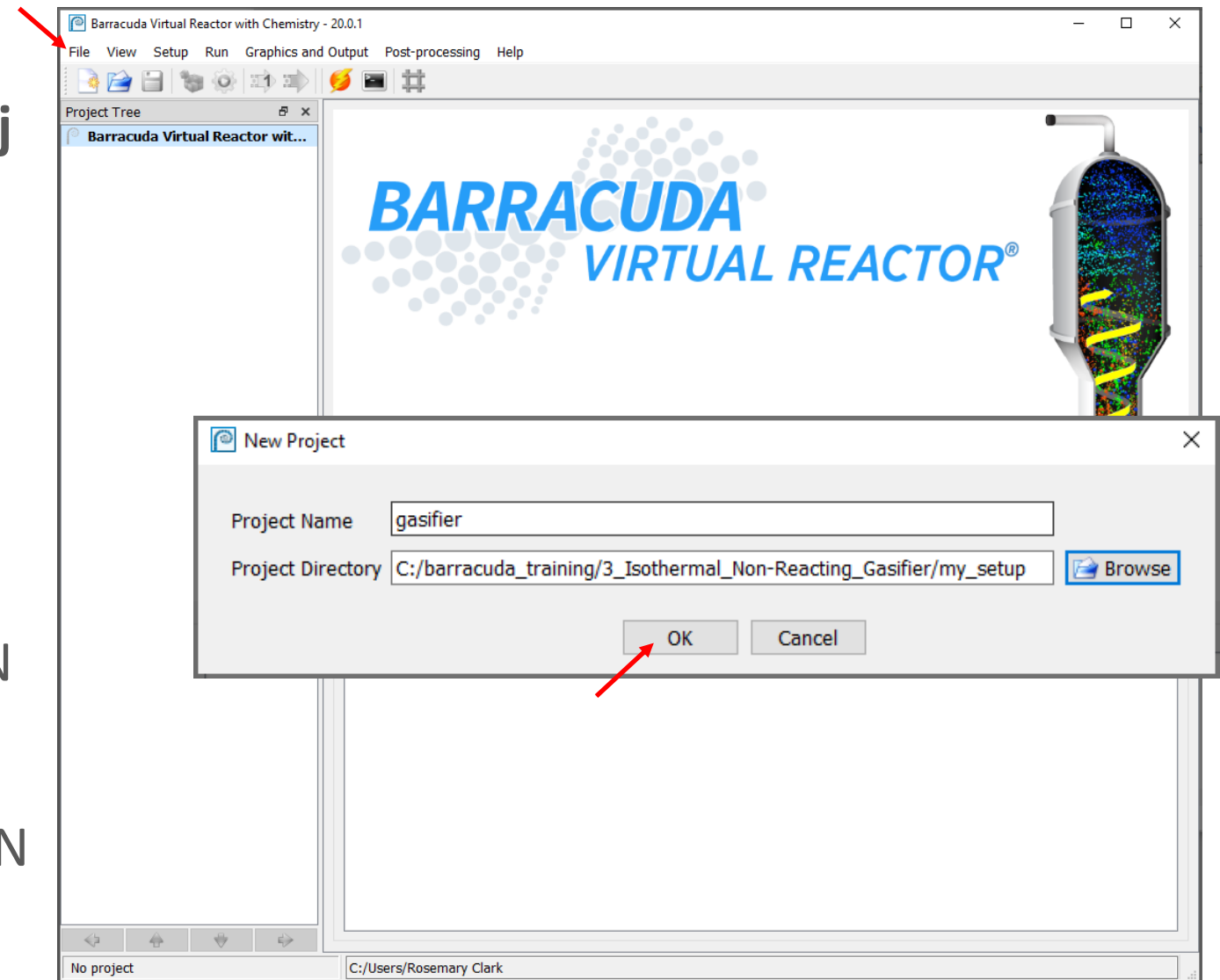
Add an STL File in the Setup Grid Window

To add the STL file to the project:

- Navigate to Setup Grid window

- Ensure you are on the Geometry tab

- Select Add Geometry

- Select the file: gasifier_isothermal_non-reacting.stl

- Click Open

**It is possible to add multiple STL files to the list, but in this case we only need one file.**

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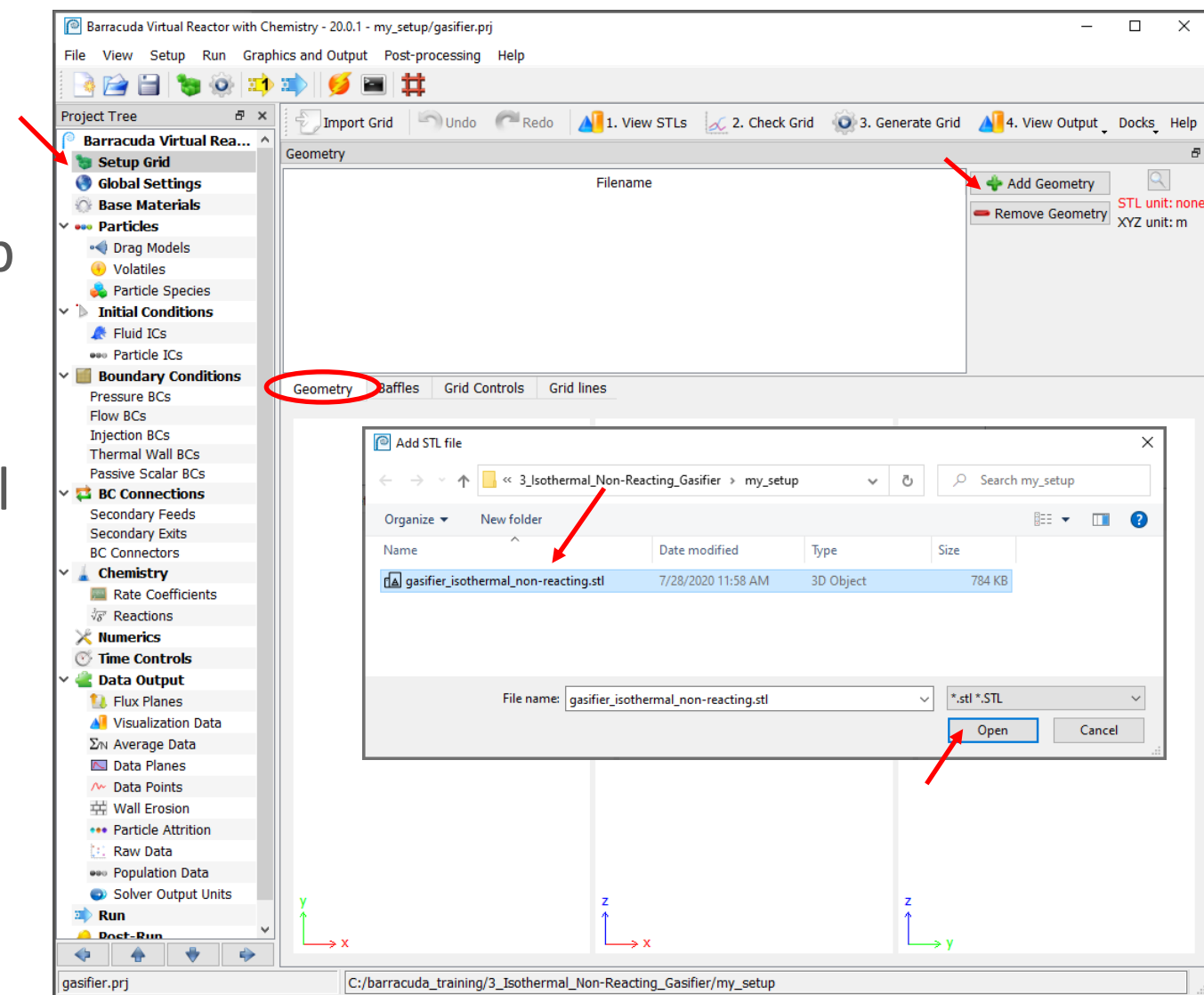
Set the Units of the STL File

STL files are unitless.

- You must tell Barracuda what the physical units of distance are.
- The units were set by the CAD designer when creating the model and exporting to STL.
- It is recommended to check STL units carefully.

Double-click the file name of the STL in the list. This will raise the STL information window.

The gasifier we are modeling is 10 feet in diameter, but the STL file has x-Min and x-Max values of -60 and +60. Therefore, the STL has units of inches.
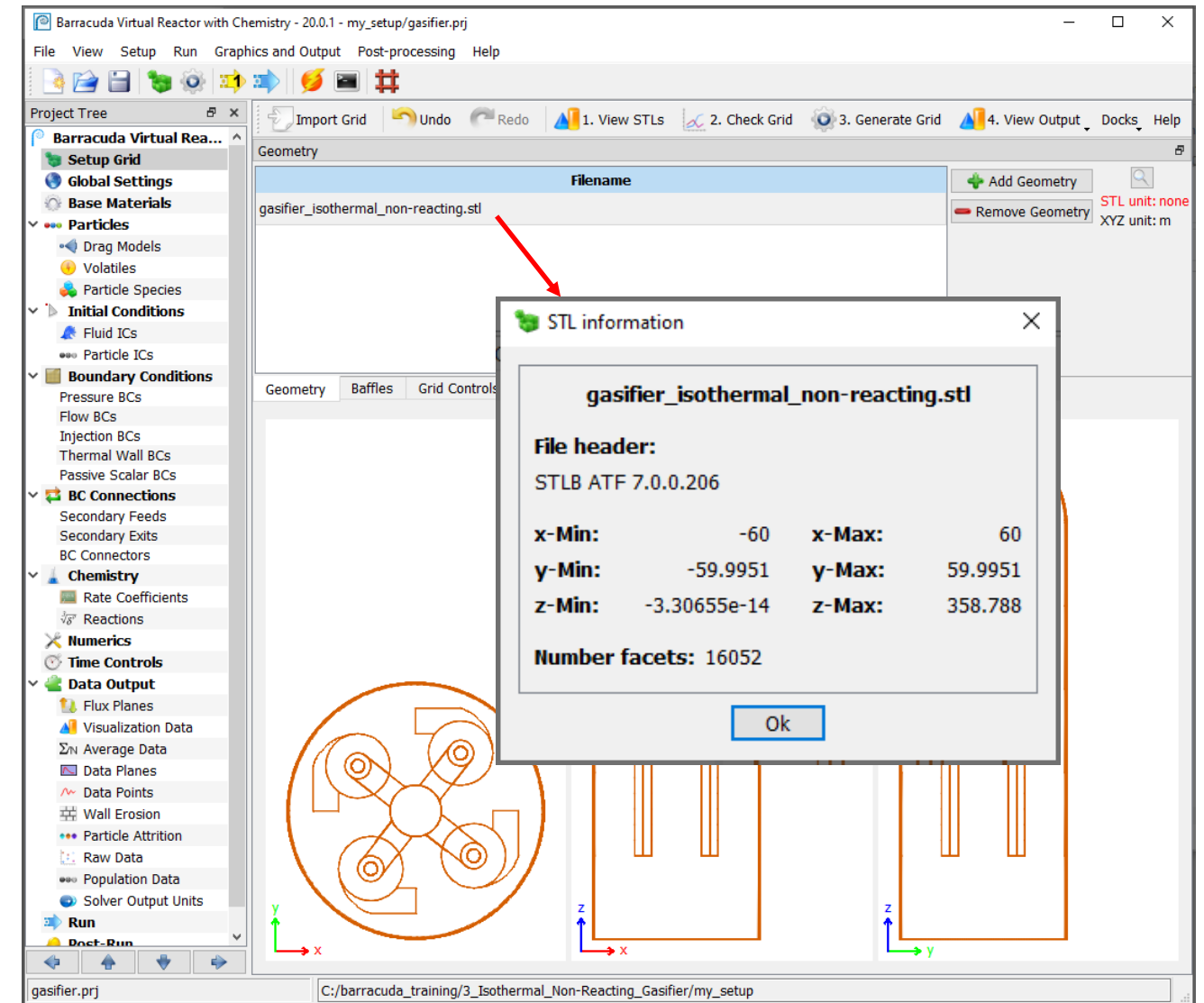
Defining and Generating a Grid

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Start with a Uniform Grid

In Barracuda, a uniform grid tends to work best. The strategy we will use for gridding this gasifier:

- Start with a uniform grid
- Use the Split Cells feature to capture important geometry.

To create a grid:

- Click to Grid Controls tab
- Verify that STL file unit and Display unit are set to in
- Click on Set uniform grid
- Enter a value of 24000 Total number of cells
- Click OK

This results in a grid with 20 cells in the x- and y-directions, and 60 cells in the z-direction. The cells are all uniformly sized with side lengths of 6 inches.
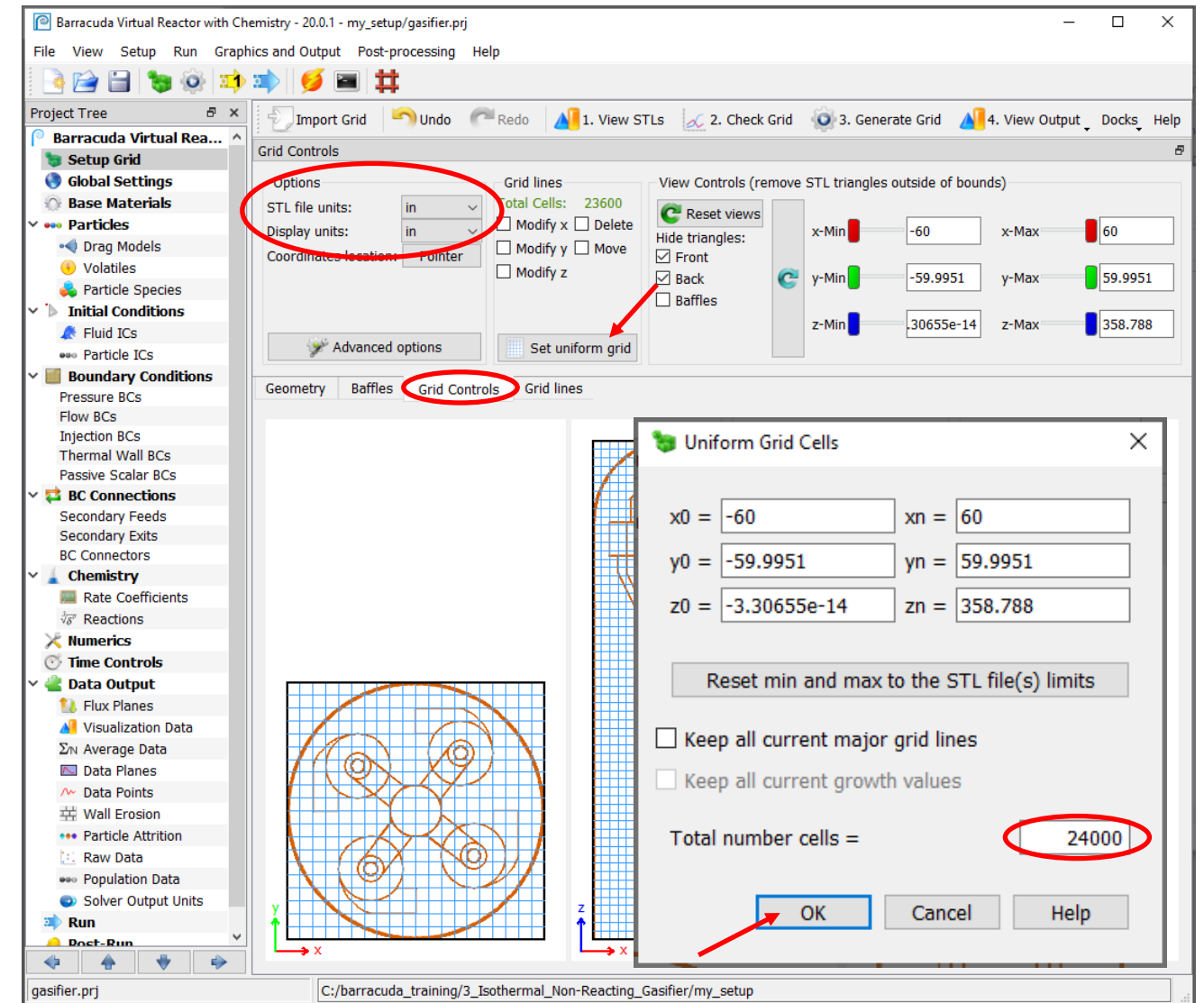
Generate the Grid

We will need to split the uniform grid at some specific locations to properly capture the internal cyclones. However, it is instructive to generate the grid with the completely uniform cells to see what it looks like.

Click Generate Grid and wait for the progress bar to reach 100%.

When defining a grid, you need to decide if the resulting geometry is close enough to the STL file geometry. We will use several shortcuts under the View Output menu to make this decision.
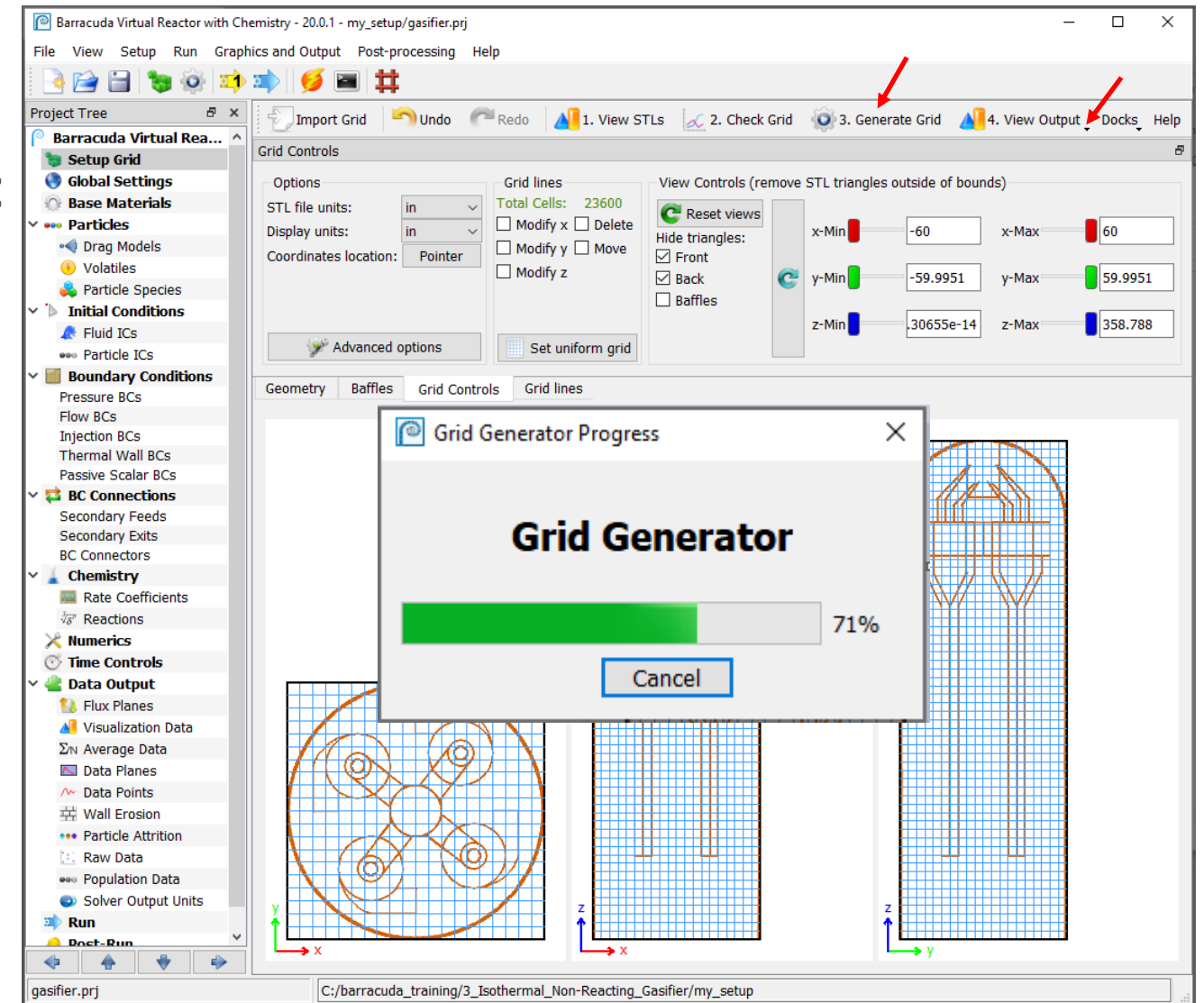
View the Original STL Geometry

To view the original STL geometry, use the shortcut View Output → View CAD.

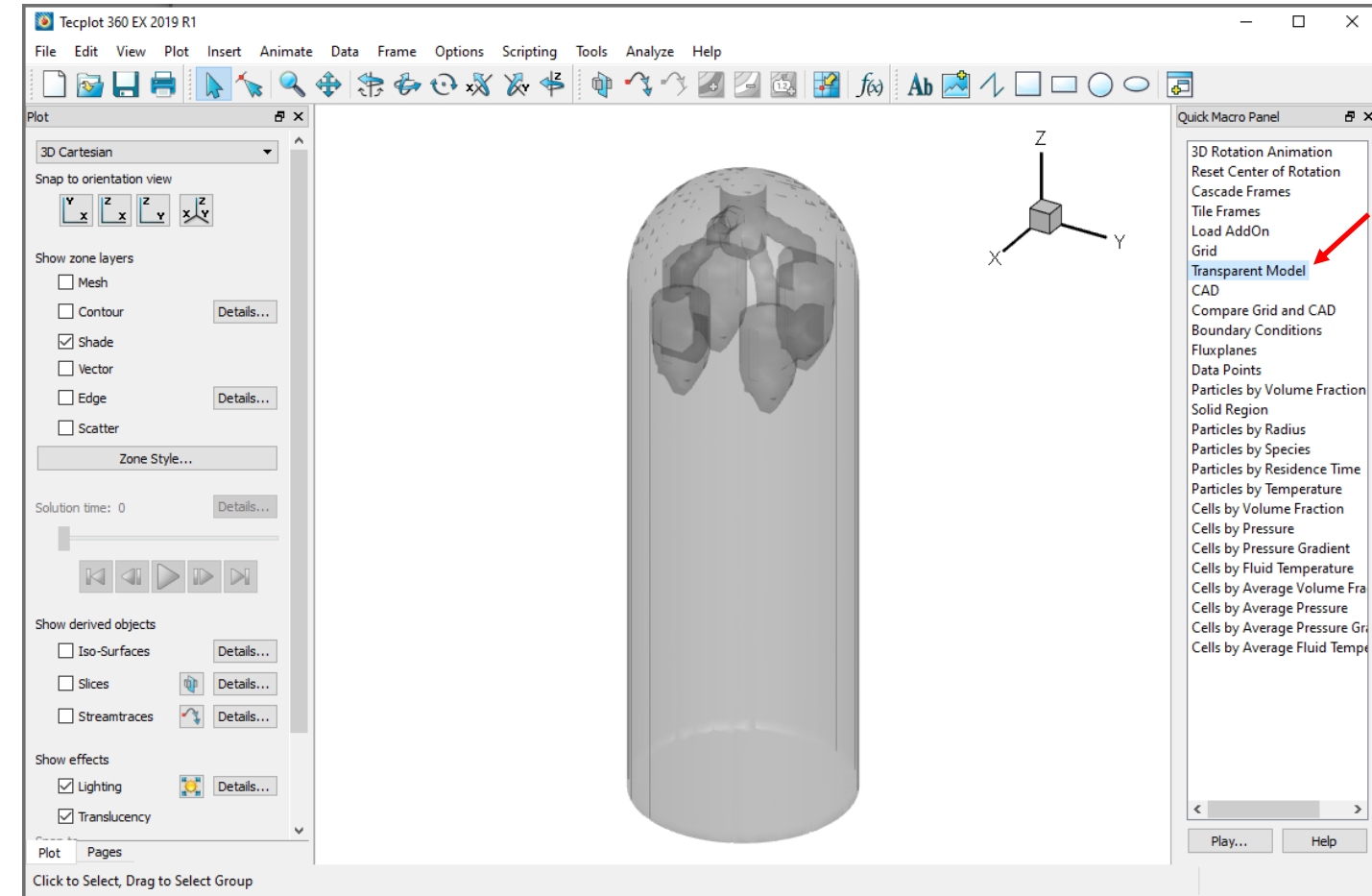This provides a Tecplot view of the STL before any cells have been created by the grid generator.
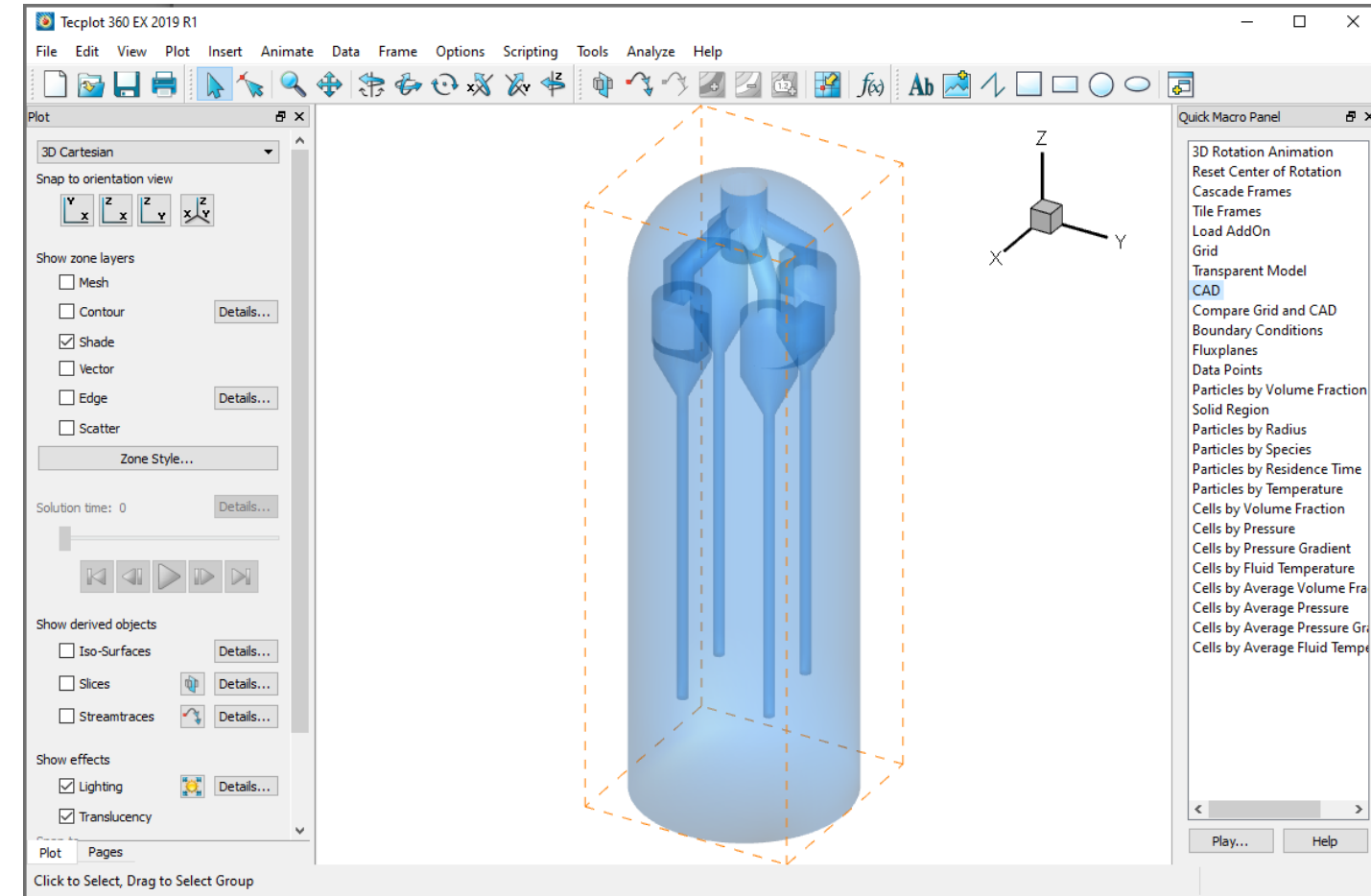
View the Gridded Geometry

To view the results of applying a uniform grid to the gasifier STL, use the Quick Macro Panel and double click on Transparent Model.

