

Gasifier Training Problem Part 3: Project Setup

February 2018

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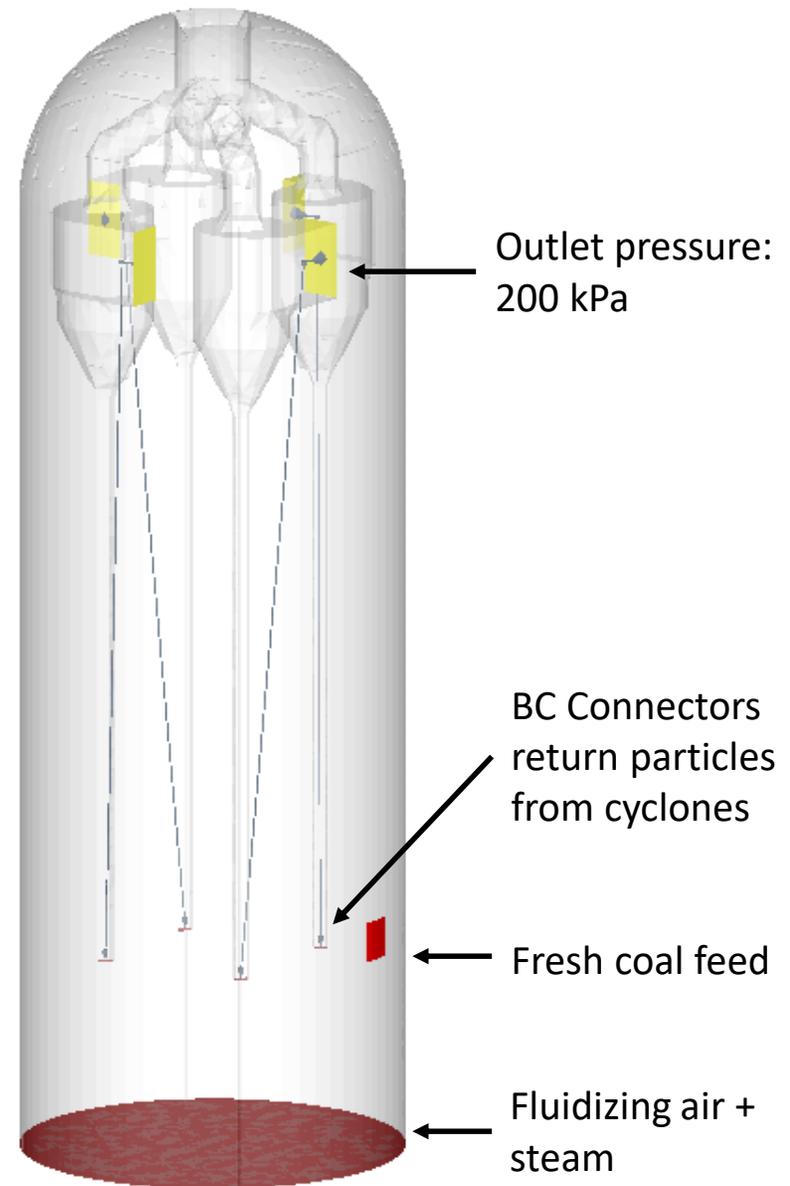
Training Objectives

- 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

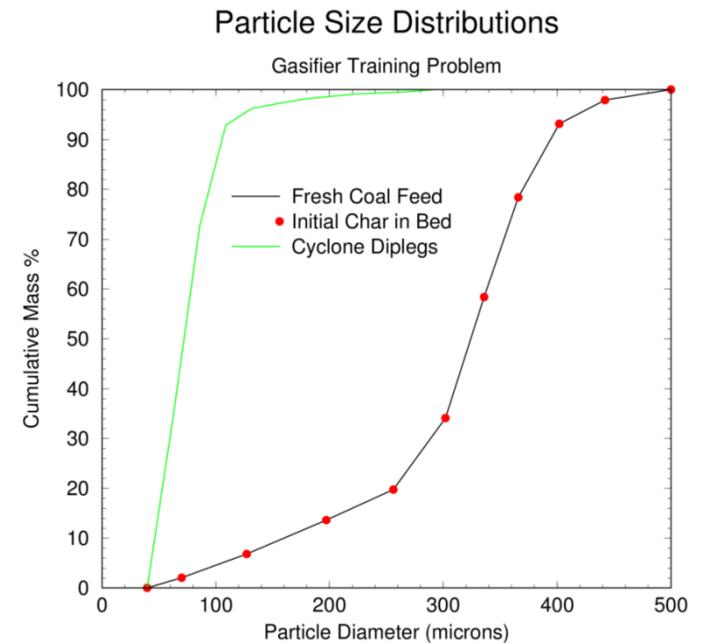
- Isothermal at 1300 K
- No chemistry in this model
- Fresh coal feed coming in at:
 - $x=1.45$ m
 - $y=0$ m
 - $z=1.75$ m

Boundary	Fluid Flow	Particle Flow
Fluidizing Air + Steam	Velocity = 0.3 m/s Gas (mass fractions): 0.3 H ₂ O, 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



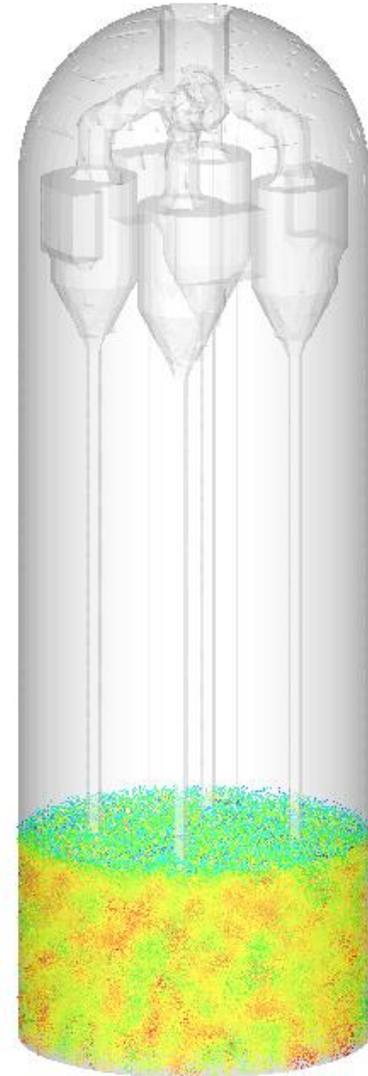
Particle Properties

- 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 CH₄, 0.1702 CO, 0.0444 CO₂, 0.1111 H₂, 0.26 H₂O
 - 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

The screenshot displays the Barracuda Virtual Reactor software interface. The title bar reads "Barracuda Virtual Reactor with Chemistry - 17.3.0 - 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 lists various settings categories: Setup Grid, Global Settings, Base Materials, Particles, Initial Conditions, Boundary Conditions, BC Connections, Chemistry, Numerics, Time Controls, and Data Output. The main panel is titled "Global Settings" and contains three sections: Gravity settings, Thermal settings, and Chemistry settings. Gravity settings include x Gravity (0 m/s²), y Gravity (0 m/s²), and z Gravity (-9.8 m/s²). Thermal settings are set to Isothermal flow at 1300 K. Chemistry settings are set to "Start with Chemistry" (On).

Global Settings

Gravity settings

x Gravity: 0 m/s²

y Gravity: 0 m/s²

z Gravity: -9.8 m/s²

Thermal settings

Isothermal flow: 1300 K

Thermal flow: Heat transfer coefficients

Thermal start options

Start with Thermal: On Off (turn on at restart)

Starting temperature: 300 K

Temperature warning limits

Minimum temperature warning (K): 100 Maximum temperature warning (K): 6000

Output minimum and maximum temperatures in system to MinMaxTemp.data log file

Chemistry settings

This feature allows chemistry to be set up, but not calculated until a later time by turning it on using time controls or a restart file. Note: This feature applies to **Volatiles** as well as all **Chemistry Reactions**.

