Gasifier Training Problem
Part 3: Project Setup

February 2018

CPFD Software LLC
10899 Montgomery Blvd. NE, Suite A
Albuquerque, NM 87111
+1.505.275.3849
www.cpfd-software.com

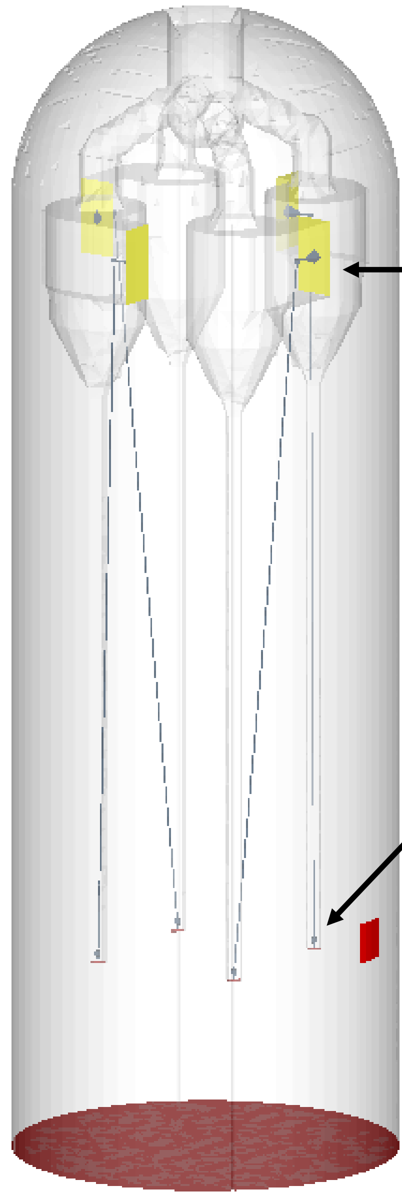
Training Objectives

- 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
  - Flux planes

Process Sheet

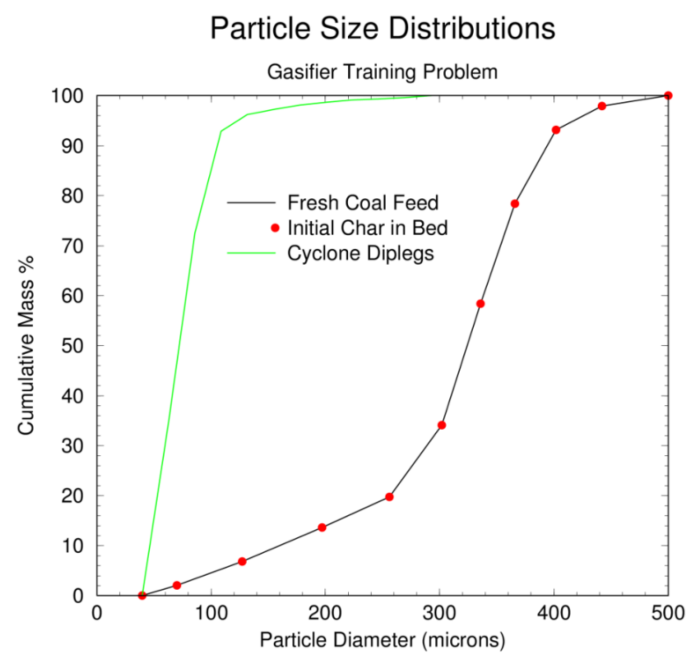
- Isothermal at 1300 K
- No chemistry in this model
- Fresh coal feed coming in at:
  - x=1.45 m
  - y=0 m
  - z=1.75 m

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	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



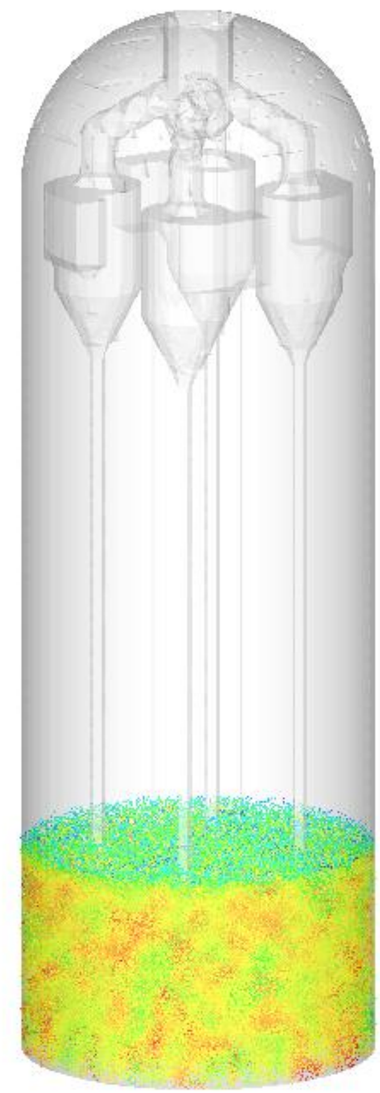
Particle Properties

- Close pack volume fraction is 0.6
- Fresh coal particles:
  - Multi-material including volatiles which are released
  - Particle composition (mass fractions):
    0.45 Carbon (solid), 0.05 Ash (solid), and 0.5 Volatiles with an overall particle density of 1450 kg/m3
  - Volatile composition (mass fractions):
    0.4144 CH_4, 0.1702 CO, 0.0444 CO_2, 0.111 H_2, 0.26 H_2O
  - Release rate of volatiles is rate = 0.05 T exp(-5500/T)
  - PSD is included in the “my_setup” folder with name **psd_fresh_coal_feed_particles.sff**
- Initial bed particles:
  - Assumed to be already devolatilized
  - Particle composition (mass fractions):
    0.8999 Carbon (solid), 0.1 Ash (solid), and 0.0001 Volatiles with an overall particle density of 725 kg/m3
  - PSD is included in the “my_setup” folder with name **psd_initial_char_in_bed.sff**



Particle Properties

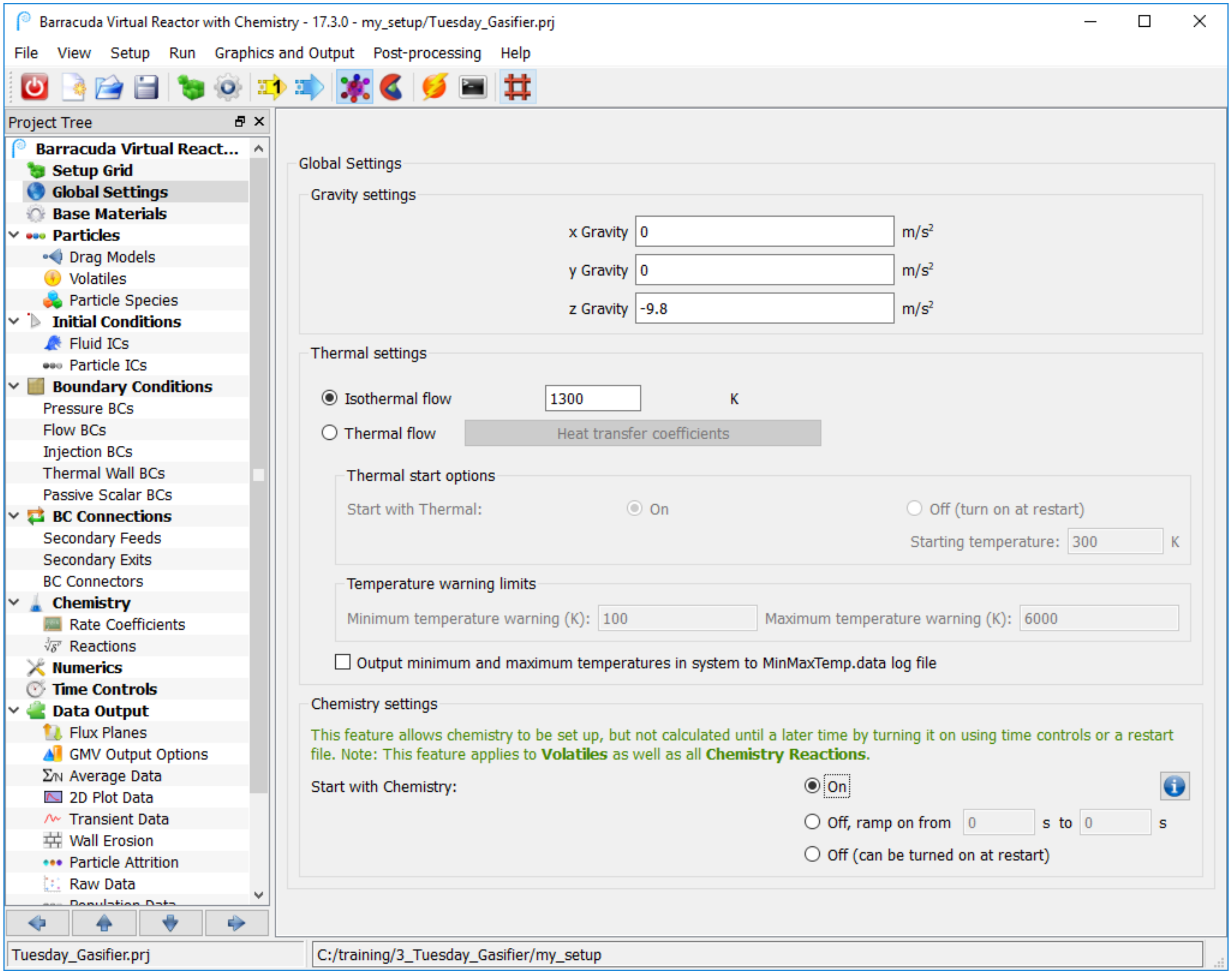
- For material properties, assume that Carbon and Ash have densities of 2150 kg/m3
- Initial Conditions
  - Initial bed mass is 4800 kg
  - Filled with Nitrogen at 200 kPa



Reminder: What do we want to learn from this model?

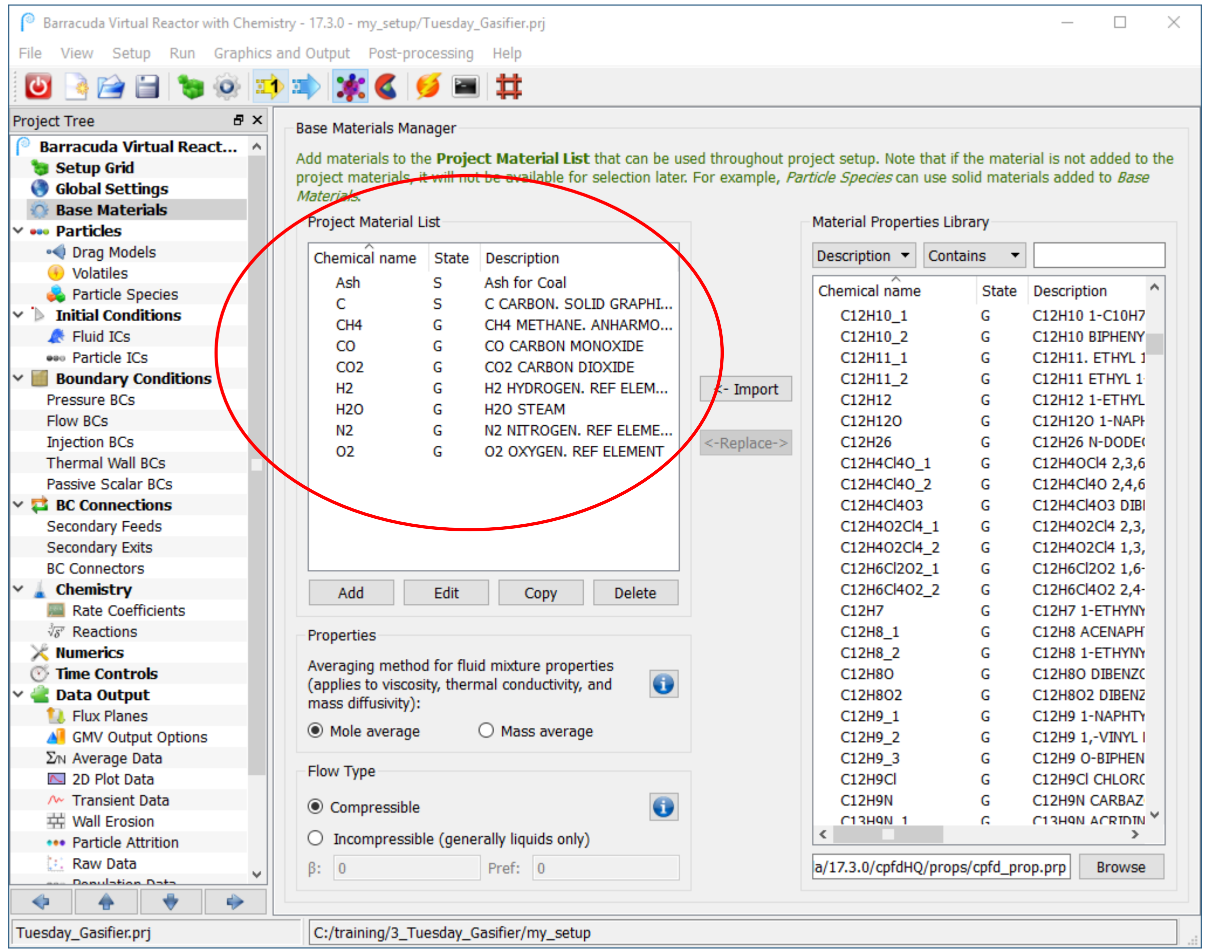
- Always keep in mind why you are running any model
- For this training problem, we want to set up and analyze the Barracuda model to learn the following:
  - General fluidization characteristics
  - Entrainment rate of particles
- This is a simplified model without chemistry or thermal calculations. Tomorrow we will add chemistry and thermal and run the more complex gasifier model