The Tecplot view will change to a transparent view of the computational cells created by the grid.

Comparing this view with that of the original STL file shows that our completely uniform grid did not capture the cyclone diplegs.

Also, the cyclone inlet horns, which will be used as boundary condition cells, need to be better resolved.

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Set View Properties to Make Gridding Easier

When modifying the grid, it is helpful to have as clear a view as possible of the geometry that you want to capture. Using the following settings can help:

- Maximize the Barracuda window so you have a large view of the grid lines

- Maximize the pane view that you are working in by moving the gray lines

- Increase the STL line widths by clicking Advanced Options, and increasing the value of Pixel width for STL lines (try 2 or 3).

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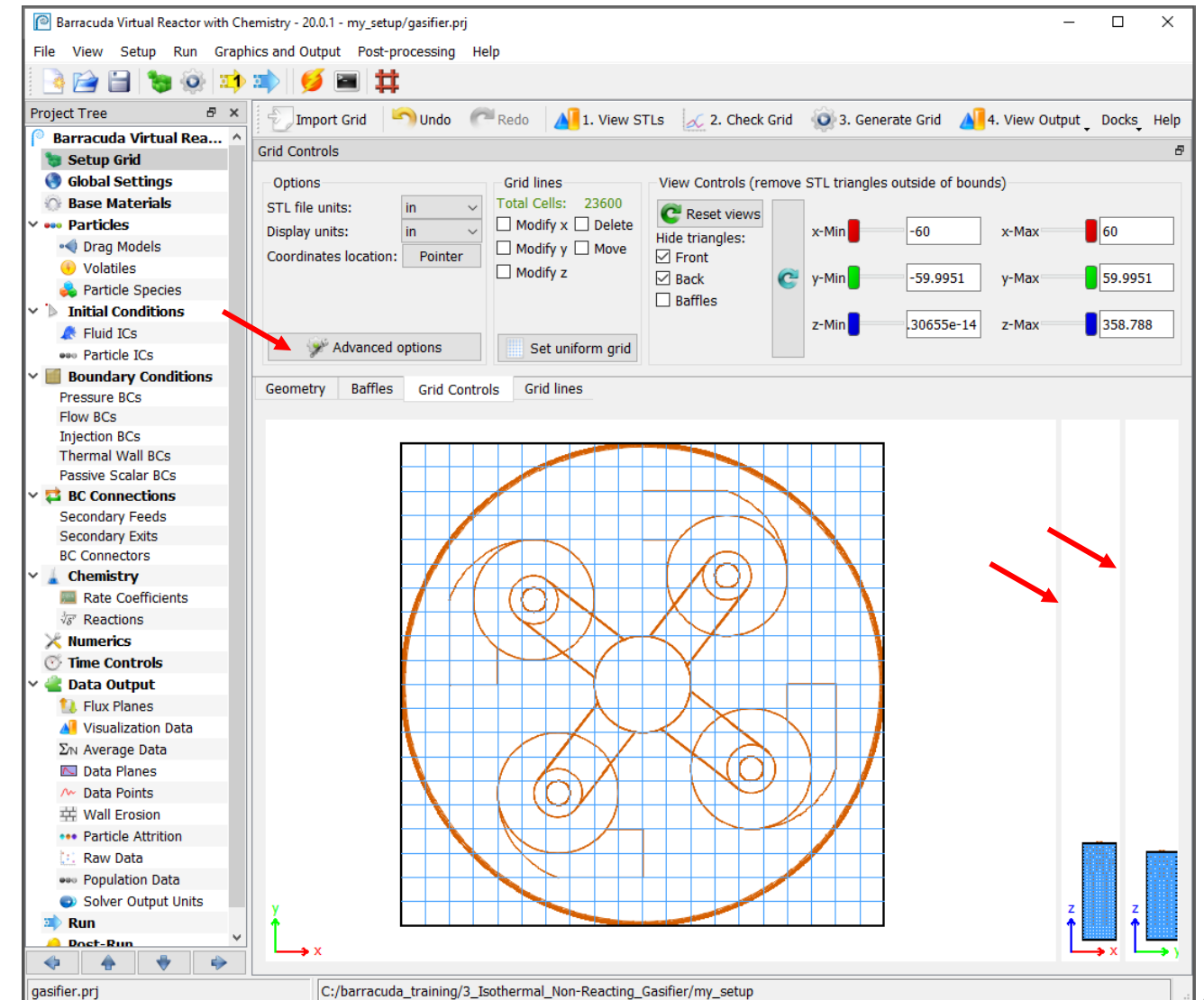
Use Modify x and y to Split Cells

We will use the method of splitting cells to modify the grid. The goal is to keep the overall grid as uniform as possible, while still capturing the important geometry of the gasifier.

Split the grid at strategic locations to capture the internal cyclones.

Start with a top (x-y) view of the reactor:

1. Select Modify x
2. Click just inside one of the cyclone horns. When you click, a pop-up will appear to ask how you want to modify the grid.
3. Select Split cells and click OK.

Repeat this process to outline all 4 cyclone inlet horns.

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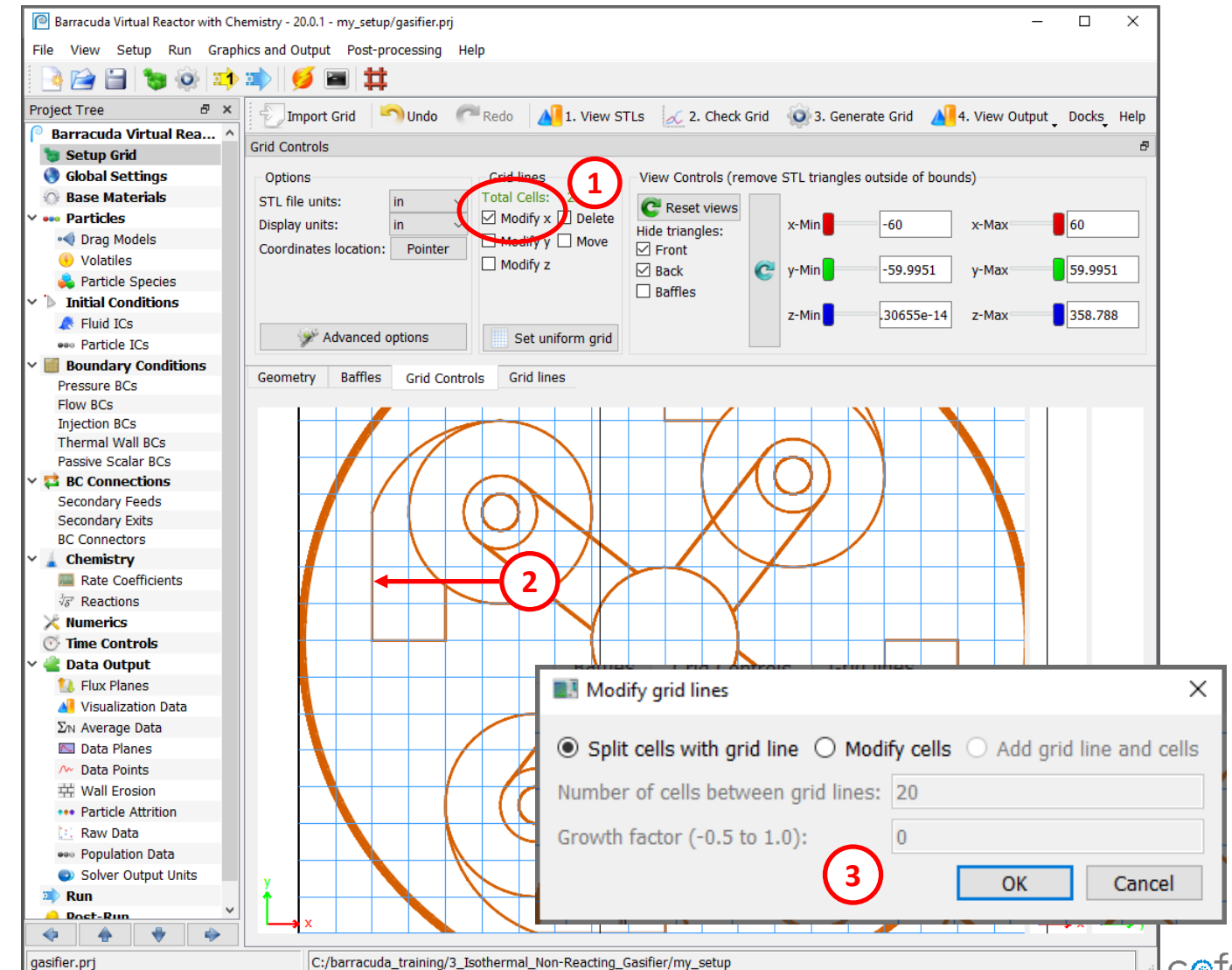
Capture Cyclone Diplegs

The cyclone diplegs are almost the same diameter as a typical cell size for this simulation.

You could capture them with either four grid lines (top, bottom, left, and right), or with two grid lines intersecting in the middle.

Because of the offset between each dipleg (none of them are exactly horizontally or vertically aligned), using the cross method is easier in this case.
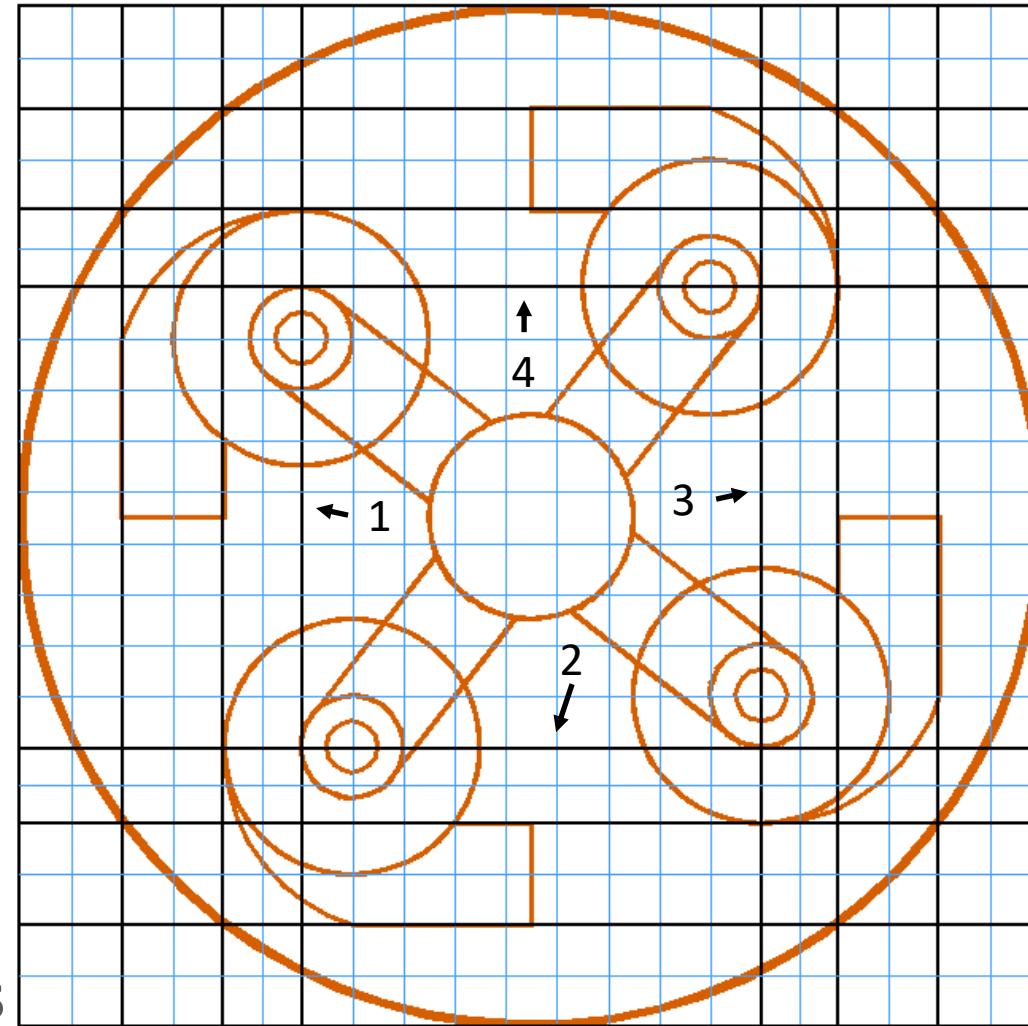
Capture Cyclone Inlet Horn Faces

A pressure BC will be applied to each inlet horn face during project setup, and a full cell is best for this procedure.

In order to capture a full cell right on the face of the inlet horn, grid lines can be placed at x=0 and y=0.

To ensure that the lines are placed exactly at the axes

- Navigate to Grid Lines tab
- Change the X-cell lines and Y-cell lines number that is closest to zero to 0
- Check to make sure there is an equal number of cells on either side of the x=0 and y=0 major grid lines.

Grid lines

X cell lines			Y cell lines		
	-60.00000			-60.00000	
2	-47.88483	0.0000	2	-47.96903	0.0000
2	-36.13155	0.0000	2	-36.02731	0.0000
2	-27.05629	0.0000	2	-26.78687	0.0000
5	0.00000	0.0000	5	0.00000	0.0000
5	26.97415	0.0000	5	27.24357	0.0000
2	36.09230	0.0000	2	36.04798	0.0000
2	47.87698	0.0000	2	47.89771	0.0000
2	59.93780	0.0000	2	59.98445	0.0000
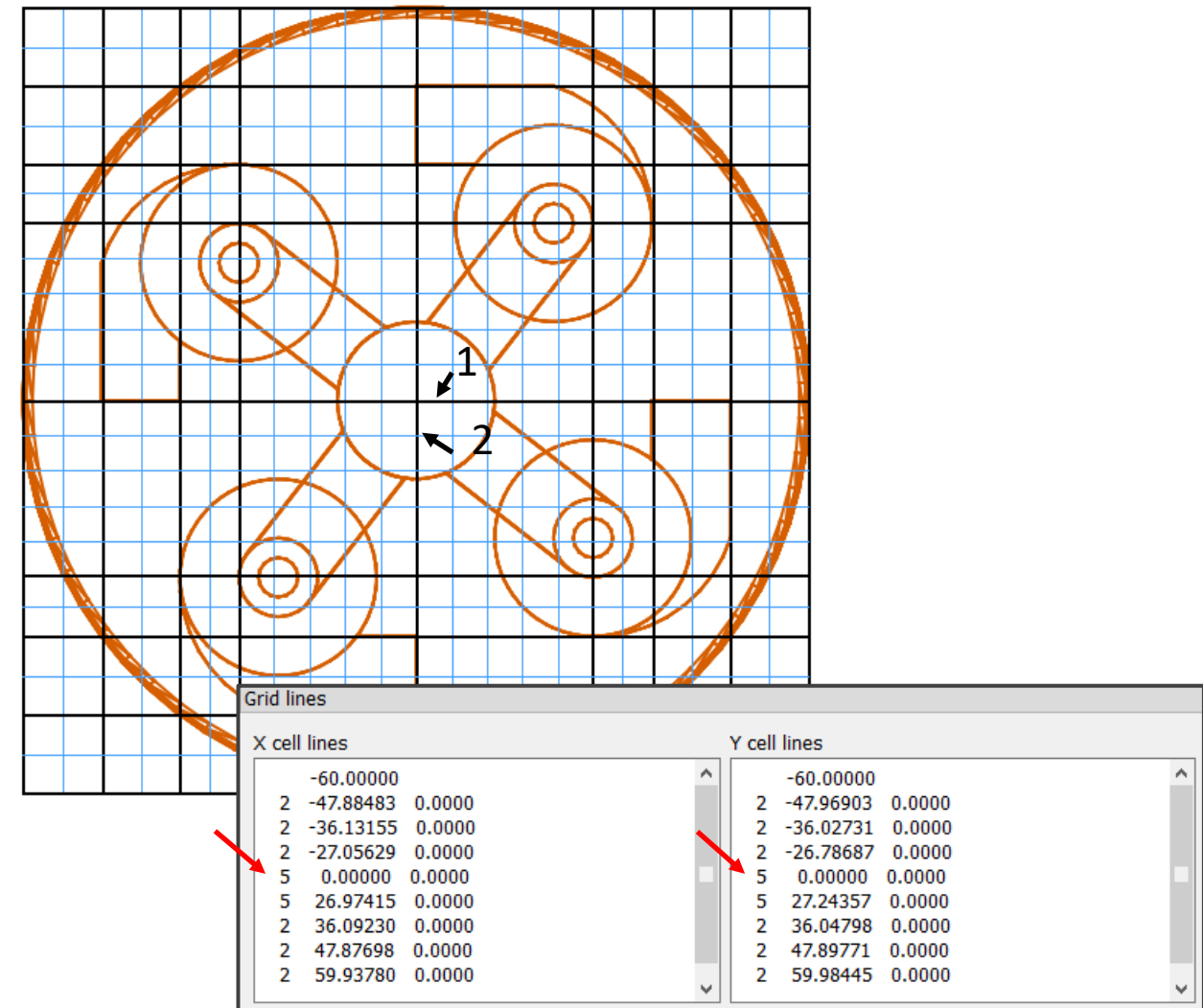
Use Modify z to Split Cells

In the vertical direction, we need to define grid lines in specific locations:

- The top and bottom surfaces of the cyclone inlet horns.
- The bottom surface of the cyclone diplegs.

In the x-z view pane, use Modify z to split the grid at the appropriate locations.
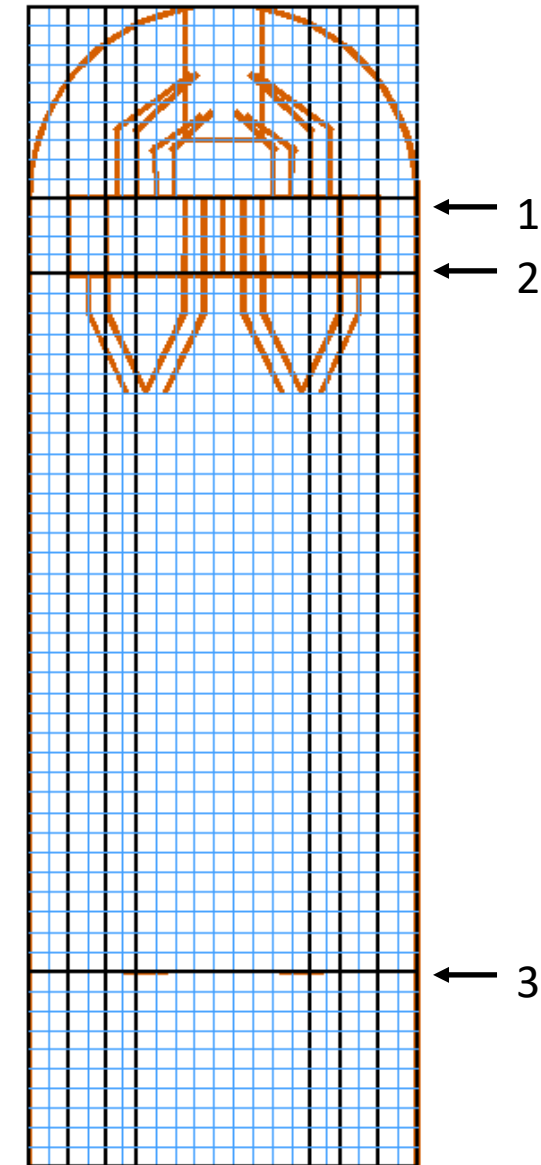
Generate the Grid

Generate the grid, and view the transparent model to see if the geometry was successfully captured.

To check the Grid:

- Select Slices and click on Details…
- In the Definition tab, change the Slice location to Z-planes.
- In the Other tab, select Show mesh.
- Click Close
- Click on the Interactive slicing tool button ⬚ . This will allow click-and-drag properties on the mesh slice. You can dynamically check your grid along the cyclone inlet horns and diplegs.

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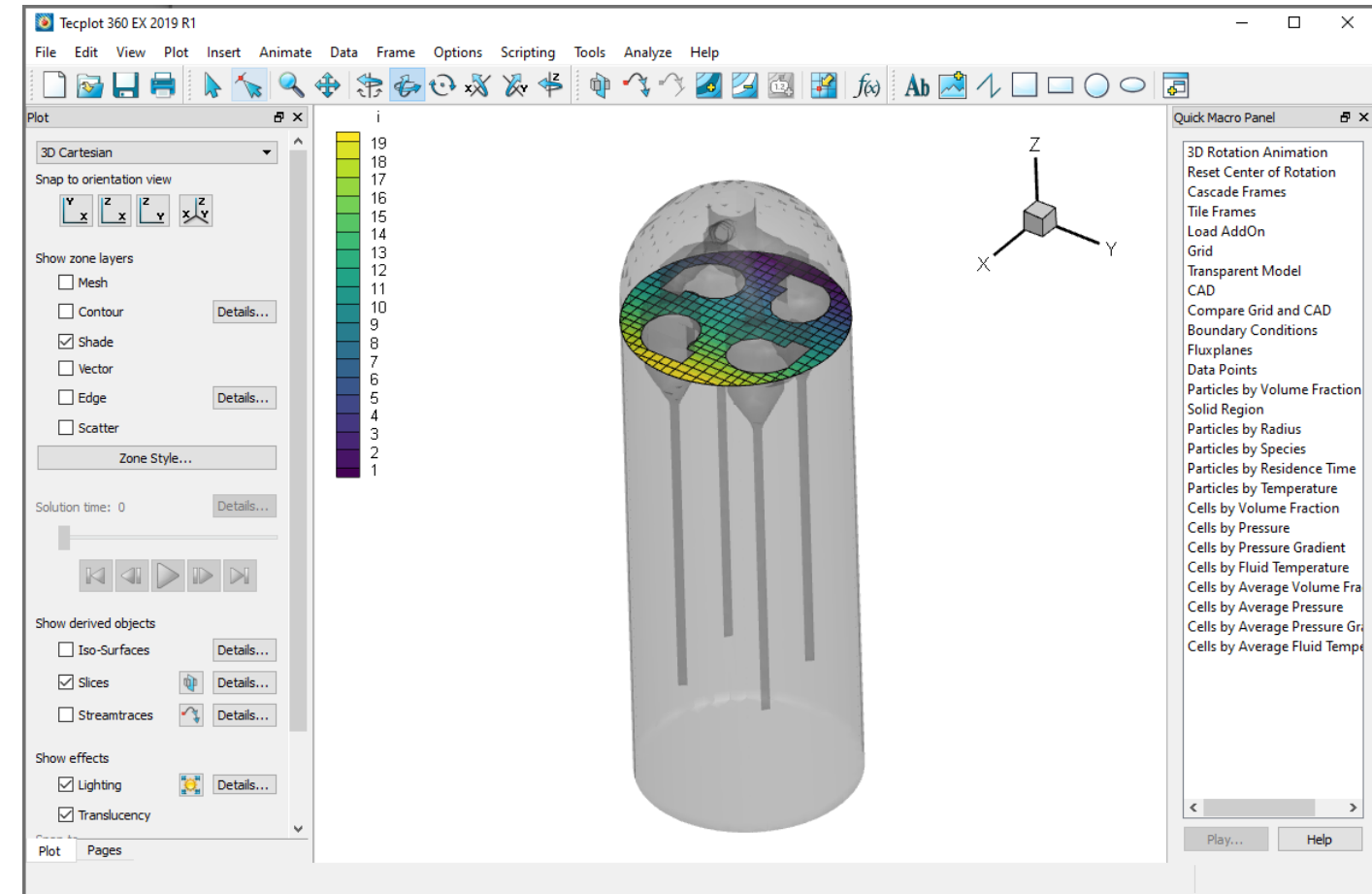
Grid Review with Instructor

Review your grid with the instructor.

Discuss any questions you have regarding the grid generation process used in Barracuda.

Once you are satisfied with the grid, move on with project setup.