Start with Chemistry: On Off, ramp on from 0 s to 0 s Off (can be turned on at restart)

Base Materials

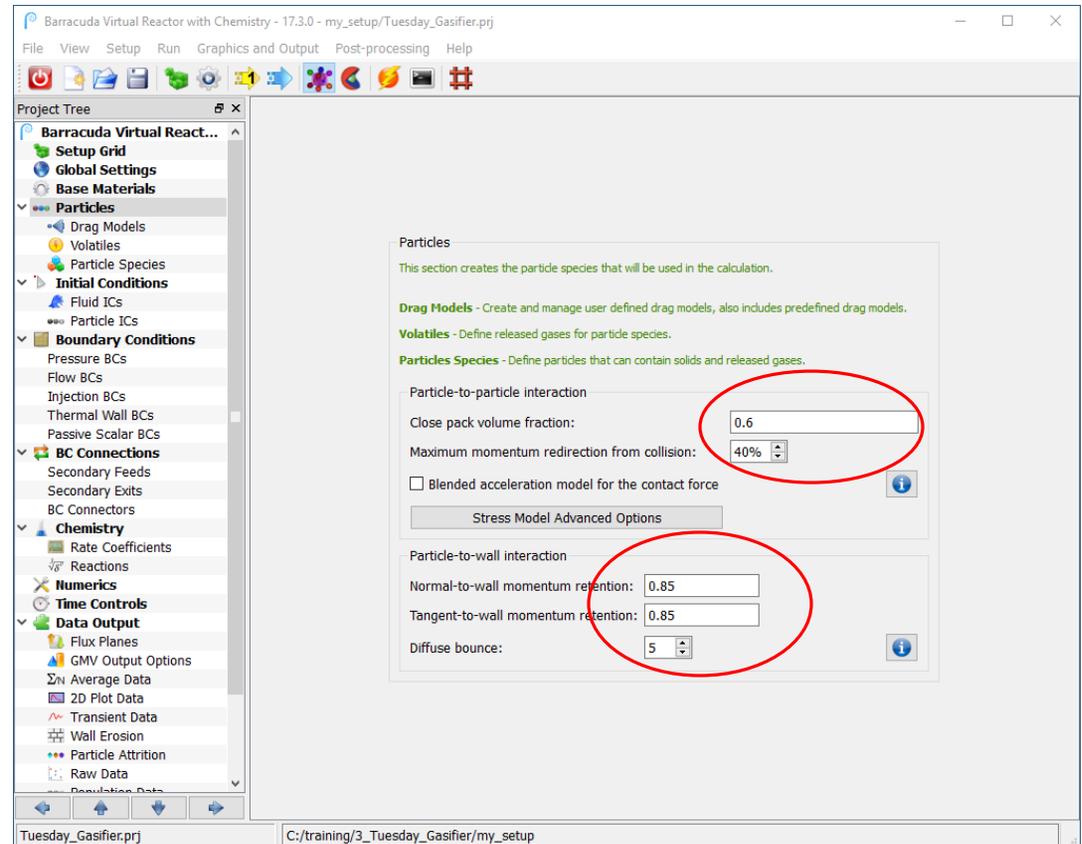
- In the **Base Materials** section, define all materials that will be used in the simulation
- Based on the process design sheet and particle properties, you will need:
 - Ash (select C_1, then rename it "Ash")
 - Carbon
 - Methane
 - Carbon Monoxide
 - Carbon Dioxide
 - Hydrogen gas
 - Steam
 - Nitrogen gas
 - Oxygen gas

The screenshot shows the Barracuda Virtual Reactor software interface. The 'Base Materials Manager' window is active, displaying a 'Project Material List' table. This table is circled in red. The table has columns for 'Chemical name', 'State', and 'Description'. Below the table are buttons for 'Add', 'Edit', 'Copy', and 'Delete'. To the right of the table are buttons for '<- Import' and '<- Replace->'. Below the table is a 'Properties' section with options for 'Averaging method for fluid mixture properties' (Mole average or Mass average) and 'Flow Type' (Compressible or Incompressible). To the right of the 'Project Material List' is a 'Material Properties Library' window with a table of materials and a 'Browse' button at the bottom.

Chemical name	State	Description
Ash	S	Ash for Coal
C	S	C CARBON. SOLID GRAPHI...
CH4	G	CH4 METHANE. ANHARMO...
CO	G	CO CARBON MONOXIDE
CO2	G	CO2 CARBON DIOXIDE
H2	G	H2 HYDROGEN. REF ELEM...
H2O	G	H2O STEAM
N2	G	N2 NITROGEN. REF ELEME...
O2	G	O2 OXYGEN. REF ELEMENT

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 CH₄, 0.1702 CO, 0.0444 CO₂, 0.111 H₂, 0.26 H₂O
- 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 screenshot shows the Barracuda Virtual Reactor software interface. The **Project Tree** on the left shows the **Volatiles** section selected. The **Volatile Editor** dialog box is open, showing the following fields:

- Name:** Volatiles
- Specific heat (Cp):** 1000 J/kg K
- Heat of devolatilization at 298.15K:** 0 J/kg
- Release gases:** CH₄, CO, CO₂, H₂, H₂O
- Rate coefficient: $k = c_0 T^{c_1} p^{c_2} p_f^{c_3} e^{-E/T+EO}$ [1/s]**
 - $c_0 = 0.05$
 - $c_1 = 1$
 - $c_2 = 0$
 - $c_3 = 0$
 - $E = 5500$
 - $EO = 0$

The **Applied materials** dialog box is also open, showing the following table:

ID	Material	State	Fraction
000	CH ₄	G	0.4144
001	CO	G	0.1702
002	CO ₂	G	0.0444
003	H ₂	G	0.111
004	H ₂ O	G	0.26

The **Applied materials** dialog box also shows the **Fraction type** set to **Mass fraction** and the **Fractions sum to:** 1.0. The **OK** button is highlighted with a red arrow.

At the bottom of the **Volatile Editor** dialog box, there is a note: "Note: Volatiles are dependent on Chemistry. If the Global Settings option Start with Chemistry is set to Off, then Volatiles will not be calculated." Below this note are buttons for **Add**, **Edit**, **Copy**, and **Delete**.

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/m³. 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 following details:

- Species-ID:** 1
- Comment:** initial char in bed
- Materials:** Applied Materials
- Drag Model:** Wen-Yu
- Table:**

Name	Link To Default	Value
c0	Linked	1
c1	Linked	0.15
c2	Linked	0.44

The **Applied Materials Manager** window is also open, showing:

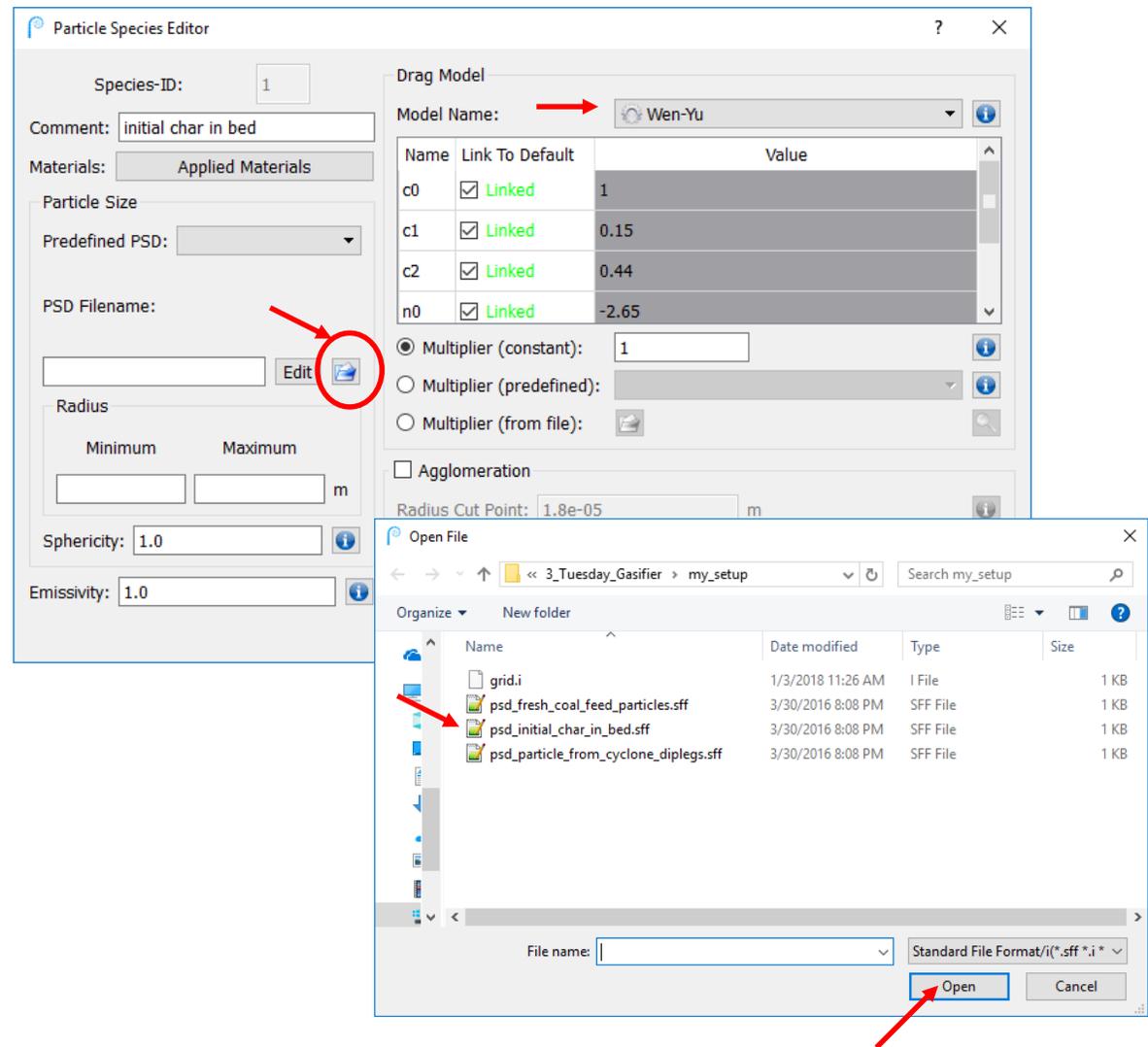
- Mass Fractions sum to:** 1.0
- Table:**