Global Settings



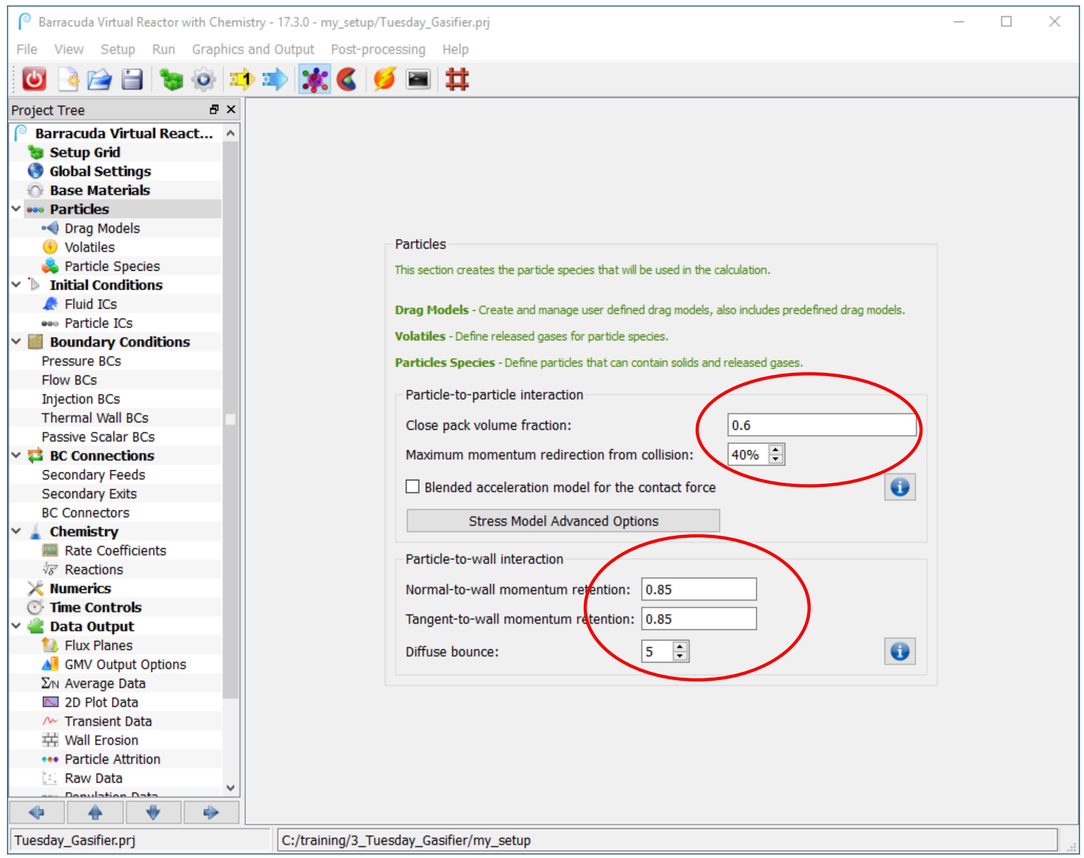
Base Materials

- 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
    - Methane
    - Carbon Monoxide
    - Carbon Dioxide
    - Hydrogen gas
    - Steam
    - Nitrogen gas
    - Oxygen gas



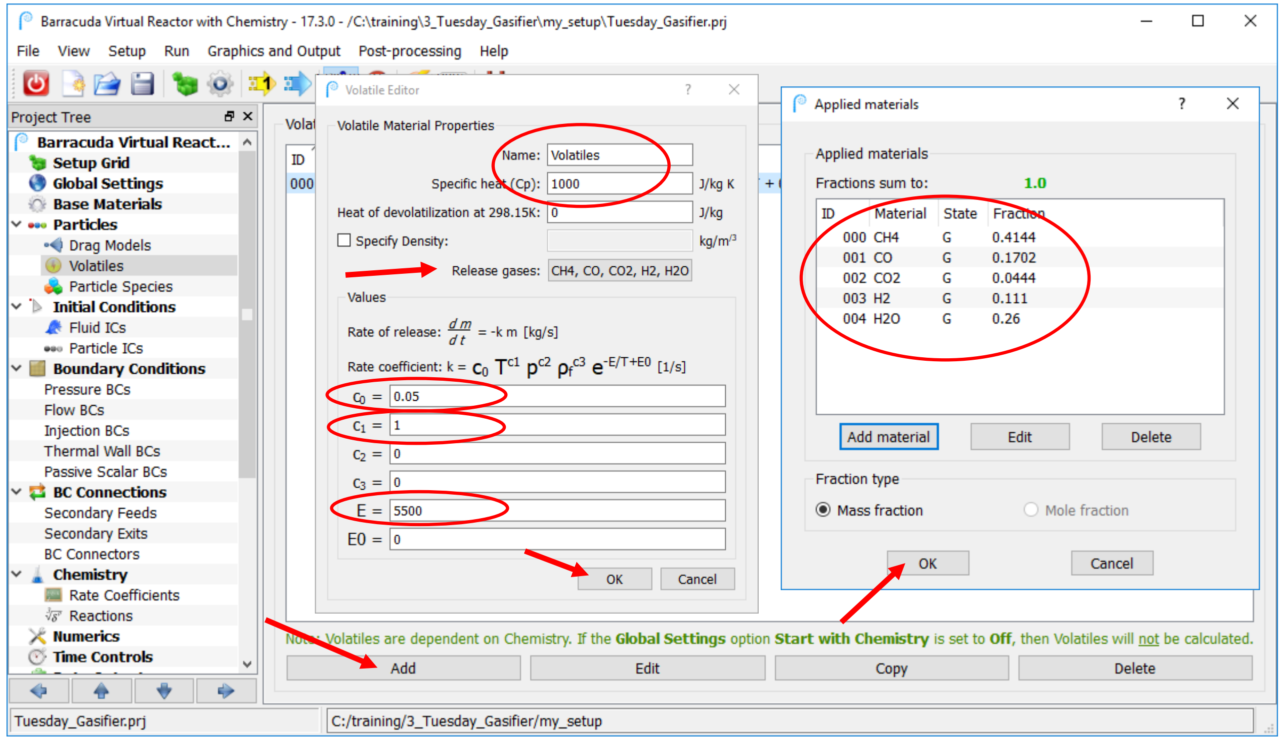
Particles

- Set the **Close pack volume fraction** to “0.6”
- Leave the **Maximum momentum redirection from collision** at “40%”
- Set the **Normal-to-wall momentum retention** to “0.85”
- Set the **Tangent-to-wall momentum retention** to “0.85”
- Leave **Diffuse bounce** at “5”



Defining Volatiles

- In the **Volatiles** section, define the volatile material trapped in the fresh coal particles, and the gases released
- Based on particle properties, the volatiles composition (by mass fraction) is 0.4144 CH_4, 0.1702 CO, 0.0444 CO_2, 0.111 H_2, 0.26 H_2O
- Click on **Add** to raise the **Volatile Editor** window
- Enter "Volatiles" for the **Name** and "1000" J/kg K for the **Specific heat**
- Click on the **Release gases** button to add the volatile materials and their mass fractions. When finished, click **OK**
- Enter "0.05" for $\mathbf{c_o}$, "1" for $\mathbf{c_1}$ and "5500" for **E**
- Click **OK**



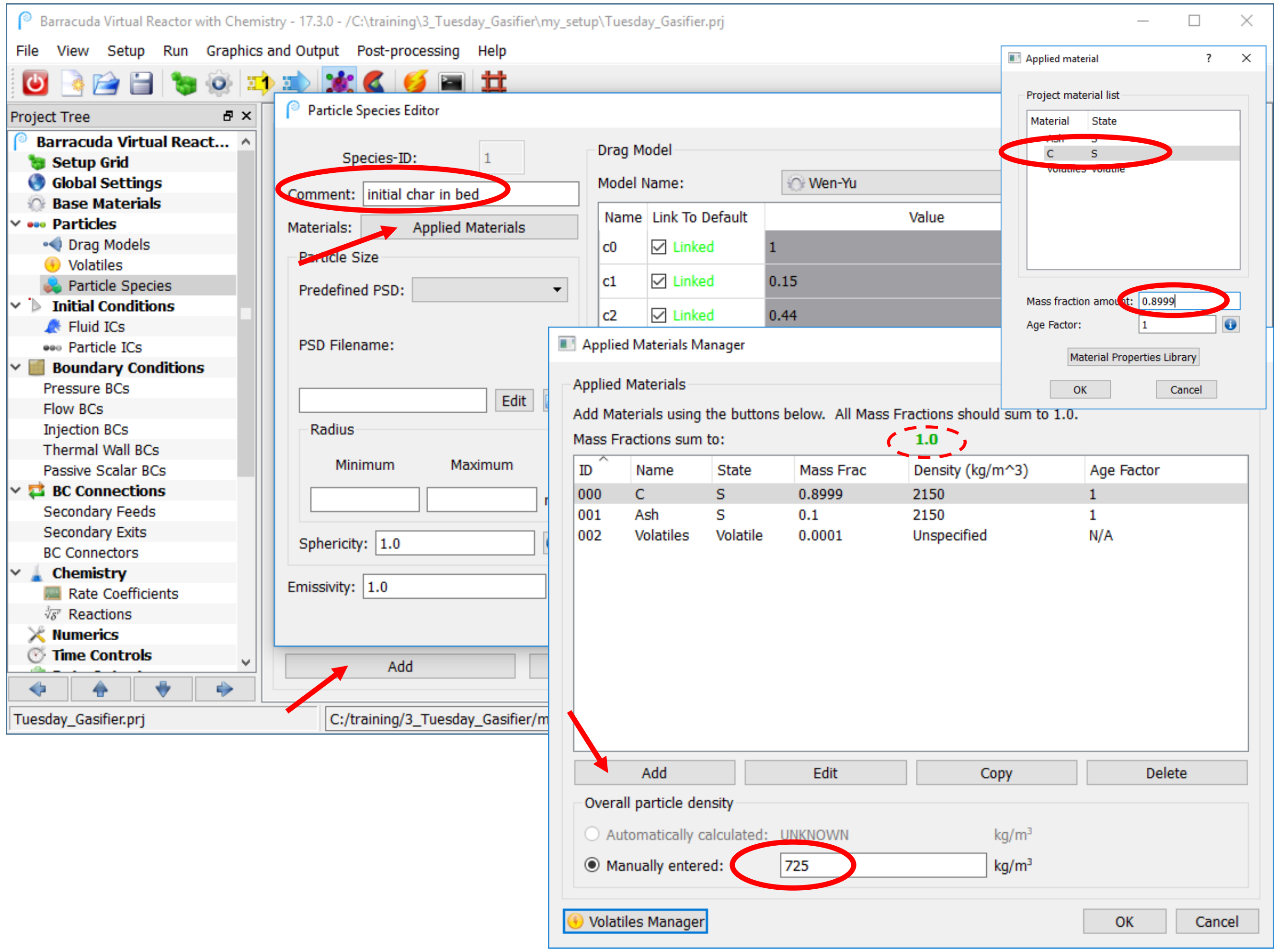
The release rate of volatiles can be specified in terms of an Arrhenius-type temperature dependence

Based on the process sheet, the release rate expression should be:

Rate = 0.05 T exp(-5500/T)

Multi-Material Particles

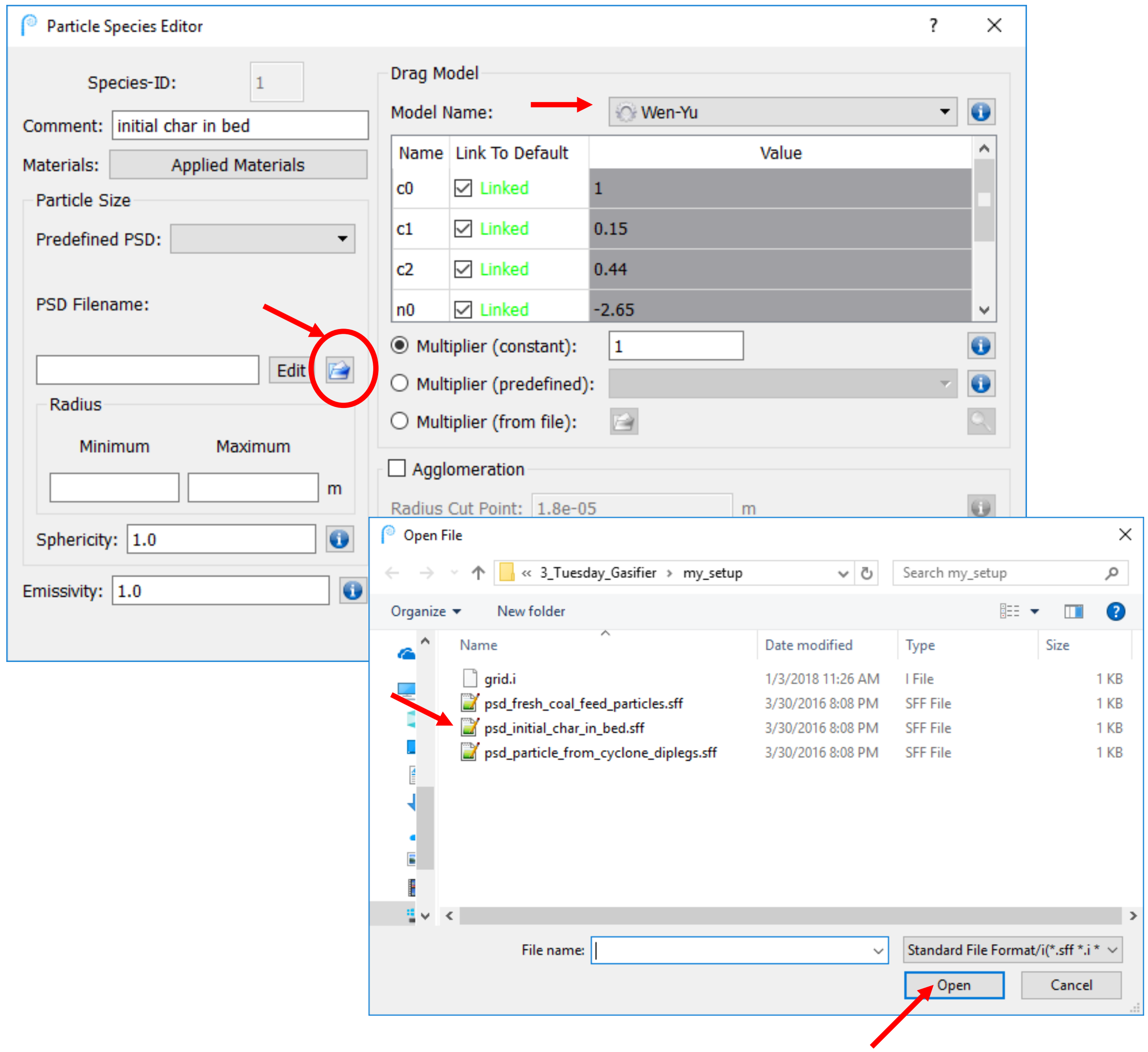
- The particles will be treated as multi-material, enabling devolatilization of the fresh coal
- To create a new particle species, click on **Add**. Then click on **Applied Materials**
- **Add** carbon and enter a **mass fraction** of “0.8999”
- **Add** ash and enter a **mass fraction** of “0.1”
- **Add** ash volatiles enter a **mass fraction** of “0.0001”
- Manually enter the overall particle density as “725” kg/m^3. Click **OK**
- Enter an appropriate description in the **Comment** field