Completing the Project Setup

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Process Sheet

Isothermal and non-reacting at 1300 K

Initial Condition	
Fluid	100 % N_2 2e5 Pa
Particles	4800 kg

Boundary	Fluid Flow	Particle Flow
Fluidizing Air + Steam	Velocity = 0.3 m/s Gas (mass fractions): 0.3 H_2O, 0.54 N_2, 0.16 O_2	None
Fresh Coal Feed x = 1.45m y = 0 m z = 1.75 m	Velocity = 0.25 m/s 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

Outlet pressure: 200 kPa

BC Connectors return particles from cyclones

Fresh coal feed

Fluidizing air + steam
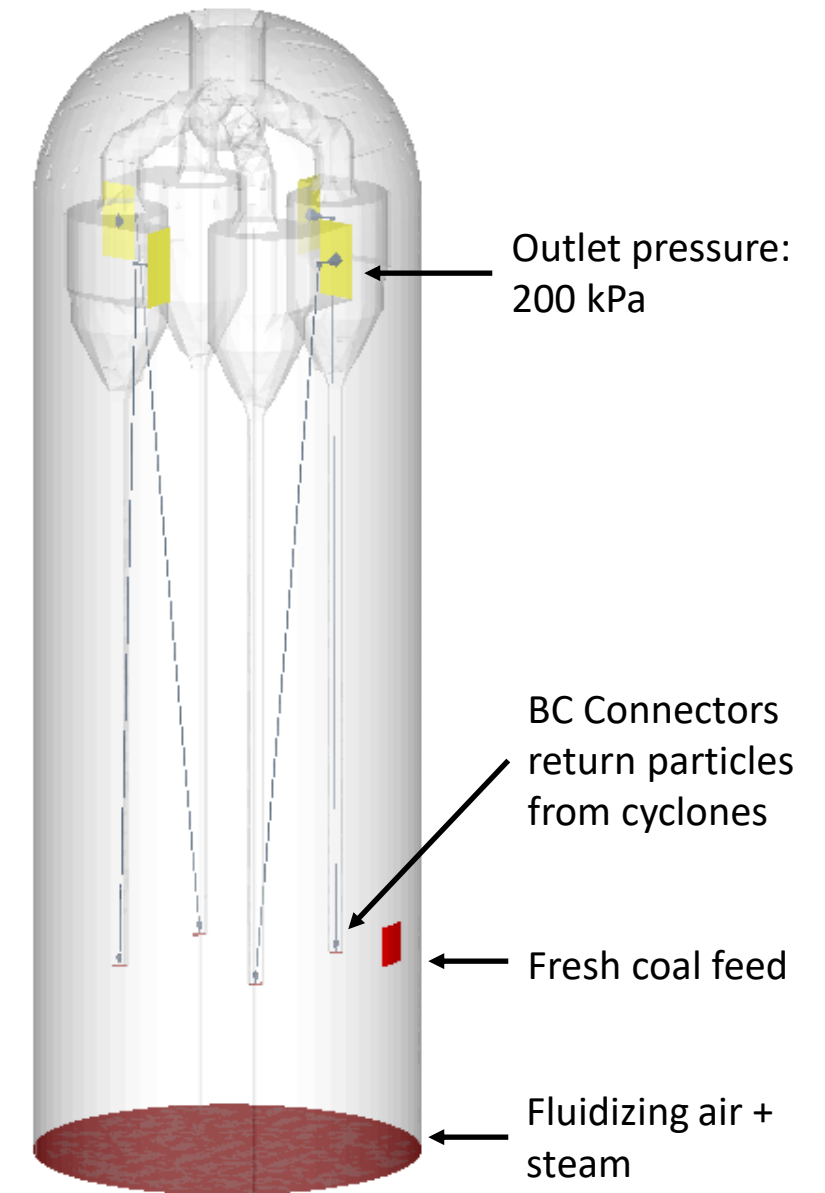
Global Settings

Set Gravity

Select Isothermal flow at 1300 K

Leave Chemistry on

- Volatiles use the chemistry solver
- We still consider this project to be non-reacting since we aren't setting up chemistry reactions
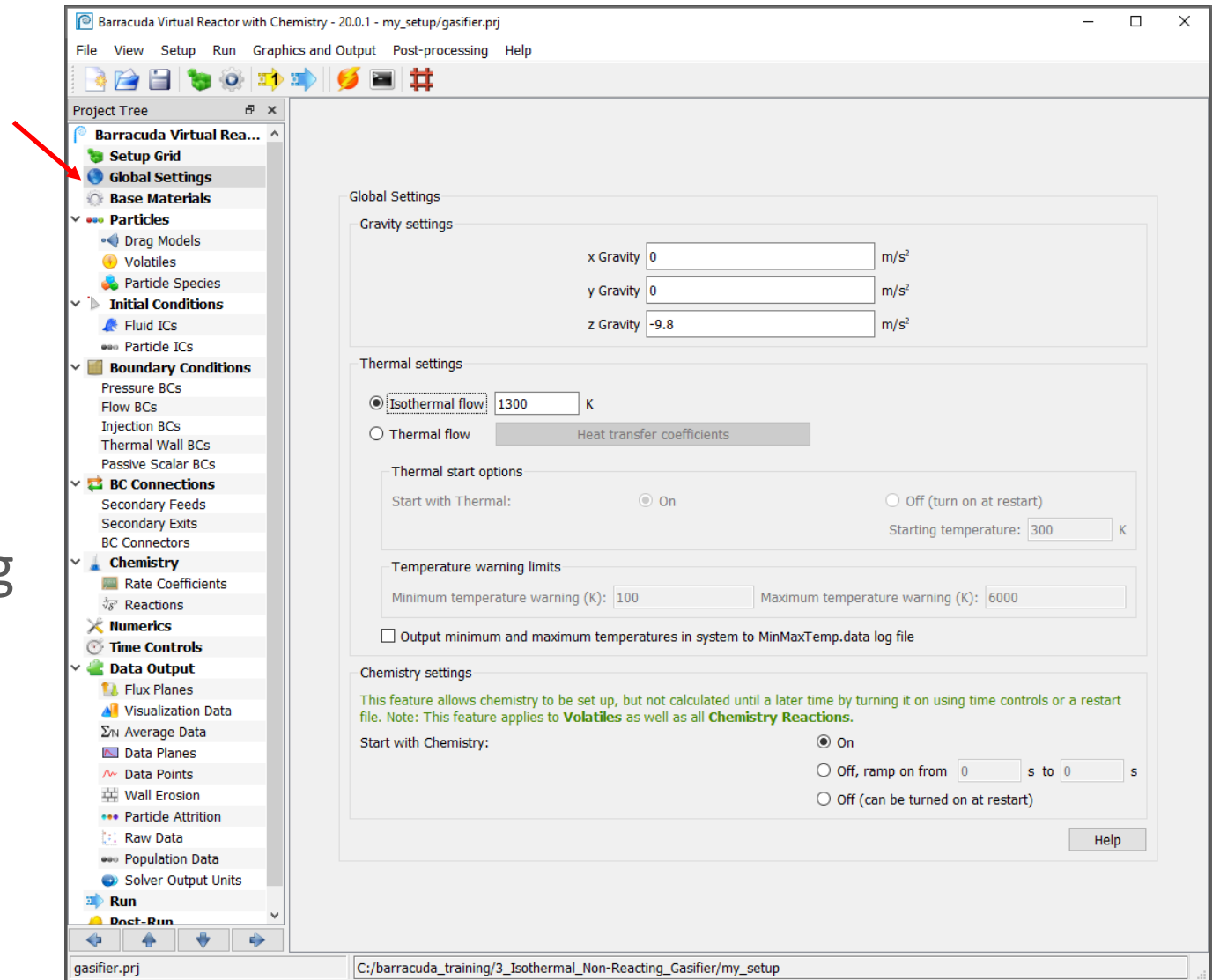
Base Materials

In the Base Materials section, define all materials that will be used in the simulation

Based on the process design sheet and particle properties, you will need:

- Ash (select C_1, then rename it "Ash")
- Carbon (C_1, then rename it "C")
- Methane (CH4_2, then rename it "CH4")
- Carbon Monoxide
- Carbon Dioxide
- Hydrogen gas
- Steam
- Nitrogen gas
- Oxygen gas
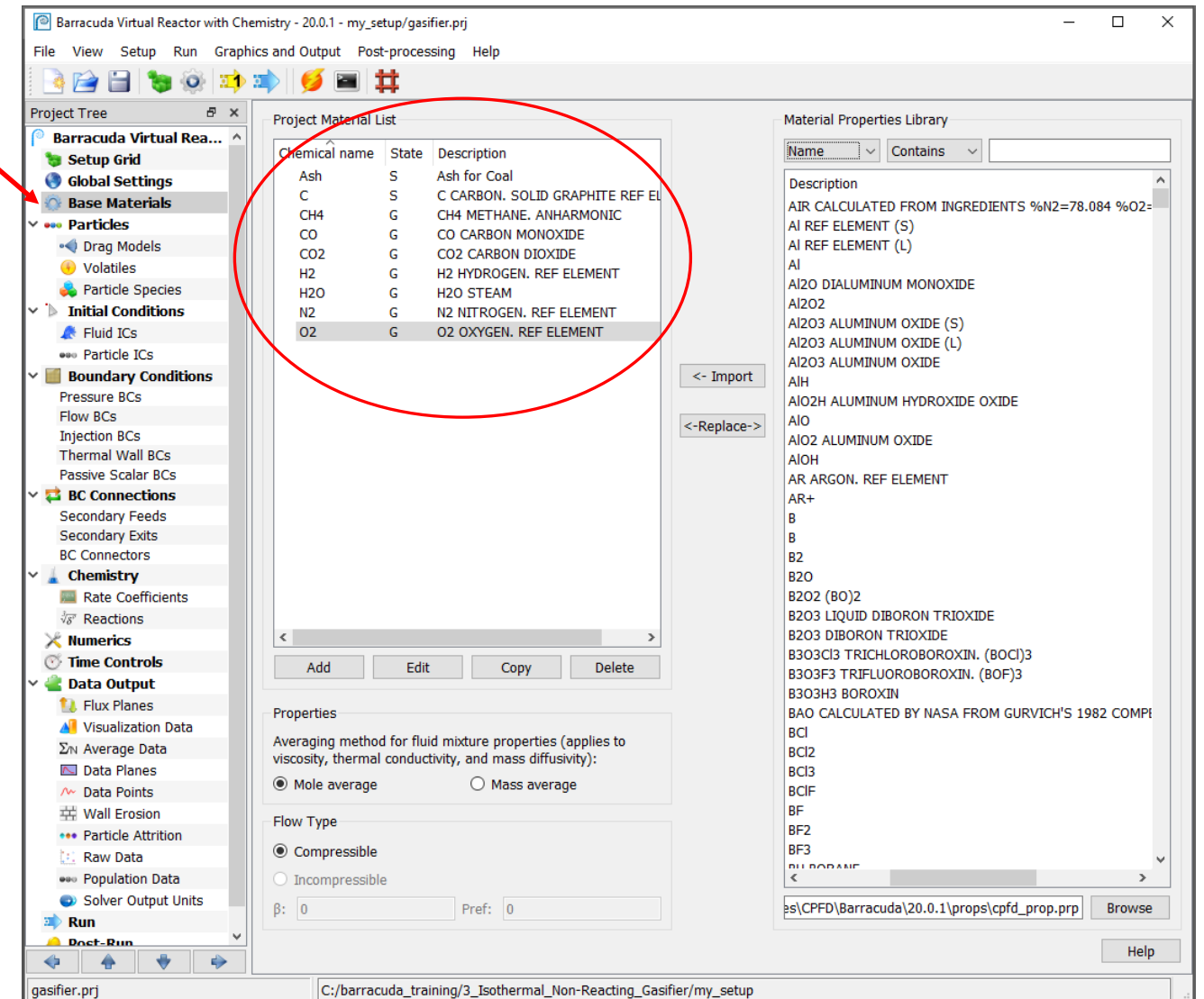
Particles

Set the Close pack volume fraction to 0.6

Set the Normal-to-wall momentum retention to 0.85

Set the Tangent-to-wall momentum retention to 0.85

Set Diffuse bounce to 5
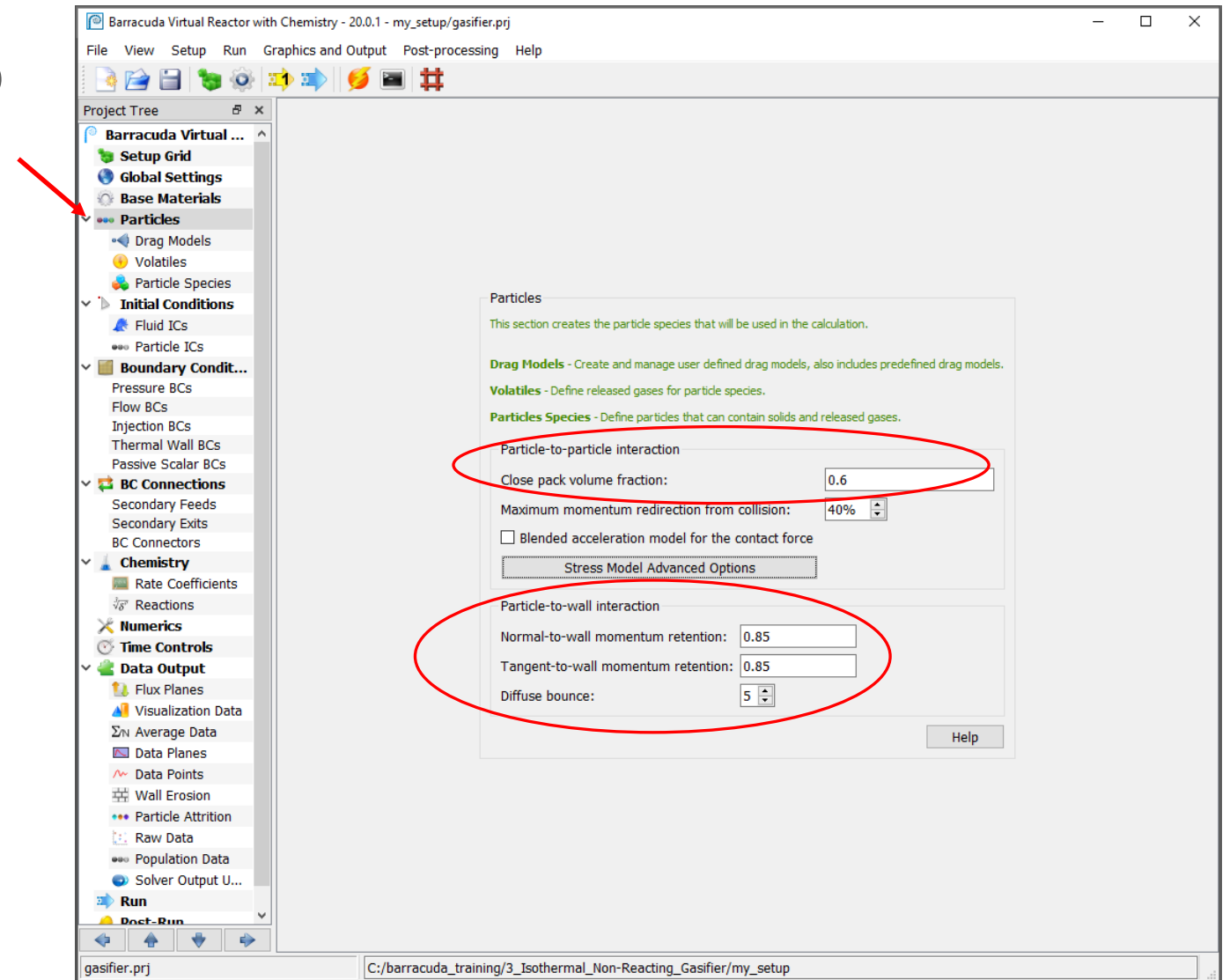
Defining Volatiles

In the Volatiles section, define the volatile material trapped in the fresh coal particles, and the gases released:

- Click on Add
- Enter a Name
- Enter 1000 J/kg K for the Specific heat
- Click on the Release gases button
- Import the gases from Available Components to Mixture using the right arrow
  - 0.4144 CH4
  - 0.1702 CO
  - 0.0444 CO2
  - 0.111 H2
  - 0.26 H2O
- Click OK in the Mixture dialog
- Enter 0.05 for c_0
- Enter 1 for c_1
- Enter 5500 for E
- Click OK

The rate of release of volatiles can be specified in terms of an Arrhenius-type temperature dependence

The release rate expression should be:

Rate = 0.05 T exp(-5500/T)

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Multi-Material Particles

The particles will be treated as multi-material, enabling devolatilization of the fresh coal. Since the initial bed particles are assumed to already be devolatilized, they consist mostly of mostly carbon and ash.

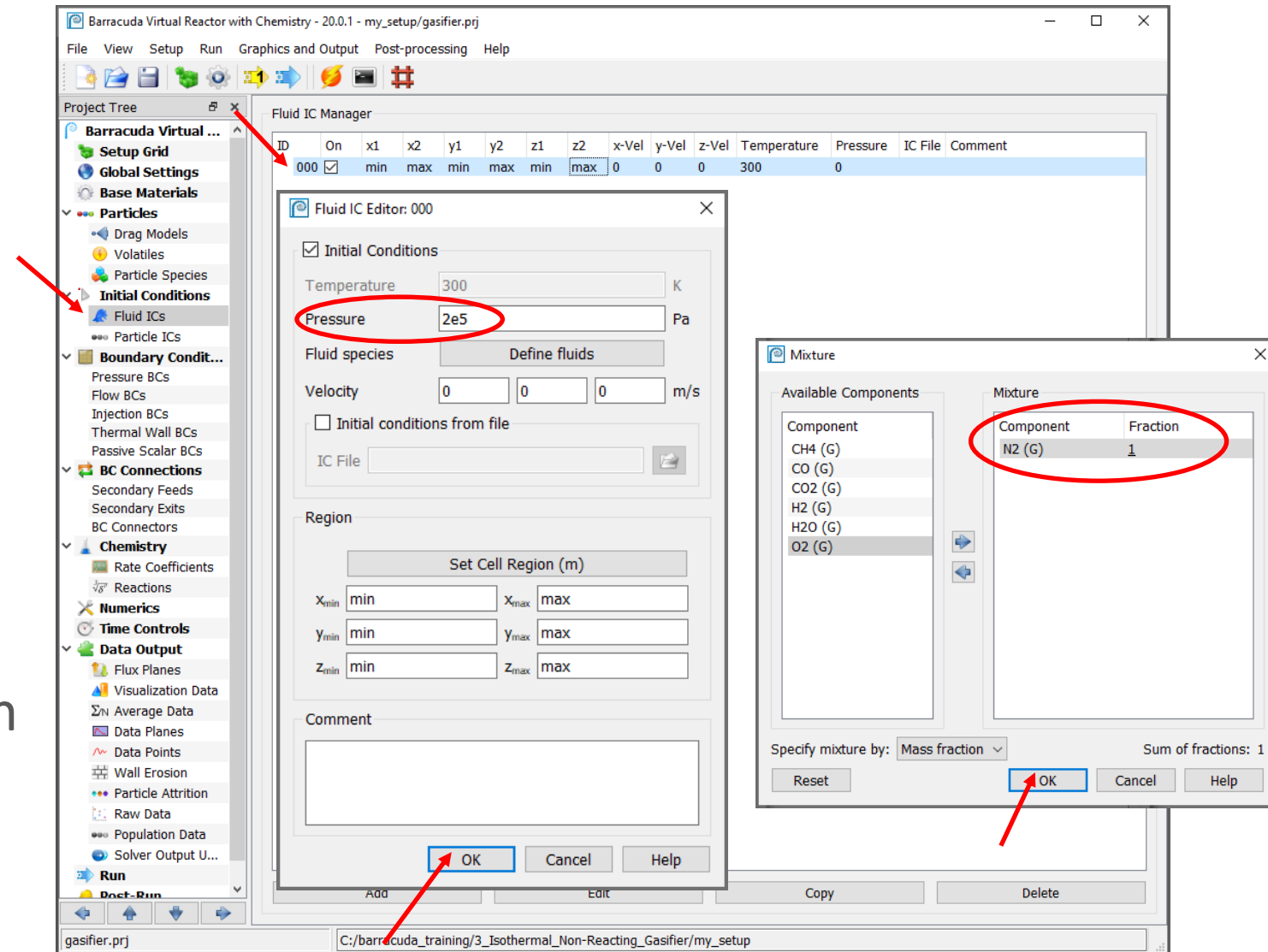**To create a new particle species:**

- Navigate to Particle Species
- Click on Add
- Enter description in Comment
- Click on Applied Materials
- Import Available Components to Mixture Components using the right arrow
  - 0.1 Ash
  - 0.8999 C
  - 0.0001 Volatiles
- Enter Particle Density as 725 kg/m^3
- Click OK

Because the density of the volatiles is unspecified, the **Particle density** must be manually entered
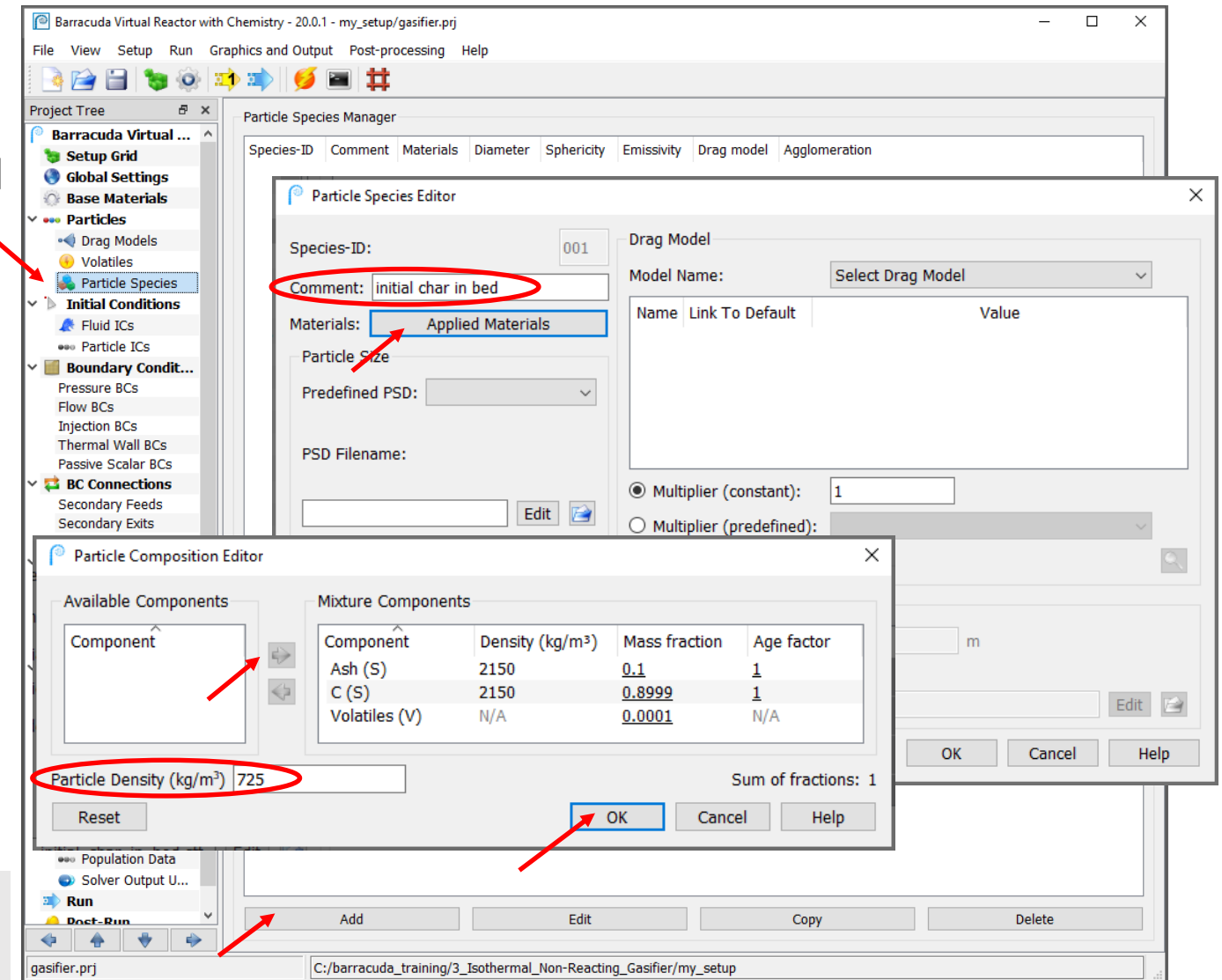
Specifying PSD

To specify the particle size distribution, click on the file directory button for PSD Filename:

- Select the file psd_initial_char_in_bed.sff
- Click Open
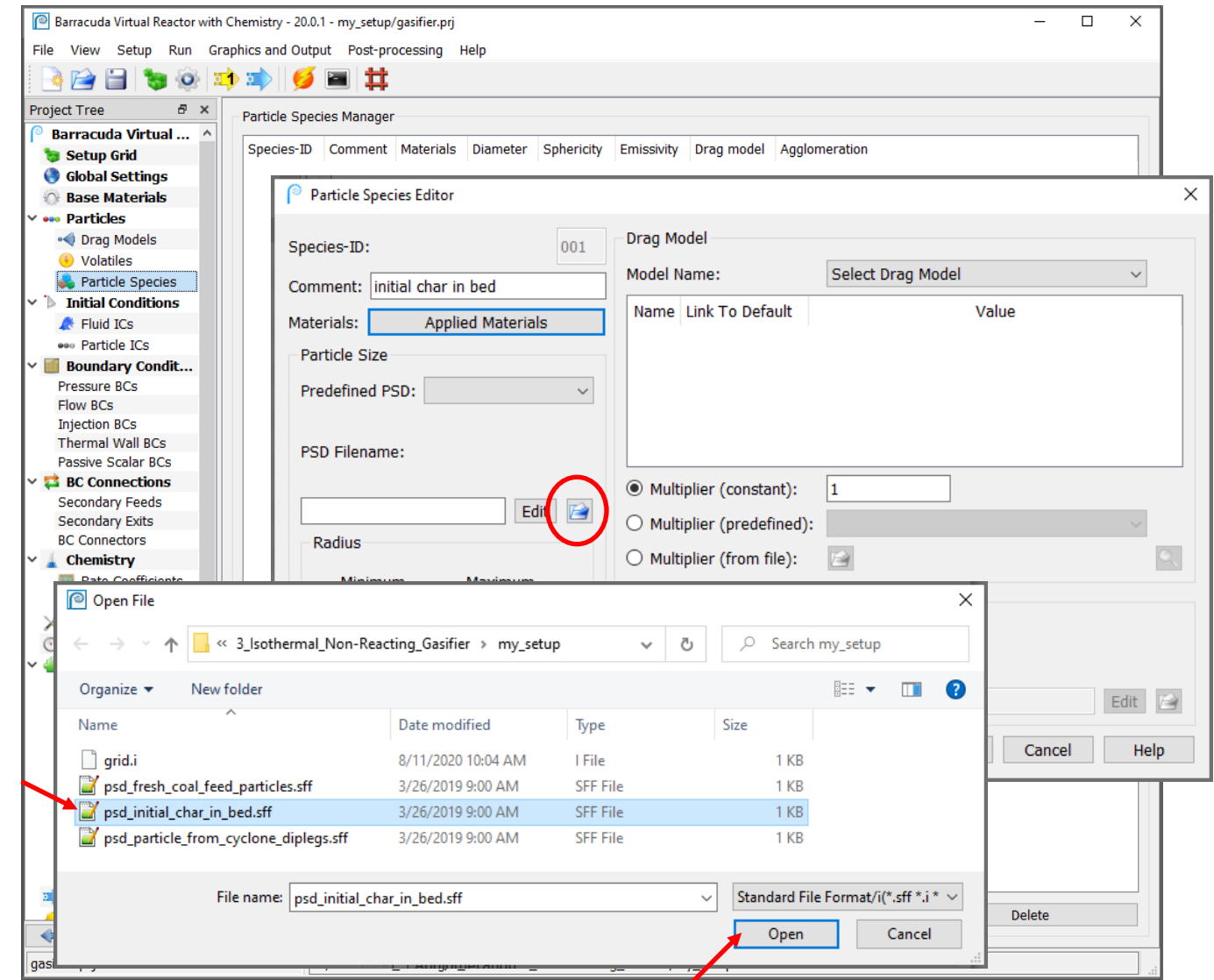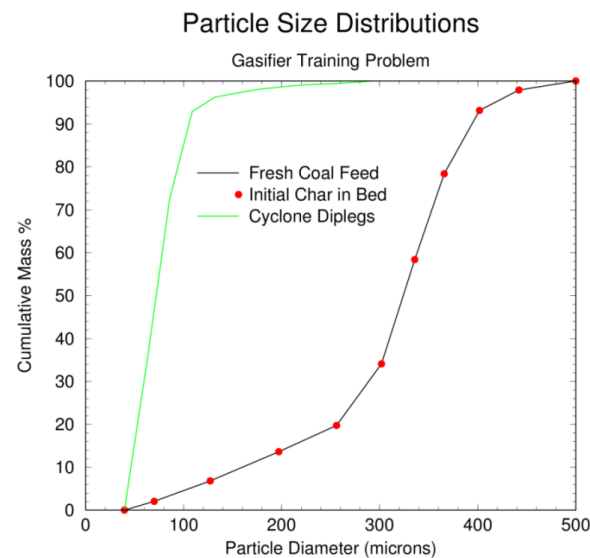
PSD File and Drag Model

To view the PSD file:

- Click on Edit
- Click on Graph to display plot of PSD
- Close Tecplot and Editor window when finished

Select the Wen-Yu drag model for all particle species in this project.