ID	Name	State	Mass Frac	Density (kg/m ³)	Age Factor
000	C	S	0.8999	2150	1
001	Ash	S	0.1	2150	1
002	Volatiles	Volatile	0.0001	Unspecified	N/A
- Overall particle density:** Manually entered: 725 kg/m³

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 Editor

Species-ID: 1
 Comment: initial char in bed
 Materials: Applied Materials
 Particle Size
 Predefined PSD: [Dropdown]
 PSD Filename: psd_initial_char_in_bed.sff **Edit**
 Radius
 Minimum [] Maximum [] m
 Sphericity: 1.0
 Emissivity: 1.0

Drag Model

Model Name: Wen-Yu

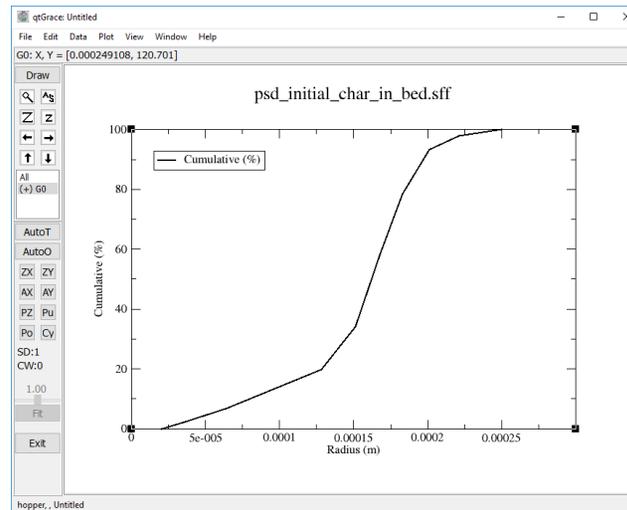
Name	Link To Default	Value
c0	<input checked="" type="checkbox"/> Linked	1
c1	<input checked="" type="checkbox"/> Linked	0.15
c2	<input checked="" type="checkbox"/> Linked	0.44
n0	<input checked="" type="checkbox"/> Linked	-2.65

Multiplier (constant): 1
 Multiplier (predefined):
 Multiplier (from file):
 Agglomeration
 Radius Cut Point: 1.8e-05 m
 Effective Particle Size Filename:

Particle Size Distributions Editor

	Cumulative (%)	Radius (m)
1	0.00	1.99E-05
2	2.05	3.50E-05
3	6.82	6.36E-05
4	13.64	9.86E-05
5	19.77	1.28E-04
6	34.09	1.51E-04
7	58.41	1.68E-04

Buttons: Add Row, Delete Row, Check Data, **Graph**, Update Simulation
 File: psd_initial_char_in_bed.sff Save Save As Close



Graphing Setup

X Axis: Radius (m)

Y Axis:

	Variable Name	Line Color	Line Style	Line Width
1	<input checked="" type="checkbox"/> Cumulative (%)	Black	Solid	Small-Medium
2	<input type="checkbox"/> Radius (m)	Red	Solid	Small-Medium

Please select your variables to graph

Close **Plot**

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**

The screenshot displays the Barracuda Virtual Reactor interface. The **Particle Species Manager** window shows a table with one entry:

Species-ID	Comment	Materials	Min radius	Max radius	Sphericity	Emissivity	Drag model	Agglomeration
001	initial char in bed	C, Ash, Volatiles	psd_initial_char_in_bed.sff		1	1	Wen-Yu	Off

The **Particle Species Editor** window shows the following fields:

- Species-ID: 2
- Comment: fresh coal feed
- Materials: Applied Materials
- Predefined PSD: (dropdown)
- PSD Filename: psd_fresh_coal_feed_particles.sff
- Radius: (Minimum/Maximum fields)
- Sphericity: 1.0
- Emissivity: 1.0
- Drag Model: Wen-Yu

The **Applied Materials Manager** window shows a table of materials:

Name	State	Mass Frac	Density (kg/m ³)	Age Factor	
000	Ash	S	0.05	2150	1
001	C	S	0.45	2150	1
002	Volatiles	Volatile	0.5	Unspecified	NA

Below the table, the **Overall particle density** is set to **Manually entered: 1450 kg/m³**.

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% N2 at 2.0×10^5 Pa
- Use [and] to select minimum and maximum extents of the domain

The screenshot displays the Barracuda Virtual Reactor interface. The Project Tree on the left shows the 'Initial Conditions' folder expanded to 'Fluid ICs'. The 'Fluid IC Manager' table lists a single fluid IC with ID 000, checked 'On', and coordinates x1: -1.524, x2: 1.52242, y1: -1.52361, y2: 1.52361, z1: 1.85943e-16, z2: 9.11321. The 'Fluid IC Editor: 000' dialog box is open, showing 'Initial Conditions' checked, Temperature 300 K, Pressure 200000 Pa (circled in red), and Velocity 0 m/s. The 'Region' section shows a 'Select region (m)' box and coordinate fields for x1, x2, y1, y2, z1, and z2. The 'Applied materials' dialog box is also open, showing 'Fractions sum to: 1.0' and a table with ID 000, Material N2, State G, and Fraction 1 (circled in red). The 'Mass fraction' radio button is selected. Red arrows point to the 'Edit' button in the Fluid IC Manager and the 'OK' button in the Applied materials dialog.

ID	On	x1	x2	y1	y2	z1	z2
000	<input checked="" type="checkbox"/>	-1.524	1.52242	-1.52361	1.52361	1.85943e-16	9.11321

ID	Material	State	Fraction
000	N2	G	1

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. The main window shows the 'Particle IC Manager' with a table for defining initial conditions. A red arrow points to the 'Add' button. The 'Particle IC' dialog box is open, showing the following settings:

- Initial conditions
- Initialize mass in region (circled in red)
- Particle species: 001 - initial char in bed (circled in red)
- Total particle mass: 4800 kg
- Temperature: 300 K
- Region (circled in red):
 - 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 (with a red arrow pointing to it).