Since the initial bed particles are assumed to already be devolatilized, they consist of mostly carbon and ash

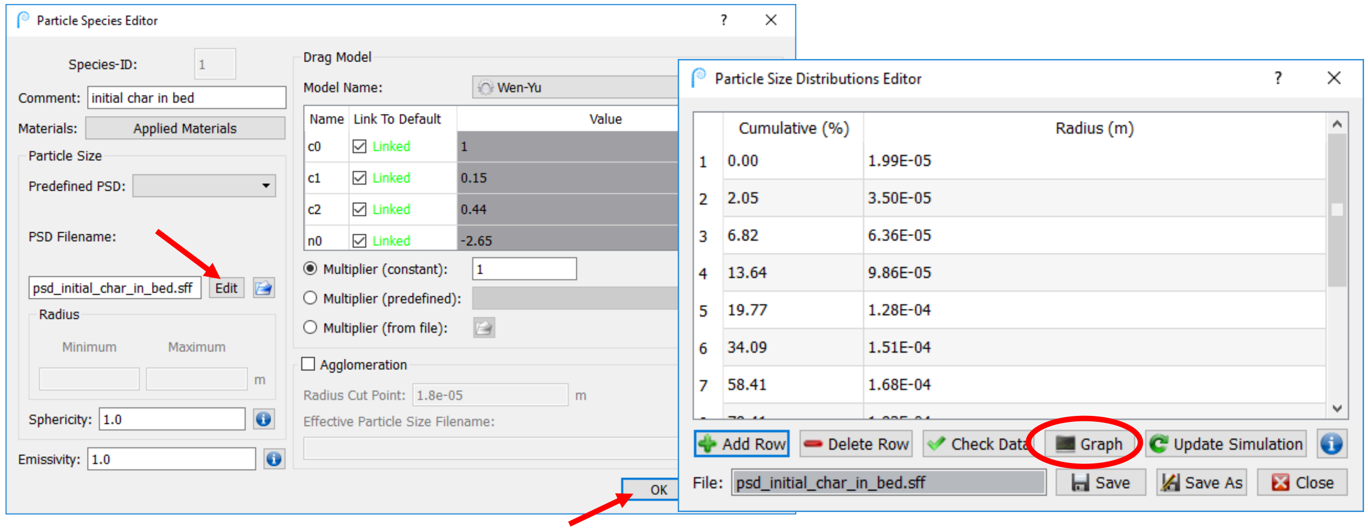
Specifying PSD

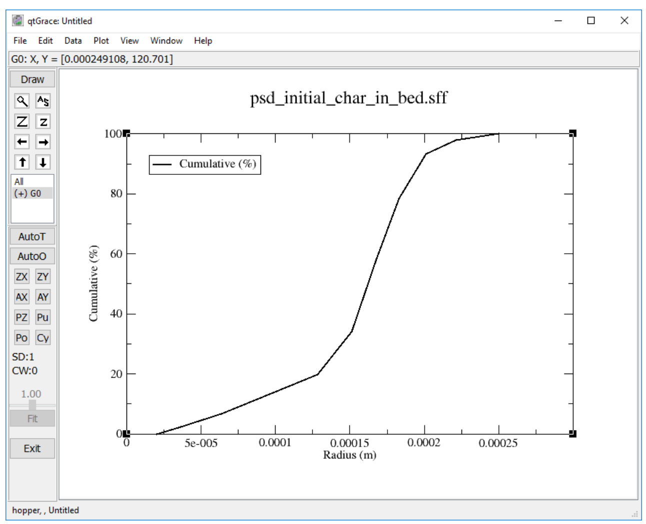
- To specify the particle size distribution, click on the file directory button for Radius Filename:
  and select the file:
  psd_initial_char_in_bed.sff
- Click **Open**
- For all particle species in this simulation, choose the Wen-Yu drag model.

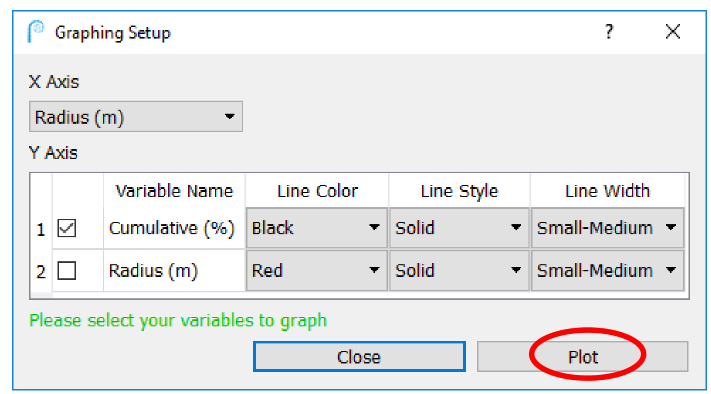


Particle Size Distribution (PSD) File

- To view the PSD file, click on **Edit**
- To display a plot of the particle size distribution, click on the graph icon on the toolbar
- When finished with the PSD file, close both the plot and file windows
- Click **OK**

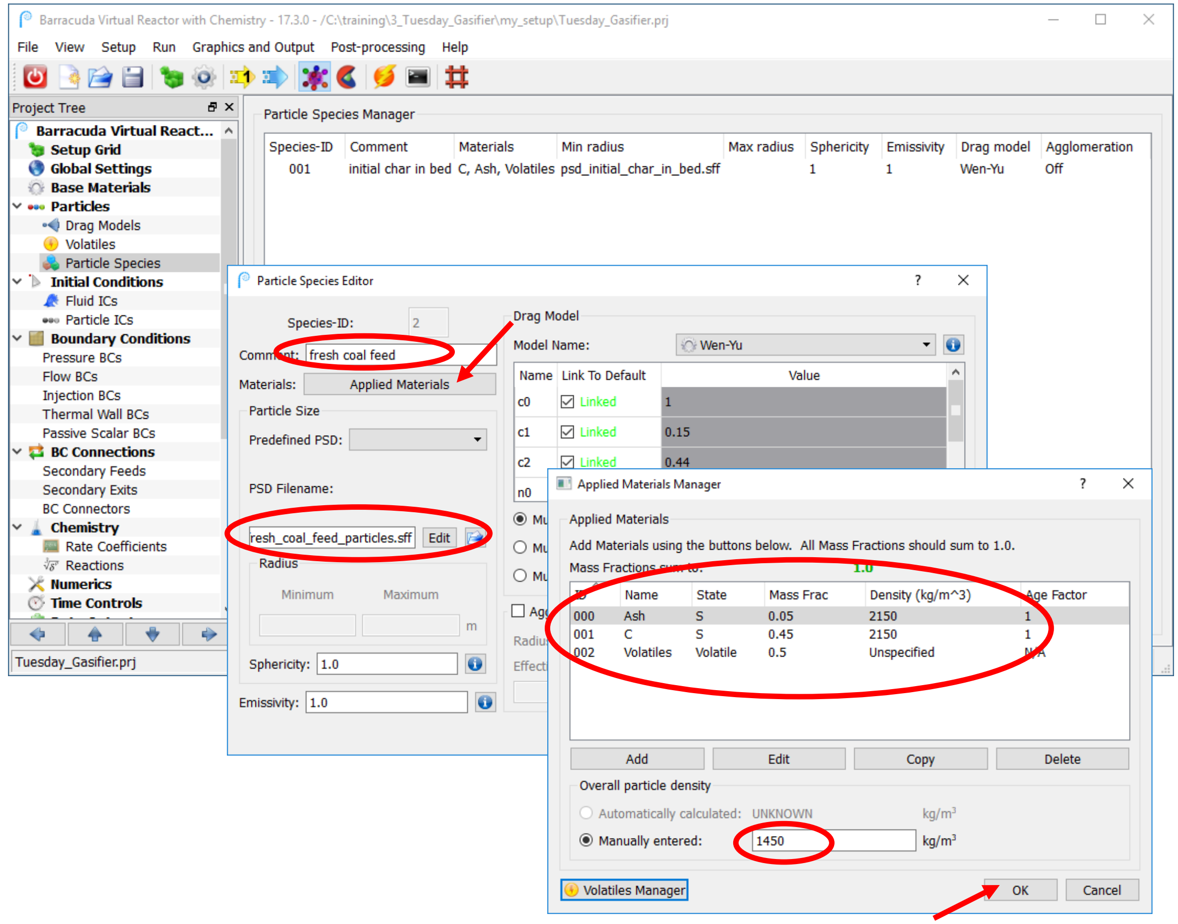






Particle Species Continued

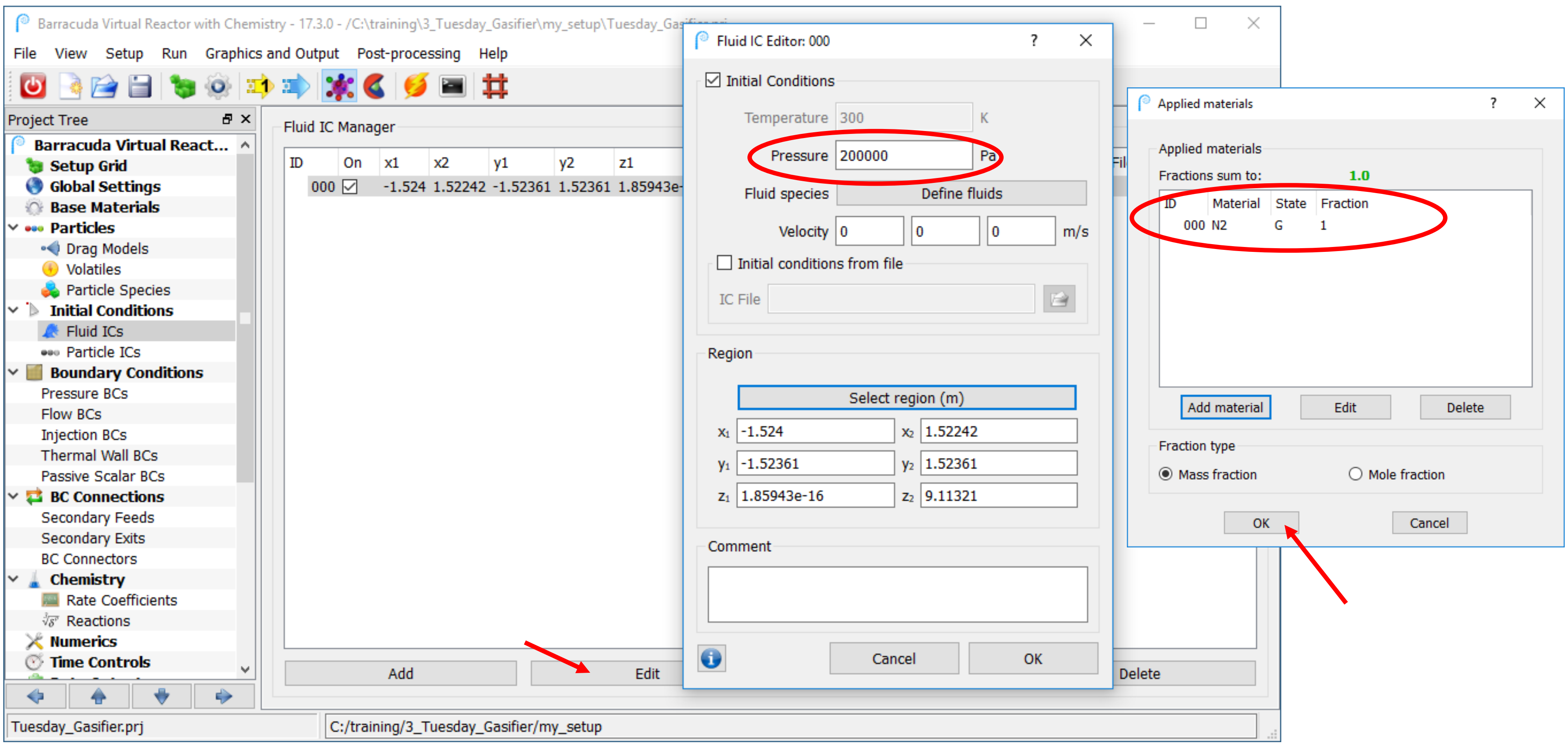
- The particle species for the particles initially in the bed has been defined
- Next, define the particle species for the fresh coal feed
- To create another particle species, click on **Add** and then click on **Applied Materials**
- In the **Applied Materials Manager** window, specify the composition of the fresh coal feed (0.05 Ash, 0.45 C, and 0.5 Volatiles by mass)
- Manually enter the overall particle density as “1450” kg/m3
- Click **OK**
- Enter an appropriate description in the **Comment** field, i.e. “Fresh coal feed”
- Specify the particle size distribution by selecting the file **psd_fresh_coal_feed_particles.sff**



Because the density of the volatiles is unspecified, the **Overall particle density** must be manually entered

