

# Gasifier Training Problem

## Part 3: Project Setup

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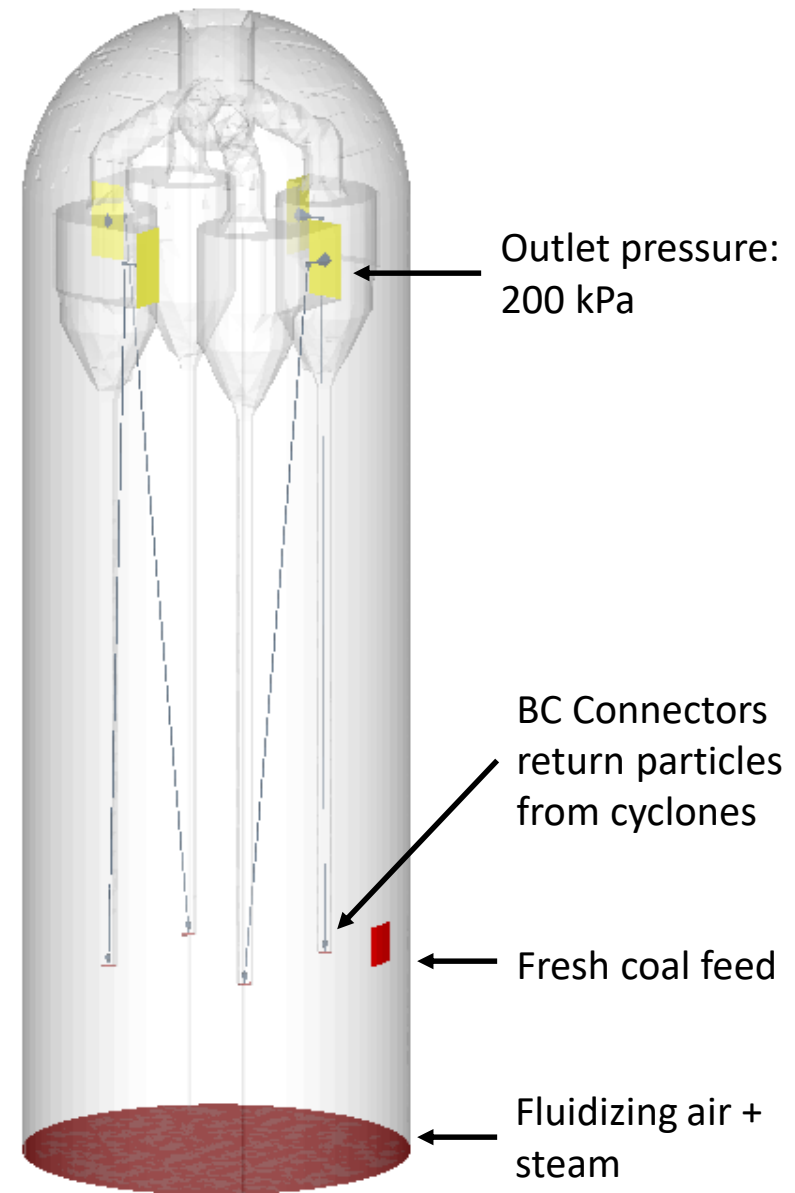
# Training Objectives

- 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

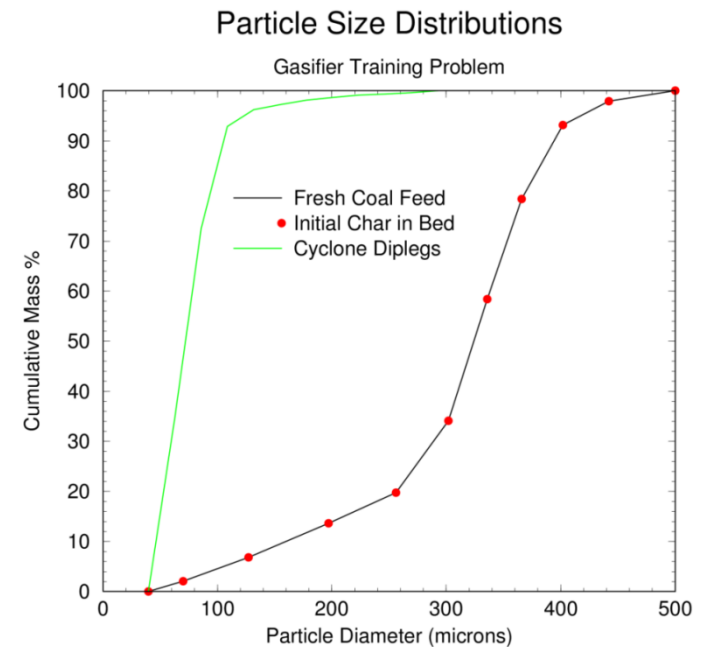
- Isothermal at 1300 K
- No chemistry in this model
- Fresh coal feed coming in at:
  - $x=1.45$  m
  - $y=0$  m
  - $z=1.75$  m

Boundary	Fluid Flow	Particle Flow
Fluidizing Air + Steam	Velocity = 0.3 m/s  Gas (mass fractions): 0.3 H <sub>2</sub> O, 0.54 N <sub>2</sub> , 0.16 O <sub>2</sub>	None
Fresh Coal Feed	Velocity = 0.25 m/s  Gas (mass fractions): 0.77 N <sub>2</sub> , 0.23 O <sub>2</sub>	Fresh coal at 1 kg/s
Cyclone Diplegs	Controlled by BC Connector	Controlled by BC Connector



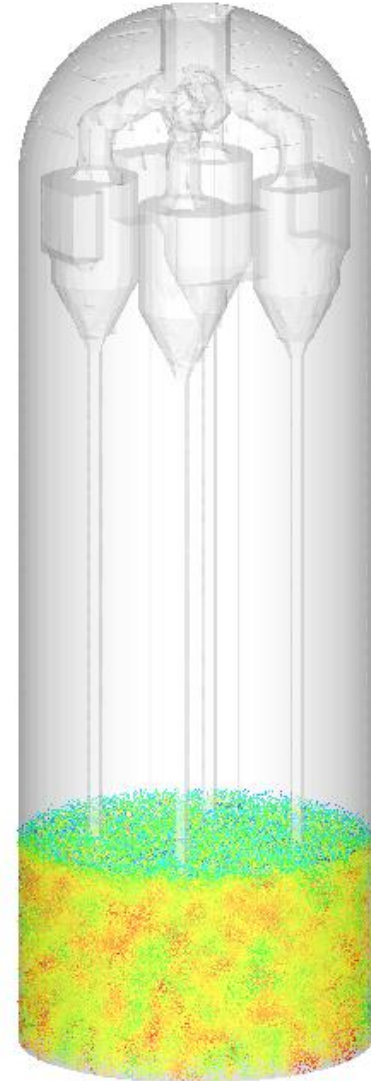
# Particle Properties

- 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/m<sup>3</sup>
  - Volatile composition (mass fractions):  
0.4144 CH<sub>4</sub>, 0.1702 CO, 0.0444 CO<sub>2</sub>, 0.111 H<sub>2</sub>, 0.26 H<sub>2</sub>O
  - Release rate of volatiles is  $\text{rate} = 0.05 T \exp(-5500/T)$
  - 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/m<sup>3</sup>
  - PSD is included in the “my\_setup” folder with name **psd\_initial\_char\_in\_bed.sff**



# Particle Properties

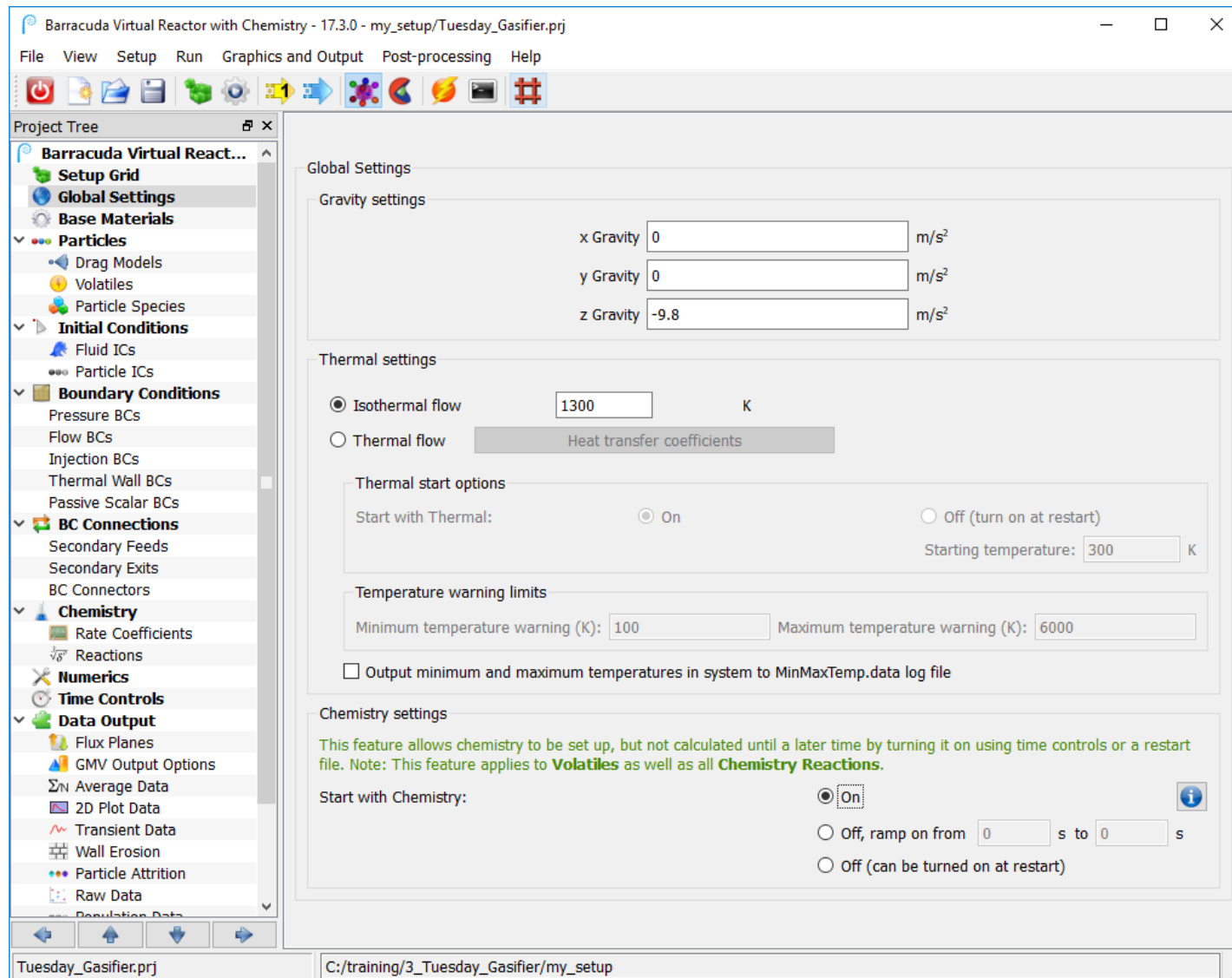
- For material properties, assume that Carbon and Ash have densities of 2150 kg/m<sup>3</sup>
- Initial Conditions
  - Initial bed mass is 4800 kg
  - Filled with Nitrogen at 200 kPa