Calculating Initial Bed Height

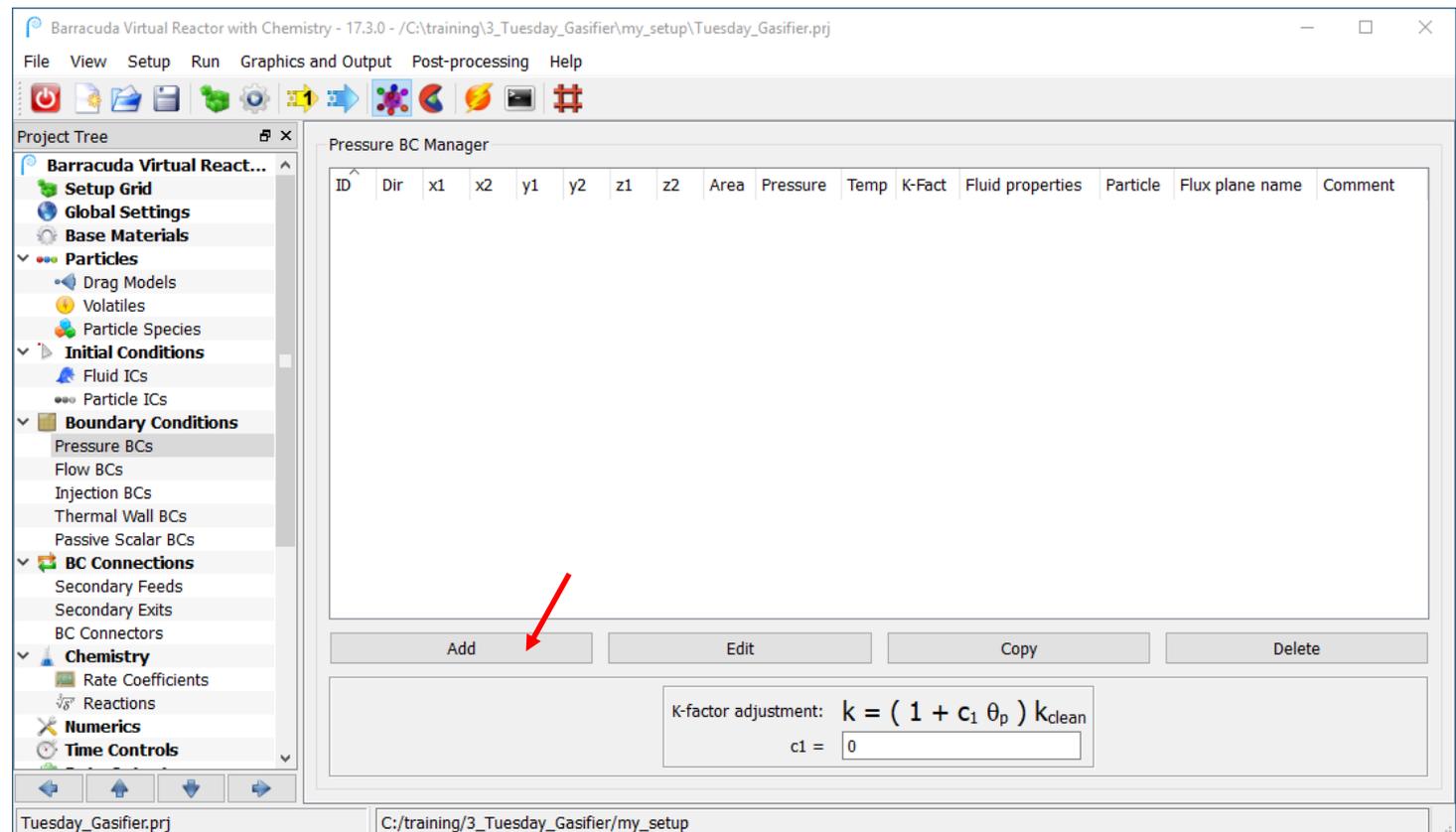
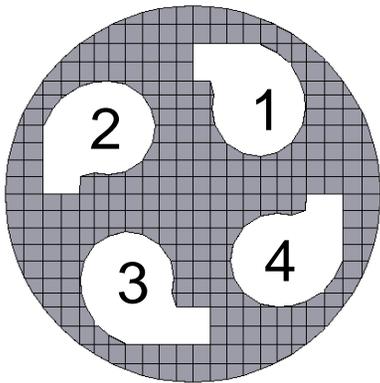
- For this problem, the target initial bed mass is 4800 kg
- In Barracuda, particles are initialized in cells specified through x, y, z locations
- For a target of 4800 kg, an initial bed height of 5.95 ft is needed. (Vessel diameter is 10 ft, particle density is 725 kg/m³, initial volume fraction is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

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

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

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.

The image shows two overlapping software windows. The top window is the 'Pressure BC Editor' and the bottom window is the 'Select Region' dialog.

Pressure BC Editor:

- Region:** Direction: z. A red arrow points to the 'Select region (m)' button.
- Fluid behavior at boundary:** Radio buttons for 'Pressure file' and 'Specify values'.
- Particle behavior at boundary:** Radio button for 'No particle exit'.
- Flux plane options:** Flux file name, Gas species flux plane behavior (Mass Fraction), Subdivide by radius, Radius divisions (100), Output raw particle data.
- Comment:** Text input field.

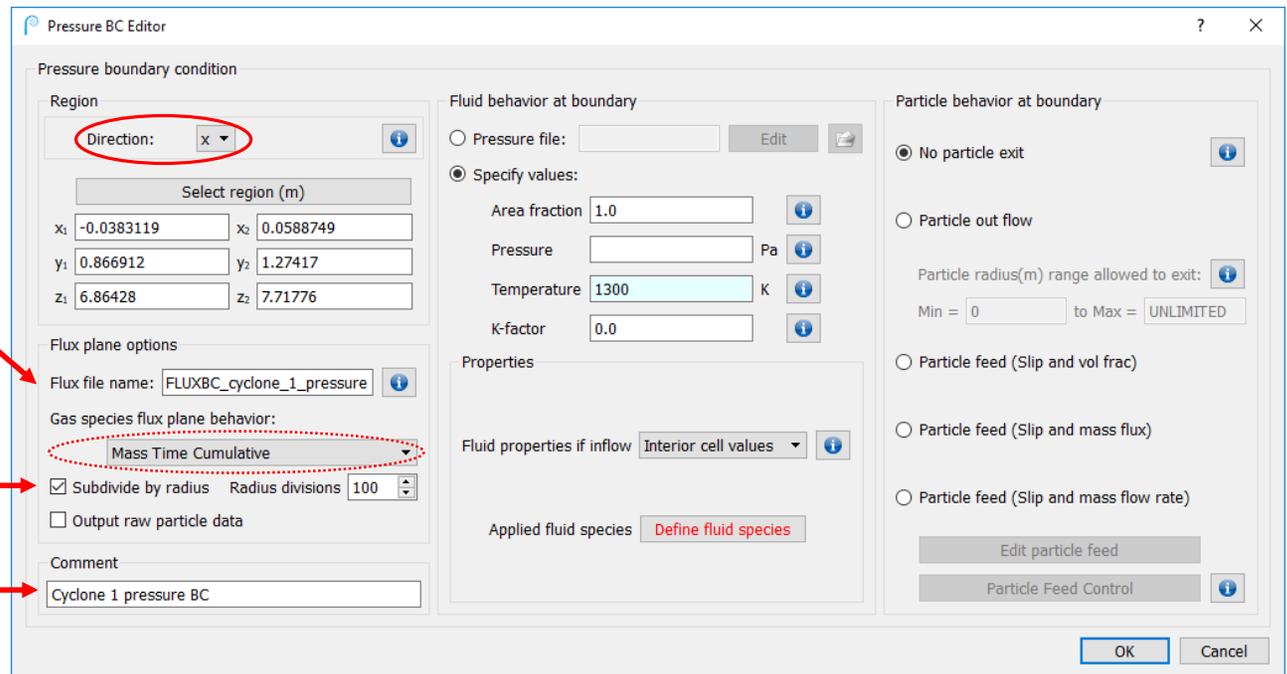
Select Region Dialog:

- Grid Controls:** Options for STL file units (in), Display units (m), Location (Pointer/Corner), and Type (Physical/Grid). Includes 'Advanced options' and 'Reset views' buttons.
- View Controls (remove STL triangles outside of bounds):** Checkboxes for 'Hide triangles: front', 'back', and 'Include Baffles'.
- Coordinate Values:**

x-min	-61.1994	x-max	61.1372
y-min	-61.1841	y-max	61.1841
z-min	-3.58788	z-max	362.376
- Baffles and Grid Controls tabs:** Three grid views showing a selection box on a grid. A red arrow points to the selection box in the first view, and another red arrow points to the selection box in the third view.
- Buttons:** 'Clear', 'View Selection', 'OK', and 'Cancel'.

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 “ 2.0×10^5 ” 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

The image shows two overlapping software windows. The top window is the 'Pressure BC Editor' and the bottom window is the 'Pressure Boundary Conditions Editor'.