Click OK
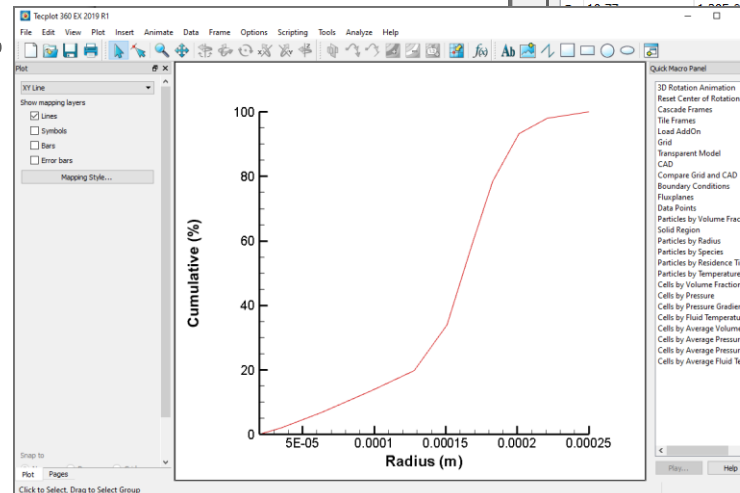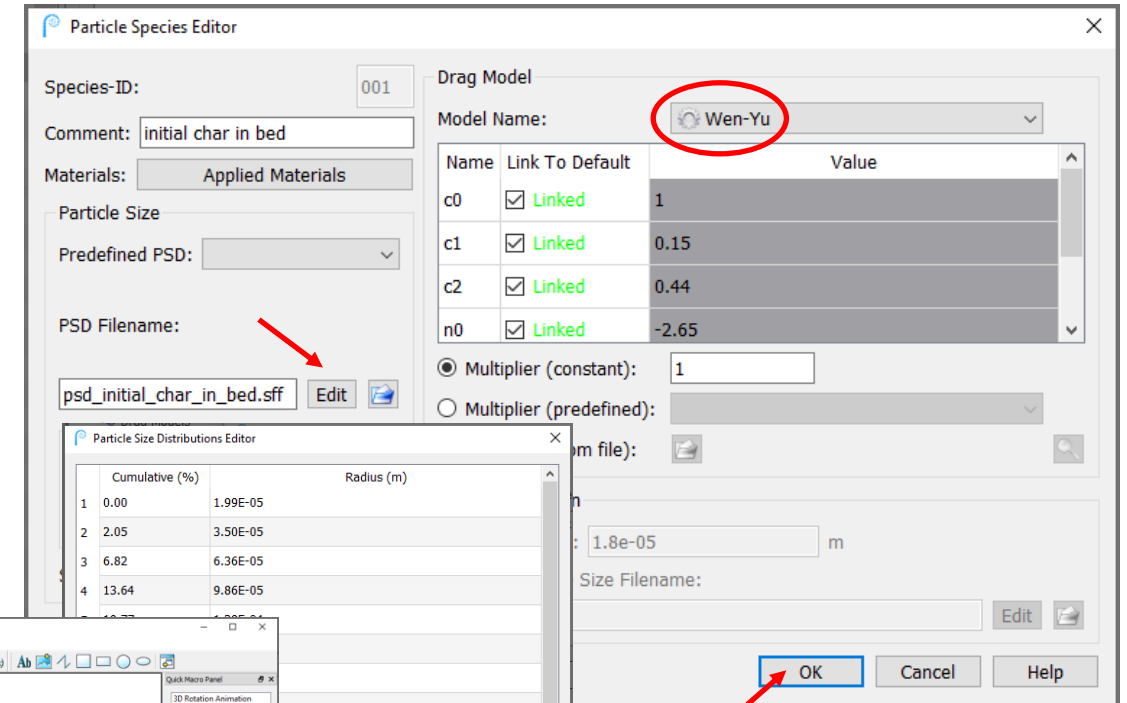
Particle Species – Fresh Coal Feed

Define the particle species for the fresh coal feed:

- Click on Add
- Enter a description in Comment
- Click on Applied Materials
- Import Available Components to Mixture Components using the right arrow
  - 0.05 Ash
  - 0.45 C
  - 0.5 Volatiles
- Manually enter the overall particle density as 1450 kg/m^3
- Click OK
- Specify the PSD by selecting the file psd_fresh_coal_feed_particles.sff
- Select Wen-Yu Drag Model
- Click OK
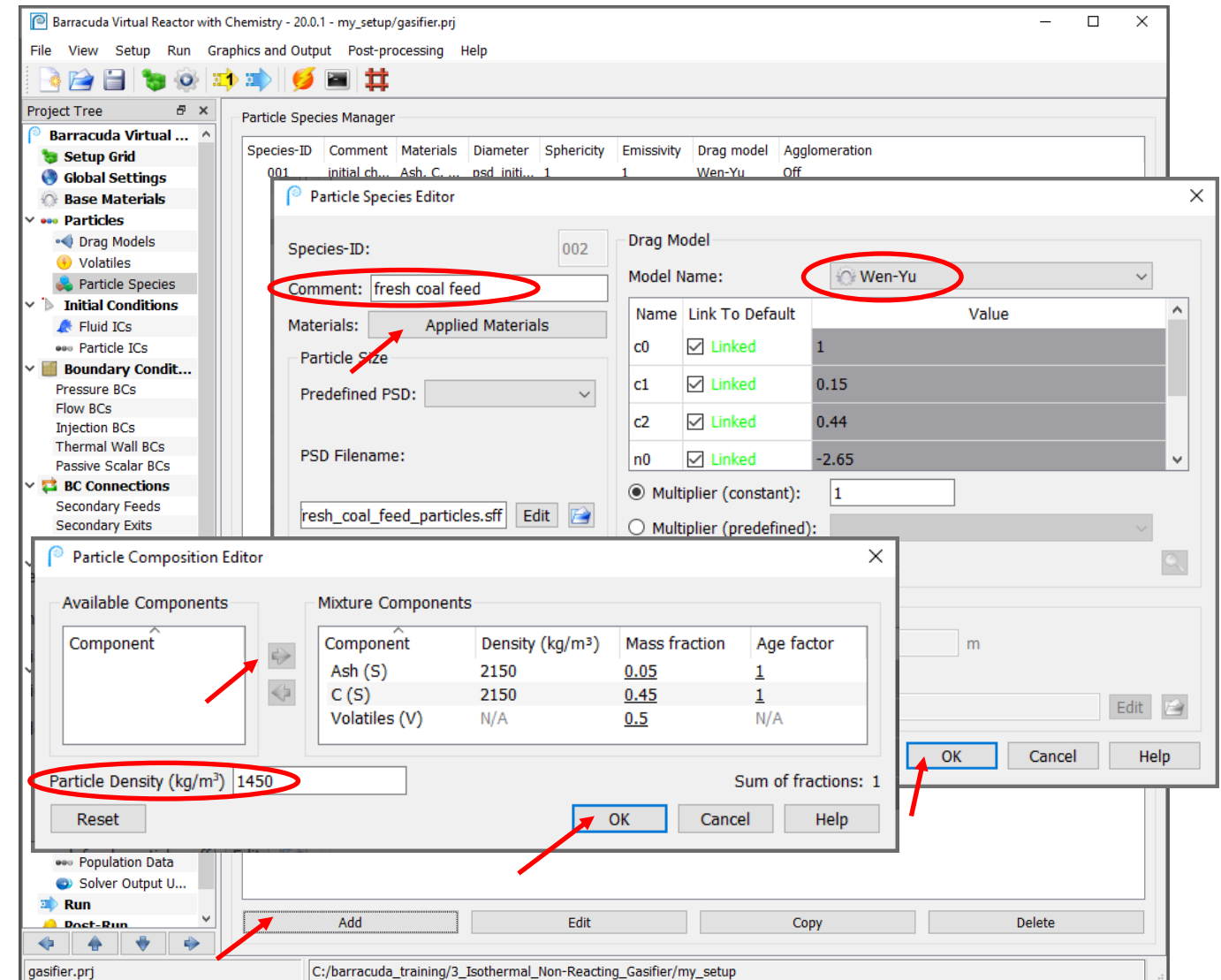
Initial Conditions: Fluid ICs

Edit the fluid initial condition

- Navigate to Fluid ICs
- Double-click on default Fluid IC
- Set Pressure to 2e5 Pa
- Click on Define fluids
- Import N2 from Available Components to Mixture
- Click OK
- Leave Region set from min to max in all directions
- Click OK

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Initial Conditions: Particle ICs

Create the initial bed:

- Navigate to Particle ICs
- Click on Add
- Choose Initialize mass in region
- Set Particle Species to 001 – initial char in bed
- Set the Region using [for min and] for max and see calculation below to determine bed height
- Click OK

$$initial\ particle\ volume = \frac{4800kg}{0.5 \times 725\frac{kg}{m^3}} = 13.24m^3 = 467.6ft^3$$

$$initial\ particle\ height = \frac{467.6ft^3}{\pi(5ft)^2} = 5.95ft = 1.815\text{m}$$

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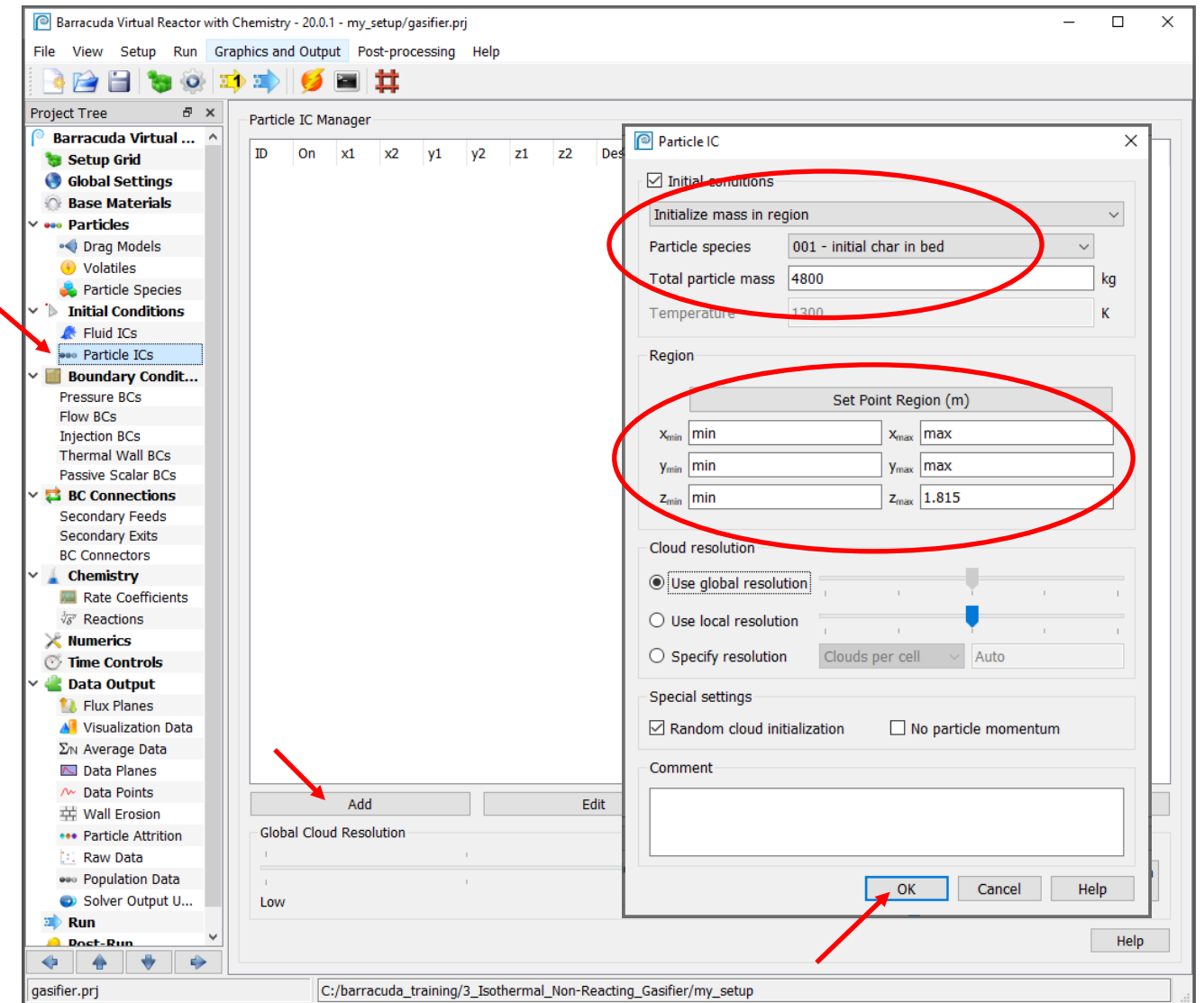
Pressure BCs: Cyclone Inlet Horns

The cyclone inlet horns will be used as pressure BCs through which particles can escape

- Note that we are not modeling the flow of particles inside the cyclones
- Each of the four cyclones will have its own pressure BC. Using the numbering convention shown below can help eliminate confusion
  - Boundary locations will need to be determined for each cyclone
  - The same pressure file can be used to specify the pressure in all cyclones

To add the first pressure BC:

- Click on Add
- Click on Select Region (m)
- (continued on next slide)
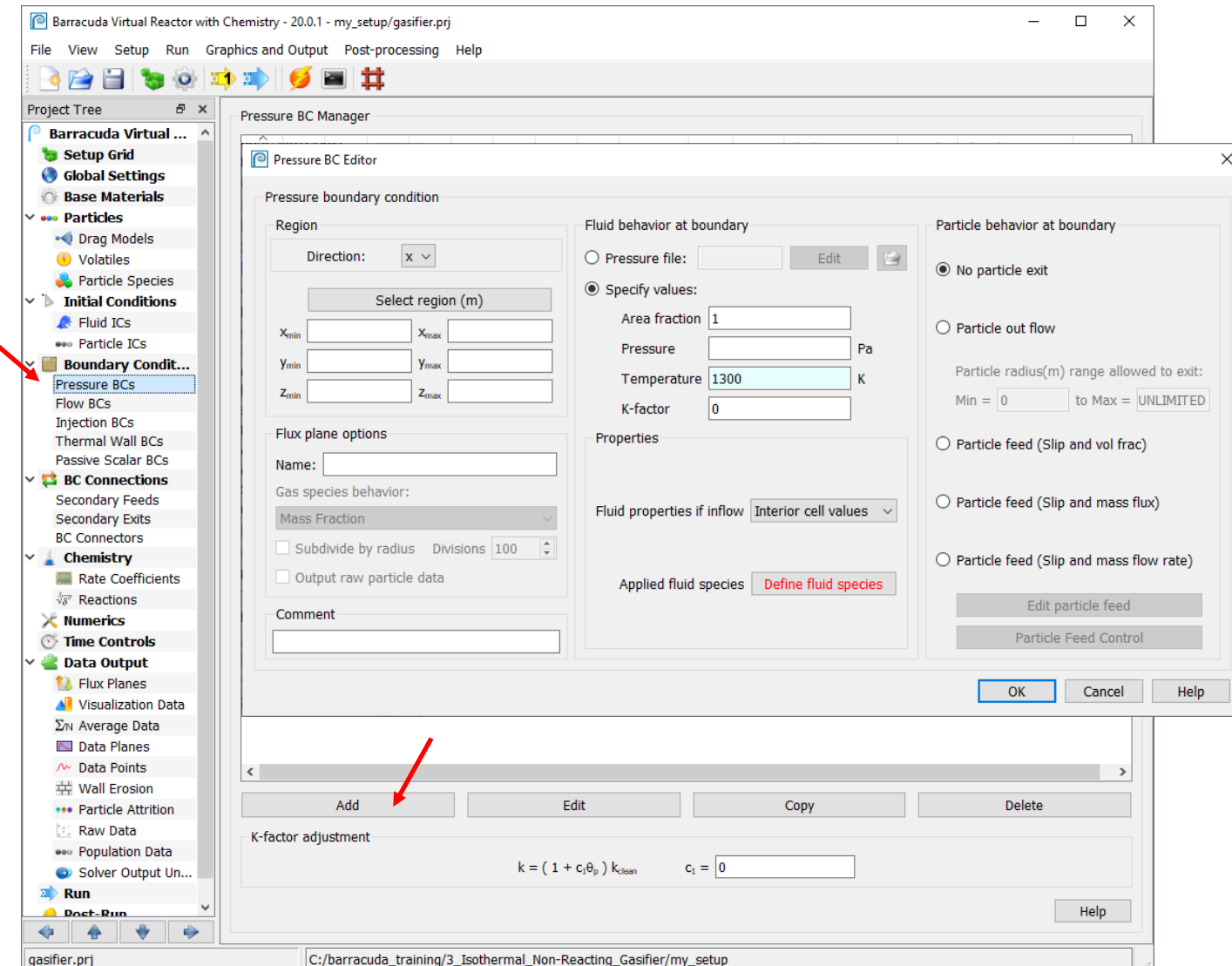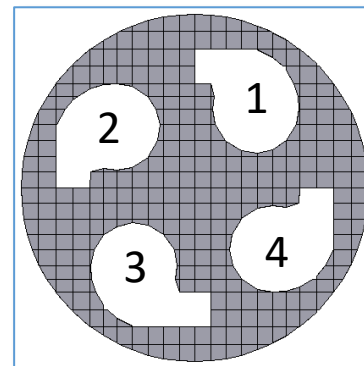
Correct Boundary Condition Location Indices

The Select Region dialog will pop up:

- Click and drag the mouse pointer to select the face for the pressure BC.

- You may need to adjust the region in each pane of the dialog in order to select the cells right around the inlet horn

- Click OK and this will populate the Region section with the x, y, z location for the pressure BC
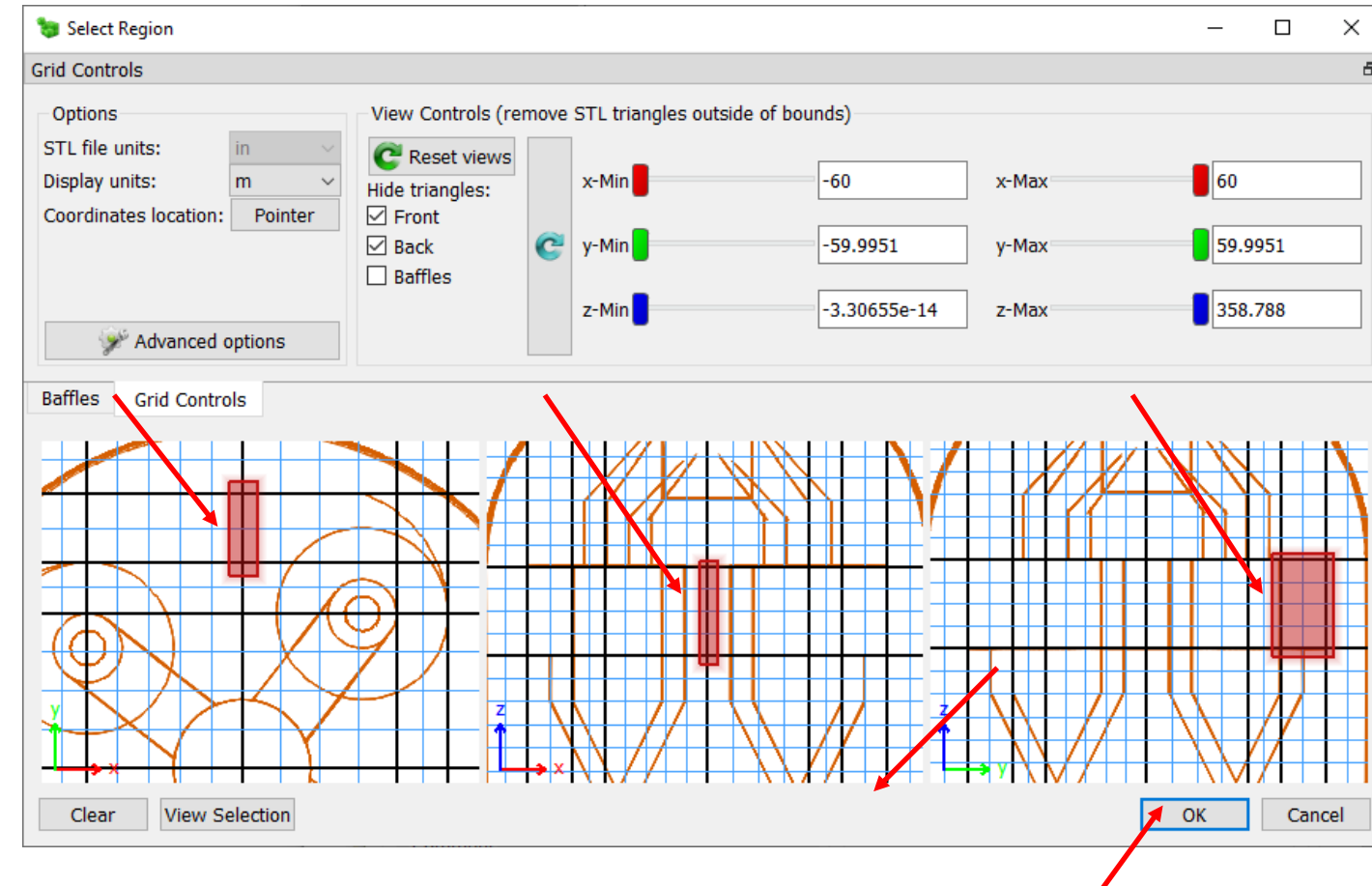
Pressure BC Flux Planes

Once you have set the cell region for the pressure BC:

- Select appropriate direction for the pressure BC of each cyclone. It should be normal to the face of the boundary
- Give each pressure BC a flux plane name that is easy to identify. We will be examining the data in these flux plane files during post-processing
  - Use a standard prefix, such as "FLUXBC_" to make the files easy to find
  - Avoid spaces in file name
- Select Mass Time Cumulative for gas species information through the flux plane. This will allow us to monitor the gas composition into the cyclones
- Enter a descriptive Comment

Pressure Boundary Conditions

The same pressure file will be used for the pressure BC of each cyclone. To create the file:

- Select Pressure file:
- Click on Edit
- Enter conditions as shown in the Pressure Boundary Conditions Editor
- Save the file as: BC_top_pressure.sff
- Click on Close

Define the fluid species as 100% N2

Select Particle out flow to allow particles to escape through the boundary

Click OK

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Pressure BCs: Cyclone Inlet Horns