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

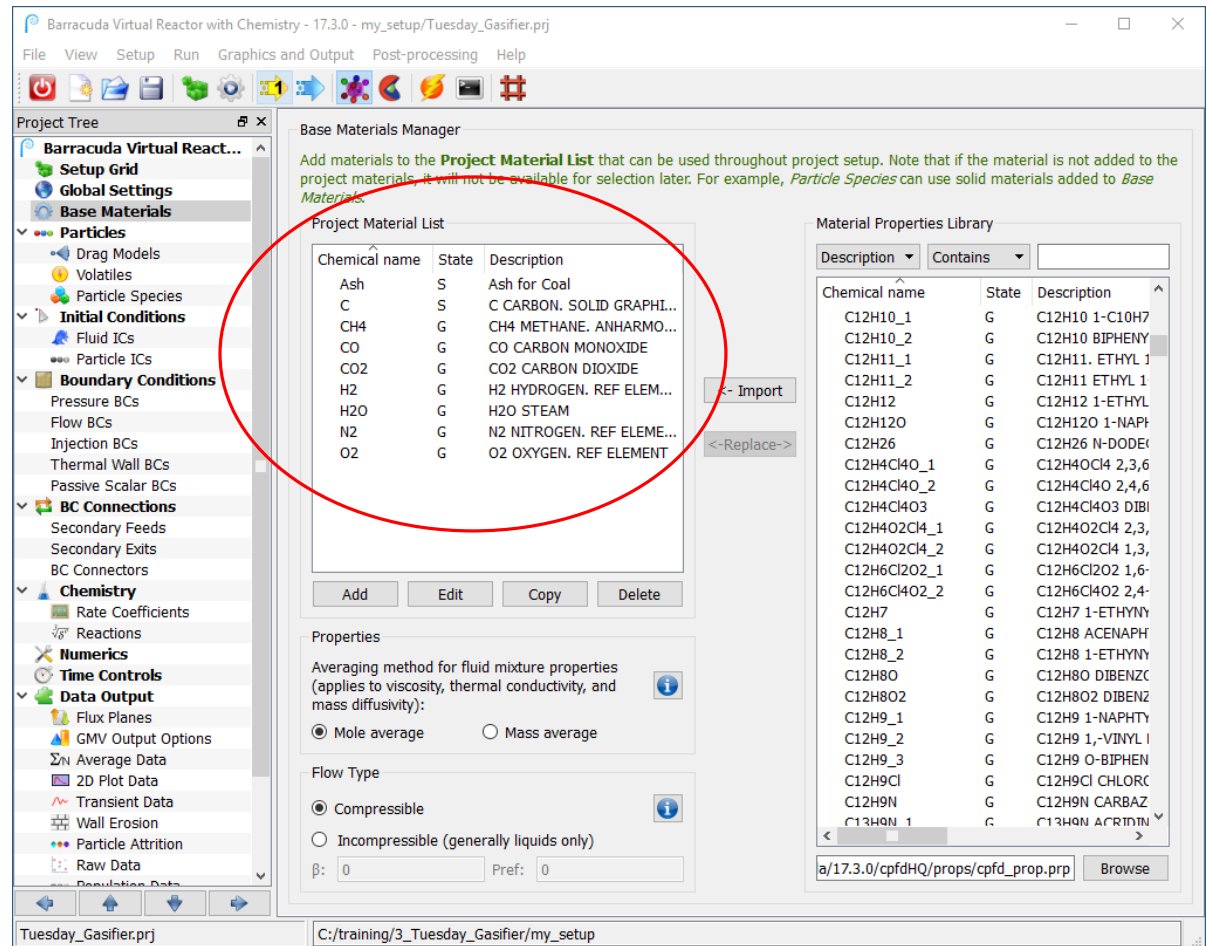
- Always keep in mind why you are running any model
- For this training problem, we want to set up and analyze the Barracuda model to learn the following:
  - General fluidization characteristics
  - Entrainment rate of particles
- This is a simplified model without chemistry or thermal calculations.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

# Global Settings



# Base Materials

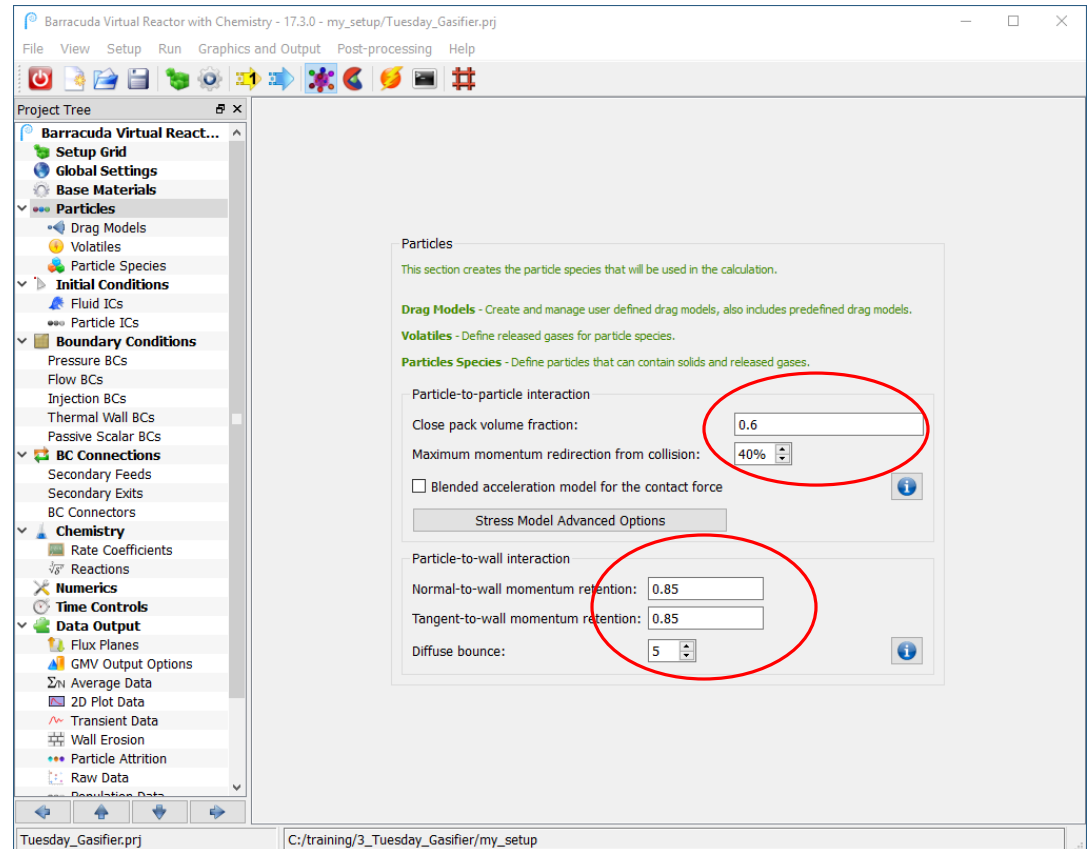
- In the **Base Materials** section, define all materials that will be used in the simulation
- Based on the process design sheet and particle properties, you will need:
  - Ash (select C\_1, then rename it "Ash")
  - Carbon
  - Methane
  - Carbon Monoxide
  - Carbon Dioxide
  - Hydrogen gas
  - Steam
  - Nitrogen gas
  - Oxygen gas





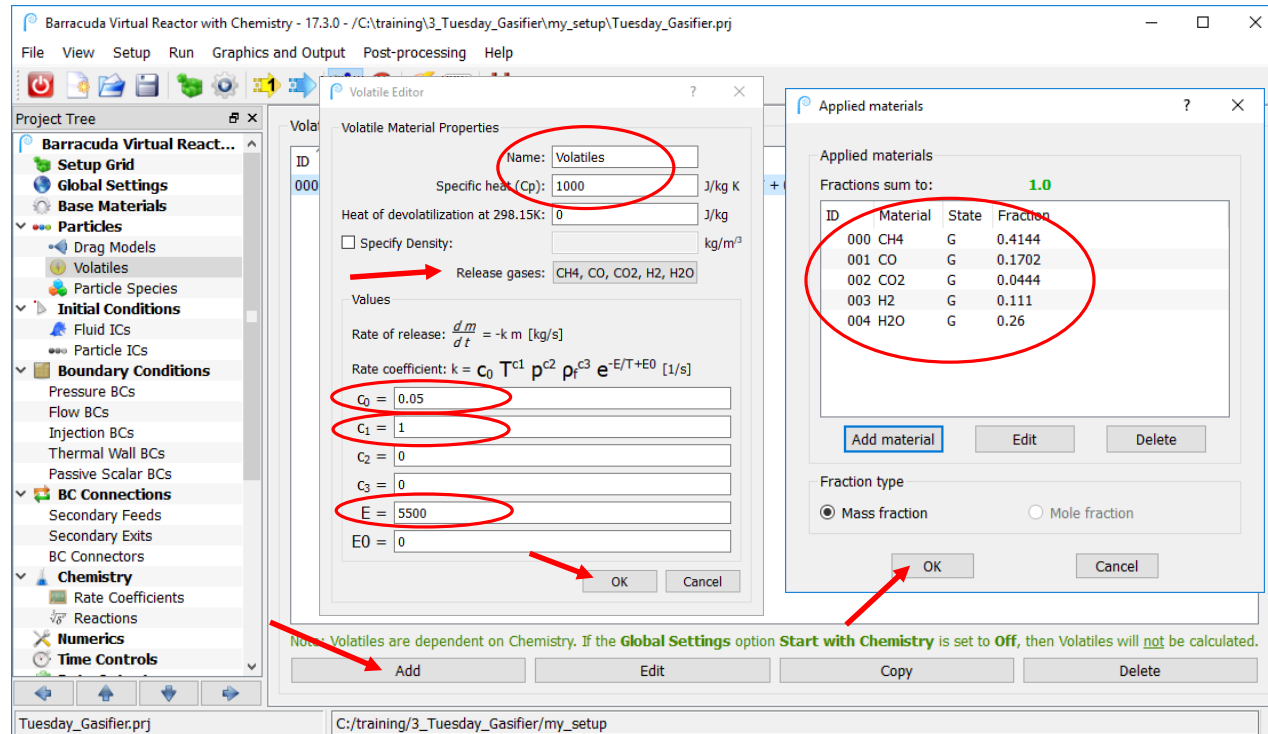
# Particles

- 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<sub>4</sub>, 0.1702 CO, 0.0444 CO<sub>2</sub>, 0.111 H<sub>2</sub>, 0.26 H<sub>2</sub>O
- 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  $c_0$ , “1” for  $c_1$  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:

$$\text{Rate} = 0.05 T \exp(-5500/T)$$

# 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<sup>3</sup>. Click **OK**
- Enter an appropriate description in the **Comment** field