Pressure BC Editor (Top Window):

- Region:** Direction: x. Select region (m) with coordinates: $x_1: -0.0383119$, $x_2: 0.0588749$, $y_1: 0.866912$, $y_2: 1.27417$, $z_1: 6.86428$, $z_2: 7.71776$.
- Fluid behavior at boundary:** Pressure file: [] Edit. Specify values: Area fraction: 1.0, Pressure: [] Pa, Temperature: 1300 K, K-factor: 0.0.
- Particle behavior at boundary:** No particle exit. Particle out flow.
- Flux plane options:** Flux file name: FLUXBC_cyclone_1_pressure. Gas species flux plane behavior: Mass Time Cumulative. Subdivide by radius (Radius divisions: 100). Output raw particle data.
- Properties:** Fluid properties if inflow: Interior cell values. Applied fluid species: Define fluid species.
- Comment:** Cyclone 1 pressure BC.

Pressure Boundary Conditions Editor (Bottom Window):

	Time (s)	Pressure (Pa)	Temperature (K)	Area Fraction	Particle Feed	K-Factor
1	0	2e5	1300	1	Off	0
2					On	

Buttons: Add Row, Delete Row, Check Data, Graph, Update Simulation. File: BC_top_pressure.sff. Buttons: Save, Save As, Close. Bottom buttons: OK, Cancel.

Pressure BCs: Cyclone Inlet Horns

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

The screenshot shows the Barracuda Virtual Reactor software interface. The Project Tree on the left is expanded to 'Boundary Conditions' > 'Pressure BCs'. The main window displays the 'Pressure BC Manager' with a table of boundary conditions. The table has columns for ID, Dir, x1, x2, y1, y2, z1, z2, Area, Pressure, Temp, K-Fact, Fluid properties, Particle, Flux plane name, and Comment. Four rows are visible, representing cyclone 1, 2, 3, and 4. Row 003 is selected. Below the table are buttons for 'Add', 'Edit', 'Copy', and 'Delete'. A K-factor adjustment section is visible at the bottom, showing the formula $k = (1 + c_1 \theta_p) k_{clean}$ and a text input field for c_1 with the value '0'.

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

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

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 displays the Barracuda Virtual Reactor software interface. The main window is titled "Flow BC Editor" and shows the configuration for a "Flow boundary condition".

Flow BC Manager Table:

ID	Dir	x1	x2	y1	y2	z1
		-1.524	1.52242	-1.524	1.52361	1.85943e-16

Flow BC Editor Configuration:

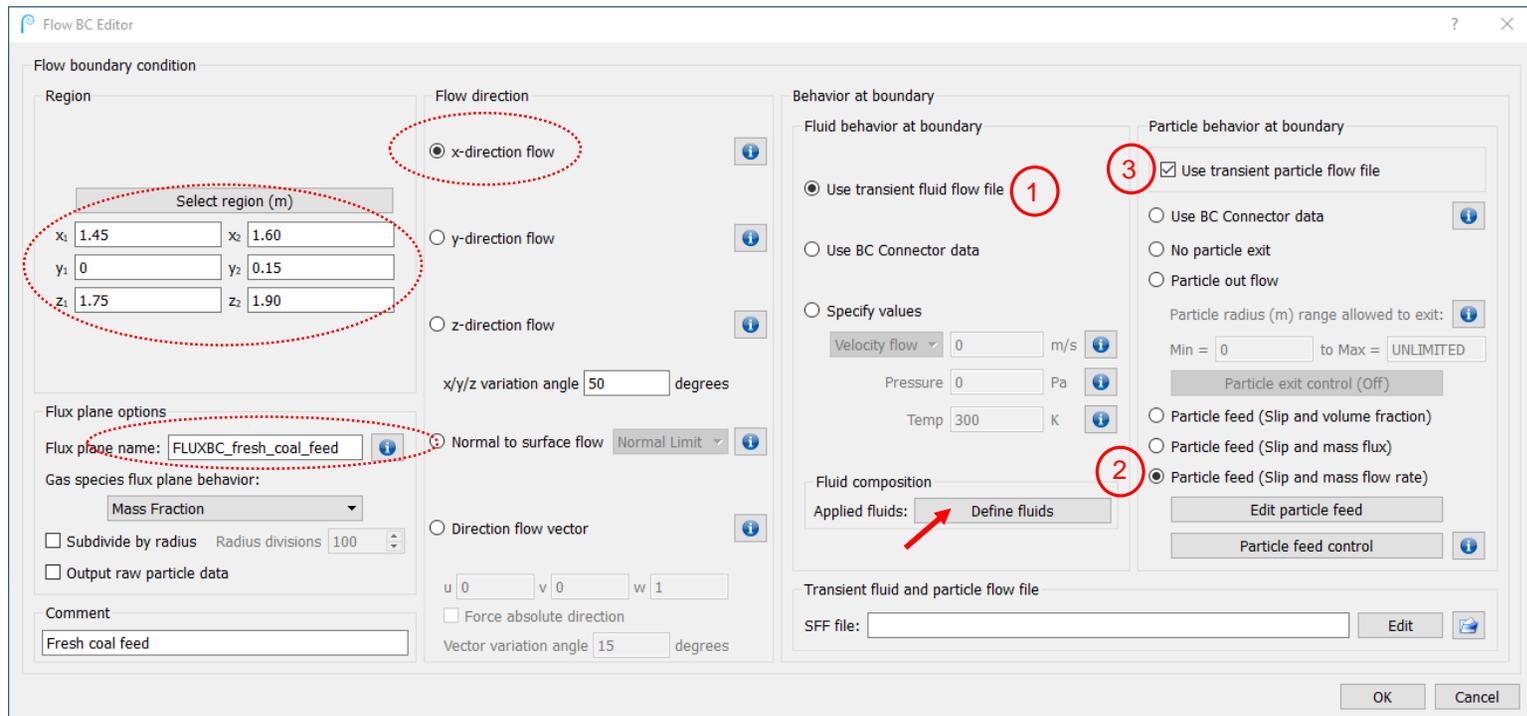
- Region:** Select region (m) with x1: -1.524, x2: 1.52242, y1: -1.524, y2: 1.52361, z1: 1.85943e-16, z2: 0.153173.
- Flow direction:** z-direction flow (selected).
- Behavior at boundary:** Use transient fluid flow file (selected).
- Particle behavior at boundary:** No particle exit (selected).
- Fluid composition:** Applied fluids: Define fluids.
- SFF file:** BC_bottom_flow.sff.

Flow Boundary Conditions Editor Table:

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

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

The image shows two overlapping dialog boxes from a software interface. The background window is the 'Flow BC Editor' with the 'Particle behavior at boundary' section selected. The foreground window is the 'Particle feed settings' dialog. Red arrows highlight the 'Edit particle feed' button in the background window and the 'OK' button in the foreground window.

Flow BC Editor - Particle behavior at boundary

- Use transient fluid flow file
- Use BC Connector data
- Specify values
- Velocity flow: 0 m/s
- Pressure: 0 Pa
- Temp: 290 K
- Fluid composition: Applied fluids: Define fluids
- Transient fluid and particle flow file: SFF file: Edit

Particle feed settings

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

Buttons: Add, Edit, Delete

Particle feed settings:

- Solid fraction: Mass Fraction
- Particle/fluid slip ratio: 0.5
- Particle feed per ave volume: 125
- Particle feed mass flow rate (kg/s): 0

Buttons: OK, Cancel

The image shows the 'Flow Boundary Conditions Editor' window with a table of boundary conditions. The table has columns for Time (s), Velocity (m/s), Temperature (K), Pressure (Pa), Particle Feed, Number Density Manual, Particle Slip, and Particle Mass Flow Rate (kg/s). The first row shows a condition at Time 0 with Velocity 0.25, Temperature 1300, Pressure 2e5, Particle Feed On, Number Density Manual 125, Particle Slip 1, and Particle Mass Flow Rate 1. The second row is empty.