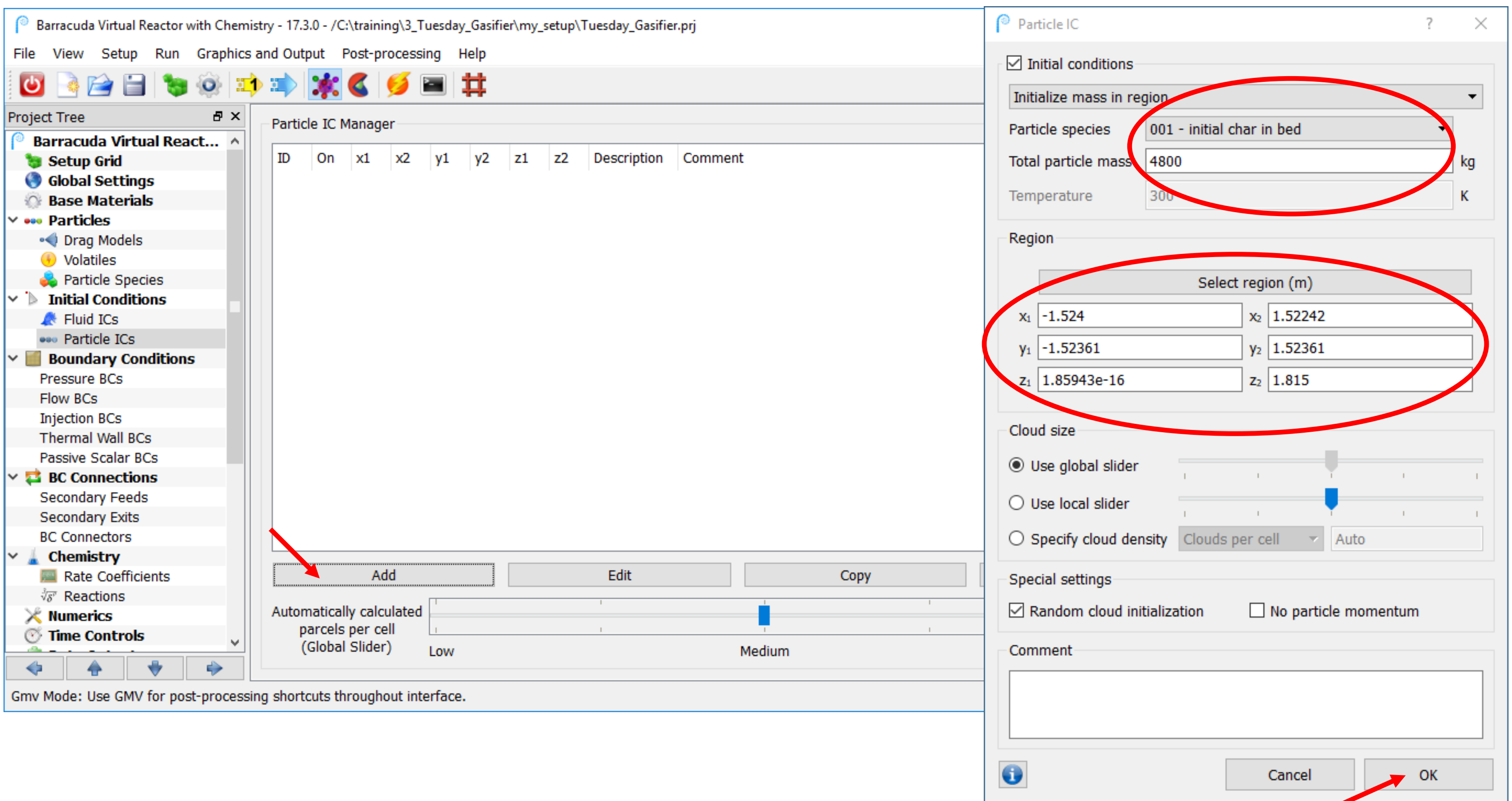
Initial Conditions: Fluid ICs

- For this simulation, set the fluid initial condition as 100% N_2 at 2.0×10^5 Pa
- Use **[** and **]** to select minimum and maximum extents of the domain



Initial Conditions: Particle ICs

- The initial particles in the bed are char (devolatilized coal)
- Initialize the particles by mass in the region
- Calculate the bed height needed for the mass (on next slide)



Calculating Initial Bed Height

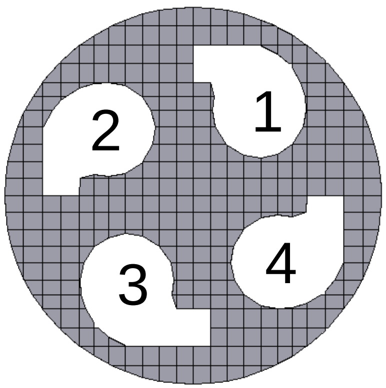
- For this problem, the target initial bed mass is 4800 kg
- In Barracuda, particles are initialized in cells specified through x, y, z locations
- For a target of 4800 kg, an initial bed height of 5.95 ft is needed. (Vessel diameter is 10 ft, particle density is 725 kg/m3, initial volume fraction is 0.5)
- For ease in setting up the particle IC, use a bed height of 5.95 ft or **1.815 m**

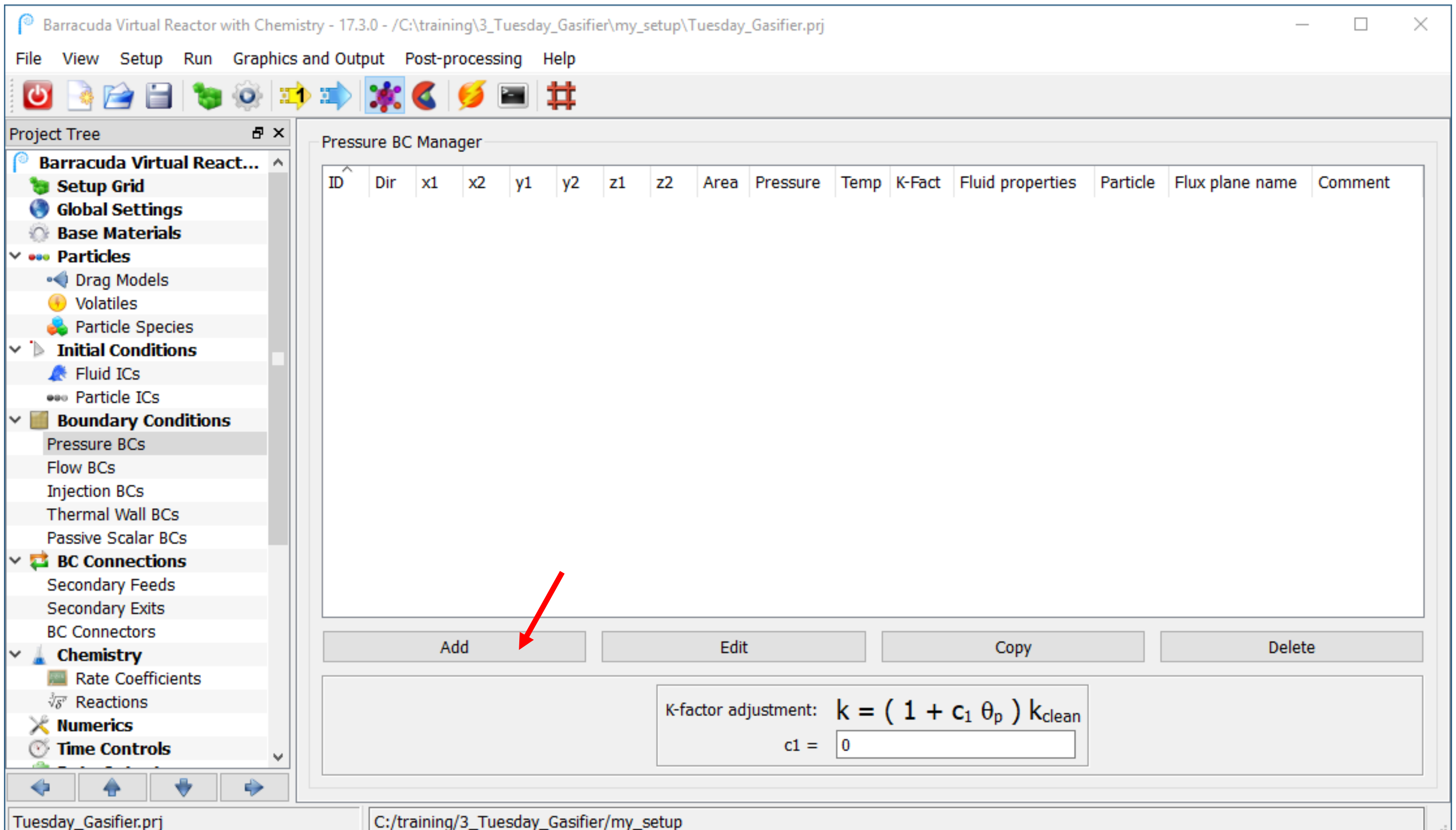
$$initial\ particle\ volume = \frac{4800kg}{0.5 \times 725\frac{kg}{m^3}} = 13.24m^3 = 467.6ft^3$$

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

Pressure BCs: Cyclone Inlet Horns

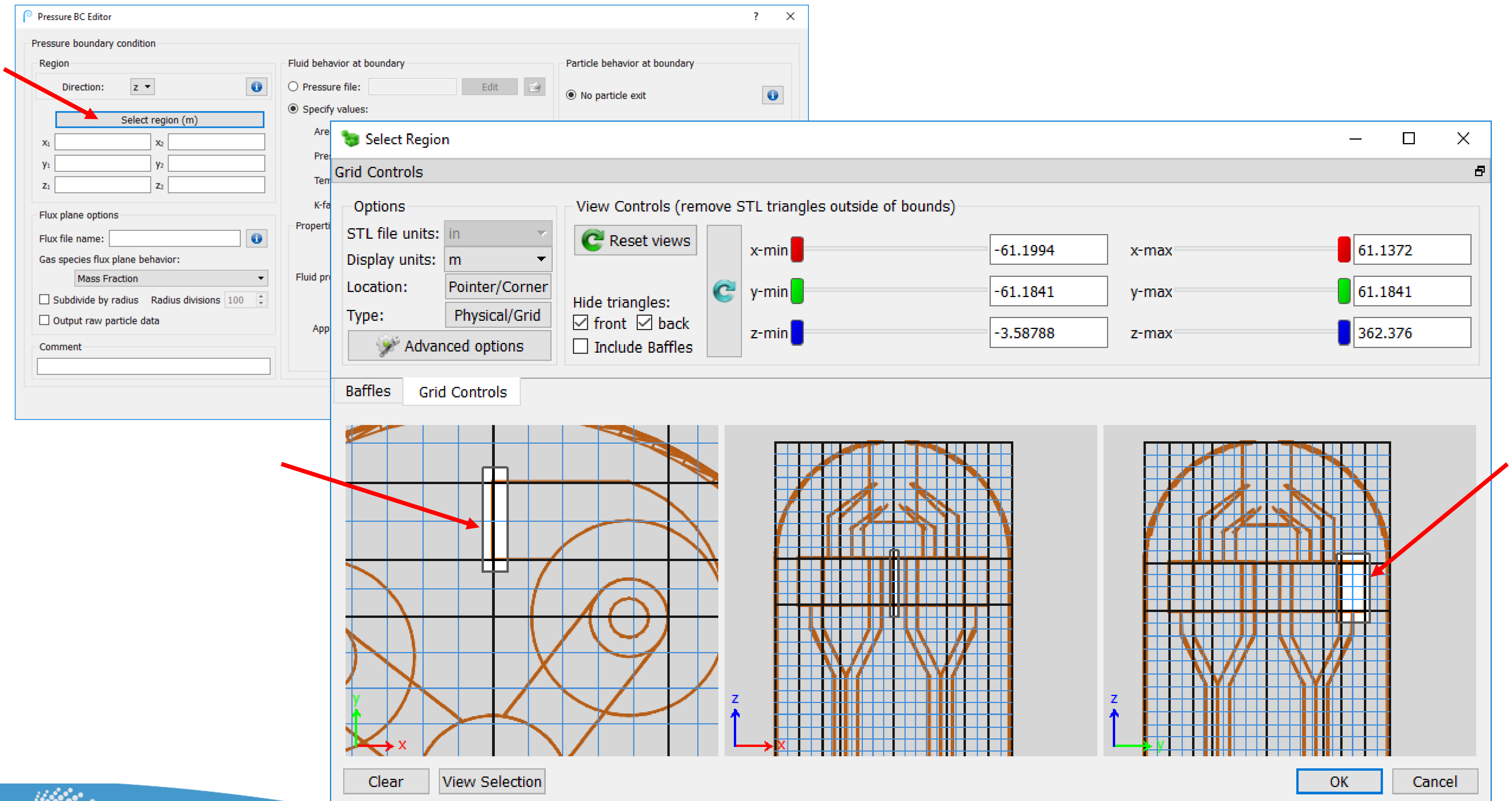
- The cyclone inlet horns will be used as pressure BCs through which particles can escape
- Note that we are not modeling the flow of particles inside the cyclones
- **Each** of the four cyclones will have its own pressure BC. Using the numbering convention shown below can help eliminate confusion
 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





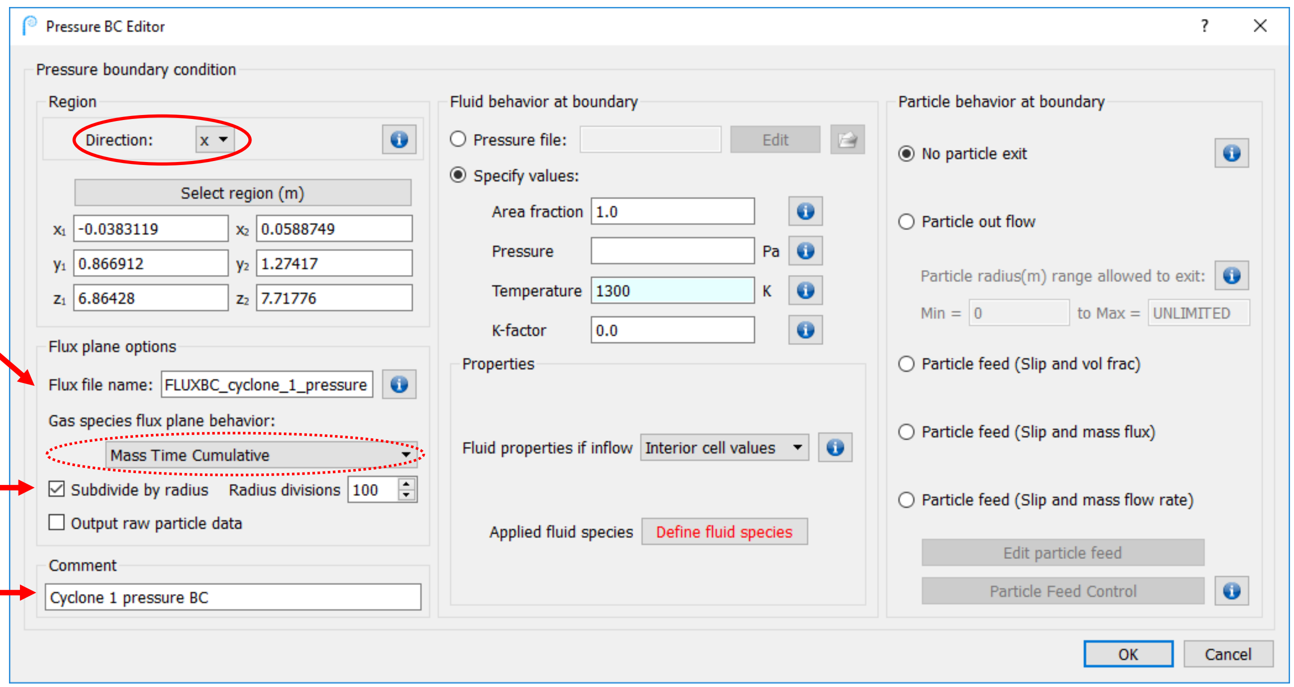
Correct Boundary Condition Location Indices

- Use the **Select region (m)** button to determine the correct boundary condition location
- Click and drag the mouse pointer to select the face for the pressure BC. This will populate the **Region** section with the x, y, z location for the pressure BC.