Follow previous steps in order to make a pressure BC for each cyclone inlet horn

Remember to browse for the pressure file created (BC_top_pressure.sff) instead of creating a new one for each pressure BC.
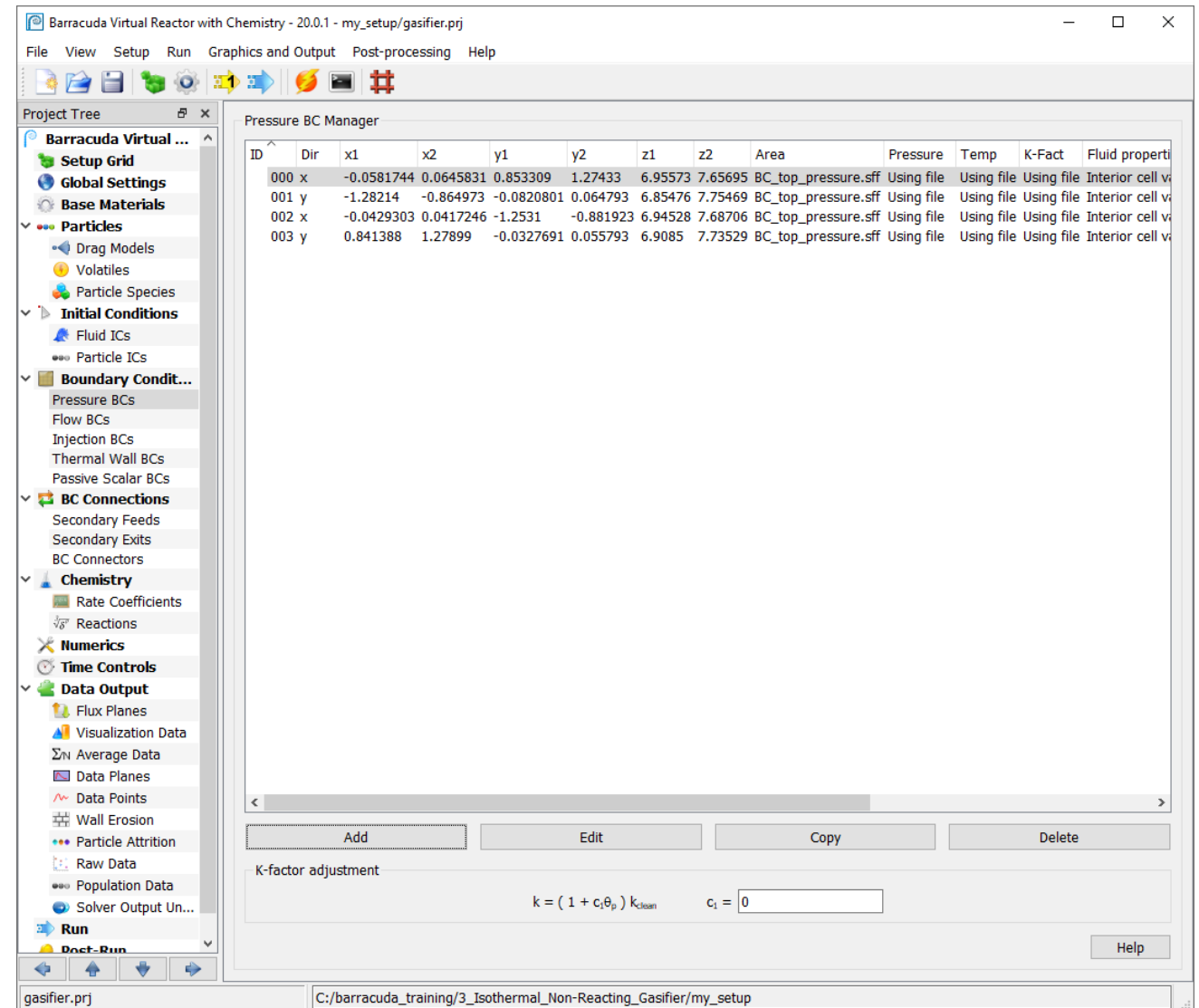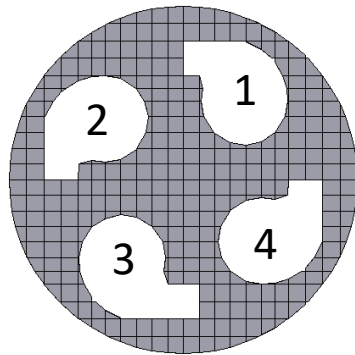
Bottom Flow BC: Simplified Sparger

Recall that the bottom uniform flow BC is being used as a simplification to introduce all fluidization gas and steam to the system. To create the flow BC:

- Click on Add
- Use [and] to specify min and max values in Region
- Enter a fluxplane name
- Enter a descriptive comment (optional)
- Select Use transient fluid flow file
- Select No particle exit
- Click on Define fluids and use values (mass fraction) from process sheet
  - 0.3 H_2O
  - 0.54 N_2
  - 0.16 O_2
- Click on Edit in Transient fluid and particle flow file
- Fill out Flow Boundary Conditions Editor using values from process sheet
  - 0.3 m/s Velocity
- Click Save to save the file as BC_bottom_flow.sff
- Click on Close
- Click on OK
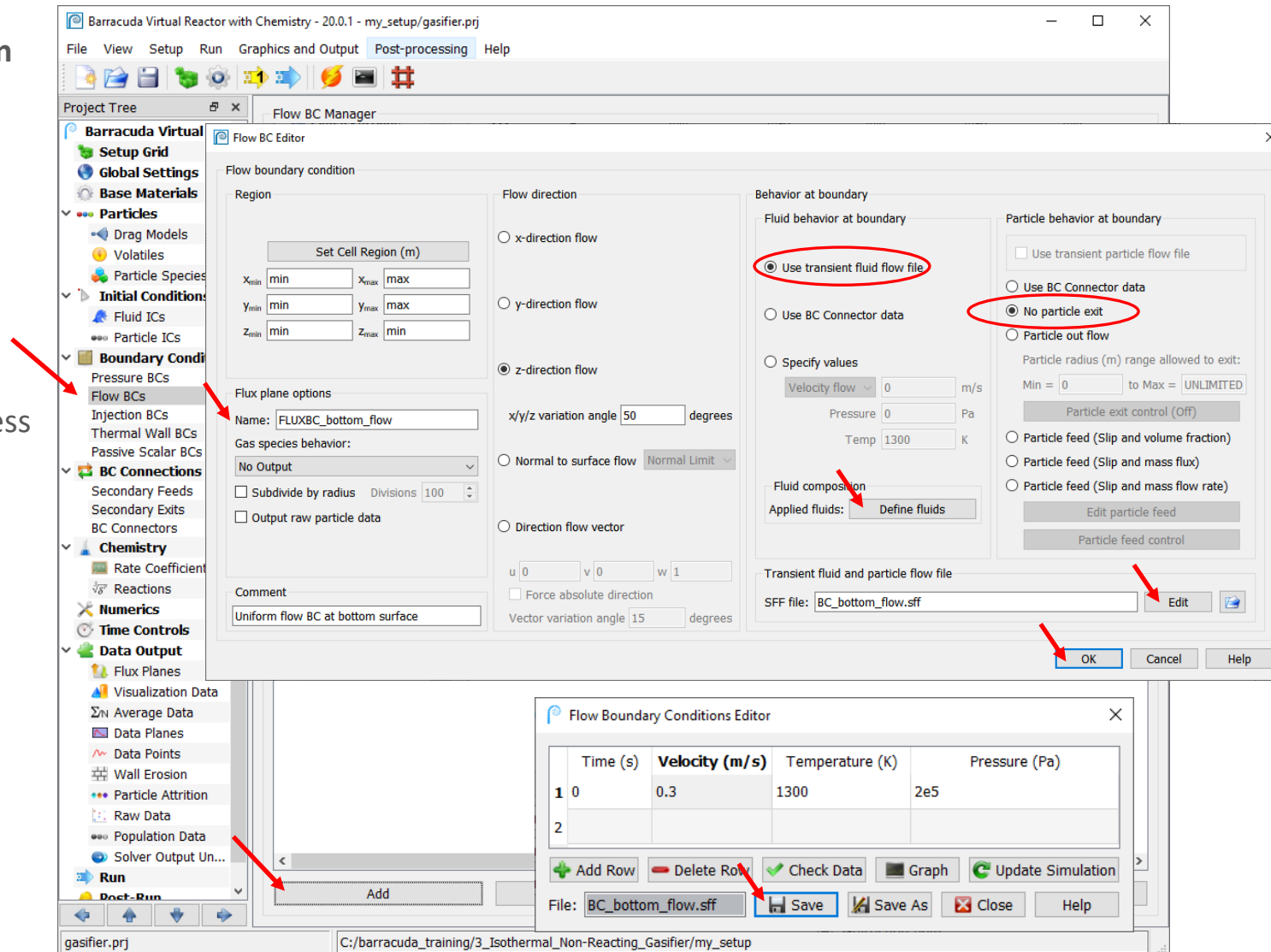
Fresh Coal Flow BC

Fresh coal is fed into the system from a side inlet location. To create this flow BC:

- Click Add
- Enter the region location
- Enter flux plane name and comment
- Select x-direction flow
- Click on Define fluids and use values (mass fraction) from process sheet
    - 0.77 N2
    - 0.23 O2

When defining flow BCs that feed both fluids and particles, keep in mind that the fluid mass flow rate and particle mass flow rate are specified separately
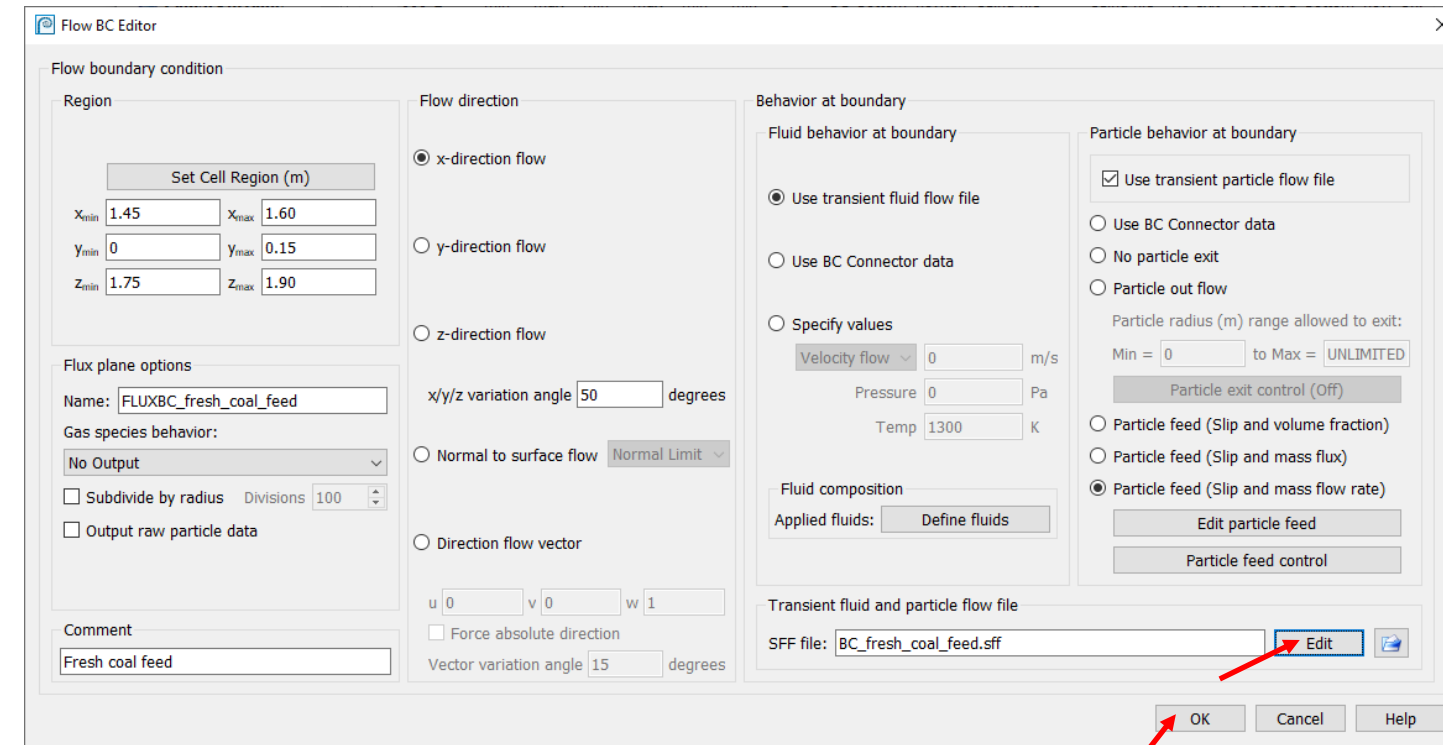
1. Select Use transient fluid flow file
2. Select Particle feed (Slip and mass flow rate)
3. Check Use transient particle flow file
4. Click on Edit particle feed
5. Import 002: fresh coal feed from Available Components to Mixture using the right arrow

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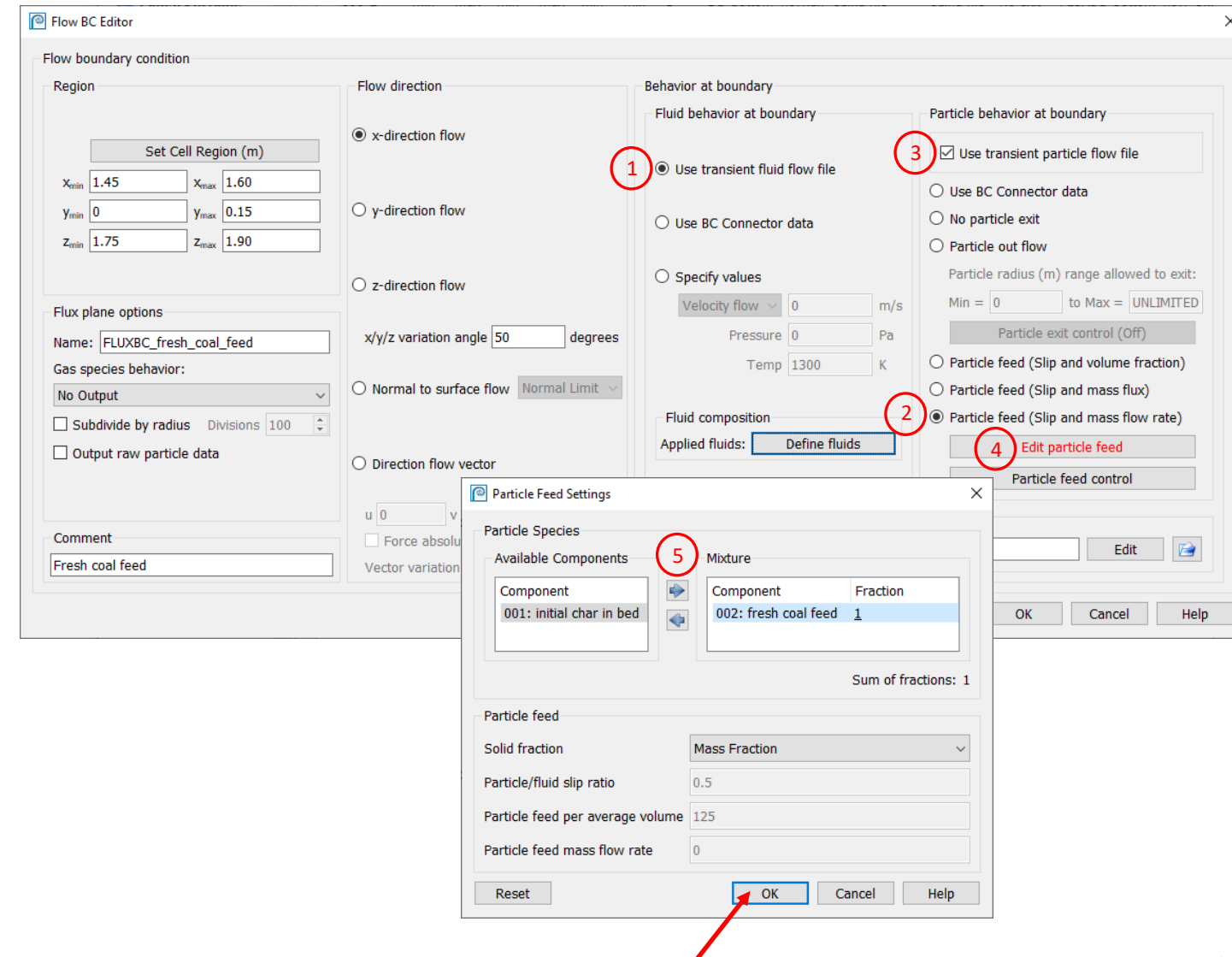
Fresh Coal Flow BC: Particle Feed

Click Edit to create a transient fluid and particle flow file using the process sheet data:

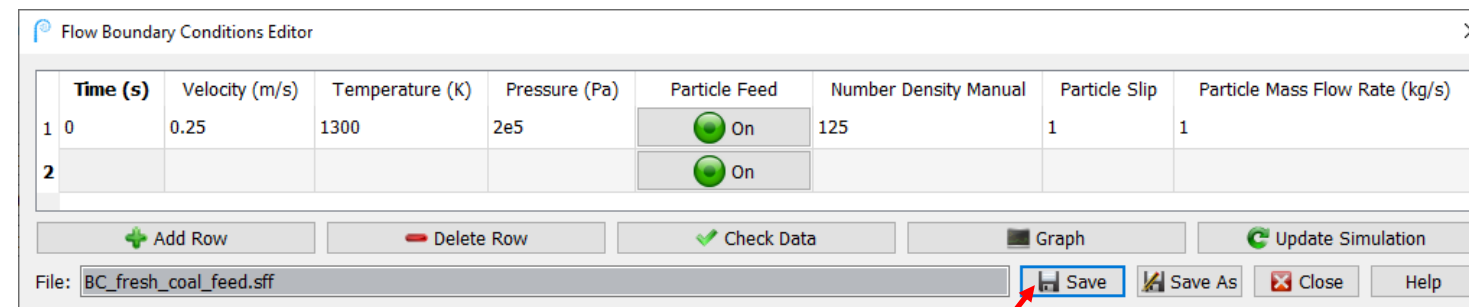- 0.25 m/s fluid velocity
- 1 kg/s particle mass flow rate

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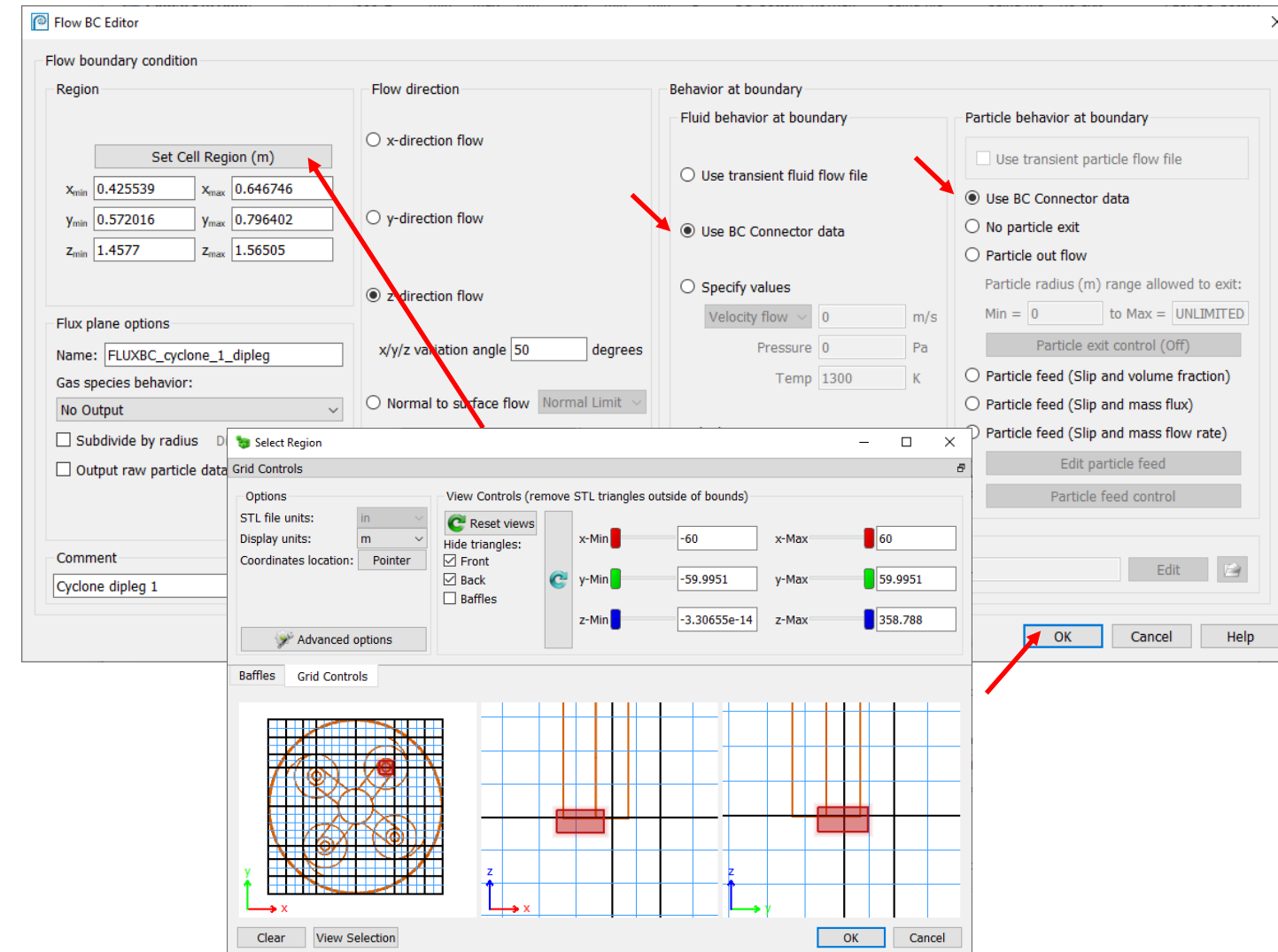
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Cyclone Dipleg Flow BCs

Flow BCs will be defined on the cyclone diplegs to maintain system mass. BC Connectors, which tie each inlet horn pressure BC to its corresponding dipleg flow BC, will be set up on subsequent slides

Each dipleg will need an individual flow BC:

- Use the Select region dialog to select the bottom face of the dipleg
- Define a good Flux plane name for each dipleg Flow BC
- Select Use BC Connector Data for both Fluid behavior at boundary and Particle behavior at boundary

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Flow BCs

Ensure that all four cyclone dipleg Flow BCs are created before moving on to the next slide
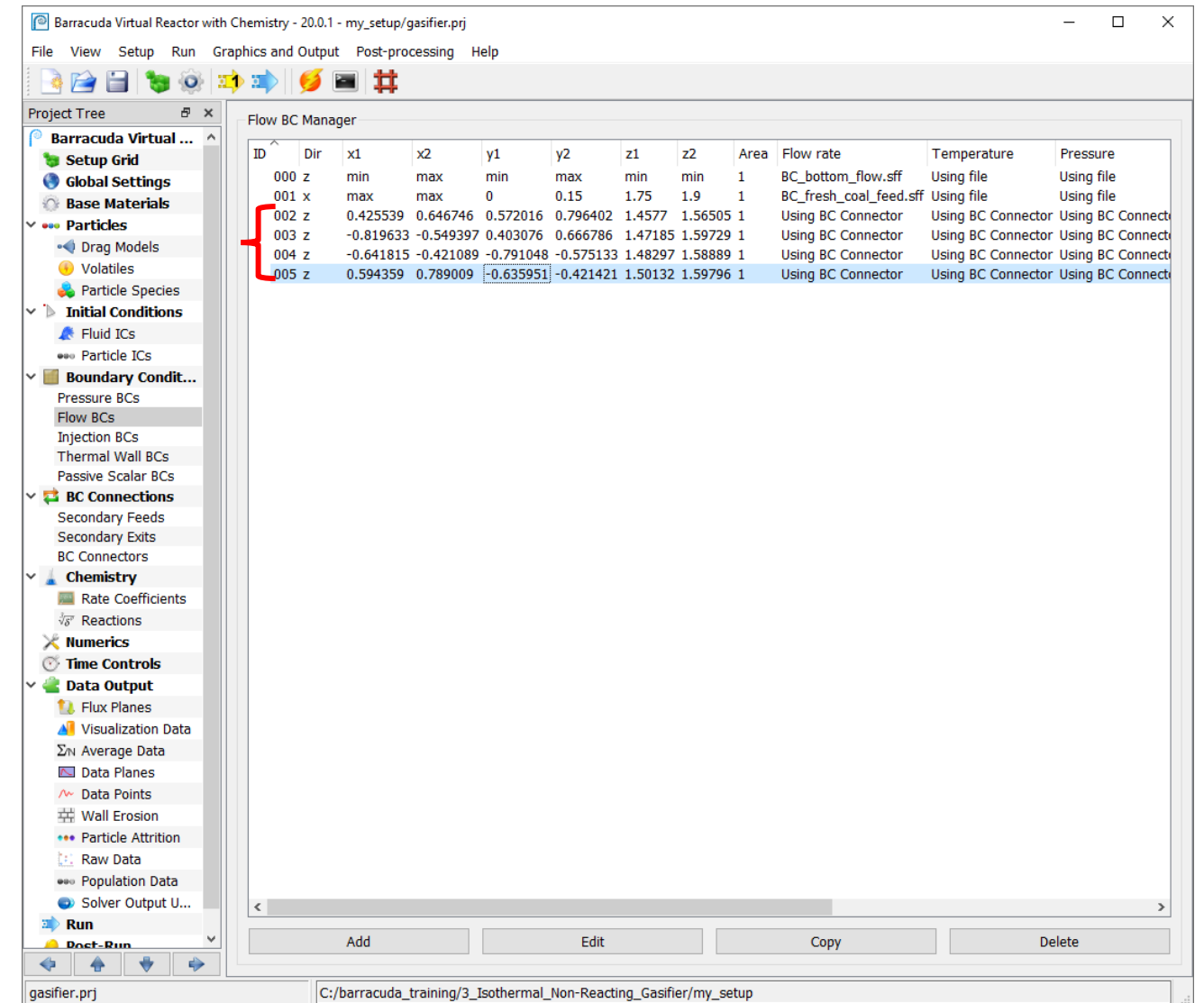
BC Connection Input from Domain