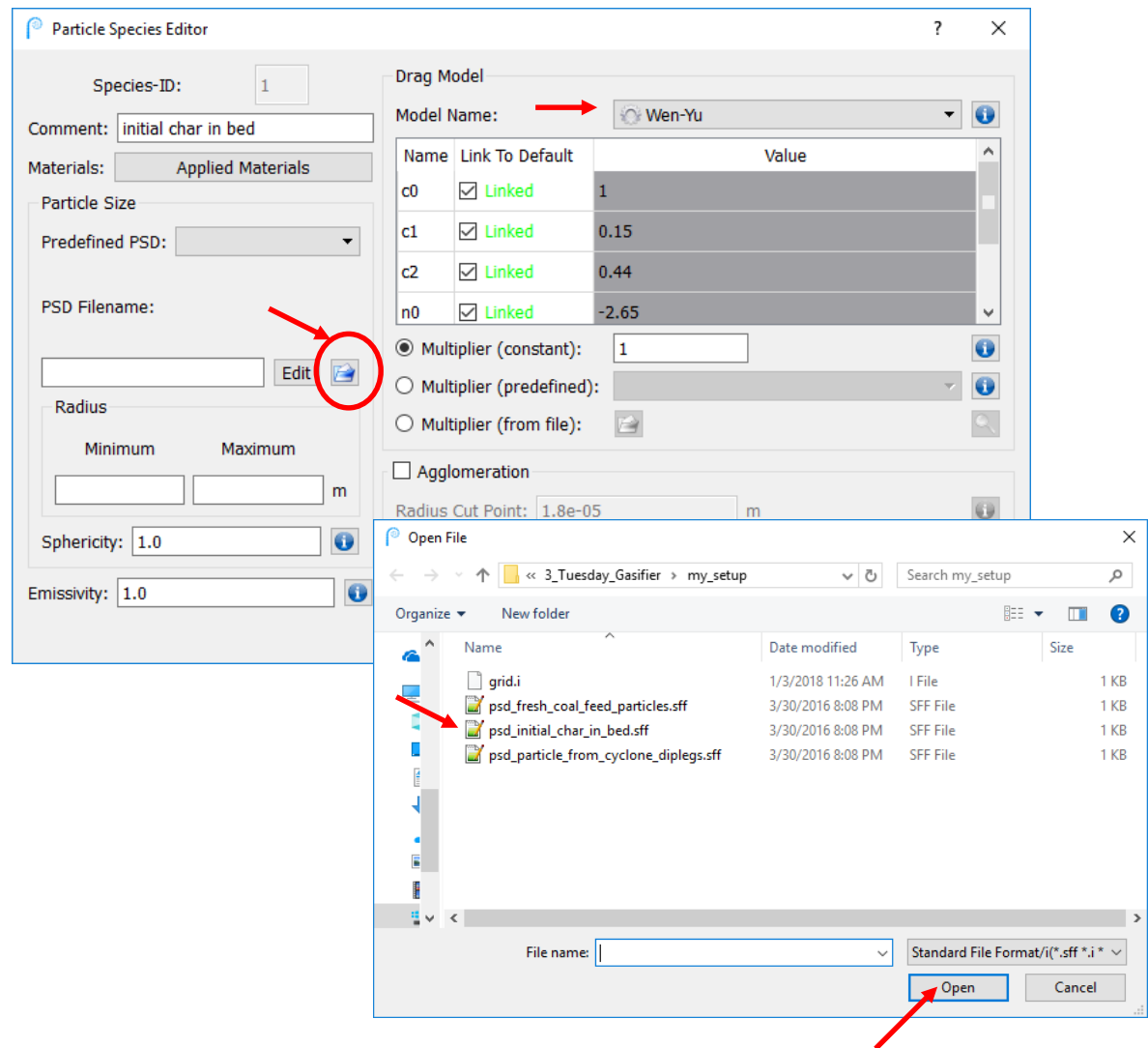
The screenshot shows the Barracuda Virtual Reactor interface. The **Particle Species Editor** window is open, showing the **Comment** field with the text "initial char in bed". The **Applied Materials Manager** window is also open, showing the **Mass Fractions sum to:** field with the value "1.0" and the **Manually entered:** field for overall particle density with the value "725". The **Applied Materials** table lists three materials: Carbon (C), Ash, and Volatiles, with their respective mass fractions and densities.

ID	Name	State	Mass Frac	Density (kg/m <sup>3</sup> )	Age Factor
000	C	S	0.8999	2150	1
001	Ash	S	0.1	2150	1
002	Volatiles	Volatile	0.0001	Unspecified	N/A

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

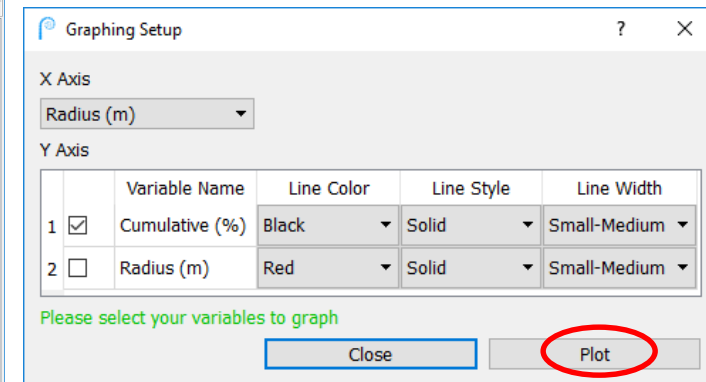
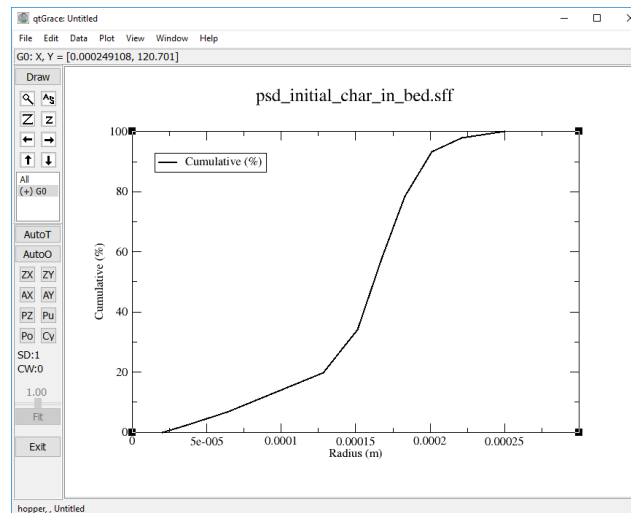
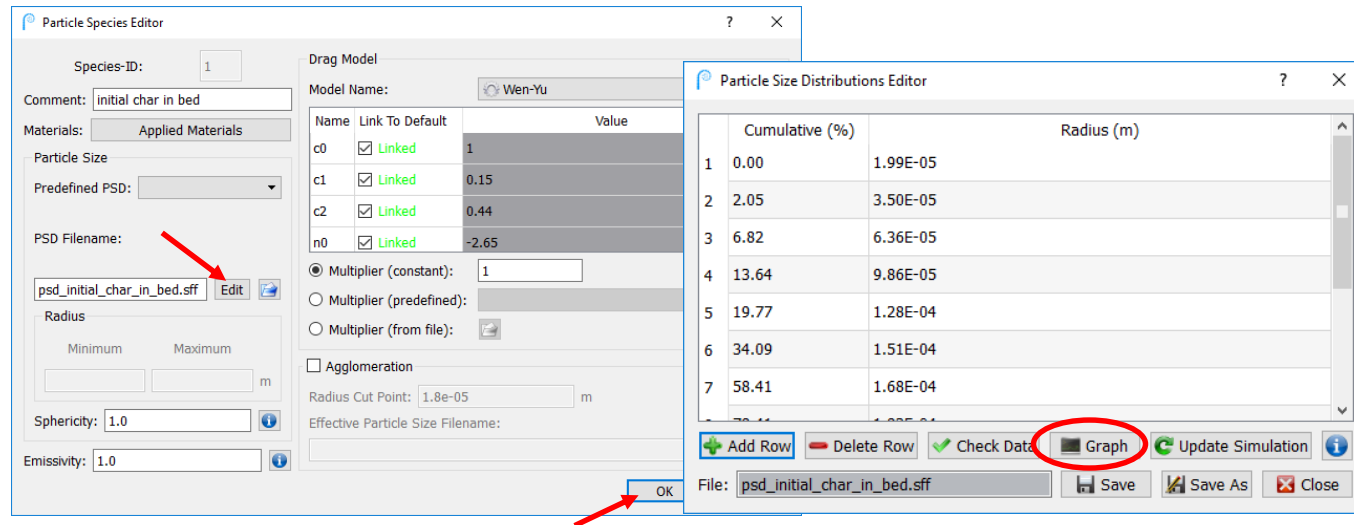
# Specifying PSD

- 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.