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			

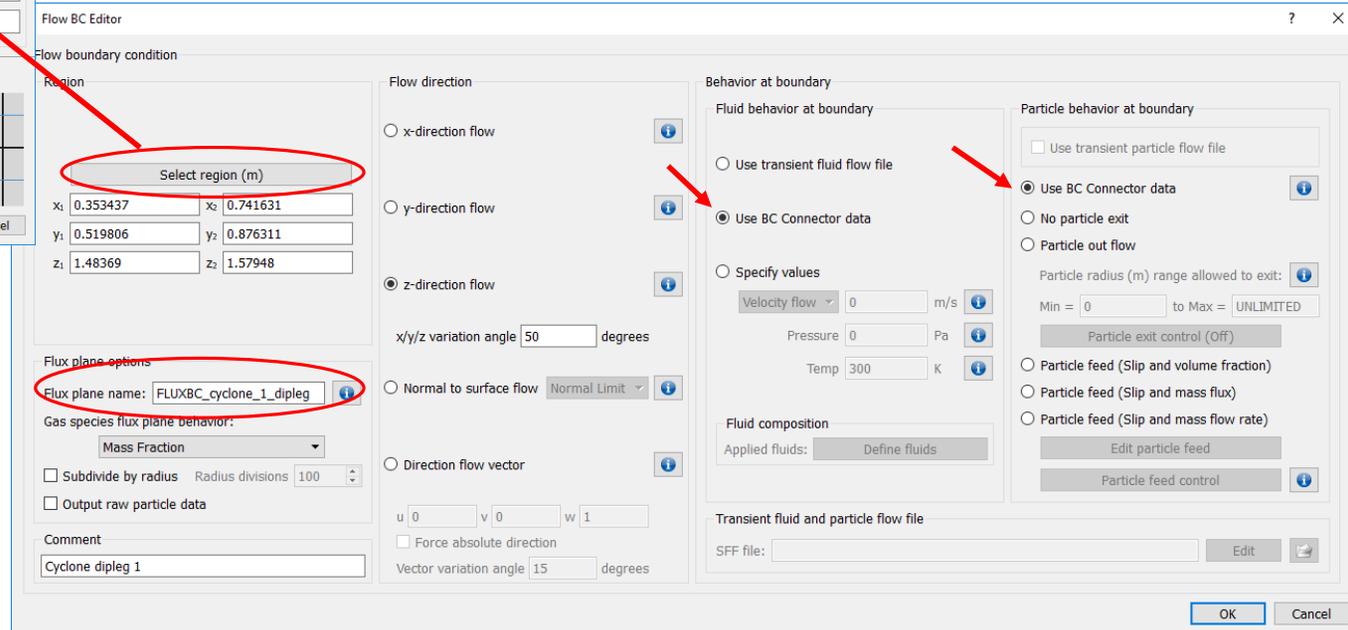
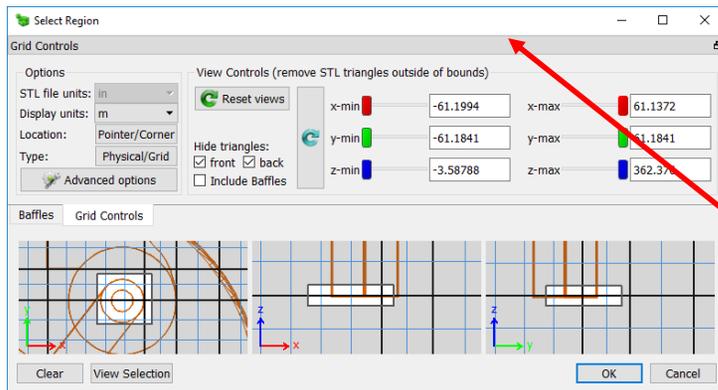
Buttons: Add Row, Delete Row, Check Data, Graph, Update Simulation

File: BC_fresh_coal_feed.sff

Buttons: Save, Save As, Close

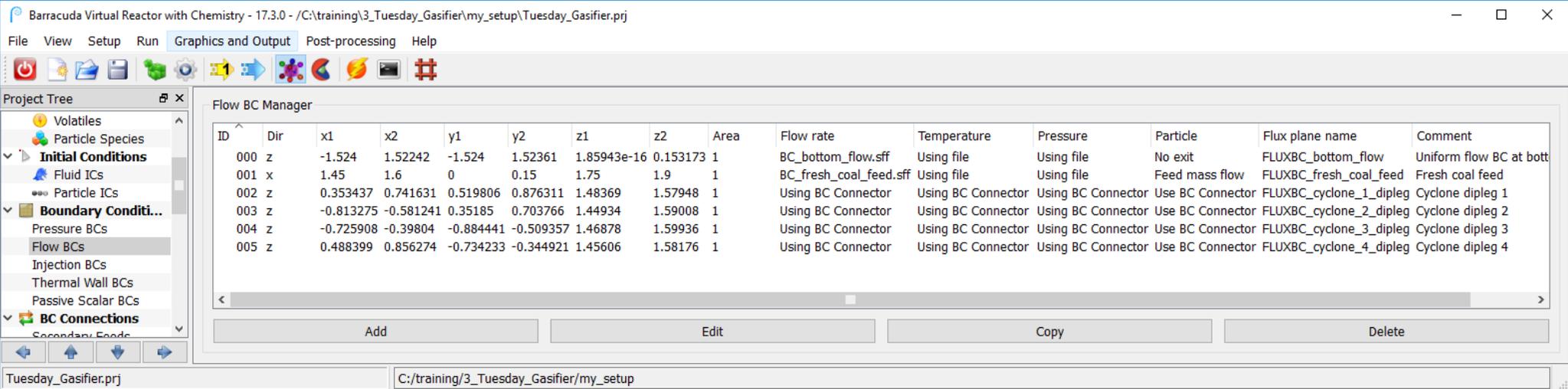
Cyclone Dipleg Flow BCs

- 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



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 "Flow BC Manager" window is open, displaying a table of boundary conditions. The table has columns for ID, Dir, x1, x2, y1, y2, z1, z2, Area, Flow rate, Temperature, Pressure, Particle, Flux plane name, and Comment. The table lists five boundary conditions, including four cyclone diplegs (IDs 002, 003, 004, and 005).

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

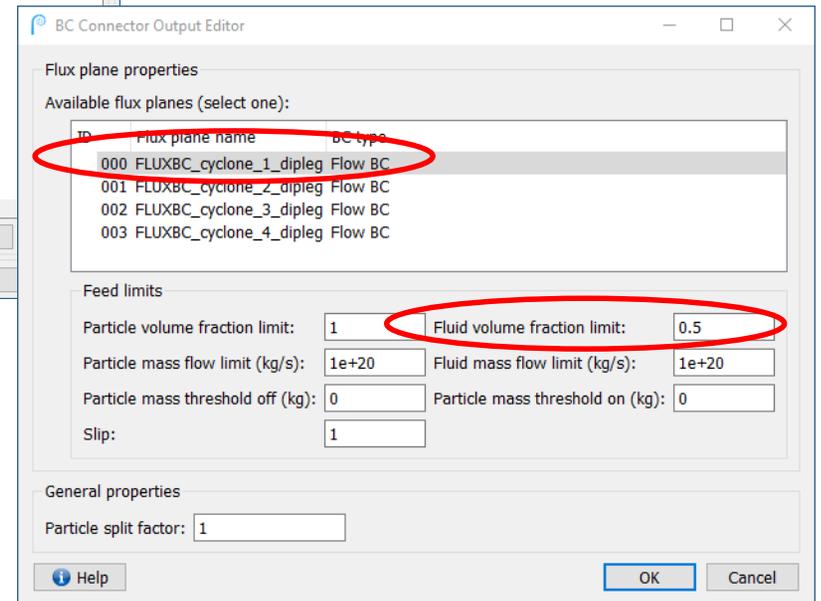
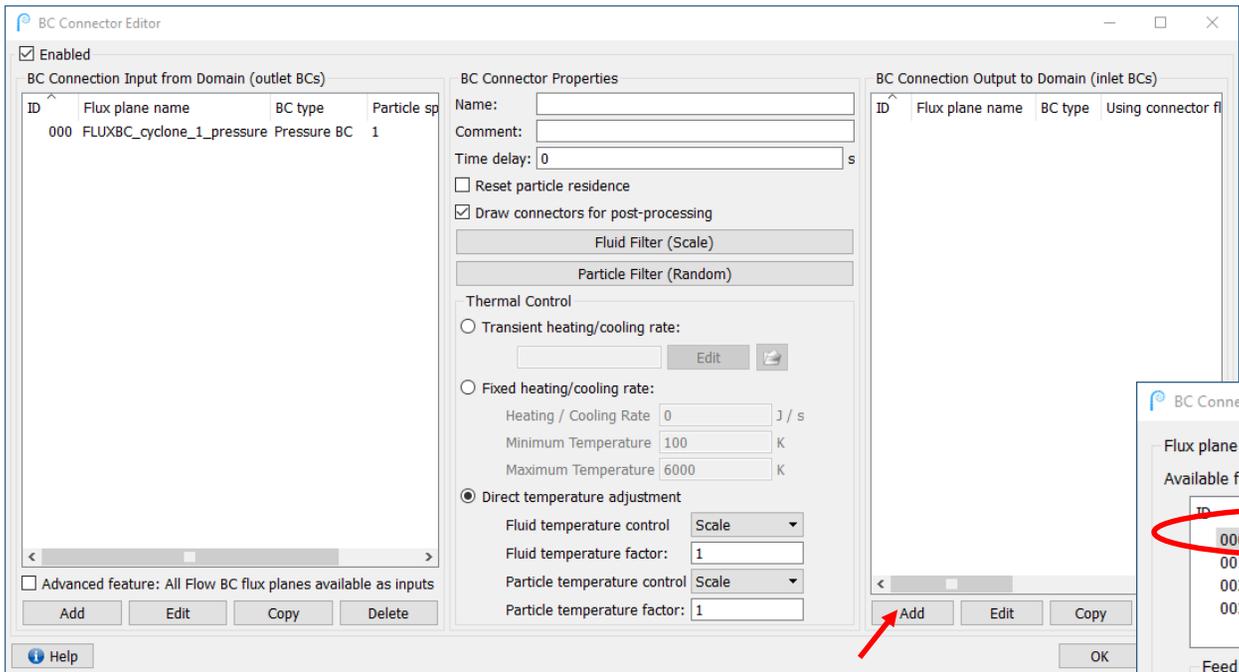
- In the **BC Connectors** section of the Barracuda VR GUI, click **Add** to define a new connection.
- On the left side, select the **BC Connector Input**, which in this case is the Pressure BC for Cyclone 1.