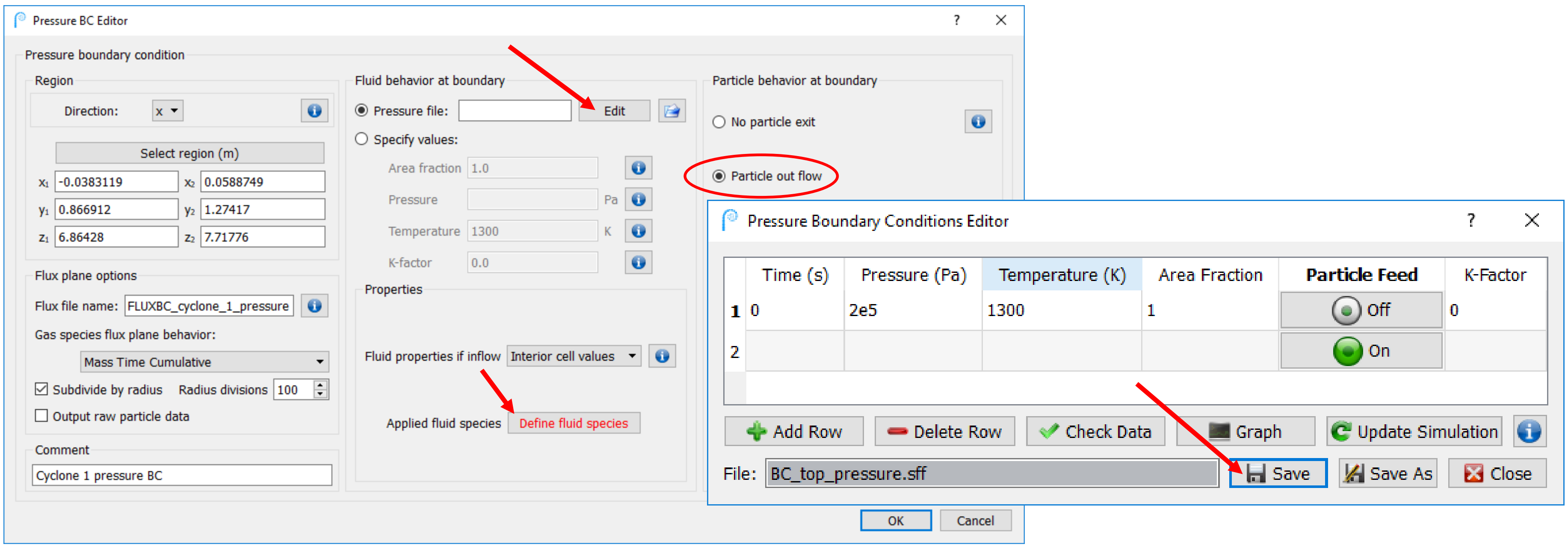
Pressure BC Flux Planes

- 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
- Use the **Subdivide by radius** feature to get particle size information for particles entrained through the flux planes
- Enter a descriptive **Comment**



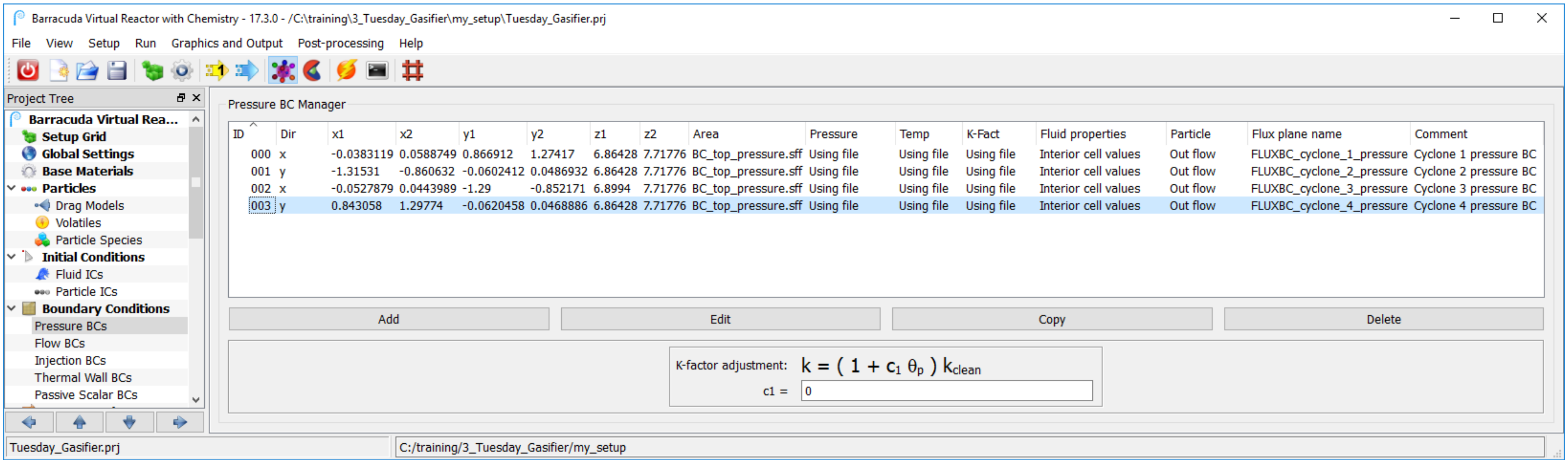
Pressure Boundary Conditions

- The same pressure file will be used for the pressure BC of each cyclone
- To create the file for cyclone 1, click on **Edit**, then enter a pressure of “2.0 x 10^5” Pa at time zero
- Save the file as: **BC_top_pressure.sff**
  - When specifying pressure for the remaining cyclones, click on the file directory button and select that file
- Define the fluid species as 100% N_2 with a mass fraction of 1
- Select **Particle out flow** to allow particles to escape through the boundary



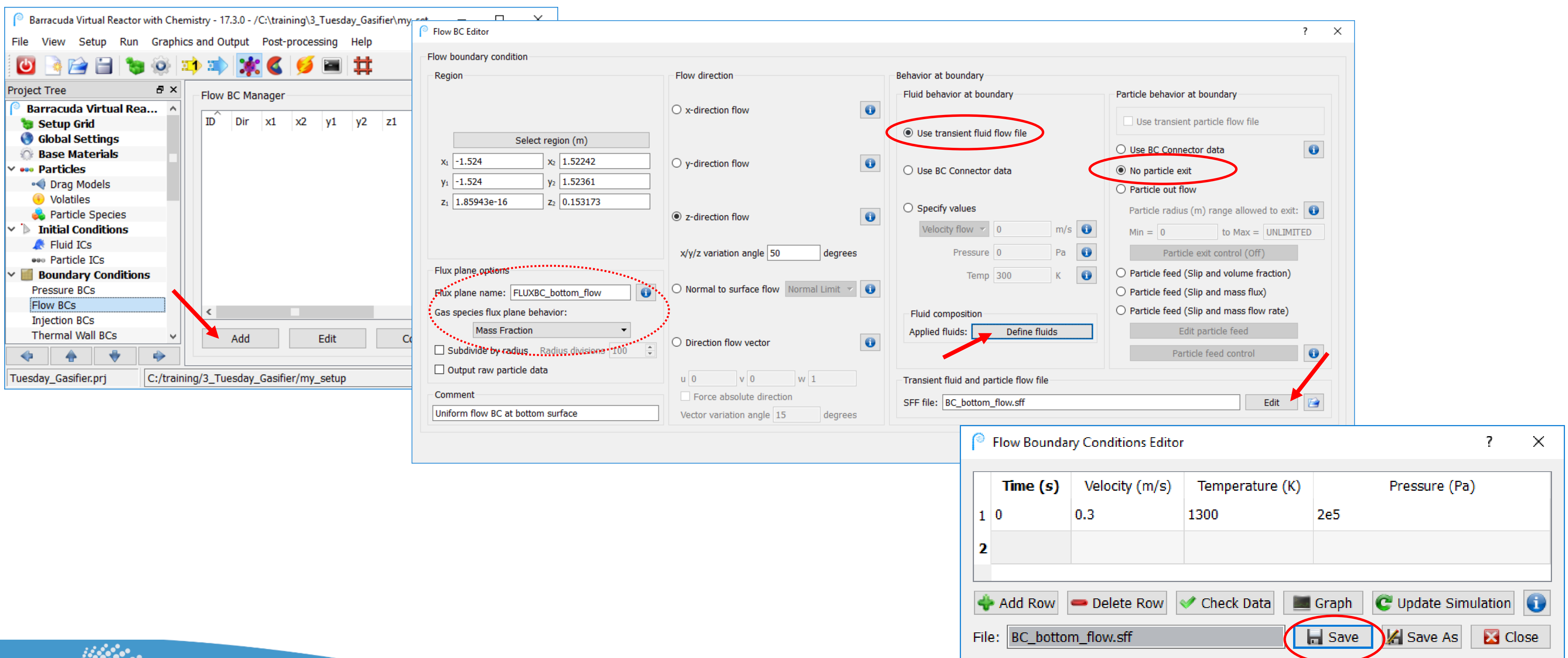
Pressure BCs: Cyclone Inlet Horns

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



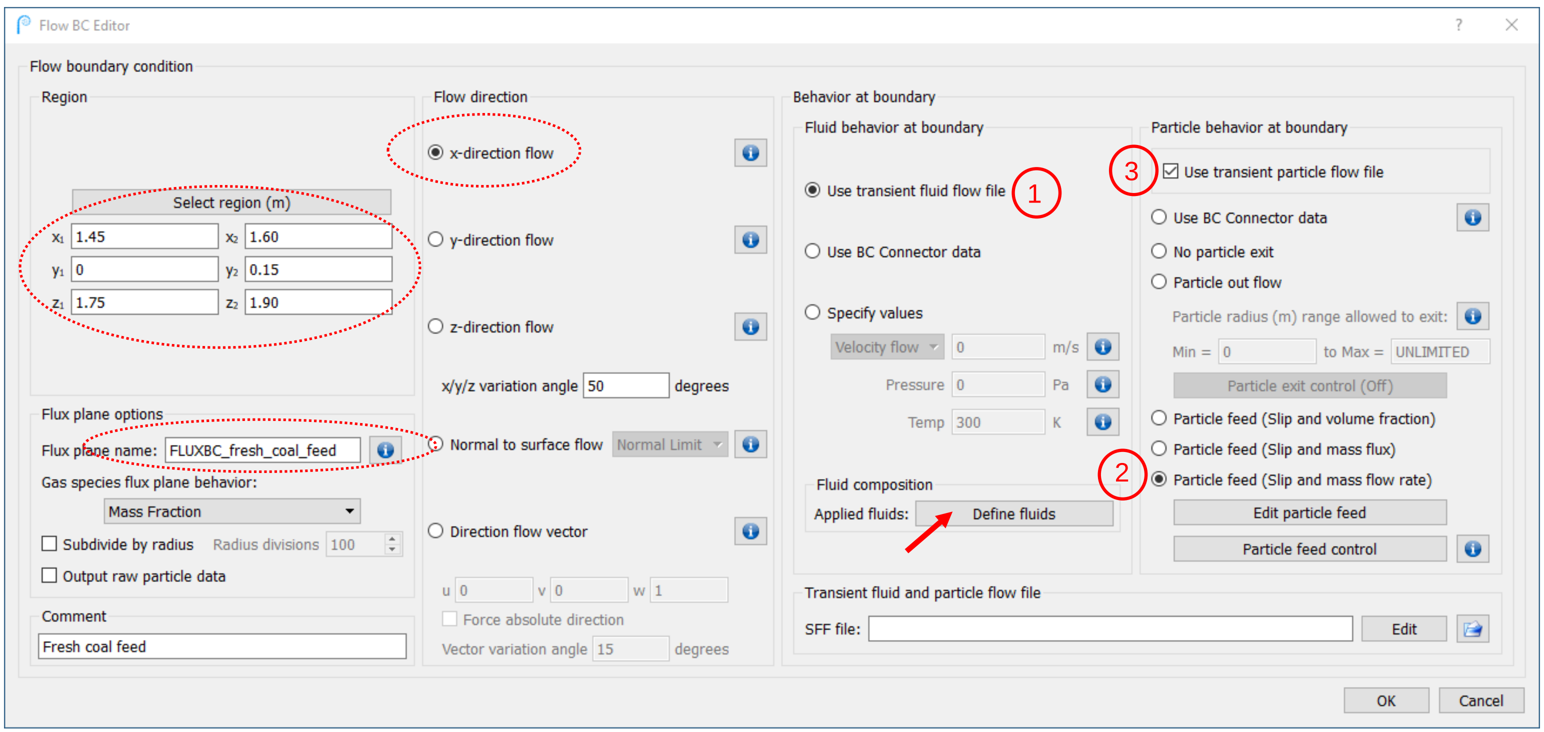
Bottom Flow BC: Simplified Sparger

- Recall that the bottom flow BC is being used to introduce all fluidization gas and steam to the system. In the real system, a gas sparger is present, but in this example a uniform boundary condition is used as a simplification. Use **[** and **]** to specify min and max values in **Region**
- Based on the process sheet, specify the flow rate and composition of gases at the bottom flow BC
- Use a transient (.sff) file to specify the fluid mass flow rate. This allows you to change the flow rate interactively if you need to do so