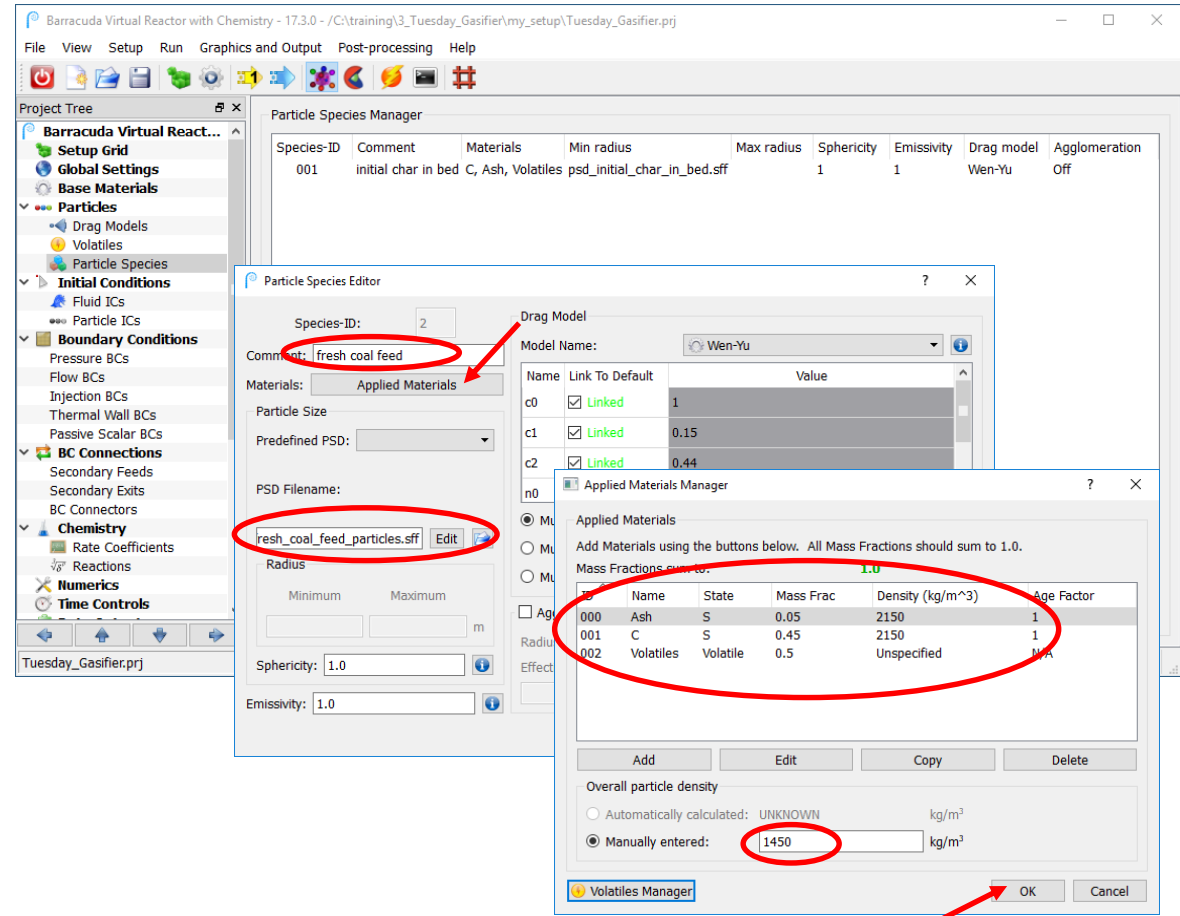
# Particle Size Distribution (PSD) File

- 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/m<sup>3</sup>
- 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<sub>2</sub> at  $2.0 \times 10^5$  Pa
- Use [ and ] to select minimum and maximum extents of the domain

The screenshot displays the Barracuda Virtual Reactor interface with two dialog boxes open. The 'Fluid IC Editor: 000' dialog box has the 'Initial Conditions' checkbox checked. The 'Pressure' field is set to 200000 Pa and is circled in red. The 'Temperature' is 300 K. The 'Fluid species' is set to 'Define fluids'. The 'Velocity' is 0 m/s. The 'Initial conditions from file' checkbox is unchecked. The 'IC File' field is empty. The 'Region' section shows a 'Select region (m)' box with coordinates: x1: -1.524, x2: 1.52242, y1: -1.52361, y2: 1.52361, z1: 1.85943e-16, z2: 9.11321. The 'Comment' field is empty. The 'Applied materials' dialog box shows 'Fractions sum to: 1.0'. The table below is circled in red:

ID	Material	State	Fraction
000	N2	G	1

The 'Fraction type' is set to 'Mass fraction'. The 'OK' button in the 'Applied materials' dialog is highlighted with a red arrow. The 'Edit' button in the 'Fluid IC Manager' is also highlighted with a red arrow.

# 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)

The screenshot displays the Barracuda Virtual Reactor interface. On the left, the Project Tree shows the hierarchy: Setup Grid, Global Settings, Base Materials, Particles, Initial Conditions, Boundary Conditions, BC Connections, and Chemistry. The 'Initial Conditions' folder is expanded, showing 'Fluid ICs' and 'Particle ICs'. The 'Particle IC Manager' window is open, showing a table with columns: ID, On, x1, x2, y1, y2, z1, z2, Description, and Comment. Below the table are buttons for 'Add', 'Edit', and 'Copy'. A red arrow points to the 'Add' button. The 'Particle IC' dialog box is also open, showing the 'Initial conditions' section with a red circle around the 'Initialize mass in region' dropdown, the 'Particle species' dropdown set to '001 - initial char in bed', and the 'Total particle mass' set to 4800 kg. The 'Region' section has a red circle around the 'Select region (m)' area, showing coordinates: x1: -1.524, x2: 1.52242, y1: -1.52361, y2: 1.52361, z1: 1.85943e-16, and z2: 1.815. The 'Cloud size' section has a red circle around the 'Use global slider' option. The 'Special settings' section has a red circle around the 'Random cloud initialization' checkbox. The 'Comment' section is empty. The 'OK' button is highlighted with a red arrow.

**Particle IC Manager Table:**

ID	On	x1	x2	y1	y2	z1	z2	Description	Comment
Automatically calculated parcels per cell (Global Slider)									
Low Medium									

**Particle IC Dialog Box:**

- ☒ Initial conditions
- Initialize mass in region (dropdown)
- Particle species: 001 - initial char in bed
- Total particle mass: 4800 kg
- Temperature: 300 K
- Region: Select region (m)
- x1: -1.524, x2: 1.52242, y1: -1.52361, y2: 1.52361, z1: 1.85943e-16, z2: 1.815
- Cloud size: ☒ Use global slider, ☐ Use local slider, ☐ Specify cloud density (Clouds per cell, Auto)
- Special settings: ☒ Random cloud initialization, ☐ No particle momentum
- Comment: (empty text box)
- Buttons: Cancel, OK



# Calculating Initial Bed Height

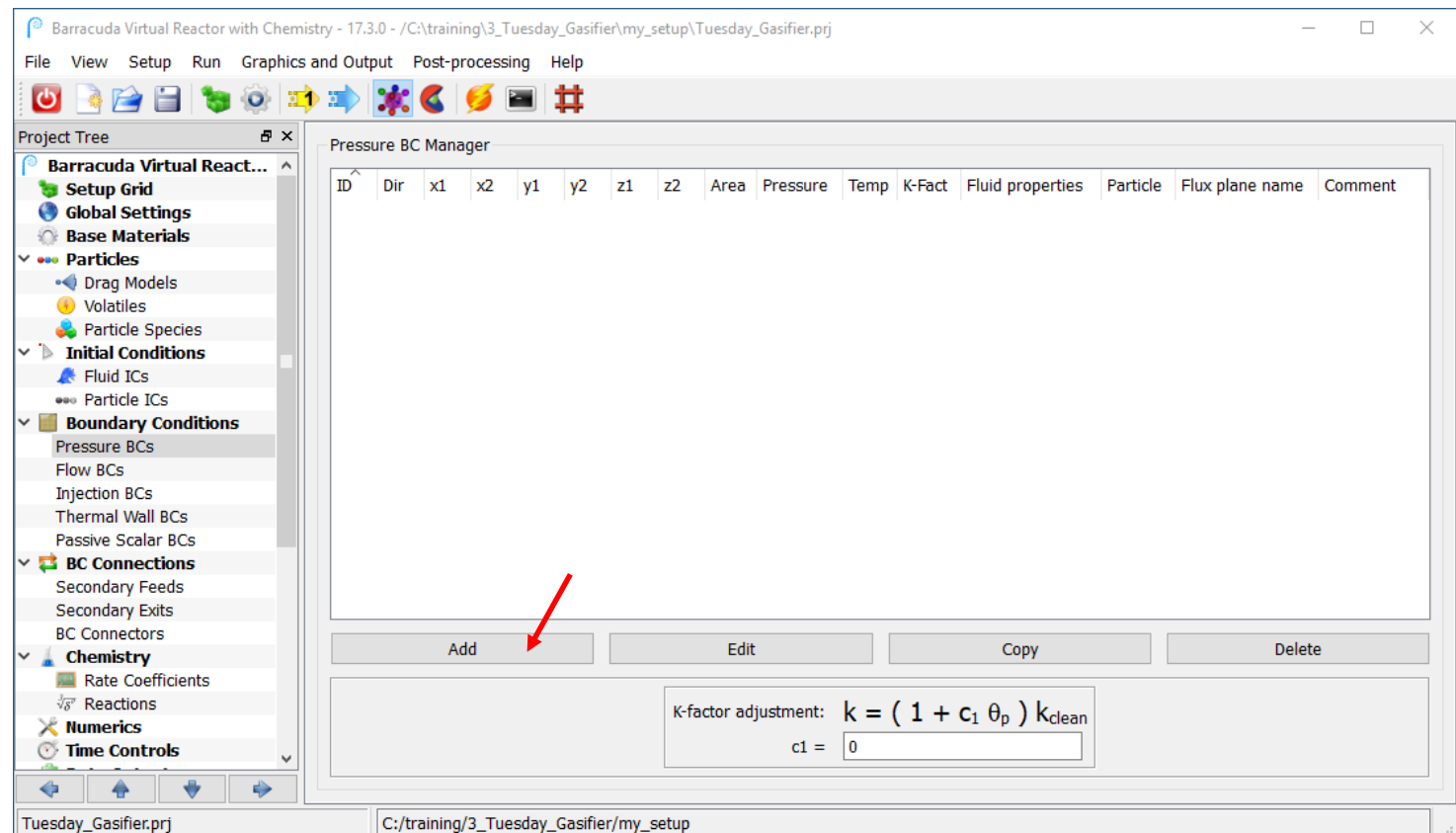
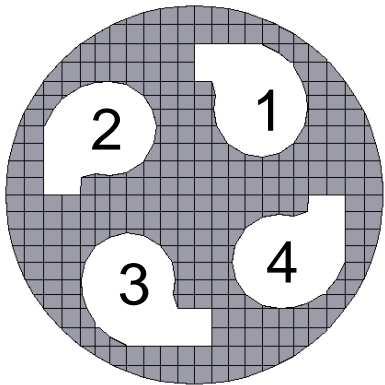
- For this problem, the target initial bed mass is 4800 kg
- In Barracuda, particles are initialized in cells specified through x, y, z locations
- For a target of 4800 kg, an initial bed height of 5.95 ft is needed. (Vessel diameter is 10 ft, particle density is 725 kg/m<sup>3</sup>, initial volume fraction is 0.5)
- For ease in setting up the particle IC, use a bed height of 5.95 ft or **1.815 m**