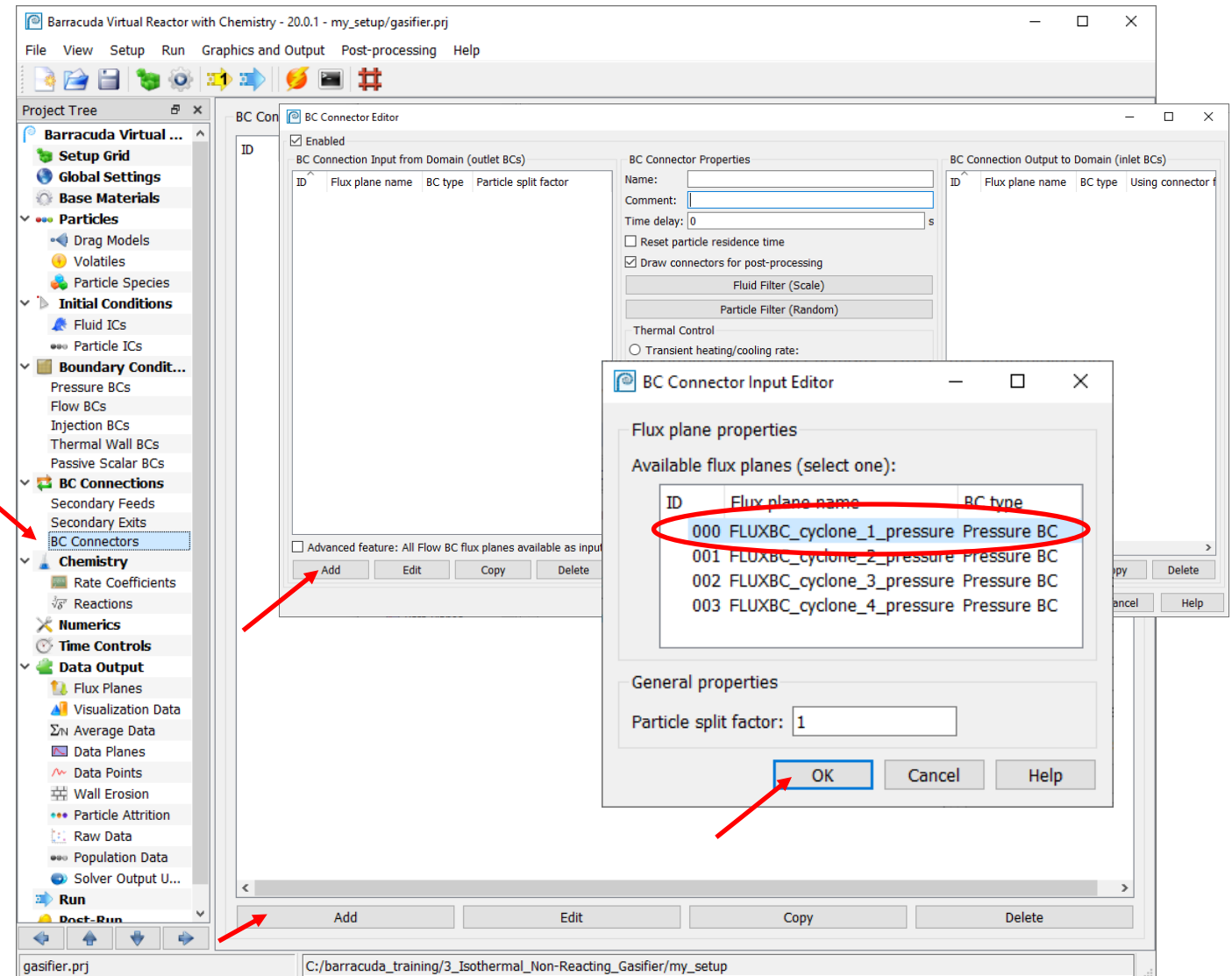**To create the BC Connections from the cyclone pressure BCs to the dipleg flow BCs:**

- Navigate to BC Connectors
- Click on Add
- Click Add on left side of BC Connector Editor
- Select the pressure BC for cyclone 1
- Click OK

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BC Connection Output to Domain

- Click add on the right side of the BC Connector Editor
- Select the flow BC for cyclone dipleg 1
- Change the Fluid volume fraction limit to 0.5. This will limit the amount of fluid that can return from the cyclone inlet horn Pressure BC to the dipleg Flow BC along with the particles
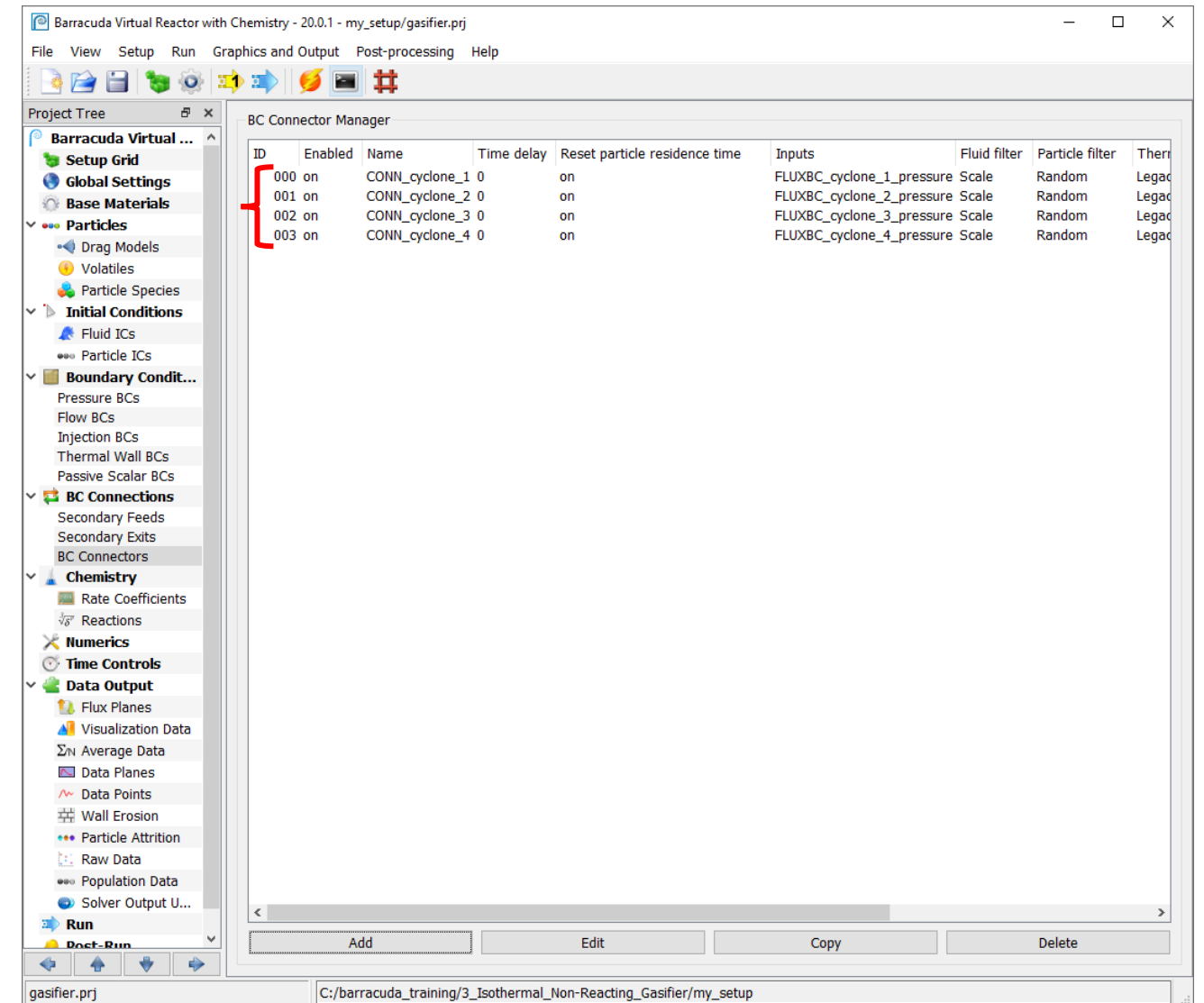- Click OK
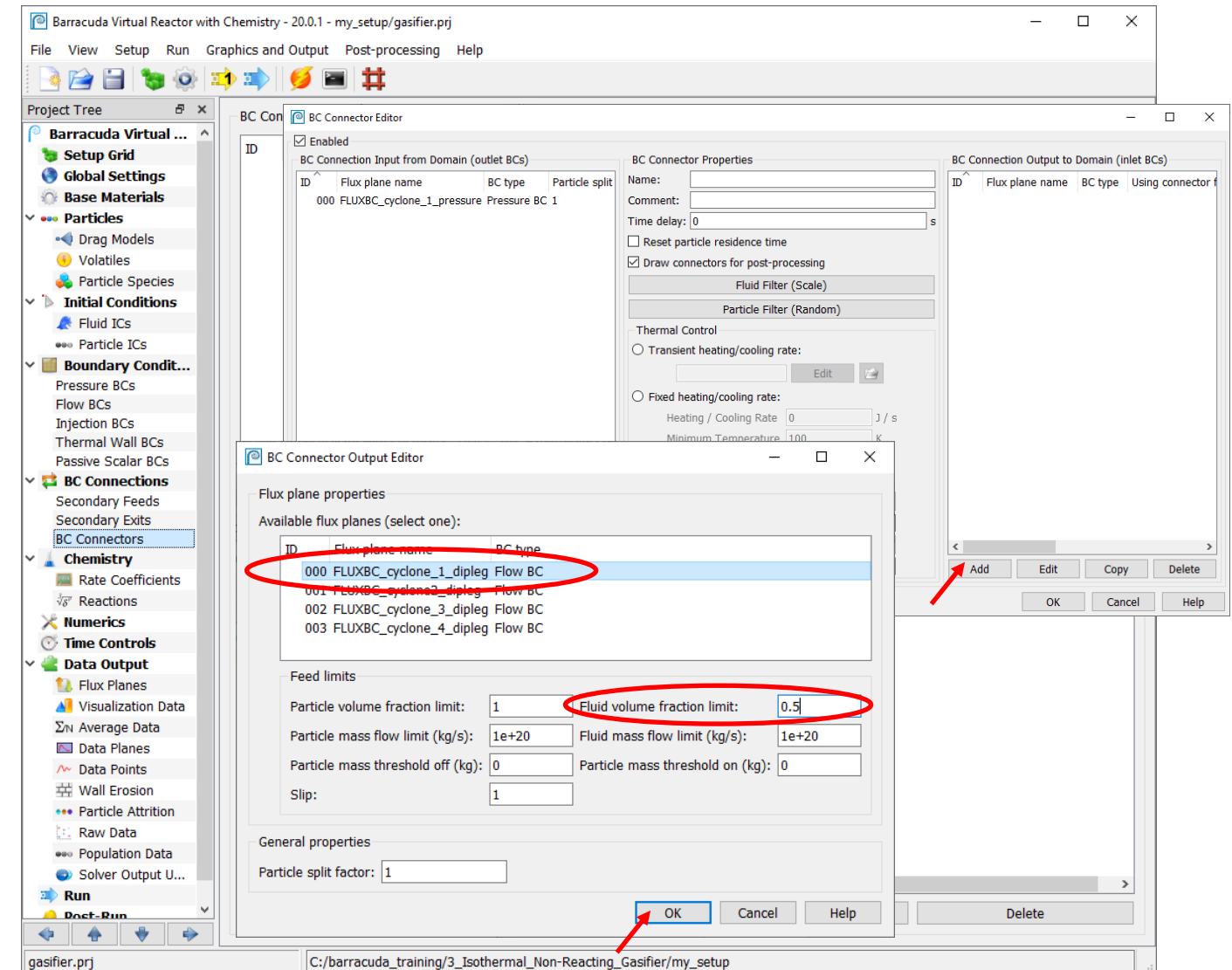
BC Connector Properties

- Enter a Name (which will be the name of a flux plane file for the BC Connection)
- Enter a Comment (optional)
- Select Reset particle residence time
- Click OK
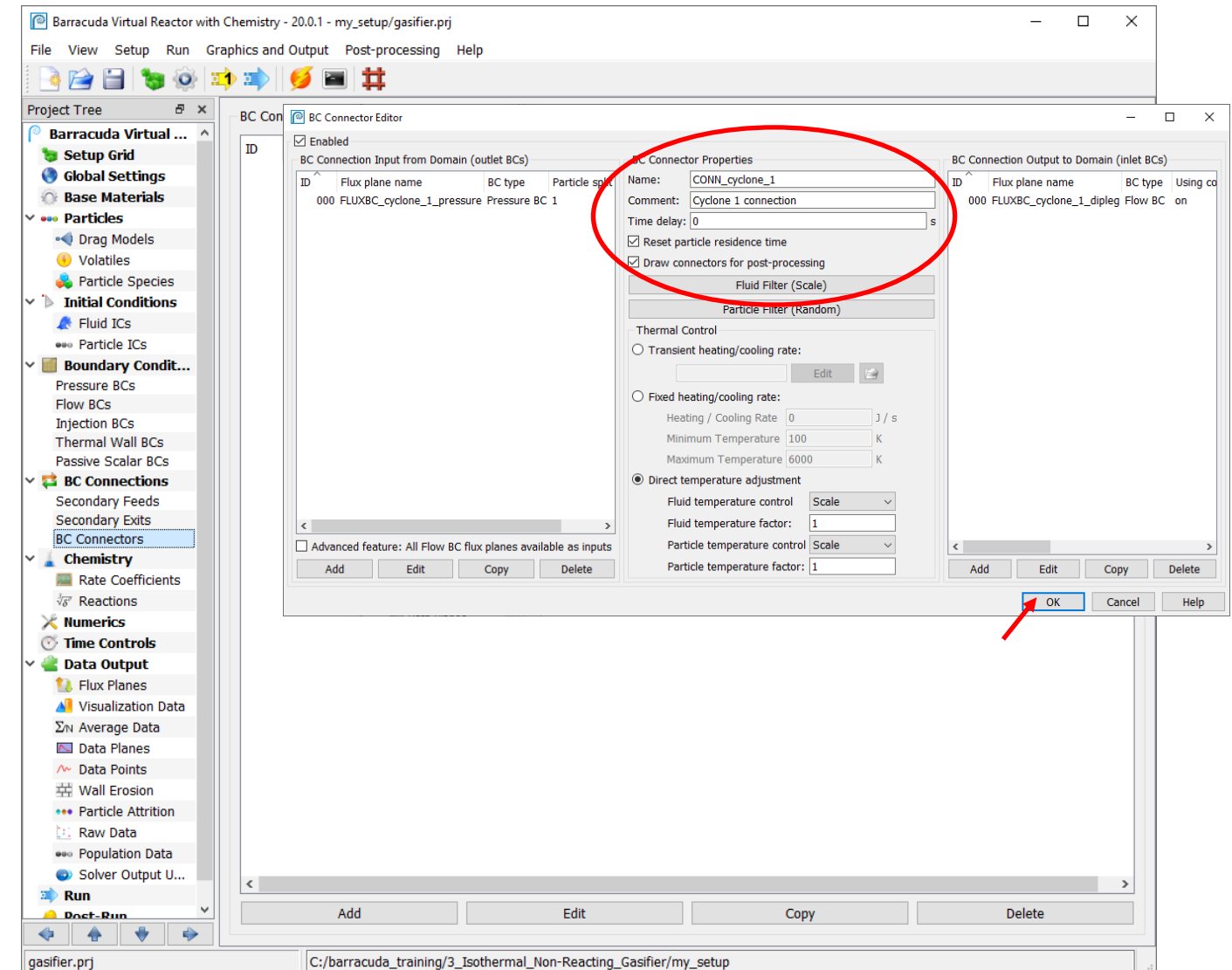
Add BC Connections for Remaining Cyclones

Repeat the above steps to define BC Connections for Cyclones 2, 3, and 4
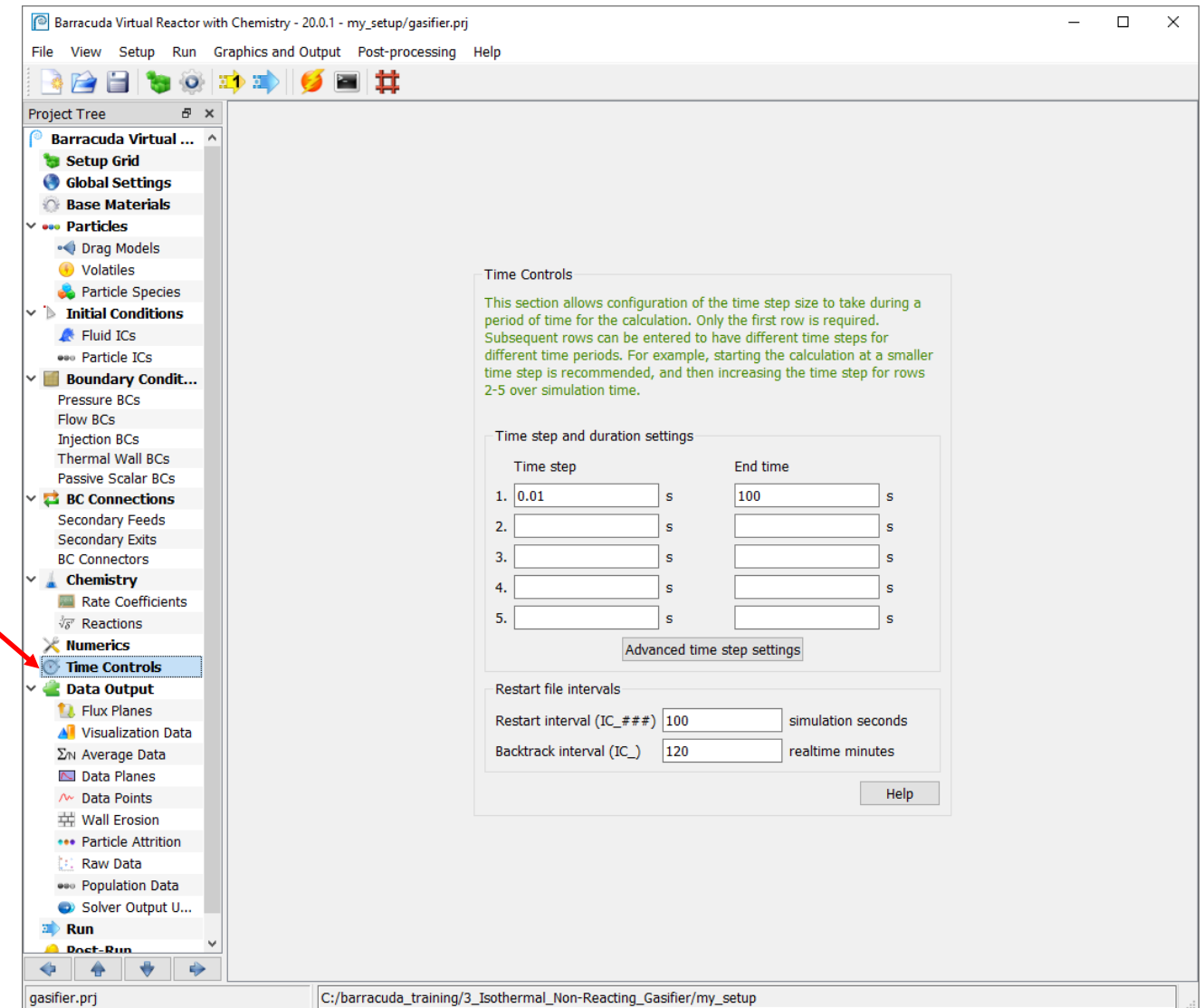
Time Controls

Set the Time step to 0.01 s

- If this initial guess is too high, the solver will automatically adjust your time-step based on built-in controls
- However, there are limits concerning how much lower it will try to go, so try to specify something reasonable

Set the End time to 100 s

Flux Planes

**Flux planes were already defined at the pressure and flow BCs.**

It is also useful to set up a flux plane lower in the freeboard to get an earlier idea of the particle entrainment rate. To set up a flux plane that spans the vessel at about the height shown in the image:

- Navigate to Flux Planes
- Click on Add
- Enter a z location
- Enter a flux plane name
- Enter a descriptive comment (optional)
- Click OK
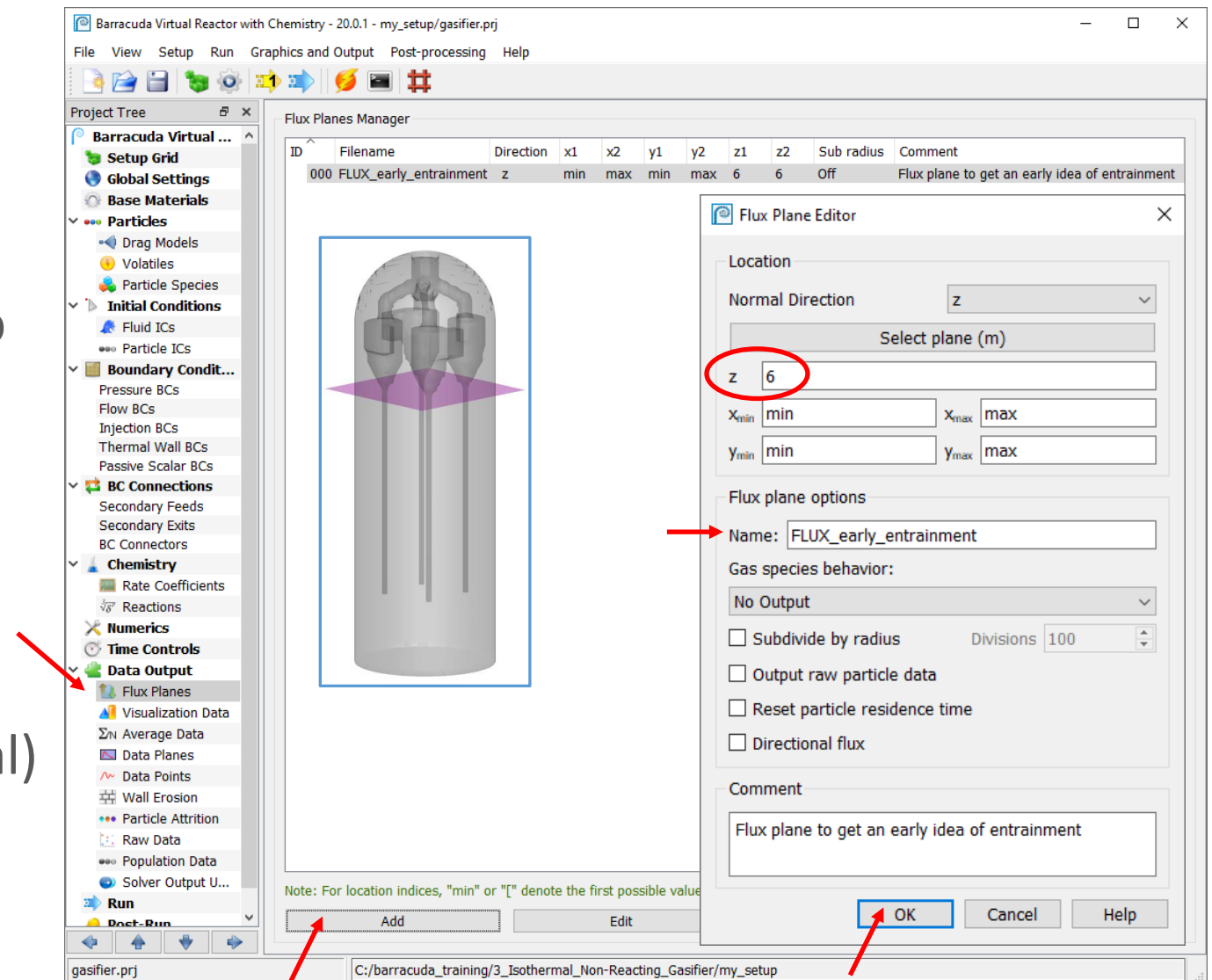
Visualization Data Output Options

By default, a minimal set of variables is selected for output to Tecplot. This is done to keep file sizes as small as possible, since Tecplot files typically take up the most space in your run directory.