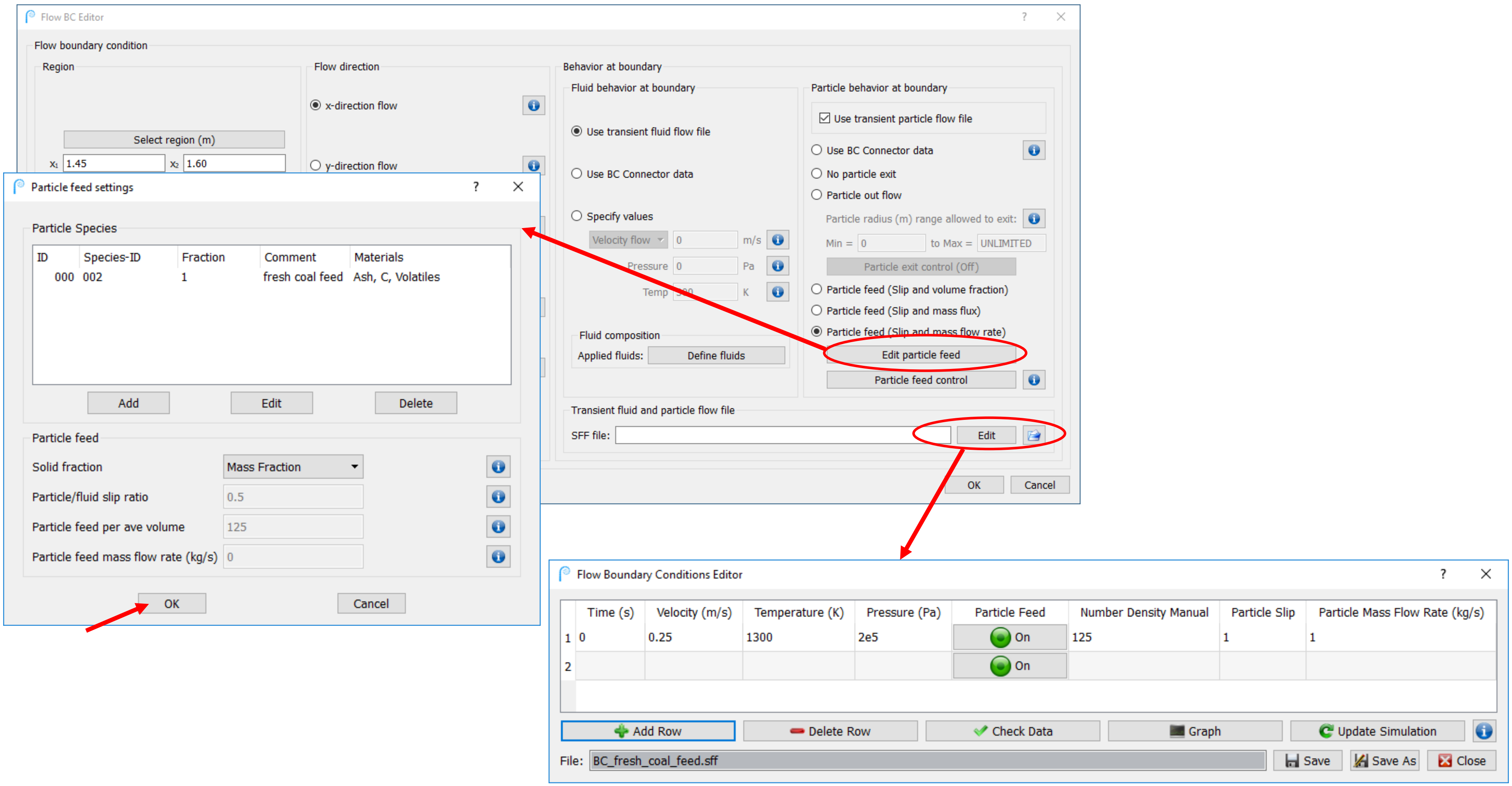
Fresh Coal Flow BC

- As shown on the process sheet, fresh coal is fed into the system from a side inlet location. Use the process sheet to define the fluids at the flow BC
- 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**



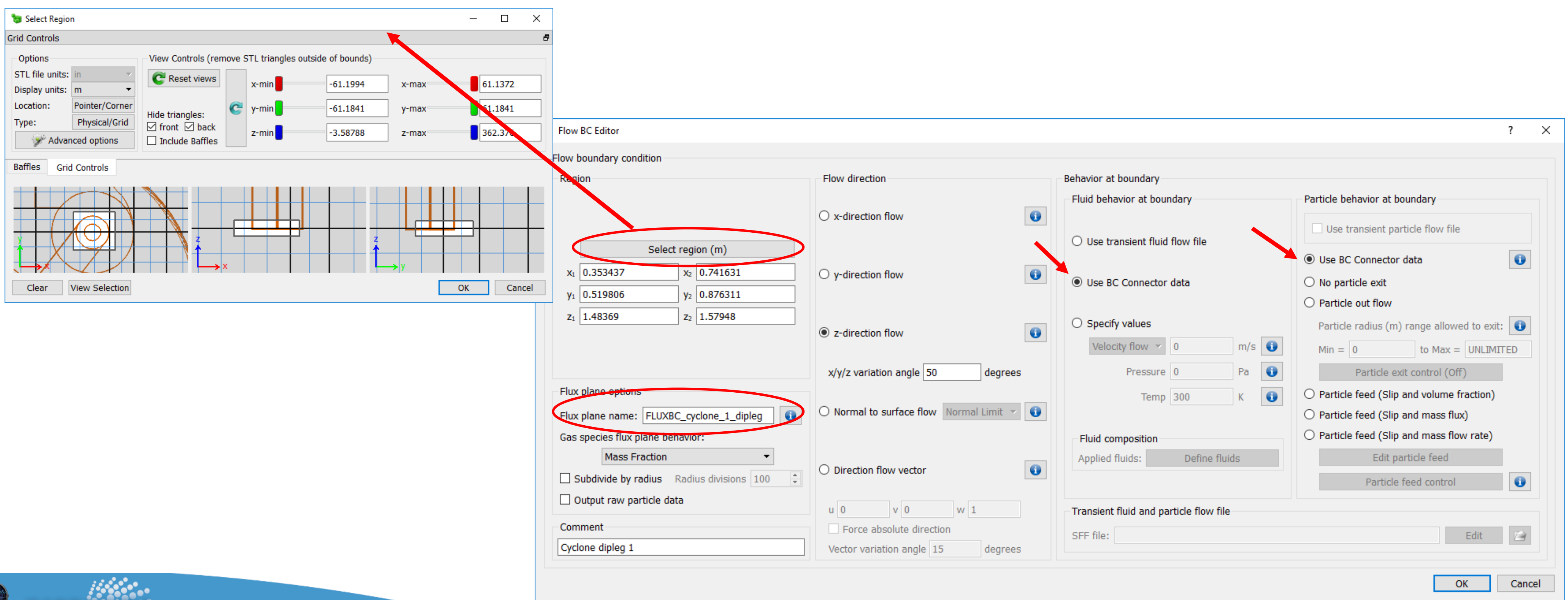
Fresh Coal Flow BC: Particle Feed

- Select **Edit particle feed** to specify particle species to feed
- Click **Edit** to create a transient fluid and particle flow file using the process sheet data



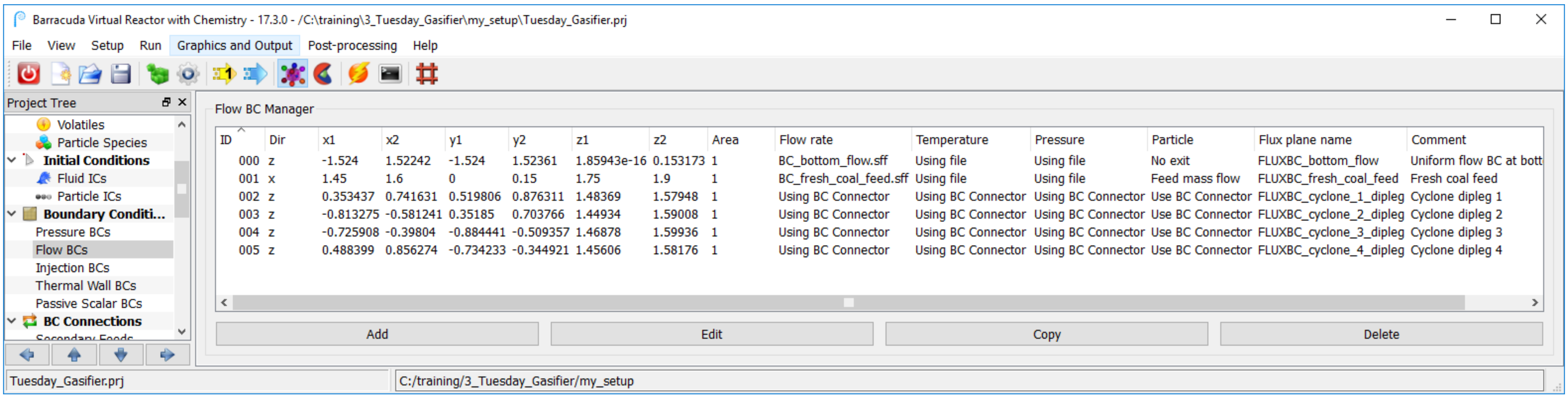
Cyclone Dipleg Flow BCs

- 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
- Be sure to 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**.



Flow BCs

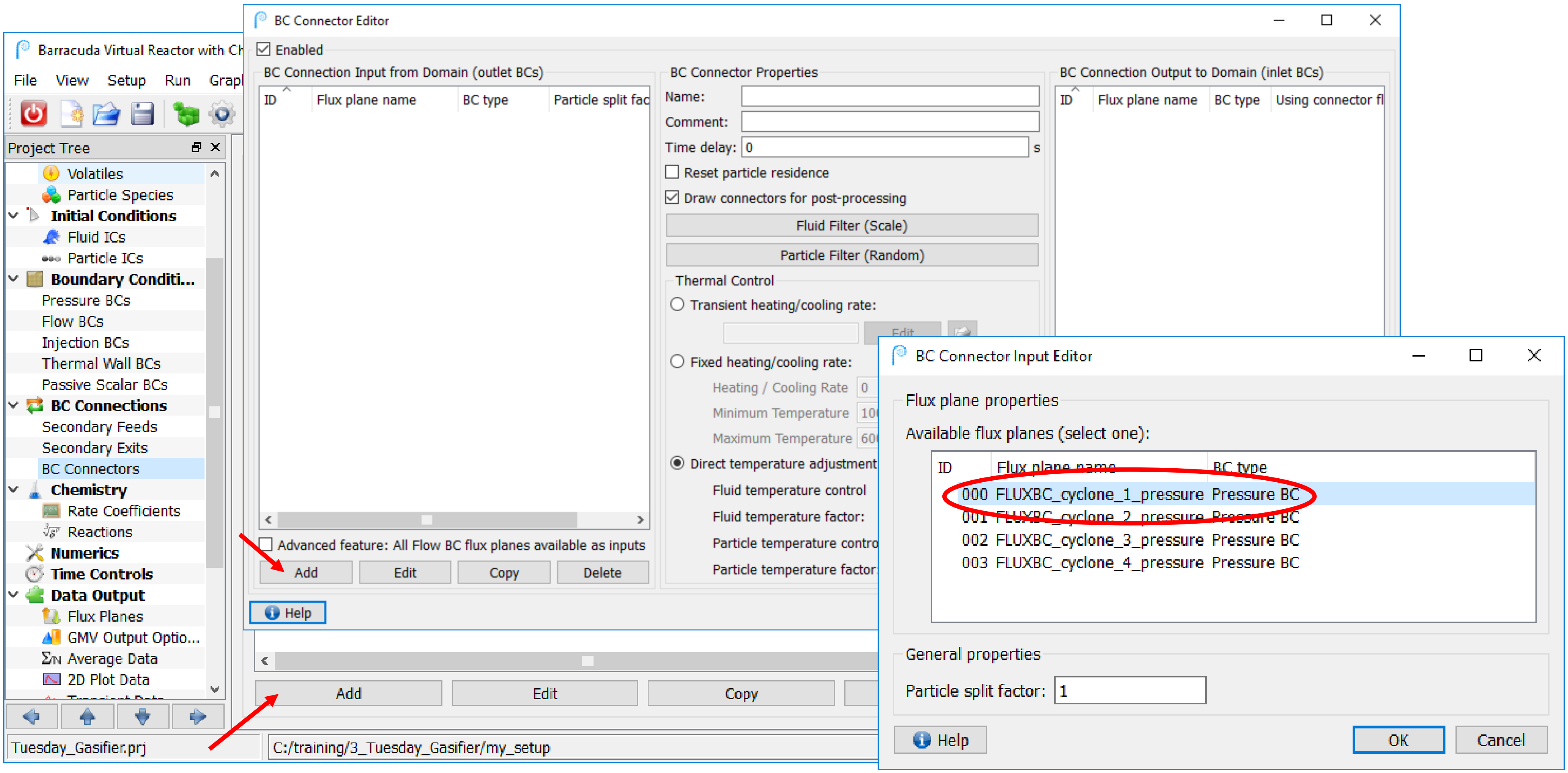
- Ensure that all four cyclone dipleg Flow BCs are created before moving on to the next slide