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

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

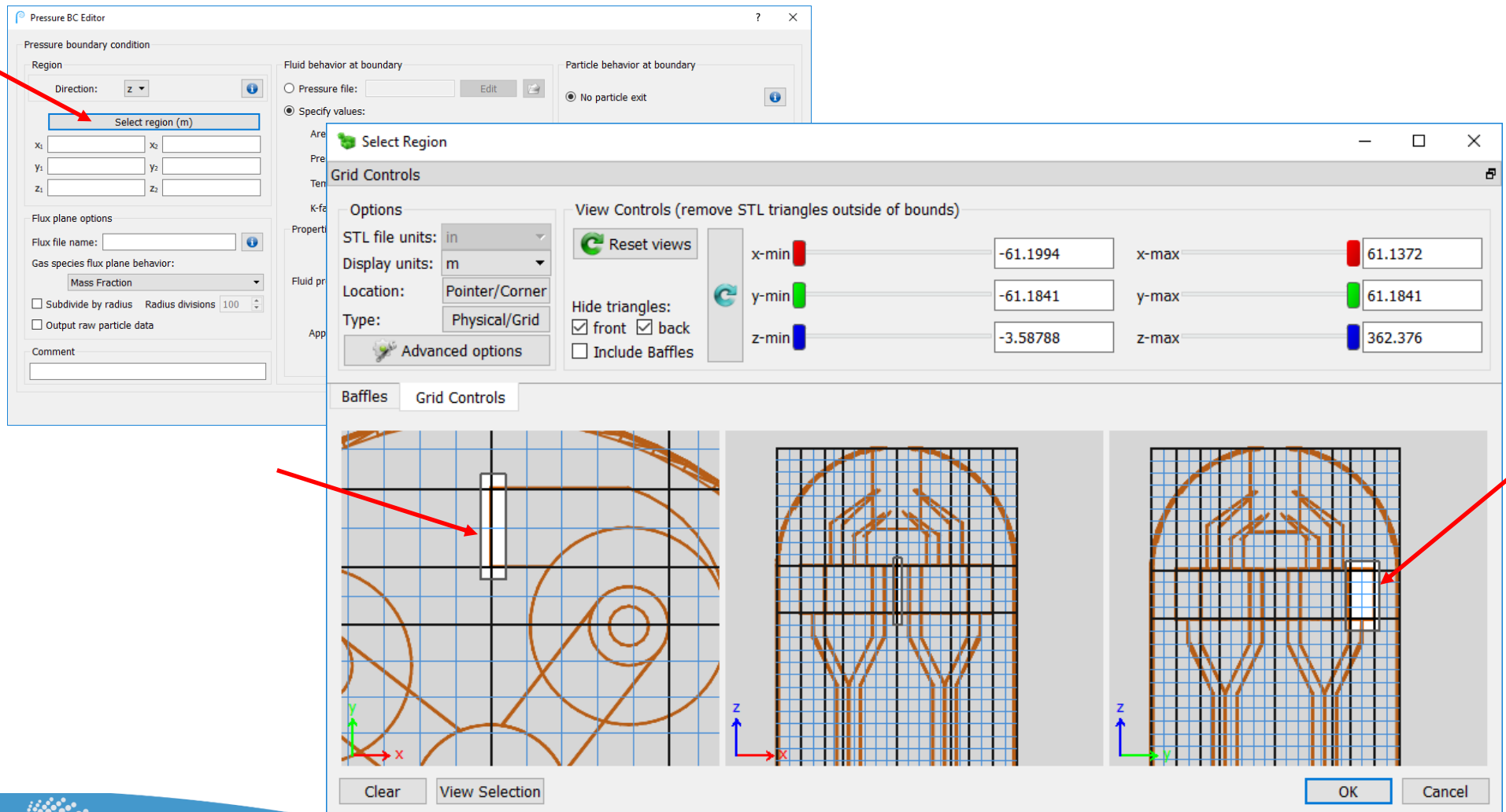
# Pressure BCs: Cyclone Inlet Horns

- 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**

The screenshot shows the 'Pressure BC Editor' dialog box with several annotations:

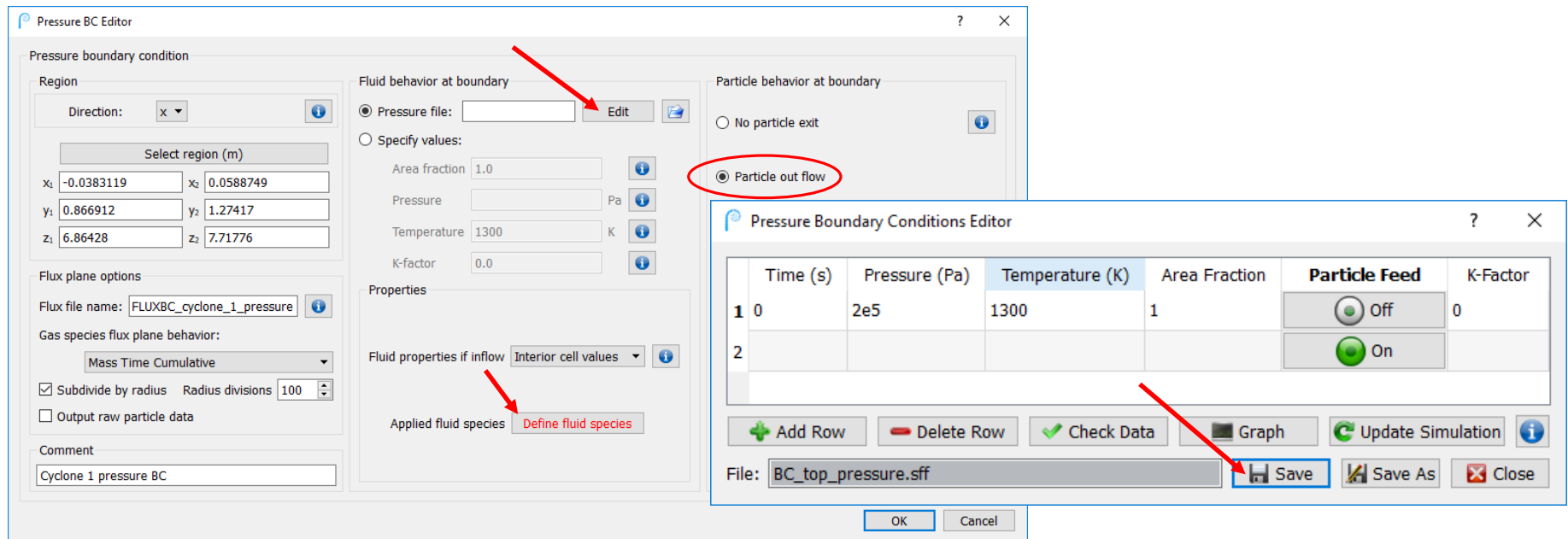
- A red circle highlights the 'Direction' dropdown menu, which is set to 'x'.
- A red arrow points to the 'Flux file name' field, which contains 'FLUXBC\_cyclone\_1\_pressure'.
- A red dotted circle highlights the 'Mass Time Cumulative' option under 'Gas species flux plane behavior'.
- A red arrow points to the 'Subdivide by radius' checkbox, which is checked.
- A red arrow points to the 'Comment' field, which contains 'Cyclone 1 pressure BC'.

The dialog box is divided into three main sections:

- Pressure boundary condition:** Includes 'Region' (Direction: x, Select region (m) coordinates), 'Flux plane options' (Flux file name, Gas species flux plane behavior, Subdivide by radius, Output raw particle data), and 'Comment'.
- Fluid behavior at boundary:** Includes 'Specify values' (Area fraction, Pressure, Temperature, K-factor) and 'Properties' (Fluid properties if inflow, Applied fluid species).
- Particle behavior at boundary:** Includes 'No particle exit', 'Particle out flow', 'Particle feed (Slip and vol frac)', 'Particle feed (Slip and mass flux)', and 'Particle feed (Slip and mass flow rate)'.

# 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 “ $2.0 \times 10^5$ ” 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<sub>2</sub> 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

Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/3\_Tuesday\_Gasifier/my\_setup/Tuesday\_Gasifier.prj

File View Setup Run Graphics and Output Post-processing Help

Project Tree

- Barracuda Virtual Rea...
- Setup Grid
- Global Settings
- Base Materials
- Particles
  - Drag Models
  - Volatiles
  - Particle Species
- Initial Conditions
  - Fluid ICs
  - Particle ICs
- Boundary Conditions
  - Pressure BCs
  - Flow BCs
  - Injection BCs
  - Thermal Wall BCs
  - Passive Scalar BCs

Pressure BC Manager

ID	Dir	x1	x2	y1	y2	z1	z2	Area	Pressure	Temp	K-Fact	Fluid properties	Particle	Flux plane name	Comment
000	x	-0.0383119	0.0588749	0.866912	1.27417	6.86428	7.71776	BC_top_pressure.sff	Using file	Using file	Using file	Interior cell values	Out flow	FLUXBC_cyclone_1_pressure	Cyclone 1 pressure BC
001	y	-1.31531	-0.860632	-0.0602412	0.0486932	6.86428	7.71776	BC_top_pressure.sff	Using file	Using file	Using file	Interior cell values	Out flow	FLUXBC_cyclone_2_pressure	Cyclone 2 pressure BC
002	x	-0.0527879	0.0443989	-1.29	-0.852171	6.8994	7.71776	BC_top_pressure.sff	Using file	Using file	Using file	Interior cell values	Out flow	FLUXBC_cyclone_3_pressure	Cyclone 3 pressure BC
003	y	0.843058	1.29774	-0.0620458	0.0468886	6.86428	7.71776	BC_top_pressure.sff	Using file	Using file	Using file	Interior cell values	Out flow	FLUXBC_cyclone_4_pressure	Cyclone 4 pressure BC

Add Edit Copy Delete

K-factor adjustment:  $k = (1 + c_1 \theta_p) k_{\text{clean}}$

c1 =

Tuesday\_Gasifier.prj C:/training/3\_Tuesday\_Gasifier/my\_setup

# 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

The screenshot shows the Barracuda Virtual Reactor interface. The main window displays the 'Flow BC Editor' for a 'Bottom Flow' boundary condition. Key settings include:

- Region:** Select region (m) with coordinates:  $x_0 = -1.524$ ,  $x_2 = 1.52242$ ,  $y_0 = -1.524$ ,  $y_2 = 1.52361$ ,  $z_0 = 1.85943e-16$ ,  $z_2 = 0.153173$ .
- Flow direction:** z-direction flow.
- Behavior at boundary:** Fluid behavior at boundary is set to 'Use transient fluid flow file' (circled in red).
- Particle behavior at boundary:** 'No particle exit' is selected (circled in red).
- Fluid composition:** 'Define fluids' is highlighted with a red arrow.
- Transient fluid and particle flow file:** SFF file is 'BC\_bottom\_flow.sff'.