The screenshot displays the Barracuda Virtual Reactor GUI with the **BC Connector Editor** window open. The **BC Connector Input Editor** window is also open, showing the **Available flux planes (select one):** table. The first row, **000 FLUXBC_cyclone_1_pressure Pressure BC**, is highlighted with a red circle. The **BC Connector Editor** window shows the **BC Connection Input from Domain (outlet BCs)** table, which is currently empty. The **BC Connector Properties** section includes fields for **Name**, **Comment**, **Time delay**, and checkboxes for **Reset particle residence** and **Draw connectors for post-processing**. The **BC Connection Output to Domain (inlet BCs)** table is also empty. The **BC Connector Input Editor** window shows the **Flux plane properties** section with the **Available flux planes (select one):** table and the **General properties** section with the **Particle split factor** set to 1.

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

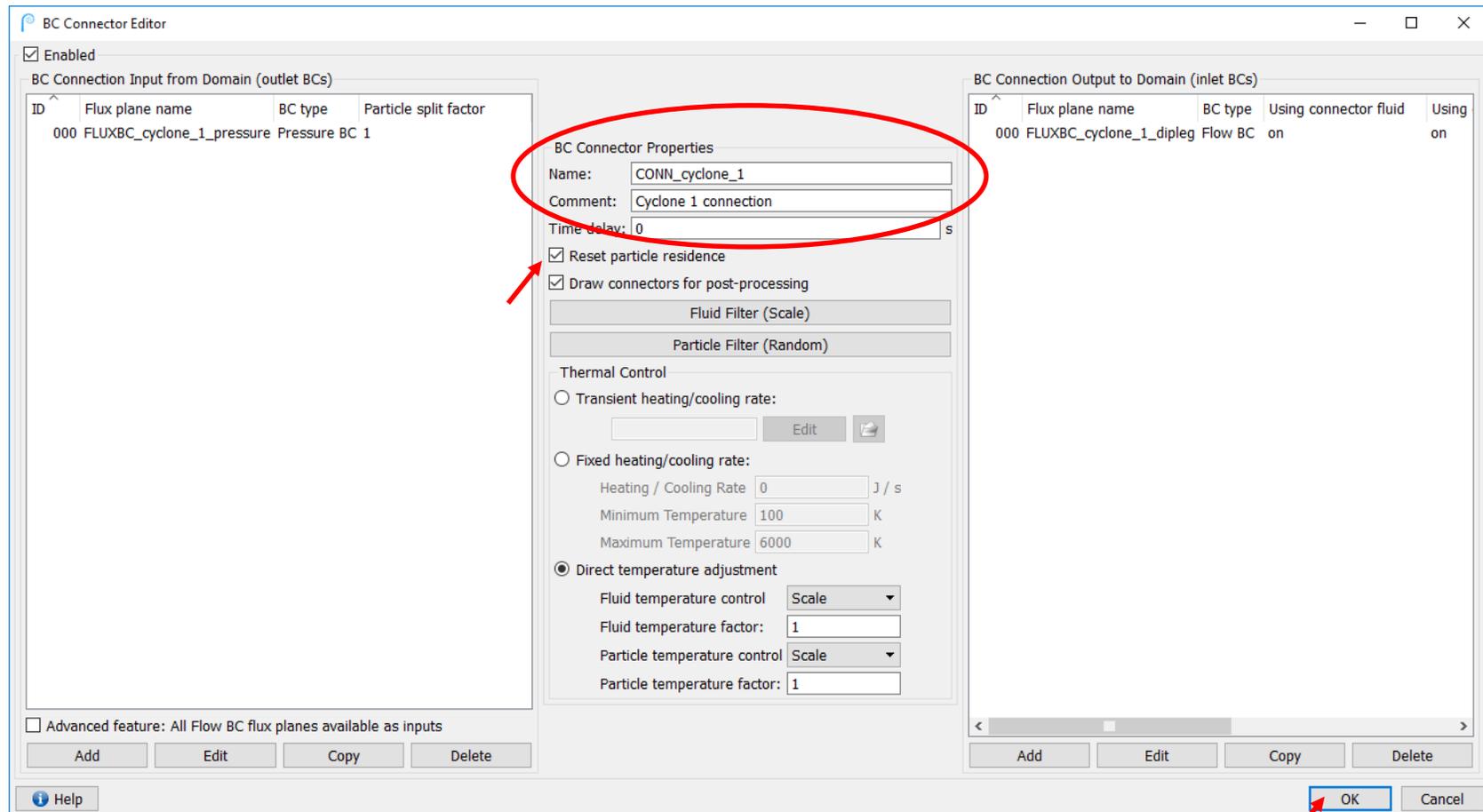
BC Connection Output to Domain

- 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

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

- Injection BCs
- Thermal Wall BCs
- Passive Scalar BCs
- BC Connections**
- Secondary Feeds
- Secondary Exits
- BC Connectors
- Chemistry**
- Rate Coefficients
- Reactions
- Numerics**
- Time Controls**

BC Connector Manager

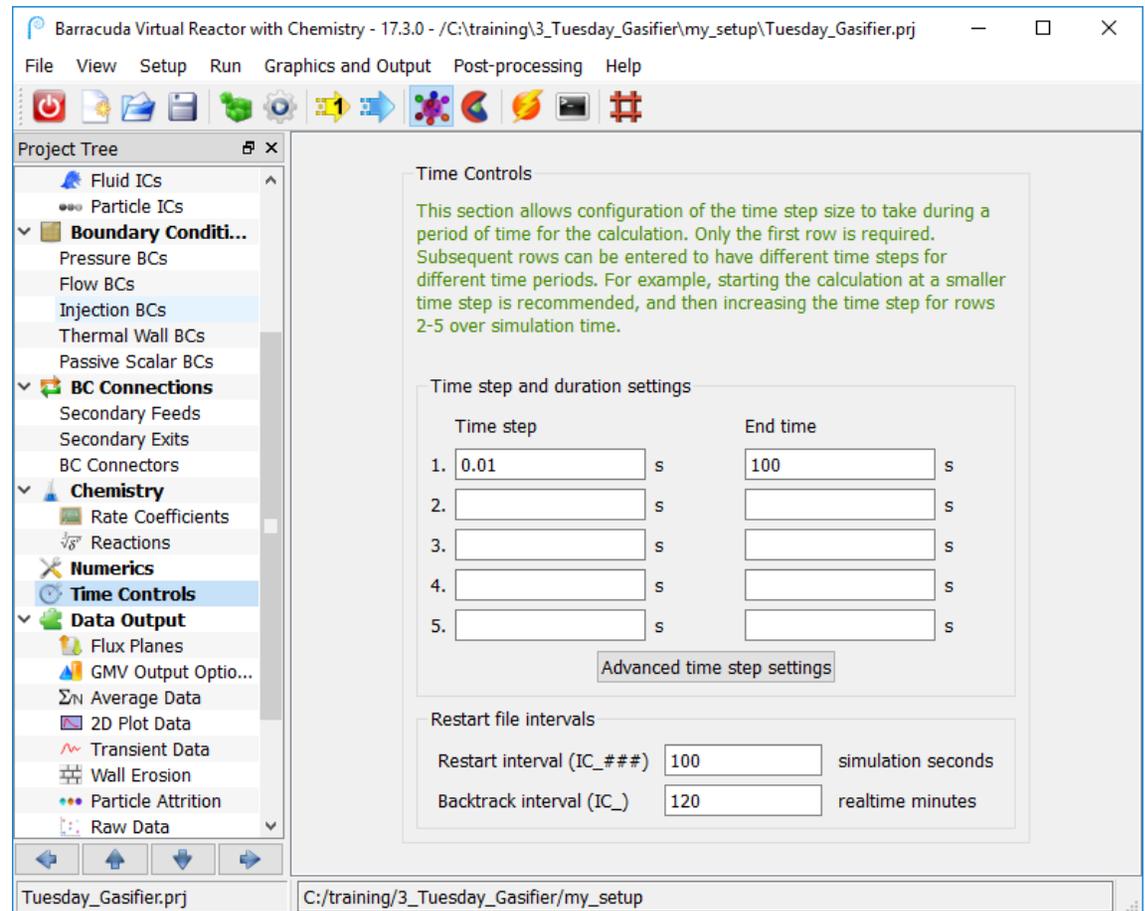
ID	Enabled	Name	Time delay	Reset residence	Inputs	Fluid filter	Particle filter	Thermal Control	Outputs	Comment
000	on	CONN_cyclone_1	0	off	FLUXBC_cyclone_1_pressure	Scale	Random	Legacy	FLUXBC_cyclone_1_dipleg	Cyclone 1 connection
001	on	CONN_cyclone_2	0	off	FLUXBC_cyclone_2_pressure	Scale	Random	Legacy	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