ID	Dir	x1	x2	y1	y2	z1	z2	Area	Flow rate	Temperature	Pressure	Particle	Flux plane name	Comment
000	z	-1.524	1.52242	-1.524	1.52361	1.85943e-16	0.153173	1	BC_bottom_flow.sff	Using file	Using file	No exit	FLUXBC_bottom_flow	Uniform flow BC at bott
001	x	1.45	1.6	0	0.15	1.75	1.9	1	BC_fresh_coal_feed.sff	Using file	Using file	Feed mass flow	FLUXBC_fresh_coal_feed	Fresh coal feed
002	z	0.353437	0.741631	0.519806	0.876311	1.48369	1.57948	1	Using BC Connector	Using BC Connector	Using BC Connector	Use BC Connector	FLUXBC_cyclone_1_dipleg	Cyclone dipleg 1
003	z	-0.813275	-0.581241	0.35185	0.703766	1.44934	1.59008	1	Using BC Connector	Using BC Connector	Using BC Connector	Use BC Connector	FLUXBC_cyclone_2_dipleg	Cyclone dipleg 2
004	z	-0.725908	-0.39804	-0.884441	-0.509357	1.46878	1.59936	1	Using BC Connector	Using BC Connector	Using BC Connector	Use BC Connector	FLUXBC_cyclone_3_dipleg	Cyclone dipleg 3
005	z	0.488399	0.856274	-0.734233	-0.344921	1.45606	1.58176	1	Using BC Connector	Using BC Connector	Using BC Connector	Use BC Connector	FLUXBC_cyclone_4_dipleg	Cyclone dipleg 4

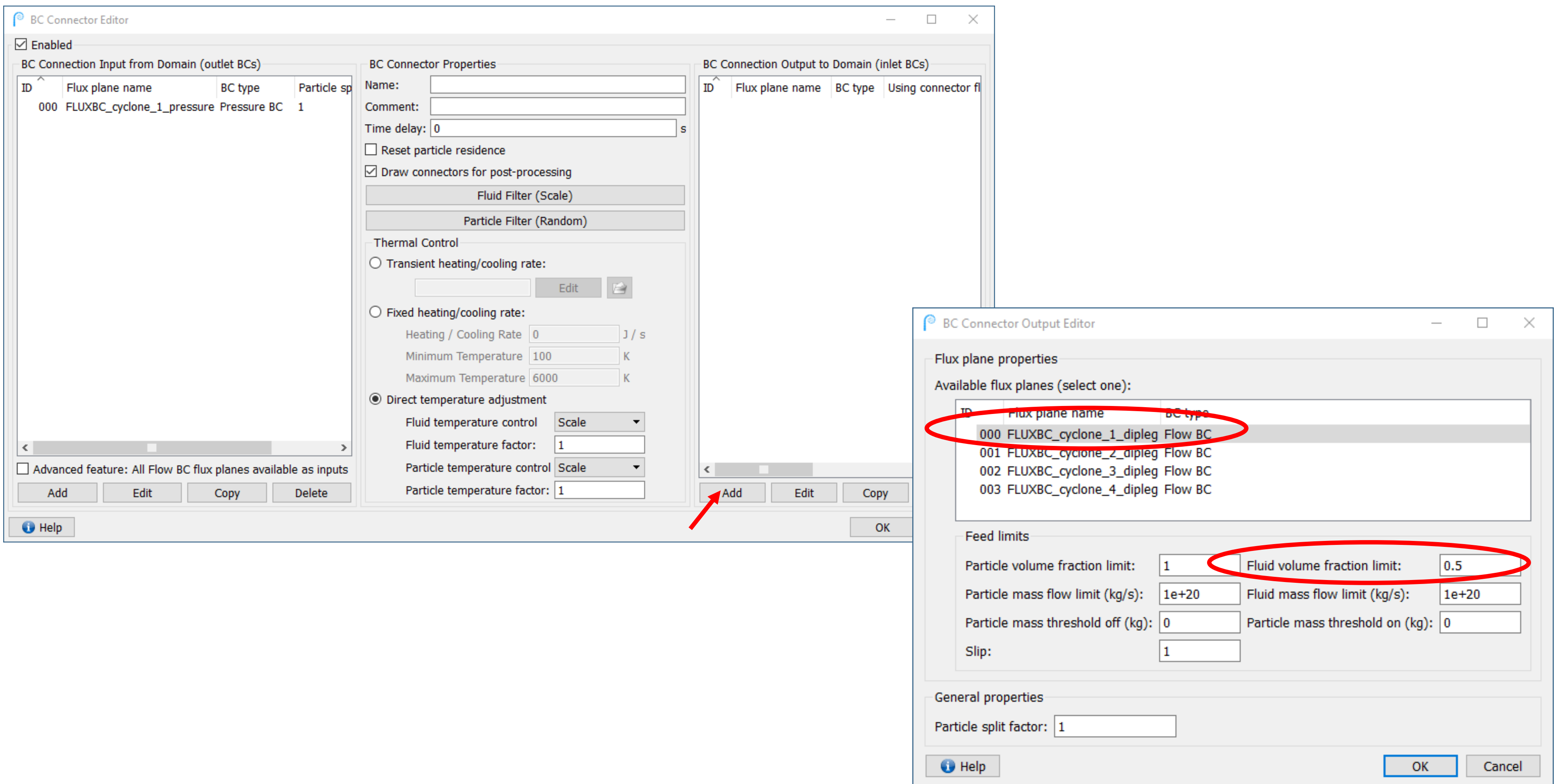
BC Connection Input from Domain

- In the **BC Connectors** section of the Barracuda VR GUI, click **Add** to define a new connection.
- On the left side, select the **BC Connector Input**, which in this case is the Pressure BC for Cyclone 1.



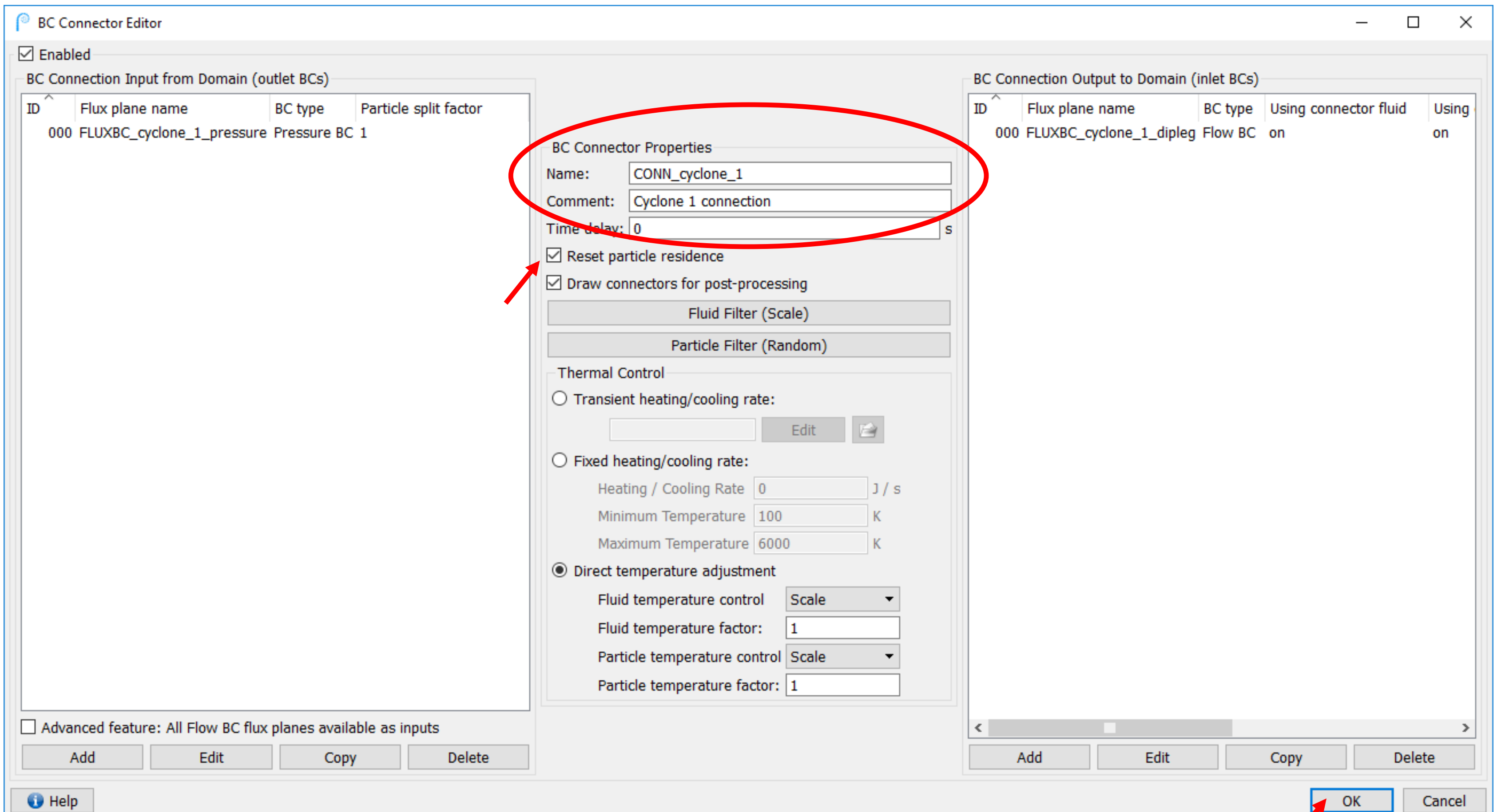
BC Connection Output to Domain

- On the right side, select the **BC Connection Output**, in this case the Flow BC for Cyclone 1 dipleg.
- 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



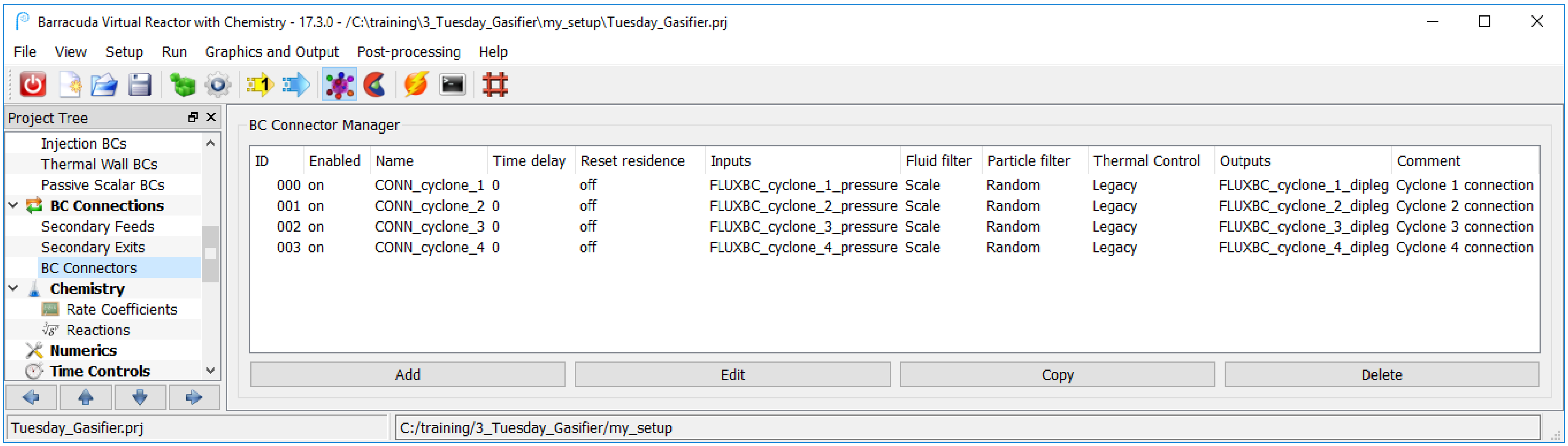
BC Connector Properties

- In the center of the dialog, define a **Name** (which will be the name of a flux plane file for the BC Connection) and a **Comment**
- Select **Reset particle residence**



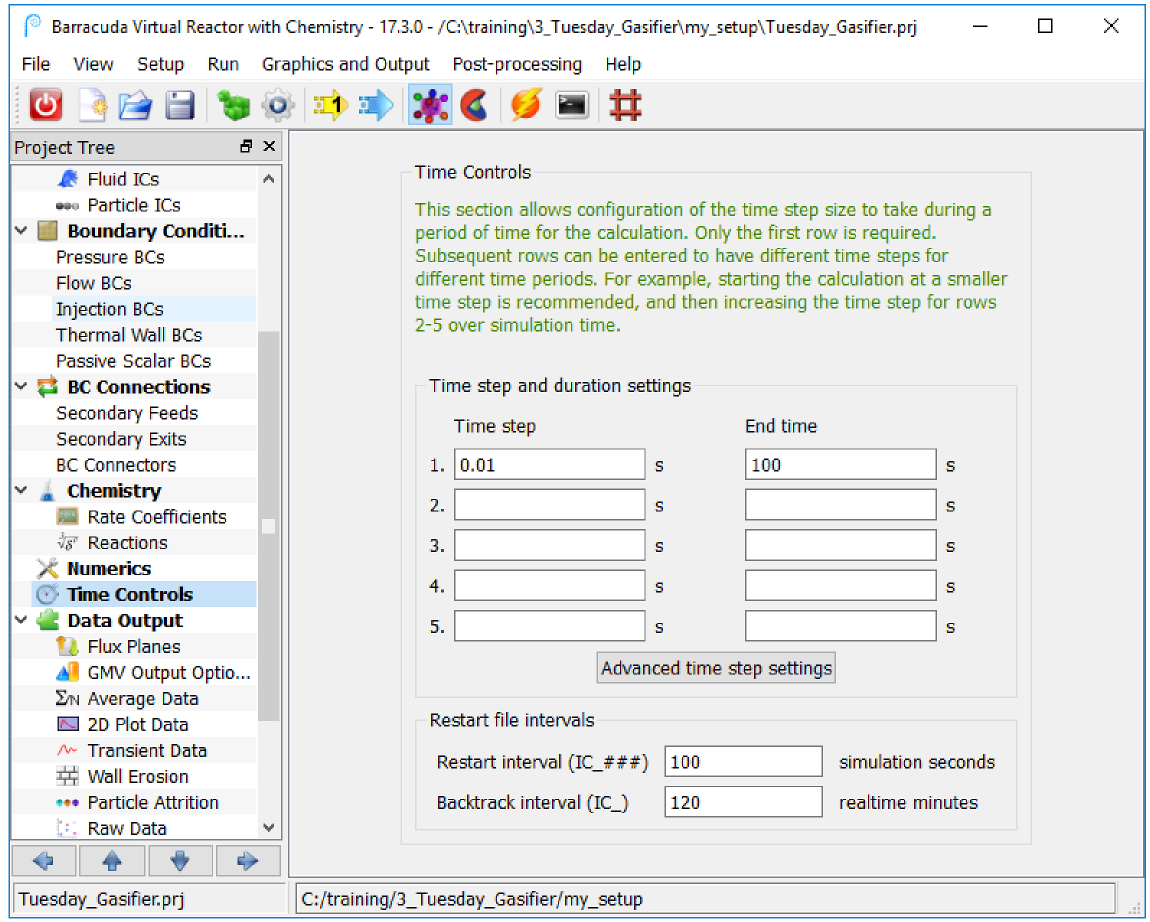
Add BC Connections for Remaining Cyclones