A secondary window, 'Flow Boundary Conditions Editor', is shown in the bottom right, displaying a table of flow conditions over time:

	Time (s)	Velocity (m/s)	Temperature (K)	Pressure (Pa)
1	0	0.3	1300	2e5
2				

The 'Save' button in the 'Flow Boundary Conditions Editor' is circled in red.

# 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**

Flow BC Editor

Flow boundary condition

Region

Select region (m)

x<sub>1</sub>: 1.45 x<sub>2</sub>: 1.60  
y<sub>1</sub>: 0 y<sub>2</sub>: 0.15  
z<sub>1</sub>: 1.75 z<sub>2</sub>: 1.90

Flux plane options

Flux plane name: FLUXBC\_fresh\_coal\_feed

Gas species flux plane behavior:

Mass Fraction

☐ Subdivide by radius Radius divisions: 100

☐ Output raw particle data

Comment

Fresh coal feed

Flow direction

☒ x-direction flow

☐ y-direction flow

☐ z-direction flow

x/y/z variation angle: 50 degrees

☒ Normal to surface flow Normal Limit

☐ Direction flow vector

u: 0 v: 0 w: 1

☐ Force absolute direction

Vector variation angle: 15 degrees

Behavior at boundary

Fluid behavior at boundary

☒ Use transient fluid flow file

☐ Use BC Connector data

☐ Specify values

Velocity flow: 0 m/s

Pressure: 0 Pa

Temp: 300 K

Fluid composition

Applied fluids: Define fluids

Particle behavior at boundary

☒ Use transient particle flow file

☐ Use BC Connector data

☐ No particle exit

☐ Particle out flow

Particle radius (m) range allowed to exit:

Min = 0 to Max = UNLIMITED

Particle exit control (Off)

☐ Particle feed (Slip and volume fraction)

☐ Particle feed (Slip and mass flux)

☒ Particle feed (Slip and mass flow rate)

Edit particle feed

Particle feed control

Transient fluid and particle flow file

SFF file: Edit

OK Cancel



# 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

**Flow BC Editor**

Flow boundary condition

Region

Flow direction

☒ x-direction flow

☐ y-direction flow

Select region (m)

$x_1$  1.45  $x_2$  1.60

**Behavior at boundary**

Fluid behavior at boundary

☒ Use transient fluid flow file

☐ Use BC Connector data

☐ Specify values

Velocity flow 0 m/s

Pressure 0 Pa

Temp 1300 K

Fluid composition

Applied fluids: Define fluids

Particle behavior at boundary

☒ Use transient particle flow file

☐ Use BC Connector data

☐ No particle exit

☐ Particle out flow

Particle radius (m) range allowed to exit:

Min = 0 to Max = UNLIMITED

Particle exit control (Off)

☐ Particle feed (Slip and volume fraction)

☐ Particle feed (Slip and mass flux)

☒ Particle feed (Slip and mass flow rate)

**Edit particle feed**

Particle feed control

Transient fluid and particle flow file

SFF file: Edit

OK Cancel

**Particle feed settings**

Particle Species

ID	Species-ID	Fraction	Comment	Materials
000	002	1	fresh coal feed	Ash, C, Volatiles

Add Edit Delete

Particle feed

Solid fraction Mass Fraction

Particle/fluid slip ratio 0.5

Particle feed per ave volume 125

Particle feed mass flow rate (kg/s) 0

OK Cancel

**Flow Boundary Conditions Editor**

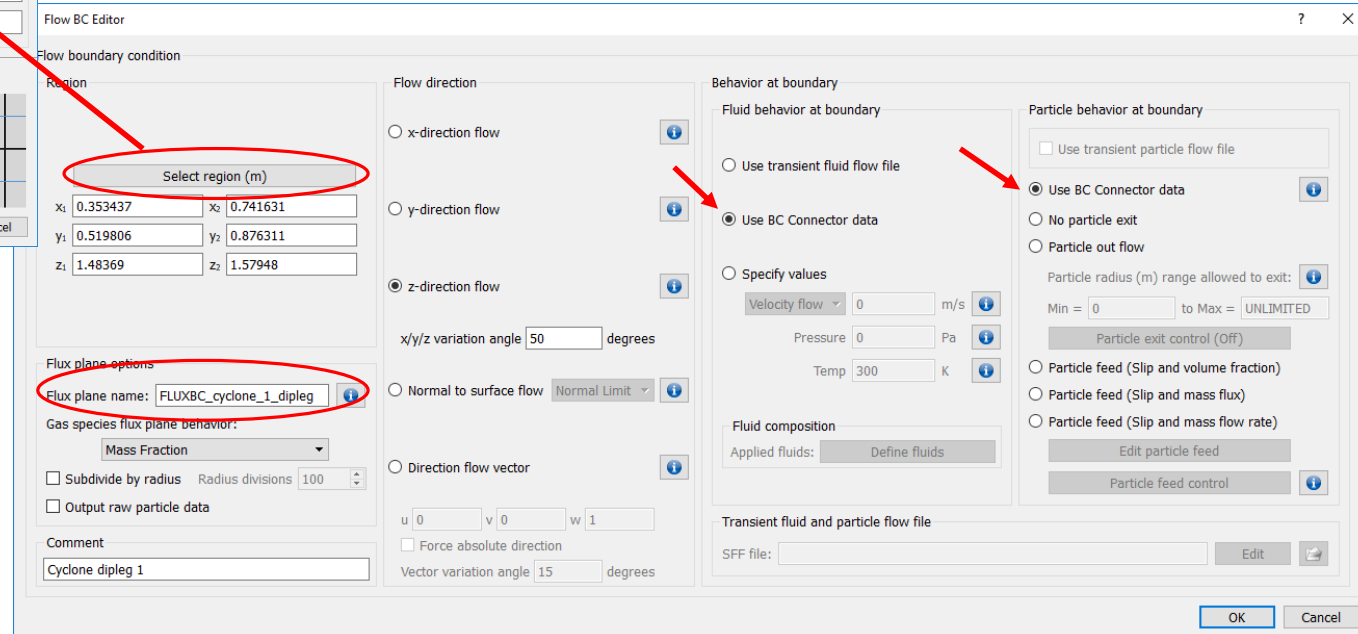
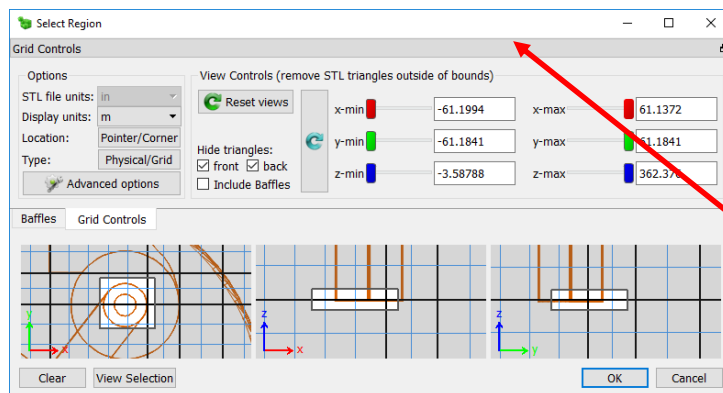
	Time (s)	Velocity (m/s)	Temperature (K)	Pressure (Pa)	Particle Feed	Number Density Manual	Particle Slip	Particle Mass Flow Rate (kg/s)
1	0	0.25	1300	2e5	On	125	1	1
2					On			

Add Row Delete Row Check Data Graph Update Simulation

File: BC\_fresh\_coal\_feed.sff Save Save As Close

# 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

Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/3\_Tuesday\_Gasifier/my\_setup/Tuesday\_Gasifier.prj

File View Setup Run Graphics and Output Post-processing Help

Project Tree

- Volatiles
- Particle Species
- Initial Conditions
  - Fluid ICs
  - Particle ICs
- Boundary Conditions
  - Pressure BCs
  - Flow BCs
  - Injection BCs
  - Thermal Wall BCs
  - Passive Scalar BCs
- BC Connections
  - Secondary Feeds

Flow BC Manager

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

Add Edit Copy Delete

Tuesday\_Gasifier.prj C:/training/3\_Tuesday\_Gasifier/my\_setup

# 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.

The screenshot displays the Barracuda Virtual Reactor GUI with the **BC Connector Editor** window open. The **Project Tree** on the left shows the **BC Connections** section expanded, with **BC Connectors** selected. The **BC Connector Editor** window has the **BC Connection Input from Domain (outlet BCs)** tab active. The **BC Connector Properties** section shows the **Enabled** checkbox checked, **Name** and **Comment** fields empty, **Time delay** set to 0, and **Draw connectors for post-processing** checked. The **BC Connection Output to Domain (inlet BCs)** tab is also visible. The **BC Connector Input Editor** window is open, showing the **Flux plane properties** section with the **Available flux planes (select one):** list. The first entry, **000 FLUXBC\_cyclone\_1\_pressure Pressure BC**, is highlighted and circled in red. The **General properties** section shows the **Particle split factor** set to 1. The **Help** button is visible in both windows.