Select all the variables shown at right for post-processing this training problem.
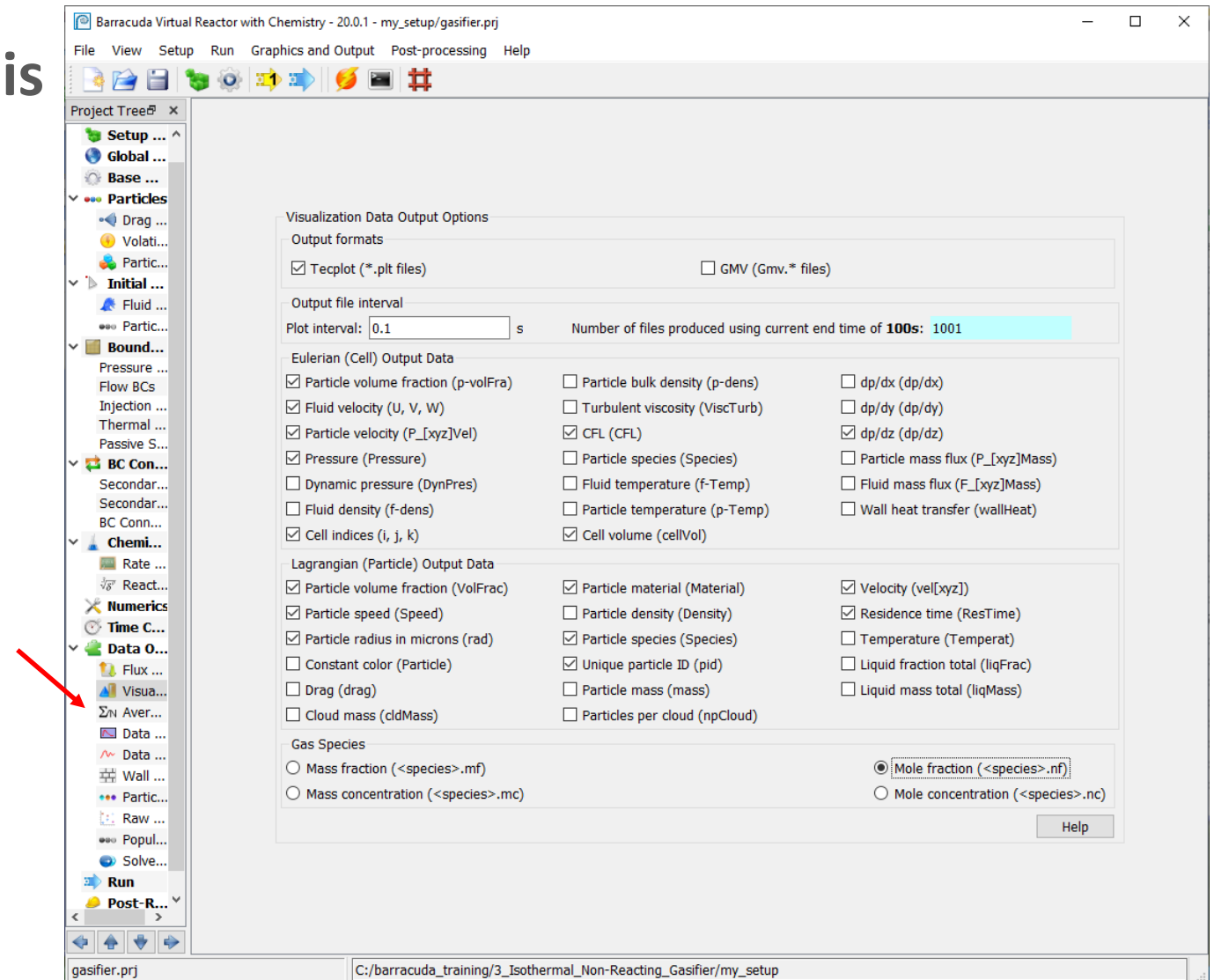
Average Data

Time-average data is very useful when analyzing particle-fluid systems. Fluidized beds, for instance, are dynamic by nature and therefore time-averaging is nice for visualizing a steady-state condition.

- Start time-averaging at 20 s
- Select the items shown for time-averaging

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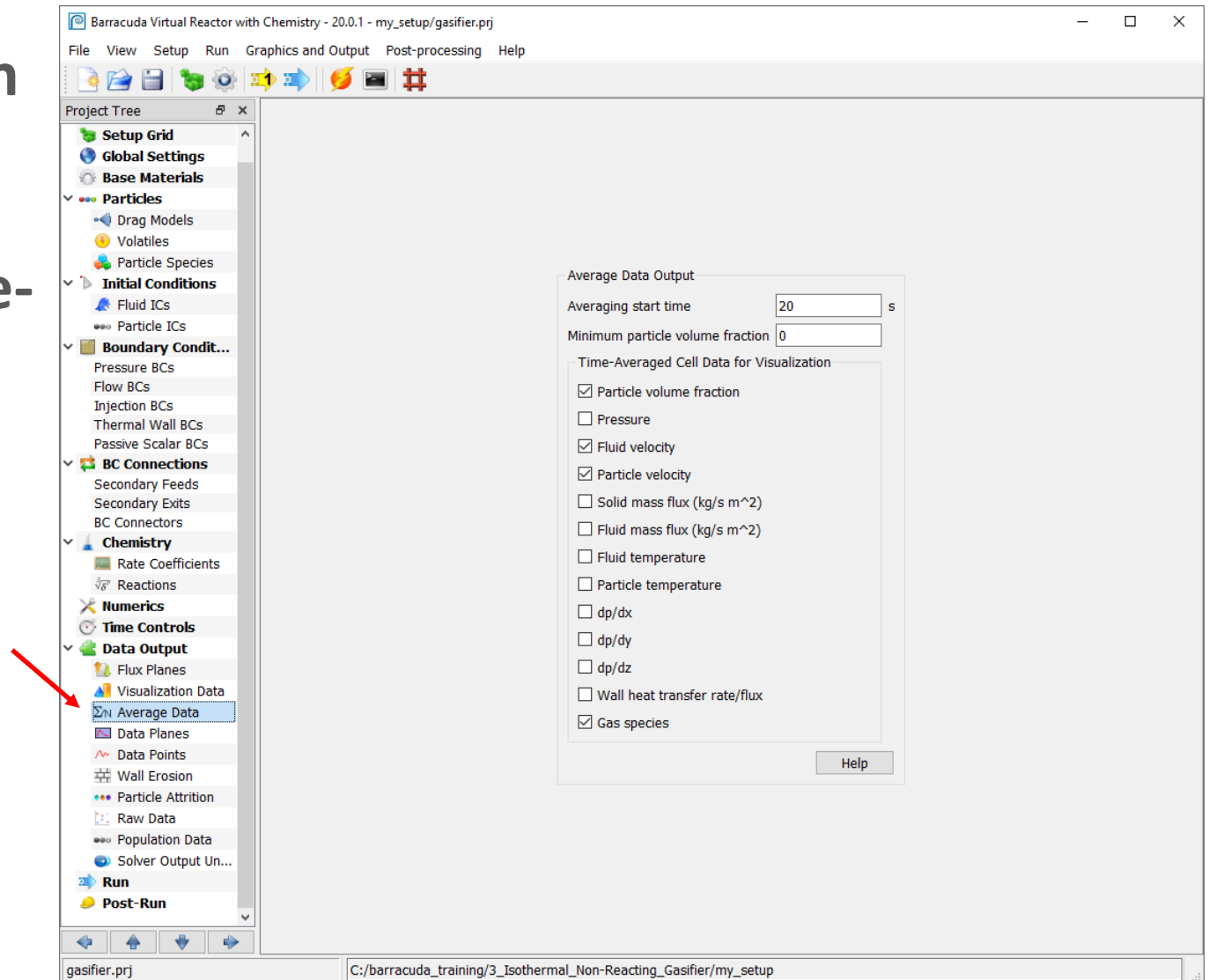
Check Model Setup

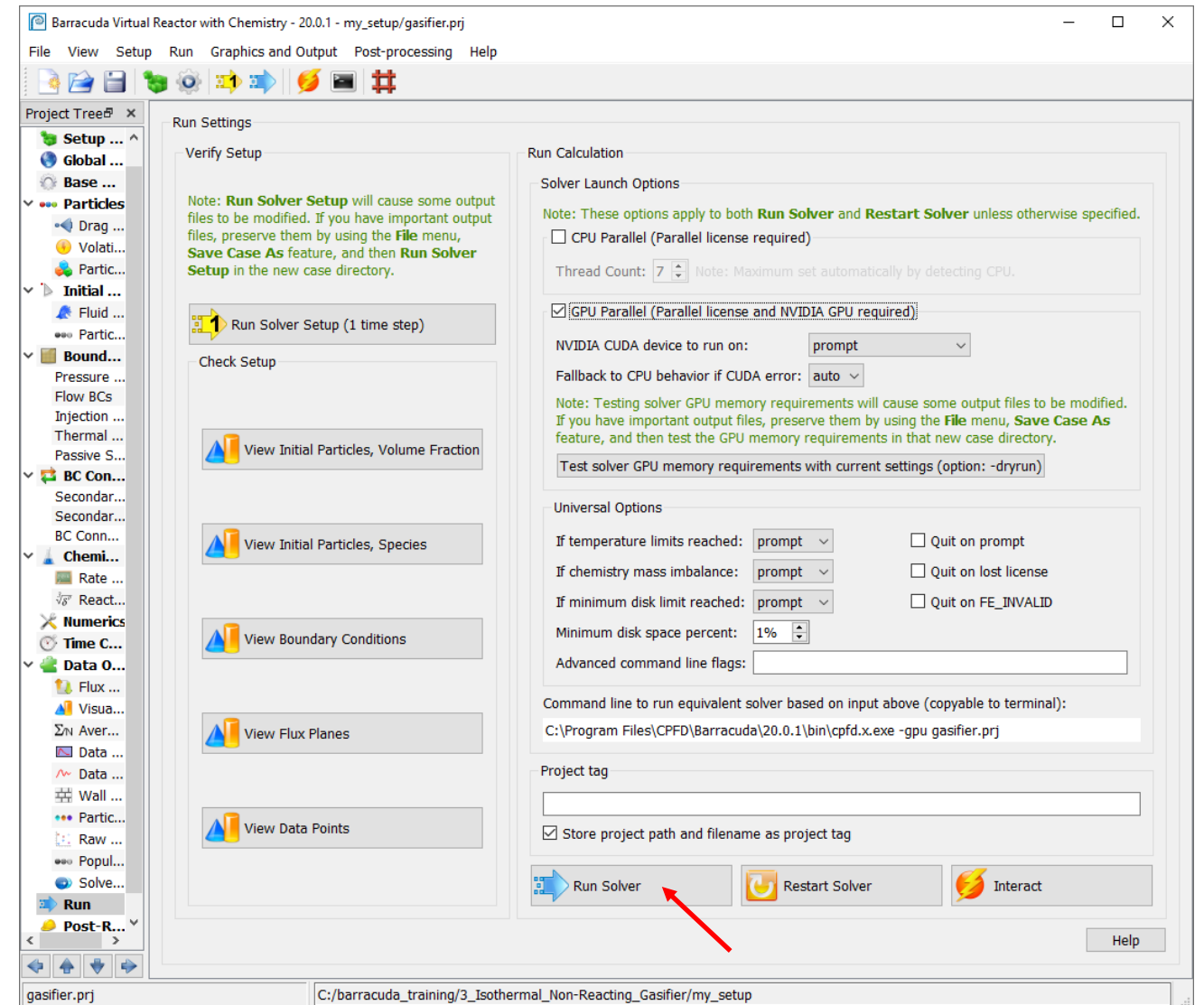**Remember to check the setup before running the project for the full 100s:**

- Navigate to Run
- Select GPU Parallel if your machine has an NVIDIA GPU card
- Run the simulation for a single time-step
- Check the initial conditions
  - Are particles initialized properly?
  - Do you have the correct initial bed mass?
- Check the boundary conditions
  - Are the flow BCs applied correctly?
  - Are the pressure BCs applied correctly?
- Do you have all desired variables in your results files? If you forgot any output variables, now is the easiest time to add them!

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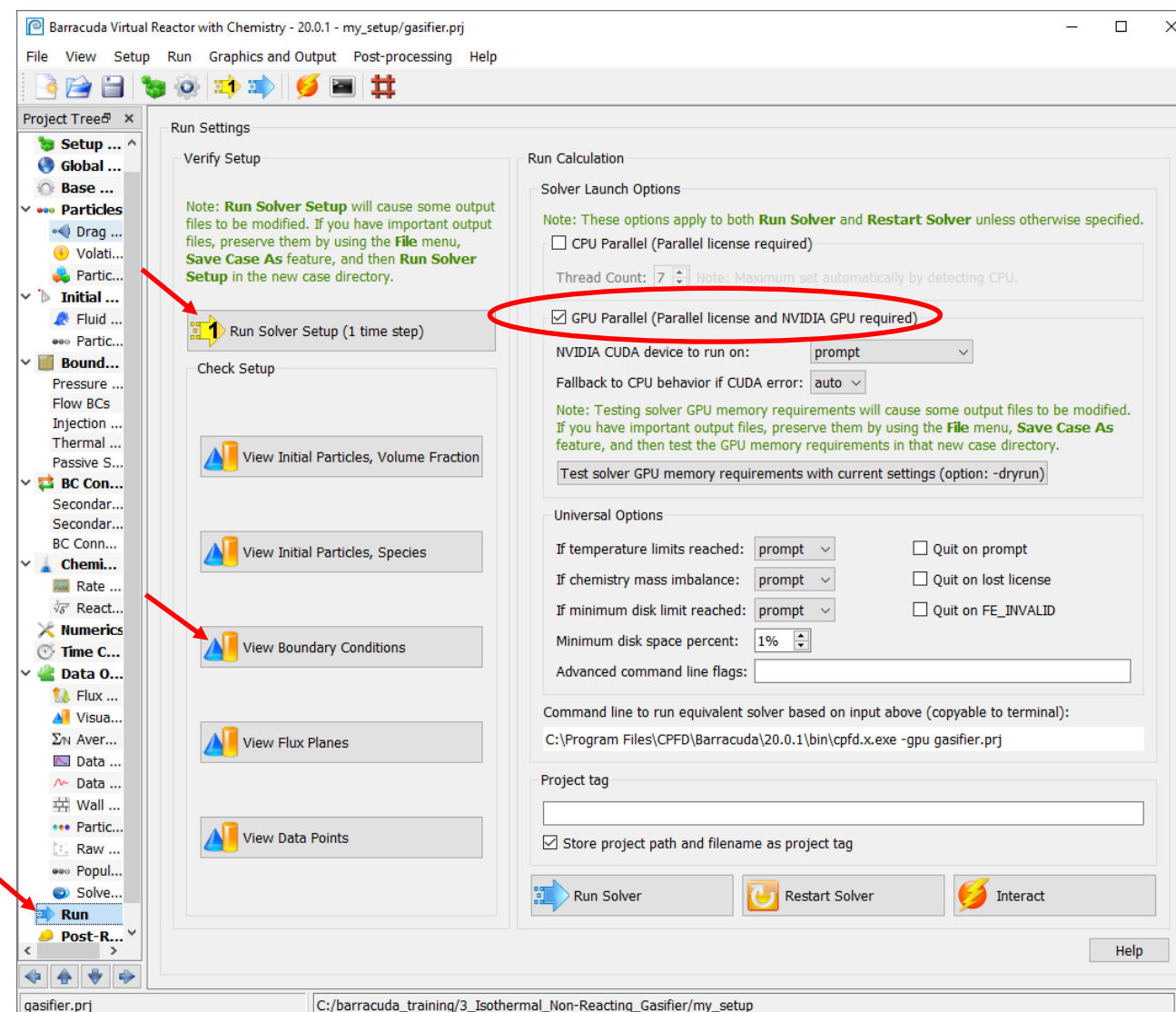
Run Solver

Have your instructor look over your boundary condition view in Tecplot.

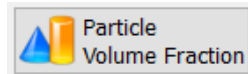**Once you are given the go-ahead, click on Run Solver.**

Post Processing

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cpfd

Post-Run

Once the simulation is running, you can begin the post-processing.
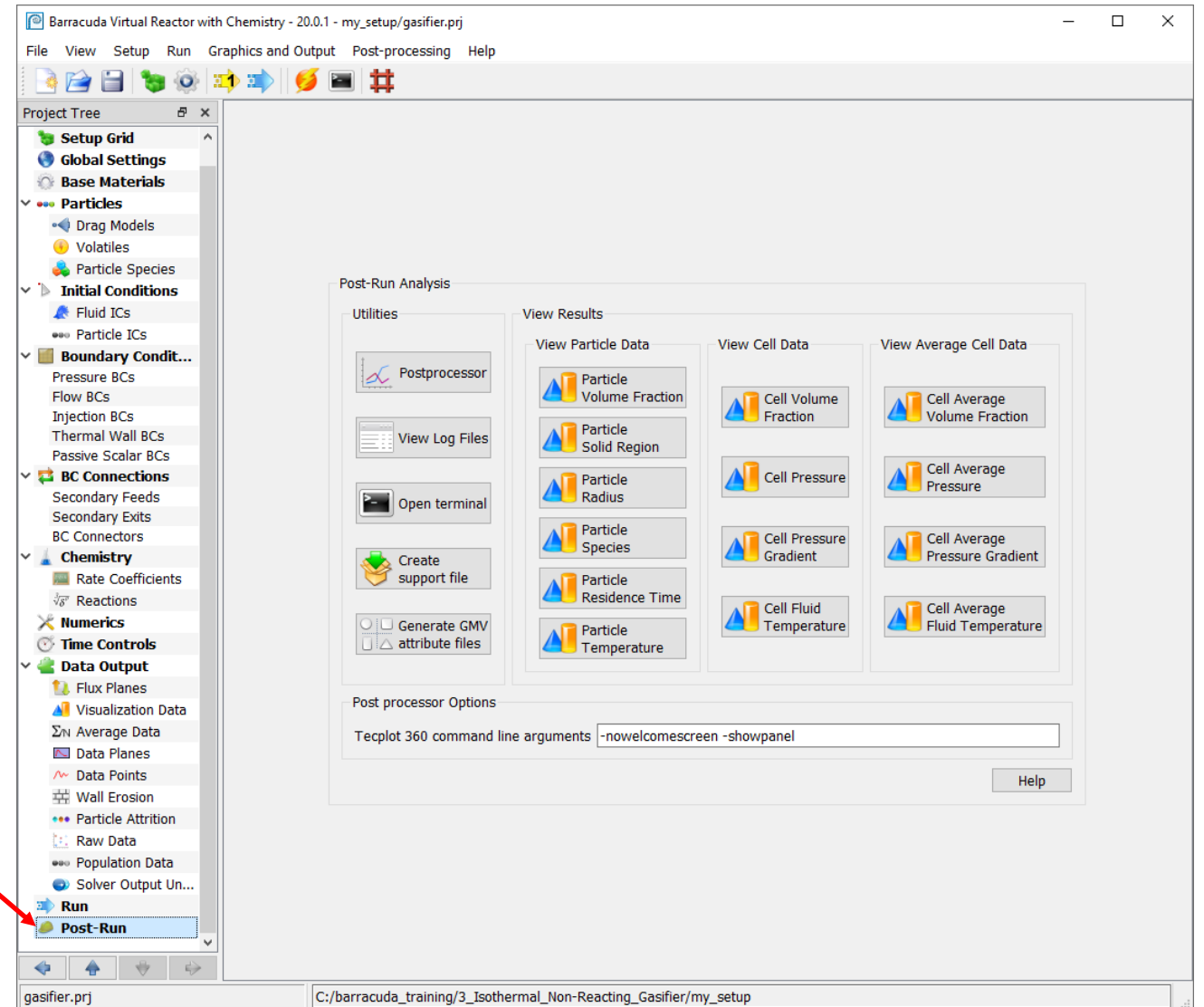
Particle Volume Fraction

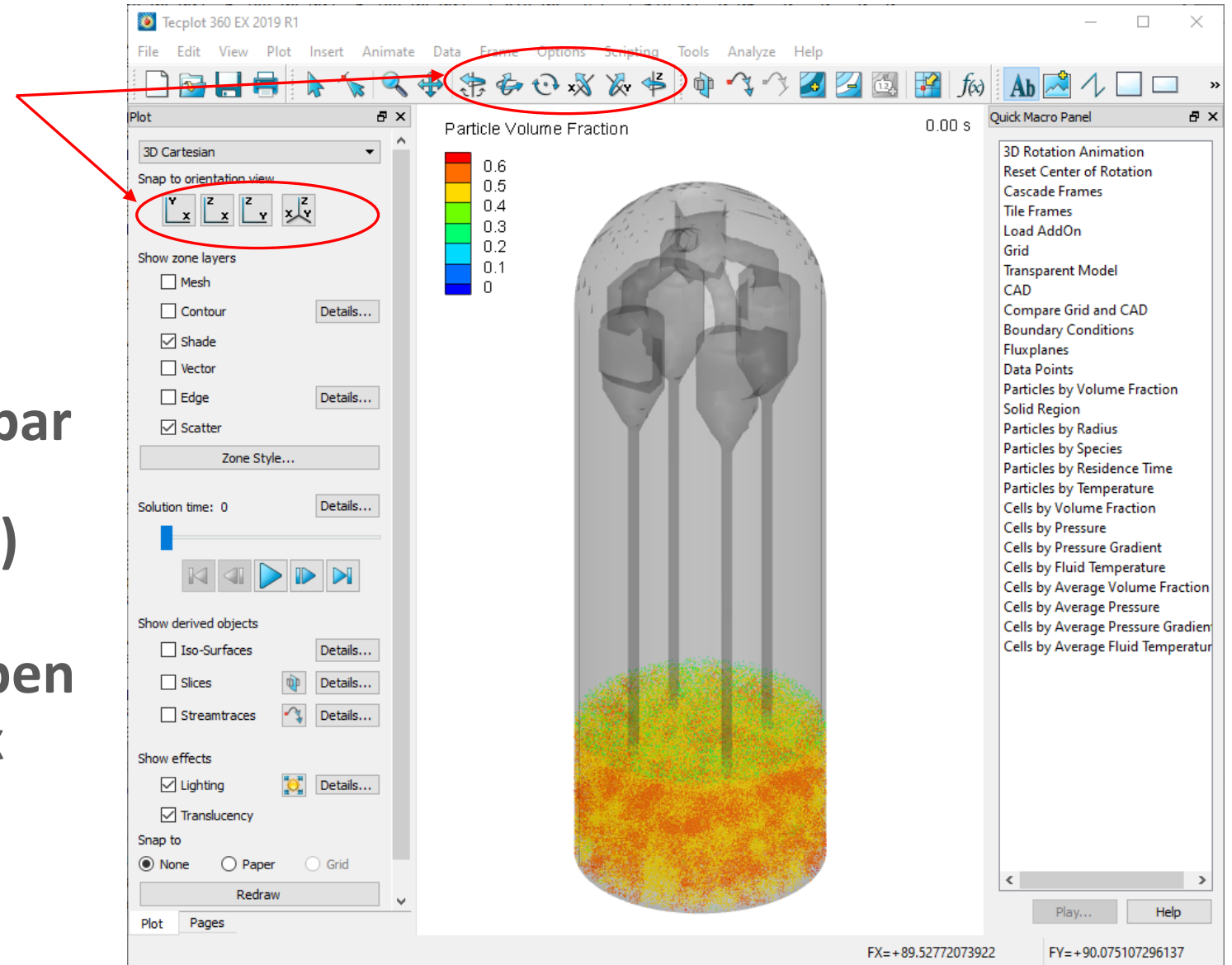**Click on** [Particle Volume Fraction]

Adjust the view angle

Adjust Data Limits and color map as desired by double-clicking on color bar

Remember to save a layout file (.lay) for each view that you would like to return to. It will be convenient to open the layout files in the more complex thermal and reacting project:

- File → Save Layout

cpfd-software.com
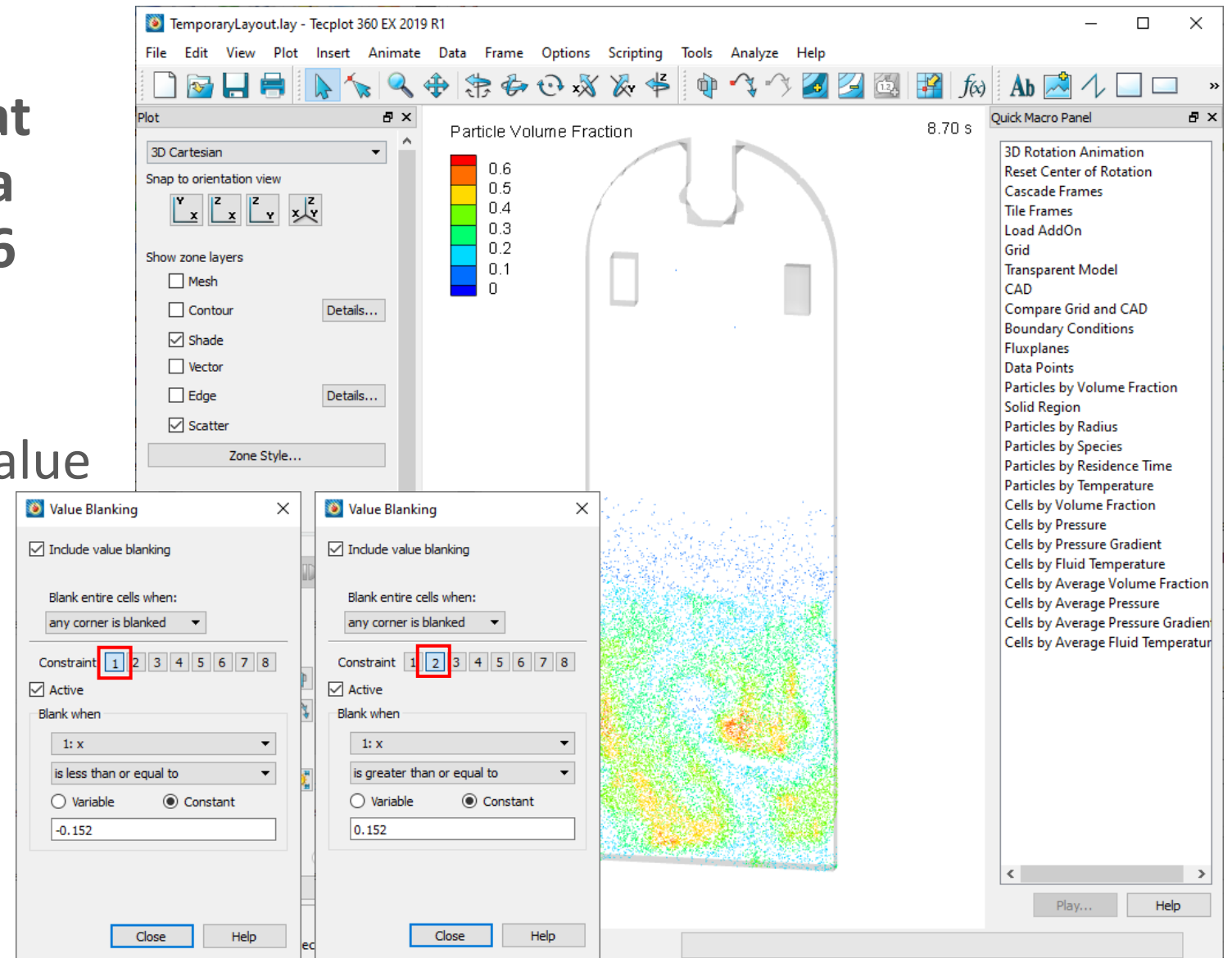
Displaying Thin Slices of the Model

Look at a thin slice of the particles at the center of the gasifier by taking a subset in the x-direction between -6 inches and +6 inches (-0.152 m to 0.152 m)

- Navigate to Plot → Blanking → Value Blanking
- Set up 2 constraints as shown

Changing Surfaces and Transparency

For this thin slice, we can change the appearance of the cells:
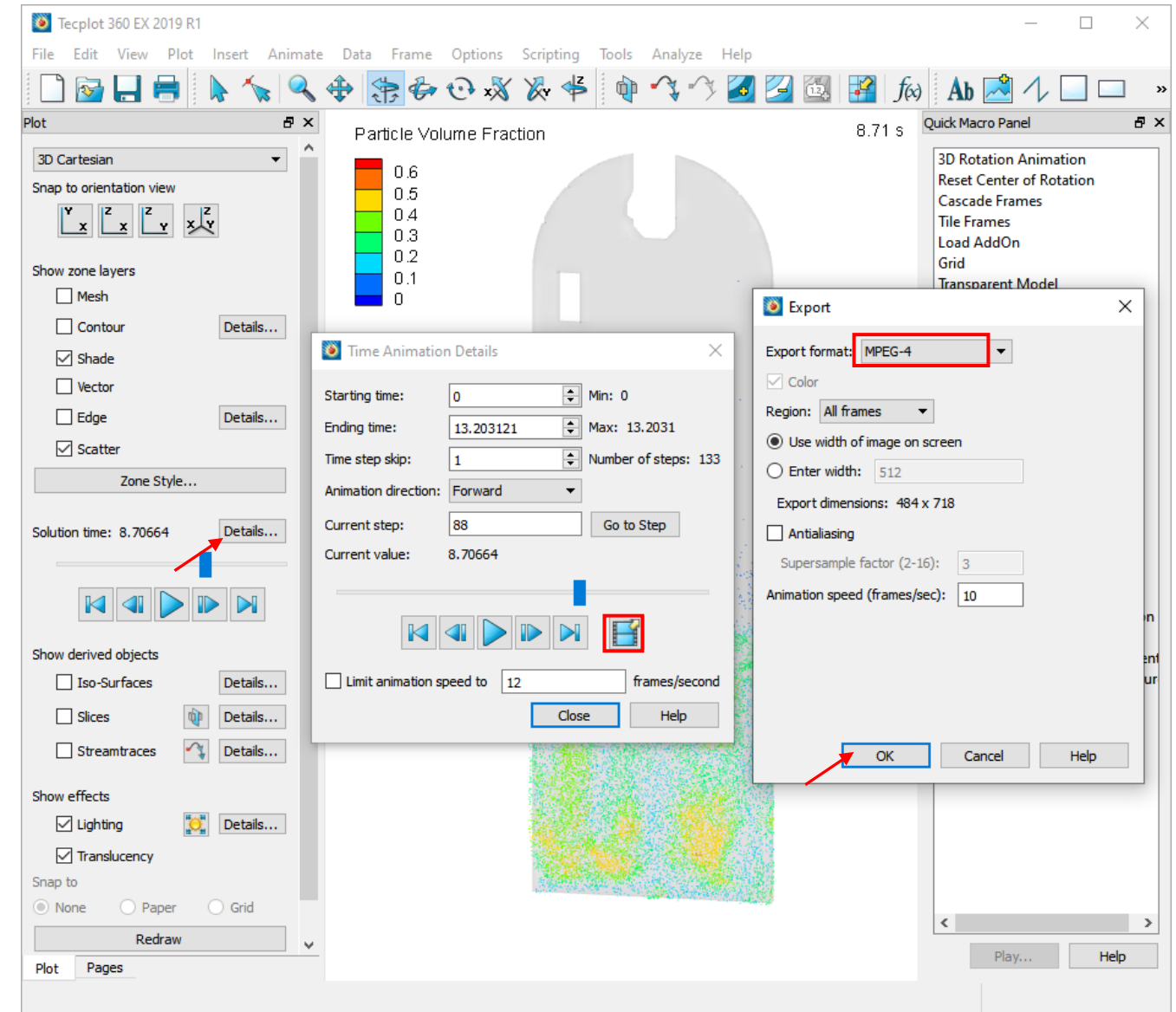
- Click on Zone Style...