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



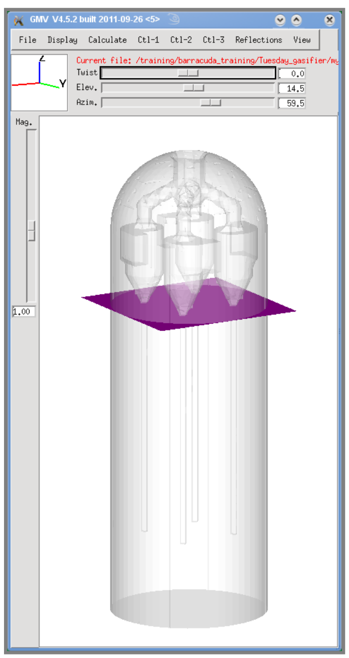
Time Controls

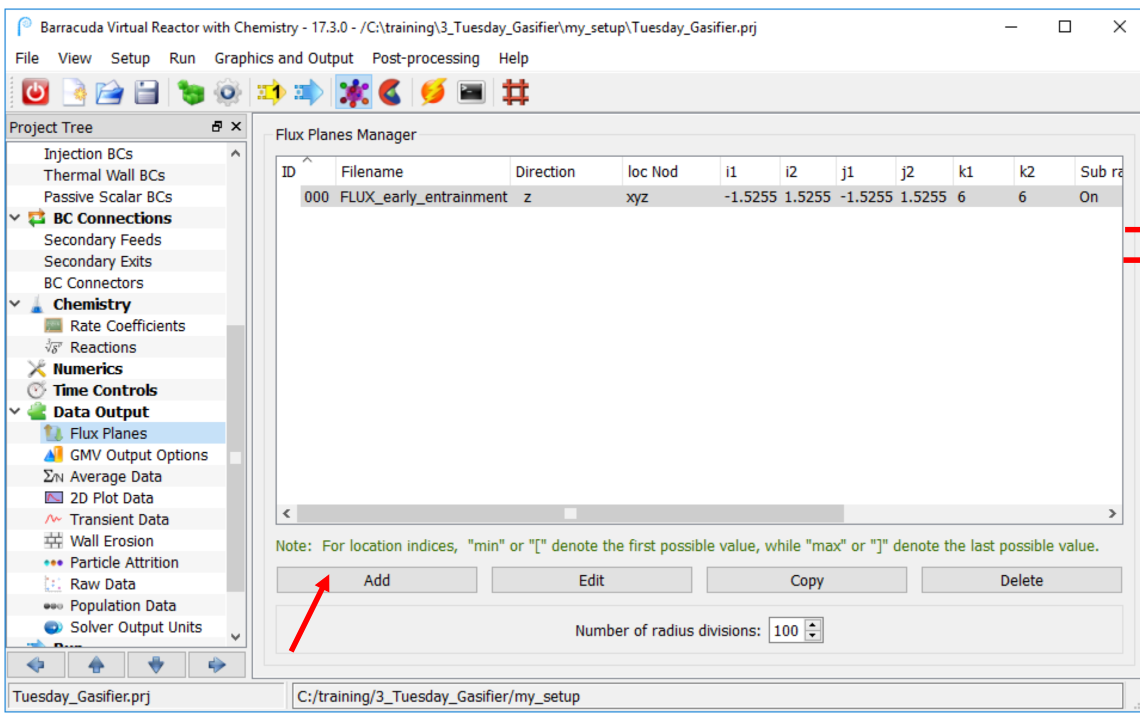
- Set the **End time** to “100” s
- When specifying an end time, take into consideration the various physical time-scales of the system. How long will the fluidization take to become steady? How long will thermal effects take? How long should chemistry take?
- Set the **Time step** to “0.01” s
  - If 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

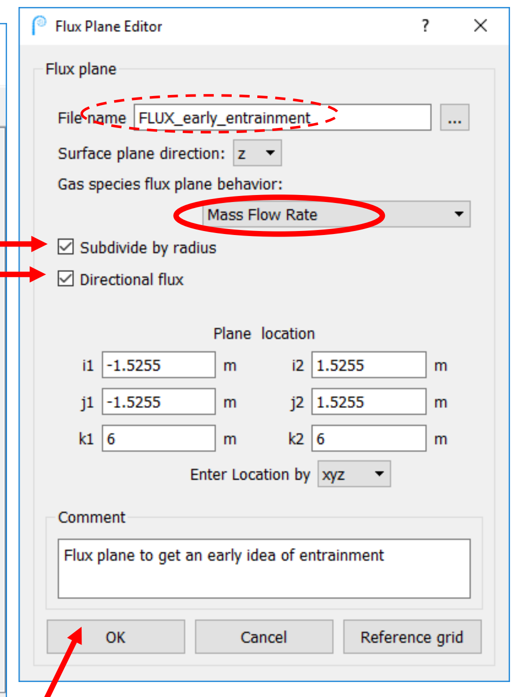


Flux Planes

- Flux planes were already defined at the pressure BCs for the cyclone inlets
- It is also useful to set up a flux plane lower in the freeboard to get an earlier idea of the particle entrainment rate. Set up a flux plane that spans the vessel at about the height shown in the image
- Select **Subdivide by radius** to get PSD information for particles passing through the flux plane
- Select **Mass Flow Rate** for gas species information from the flux plane

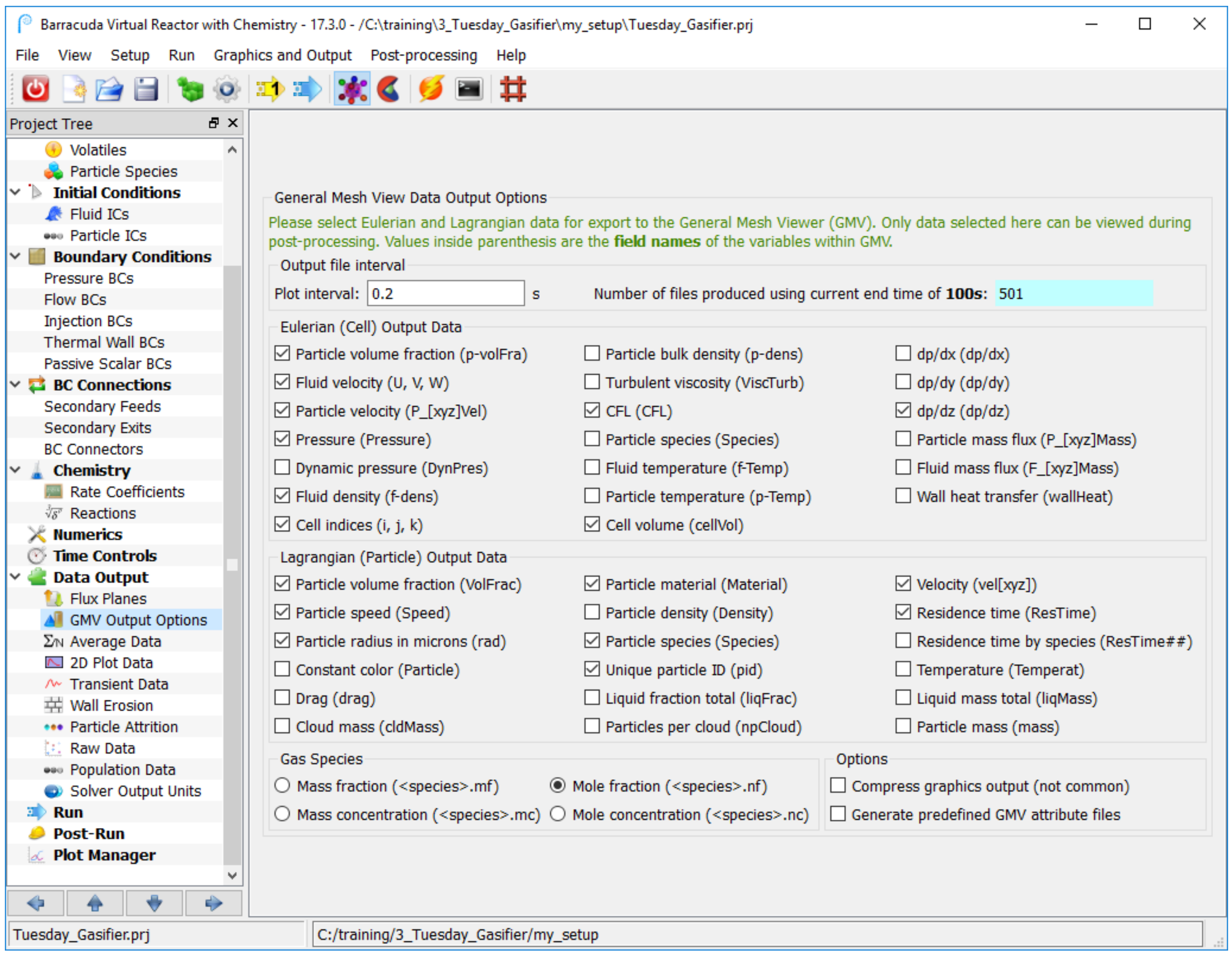






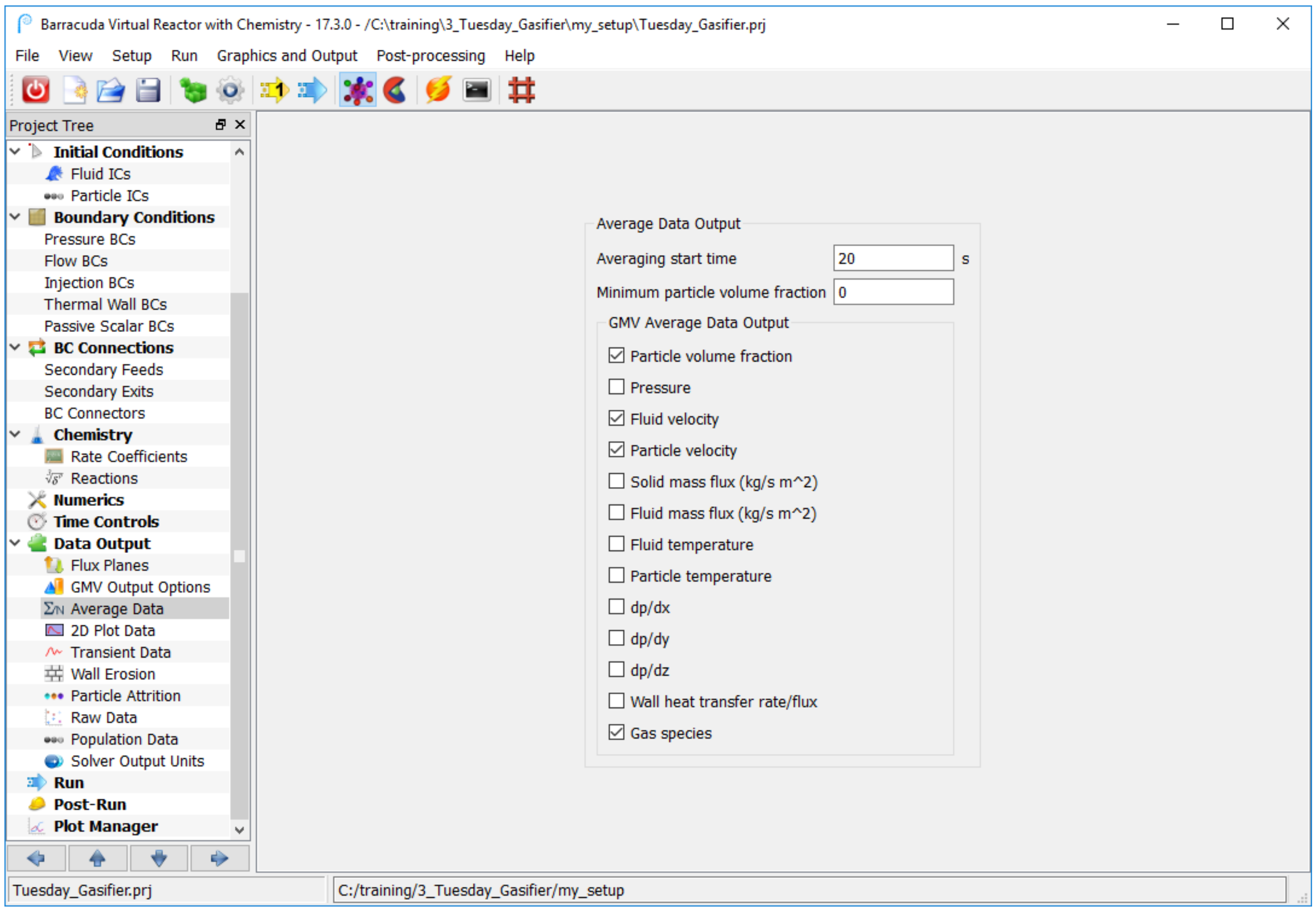
GMV Output Options

- By default, a minimal set of variables is selected for output to GMV. This is done to keep file sizes as small as possible, since GMV files typically take up the most space in your run directory
- When setting up your project, make sure that you check the boxes next to any other variables of importance to your analysis of the simulation. Suggested variables, for this training project, are shown below



Average Data

- Time-average data is very useful when analyzing particle-fluid systems. Fluidized beds, for instance, are dynamic by nature and will not reach a traditional “steady-state” condition
- Start time-averaging at “20” s
- Select the items for time-averaging shown below



Check Model Setup

- Select **GPU Parallel**
- **Save** your project
- 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 the Gmv.00000 file? If you forgot any output variables, now is the easiest time to add them!