**BC Connector Editor**

**BC Connection Input from Domain (outlet BCs)**

ID	Flux plane name	BC type	Particle split fac
----	-----------------	---------	--------------------

**BC Connector Properties**

Name:

Comment:

Time delay: 0 s

☐ Reset particle residence

☒ Draw connectors for post-processing

Fluid Filter (Scale)

Particle Filter (Random)

Thermal Control

☐ Transient heating/cooling rate:

☐ Fixed heating/cooling rate:

Heating / Cooling Rate: 0

Minimum Temperature: 10

Maximum Temperature: 60

☒ Direct temperature adjustment

Fluid temperature control

Fluid temperature factor:

Particle temperature control

Particle temperature factor:

☐ Advanced feature: All Flow BC flux planes available as inputs

Add Edit Copy Delete

Help

**BC Connection Output to Domain (inlet BCs)**

ID	Flux plane name	BC type	Using connector fl
----	-----------------	---------	--------------------

**BC Connector Input Editor**

**Flux plane properties**

Available flux planes (select one):

ID	Flux plane name	BC type
000	FLUXBC_cyclone_1_pressure	Pressure BC
001	FLUXBC_cyclone_2_pressure	Pressure BC
002	FLUXBC_cyclone_3_pressure	Pressure BC
003	FLUXBC_cyclone_4_pressure	Pressure BC

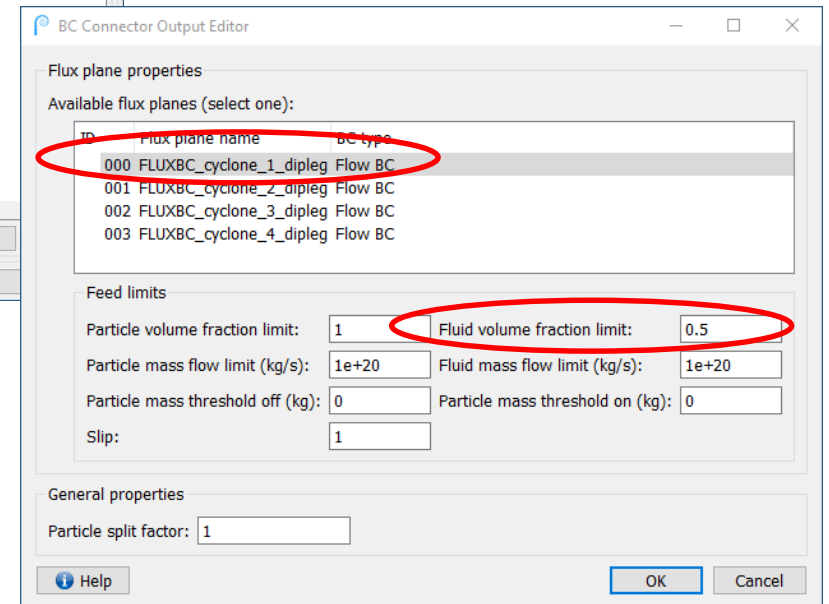
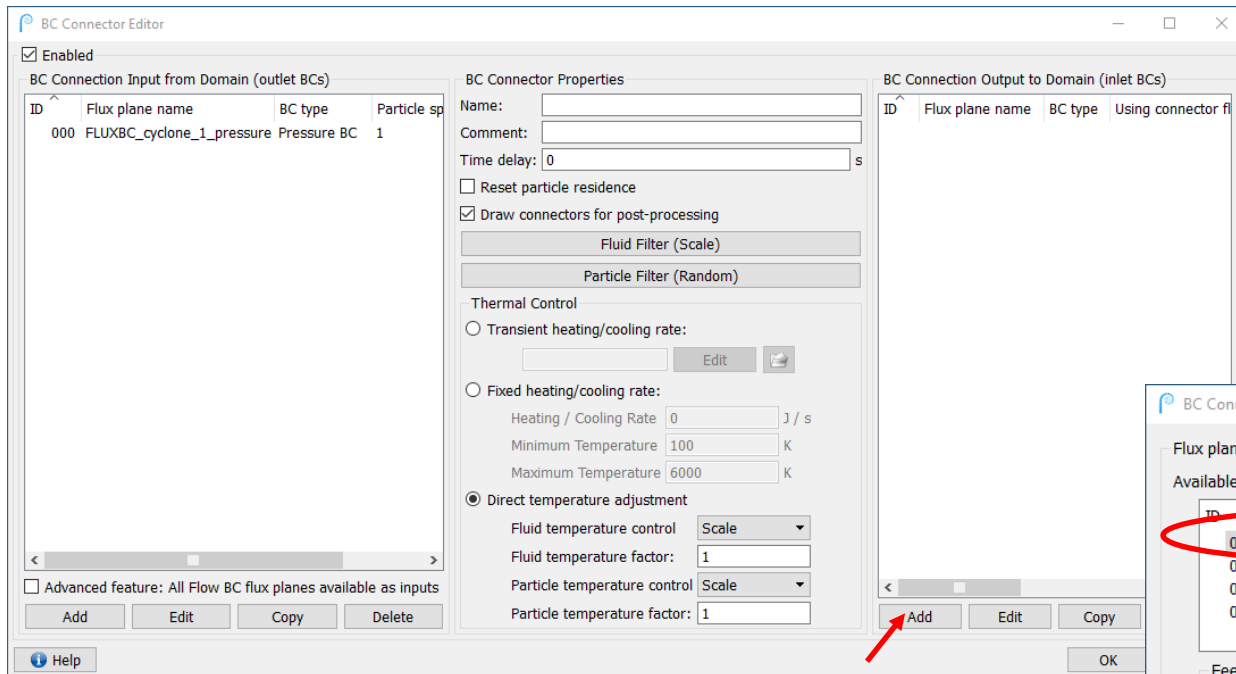
**General properties**

Particle split factor: 1

Help OK Cancel

# 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**

BC Connector Editor

☒ Enabled

BC Connection Input from Domain (outlet BCs)

ID	Flux plane name	BC type	Particle split factor
000	FLUXBC_cyclone_1_pressure	Pressure BC	1

BC Connector Properties

Name:

Comment:

Time delay:  s

☒ Reset particle residence

☒ Draw connectors for post-processing

Fluid Filter (Scale)

Particle Filter (Random)

Thermal Control

☐ Transient heating/cooling rate:

Edit

☐ Fixed heating/cooling rate:

Heating / Cooling Rate  J / s

Minimum Temperature  K

Maximum Temperature  K

☒ Direct temperature adjustment

Fluid temperature control

Fluid temperature factor:

Particle temperature control

Particle temperature factor:

☐ Advanced feature: All Flow BC flux planes available as inputs

Add Edit Copy Delete

Help

BC Connection Output to Domain (inlet BCs)

ID	Flux plane name	BC type	Using connector fluid	Using
000	FLUXBC_cyclone_1_dipleg	Flow BC	on	on

Add Edit Copy Delete

OK Cancel

# Add BC Connections for Remaining Cyclones

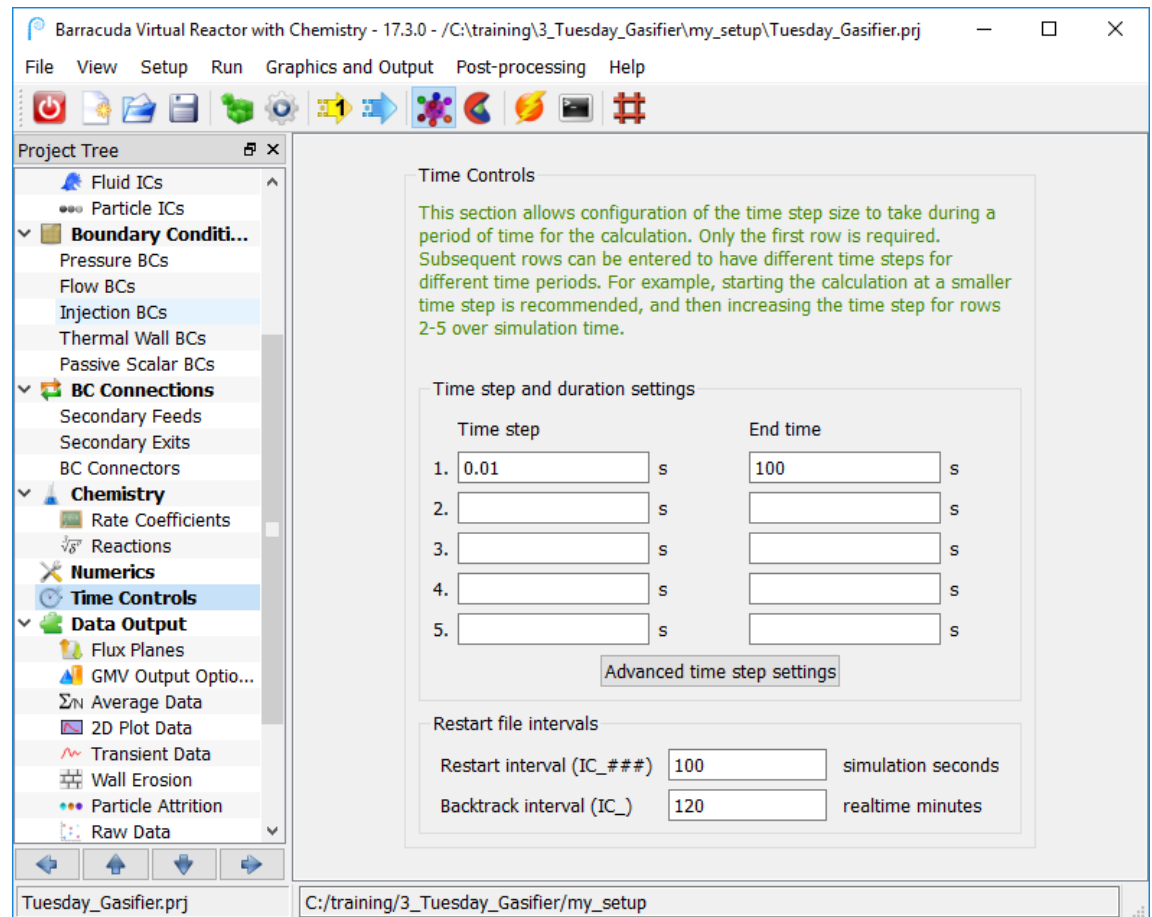
- Repeat the above steps to define BC Connections for Cyclones 2, 3, and 4

The screenshot shows the Barracuda Virtual Reactor software interface. The main window is titled "Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/3\_Tuesday\_Gasifier/my\_setup/Tuesday\_Gasifier.prj". The menu bar includes File, View, Setup, Run, Graphics and Output, Post-processing, and Help. The Project Tree on the left shows a hierarchy of settings: Injection BCs, Thermal Wall BCs, Passive Scalar BCs, BC Connections (selected), Secondary Feeds, Secondary Exits, BC Connectors, Chemistry (expanded), Rate Coefficients, Reactions, Numerics, and Time Controls. The BC Connector Manager window is open, displaying a table of connections for four cyclones. The table has columns for ID, Enabled, Name, Time delay, Reset residence, Inputs, Fluid filter, Particle filter, Thermal Control, Outputs, and Comment. Below the table are buttons for Add, Edit, Copy, and Delete. The status bar at the bottom shows the project name "Tuesday\_Gasifier.prj" and the file path "C:/training/3\_Tuesday\_Gasifier/my\_setup".