- Click on Surfaces tab

- Right click on Boundary cell faces and change it to Exposed cell faces

- Click on Effects tab

- Right click on Surface Translucency for the Cells and change to 90
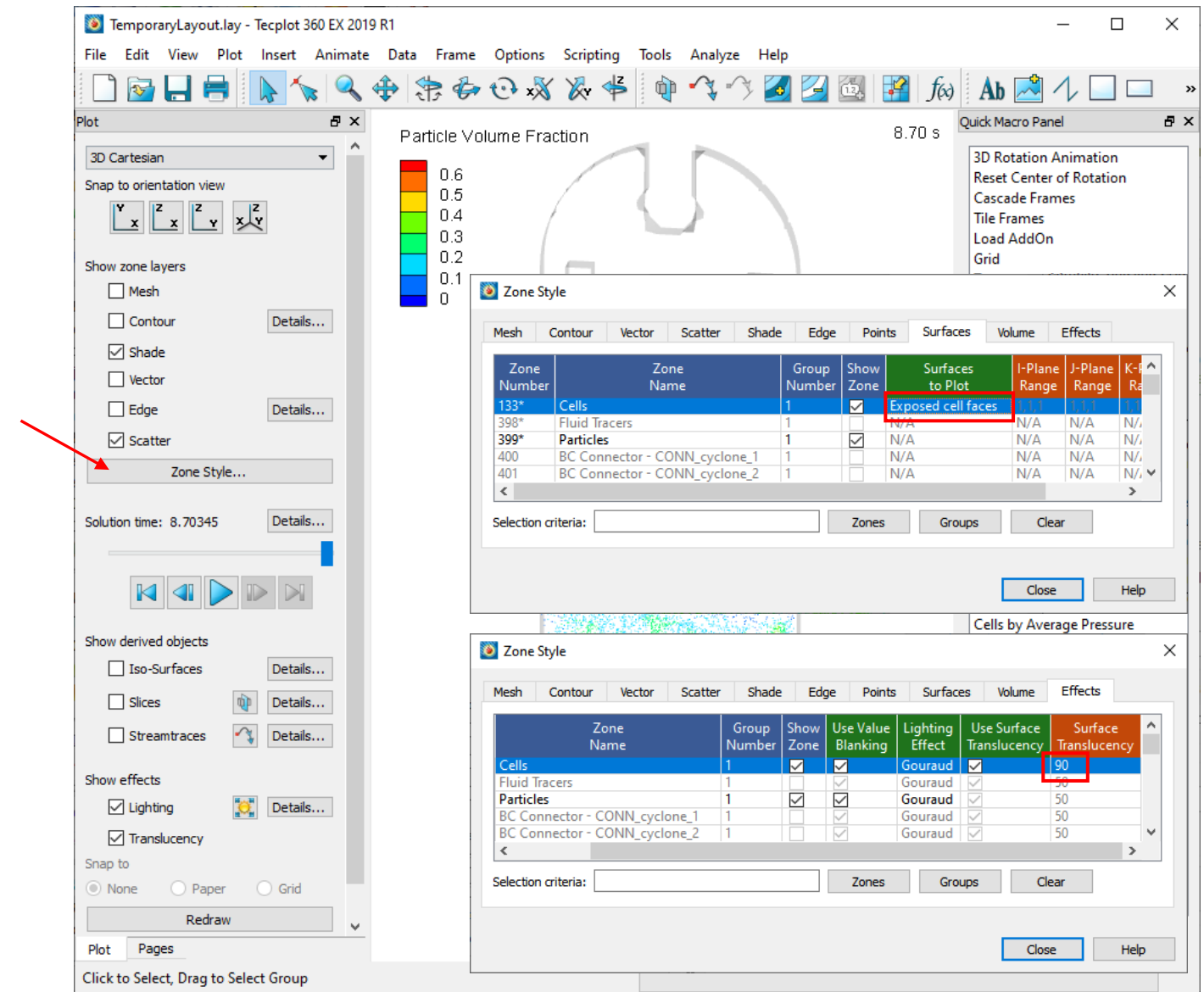
Animation of Gasifier Fluidization

Create an animation showing the gasifier fluidization

- Click on Details… button next to Solution time
- Make any desired changes to Time Animation Details editor
- Click on Export to File button
- Pick the Export format you want
- Click OK
- Enter a File name for animation
- Click Save

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View Animation of Gasifier Fluidization

Once the animation is created, you can view it by double-clicking on file in the simulation directory
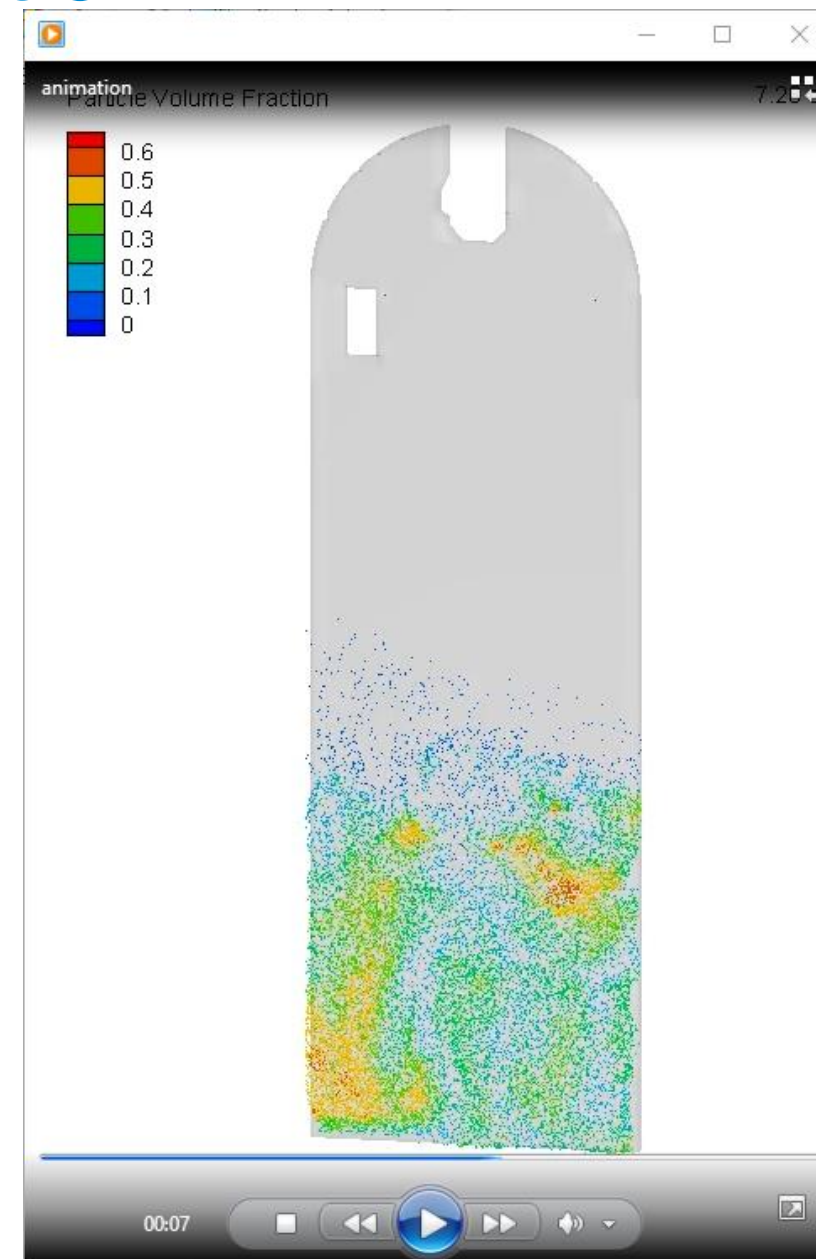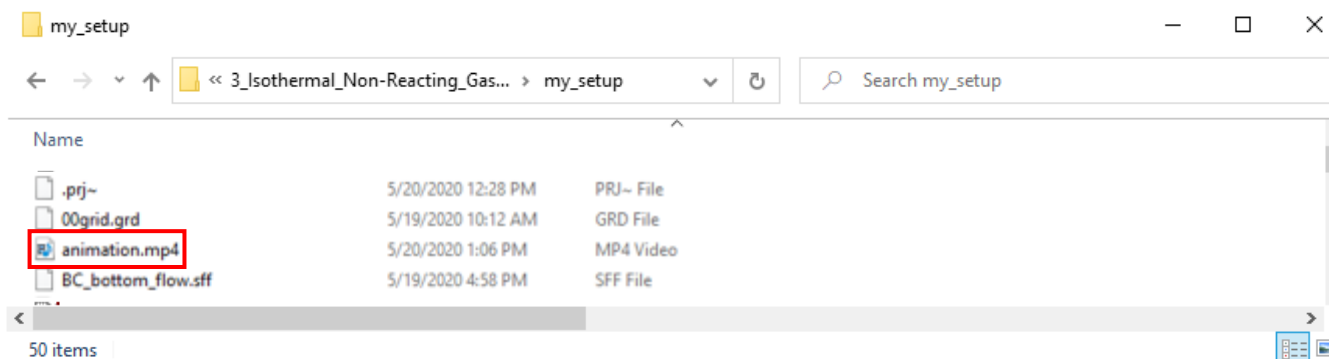
Residence Time of Particles

Double click on Particles by Residence Time in Quick Macro Panel

Use Plot → Blanking → Value Blanking to display only the particles with a volatile mass fraction (mf-volatile) between 0.01 and 0.5

Change the particle from Point to Sphere with Zone Style... -> Scatter -> Symbol Shape and Scatter Size to 1.00%

Adjust the Residence Time Contour Levels to show residence times between 0 and 5 seconds

What does this tell us about devolatilization?

How can Barracuda be used to optimize the coal feed location?
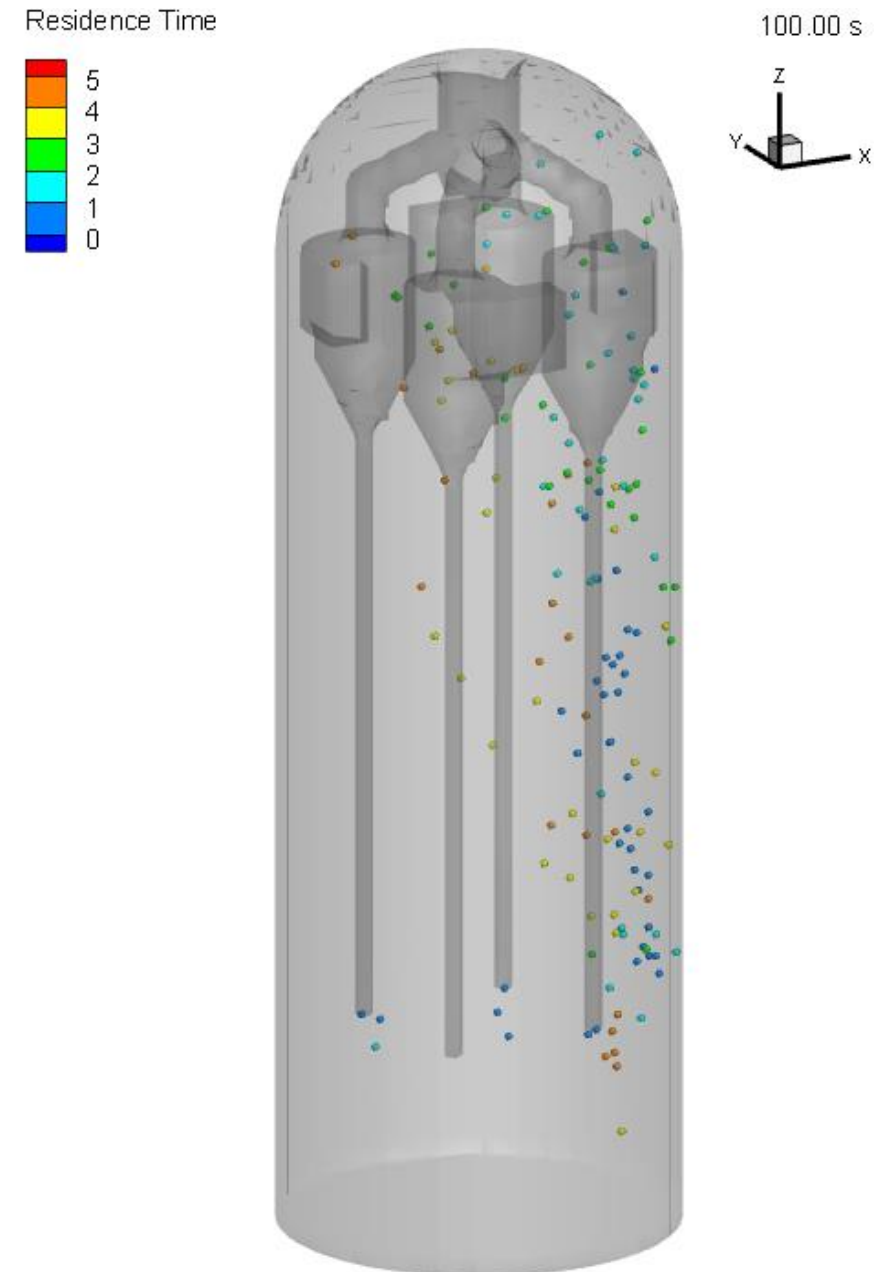
Devolatilization of Methane

Follow along with this video to create an isovolume of high mole fraction of methane:

- https://cpfd-software.com/customer-support/knowledge-base/tecplot-for-barracuda-creating-an-isovolume

**What does this tell us about the mixing of gases within the bed?**

Plotting Total Bed Mass

From the Post-Run window, click on
to plot the total bed mass from the history.log
file:

- Load data using File → Load Barracuda data… → Load Data File → history.log

- Tecplot will automatically load column 1 on the x-axis and column 2 on the y-axis for all XY Line plots

- To change the data shown, click on Mapping Style…

- Select on particle mass (kg) and de-select dt (s)

- The plot will look empty, to rescale the axes click in the plot area and then press Ctrl+F to auto-scale the plot

- This video shows how to create xy plots in Tecplot
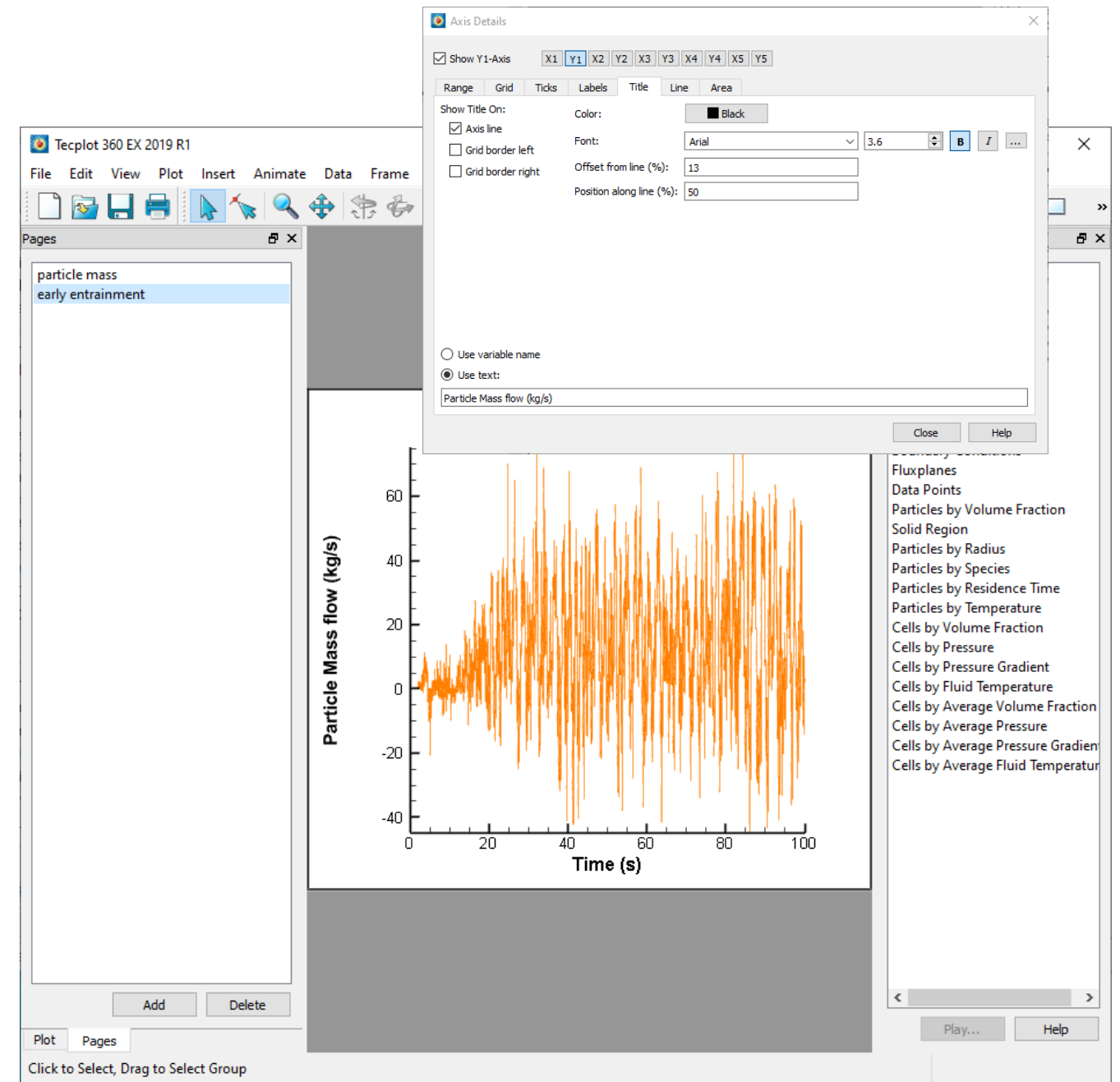
Are the BC Connectors working?
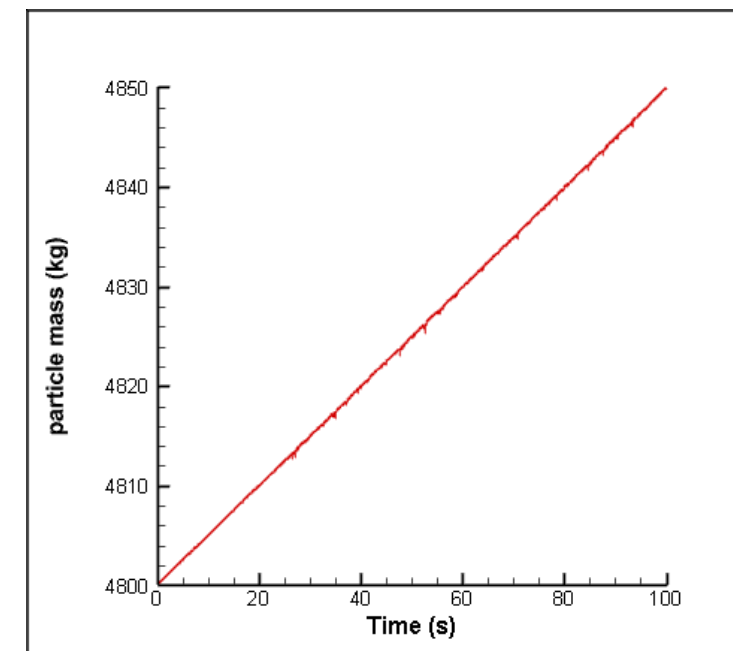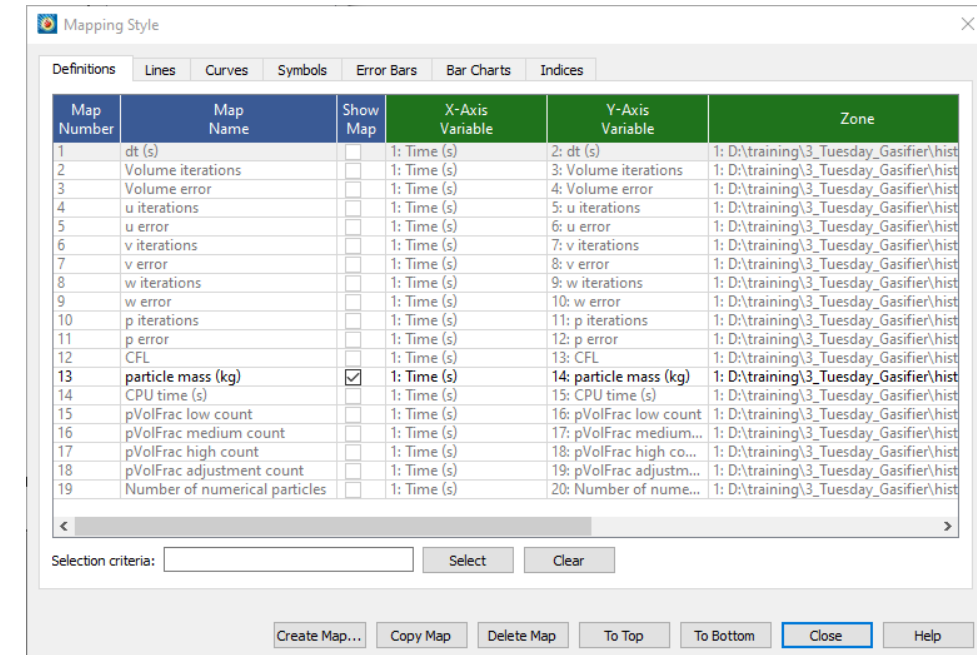
Plotting Early Entrainment

One way to add another xy plot:

- Click on Pages tab
- Double click on Untitled and give your plot page an appropriate name
- Click on Add
- Give that new page an appropriate name as well

Plot the particle mass flow through the early entrainment flux plane from the FLUX_early_entrainment file

- Follow the load data instructions from the previous slide
- Click on Plot tab → Mapping Styles…
- Select on Particle mass flow rate of all species (5 time step average) (kg/s) and de-select Fluid mass flow rate (kg/s)
- Don't forget to auto-scale the plot! Ctrl+F
- The axes labels can be adjusted by double clicking on them
- Select Use text: in the Axis Details dialog and enter an appropriate axis legend

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Conclusion of Gasifier Example

A basic coal gasifier was set up including

- Multi material particles
- Volatile components

A coarse grid was used and boundary condition assumptions were made to obtain a fast running model

Basic post processing was performed to study the fluidization and entrainment in the model

This work serves as the basis for a more complex model.