Add Edit Copy Delete

Tuesday_Gasifier.prj C:/training/3_Tuesday_Gasifier/my_setup

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

The screenshot displays the Barracuda Virtual Reactor interface. On the left, a 3D model of a reactor vessel is shown with a purple horizontal flux plane positioned in the freeboard. The main window shows the 'Flux Planes Manager' table with the following data:

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

The 'Flux Plane Editor' dialog box is open, showing the following settings:

- 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

Red arrows point from the 'Add' button in the Flux Planes Manager to the 'Add' button in the Flux Plane Editor, and from the 'Subdivide by radius' and 'Directional flux' checkboxes in the Flux Plane Editor to the corresponding settings in the dialog box.

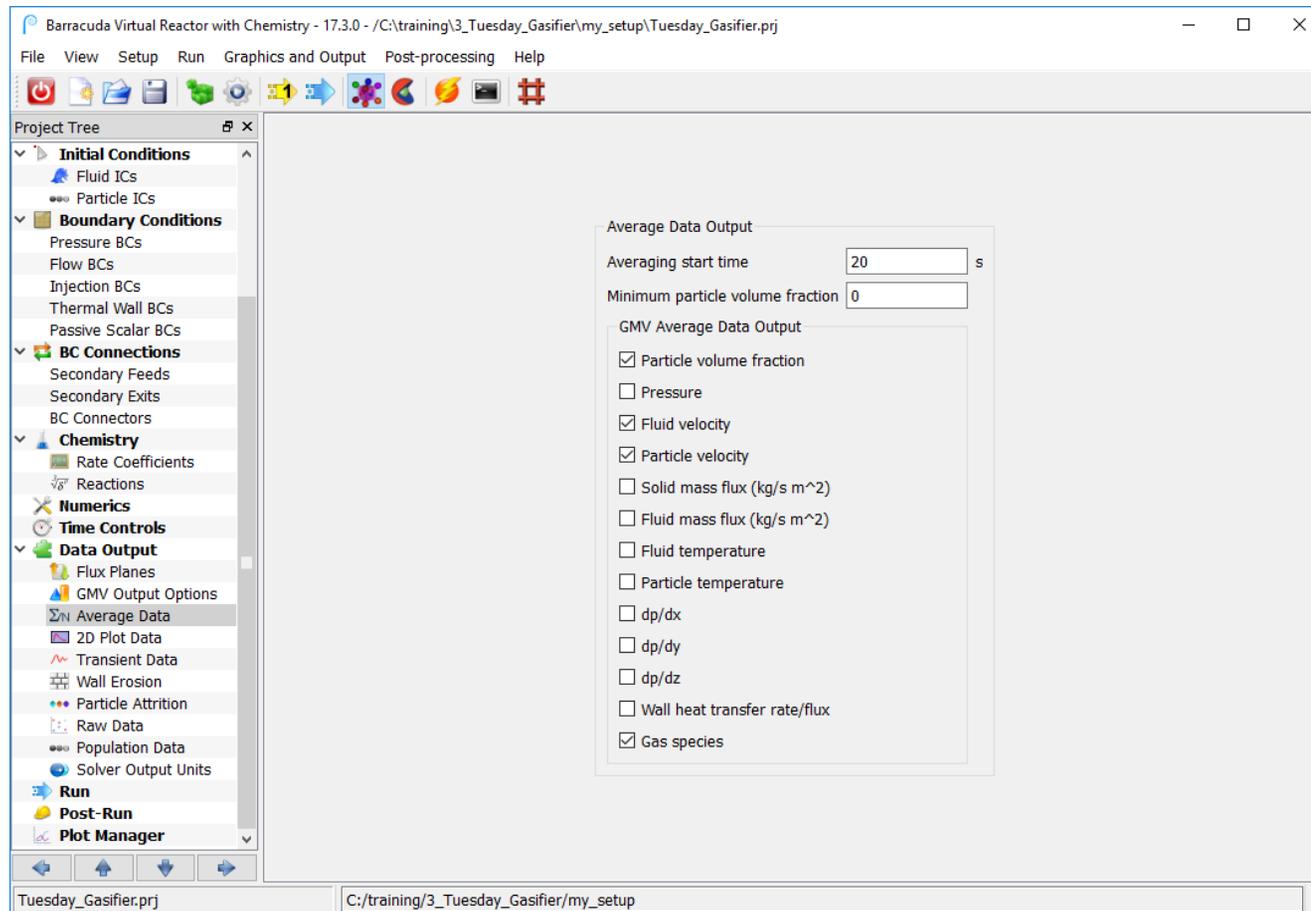
GMV Output Options

- 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

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 interface includes a menu bar (File, View, Setup, Run, Graphics and Output, Post-processing, Help) and a toolbar with various icons. On the left, there is a "Project Tree" with categories like Volatiles, Particle Species, Initial Conditions, Boundary Conditions, BC Connections, Chemistry, Numerics, Time Controls, and Data Output. The "Data Output" category is expanded, showing "GMV Output Options" selected. The main panel displays the "General Mesh View Data Output Options" dialog box. It contains a warning message: "Please select Eulerian and Lagrangian data for export to the General Mesh Viewer (GMV). Only data selected here can be viewed during post-processing. Values inside parenthesis are the field names of the variables within GMV." Below this, there are sections for "Eulerian (Cell) Output Data" and "Lagrangian (Particle) Output Data". The "Eulerian" section has checkboxes for Particle volume fraction (p-volFra), Fluid velocity (U, V, W), Particle velocity (P_[xyz]Vel), Pressure (Pressure), Dynamic pressure (DynPres), Fluid density (f-dens), Cell indices (i, j, k), Particle bulk density (p-dens), Turbulent viscosity (ViscTurb), CFL (CFL), Particle species (Species), Fluid temperature (F-Temp), Particle temperature (p-Temp), and Cell volume (cellVol). The "Lagrangian" section has checkboxes for Particle volume fraction (VolFrac), Particle speed (Speed), Particle radius in microns (rad), Constant color (Particle), Drag (drag), Cloud mass (cldMass), Particle material (Material), Particle density (Density), Particle species (Species), Unique particle ID (pid), Liquid fraction total (liqFrac), Particles per cloud (npCloud), Velocity (vel[xyz]), Residence time (ResTime), Residence time by species (ResTime##), Temperature (Temperat), Liquid mass total (liqMass), and Particle mass (mass). At the bottom, there are radio buttons for "Gas Species" (Mass fraction, Mole fraction, Mass concentration, Mole concentration) and checkboxes for "Options" (Compress graphics output, Generate predefined GMV attribute files). The status bar at the bottom shows the file name "Tuesday_Gasifier.prj" and the path "C:/training/3_Tuesday_Gasifier/my_setup".

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!