ID	Enabled	Name	Time delay	Reset residence	Inputs	Fluid filter	Particle filter	Thermal Control	Outputs	Comment
000	on	CONN_cyclone_1	0	off	FLUXBC_cyclone_1_pressure	Scale	Random	Legacy	FLUXBC_cyclone_1_dipleg	Cyclone 1 connection
001	on	CONN_cyclone_2	0	off	FLUXBC_cyclone_2_pressure	Scale	Random	Legacy	FLUXBC_cyclone_2_dipleg	Cyclone 2 connection
002	on	CONN_cyclone_3	0	off	FLUXBC_cyclone_3_pressure	Scale	Random	Legacy	FLUXBC_cyclone_3_dipleg	Cyclone 3 connection
003	on	CONN_cyclone_4	0	off	FLUXBC_cyclone_4_pressure	Scale	Random	Legacy	FLUXBC_cyclone_4_dipleg	Cyclone 4 connection

# 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

**Flux Planes Manager**

ID	Filename	Direction	loc	Nod	i1	i2	j1	j2	k1	k2	Sub r
000	FLUX_early_entrainment	z	xyz		-1.5255	1.5255	-1.5255	1.5255	6	6	On

Note: For location indices, "min" or "[ " denote the first possible value, while "max" or "]" denote the last possible value.

**Flux Plane Editor**

Flux plane

File name: FLUX\_early\_entrainment

Surface plane direction: z

Gas species flux plane behavior: Mass Flow Rate

☒ Subdivide by radius

☒ Directional flux

Plane location

i1: -1.5255 m, i2: 1.5255 m

j1: -1.5255 m, j2: 1.5255 m

k1: 6 m, k2: 6 m

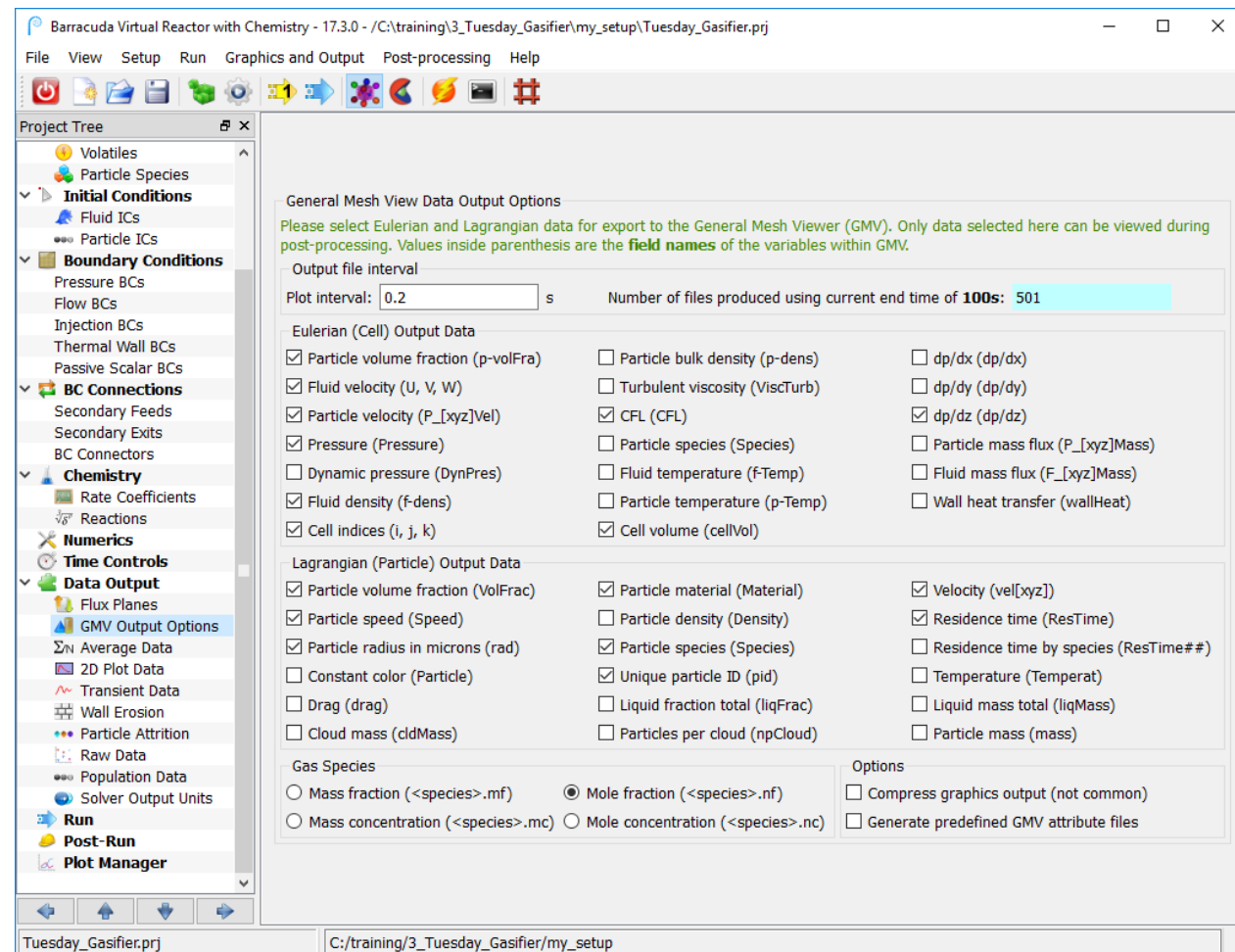
Enter Location by: xyz

Comment: Flux plane to get an early idea of entrainment

OK Cancel Reference grid

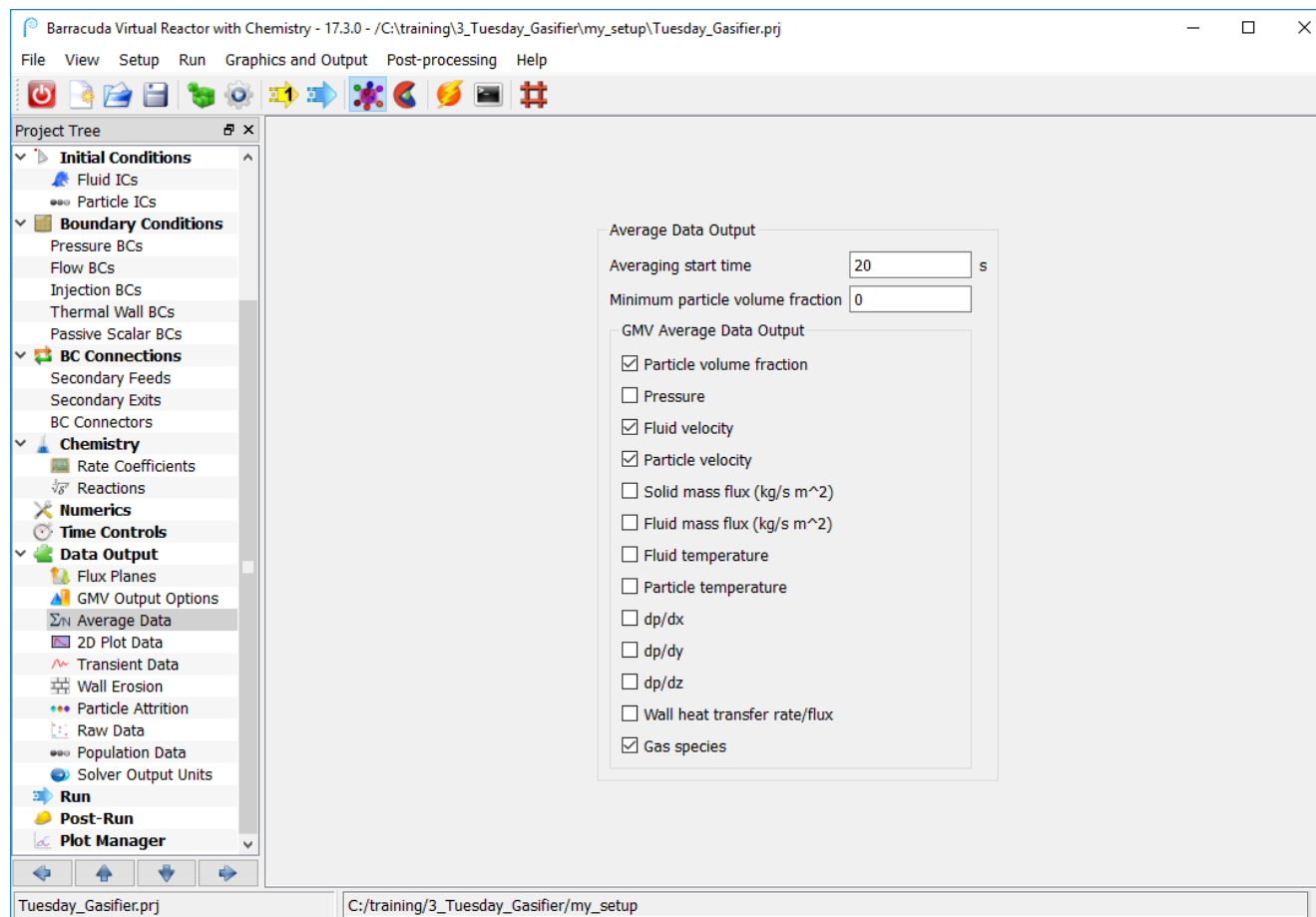
# GMV Output Options

- 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!

