

Thermal Reacting Gasifier Training Problem Part 2: Project

August 2020

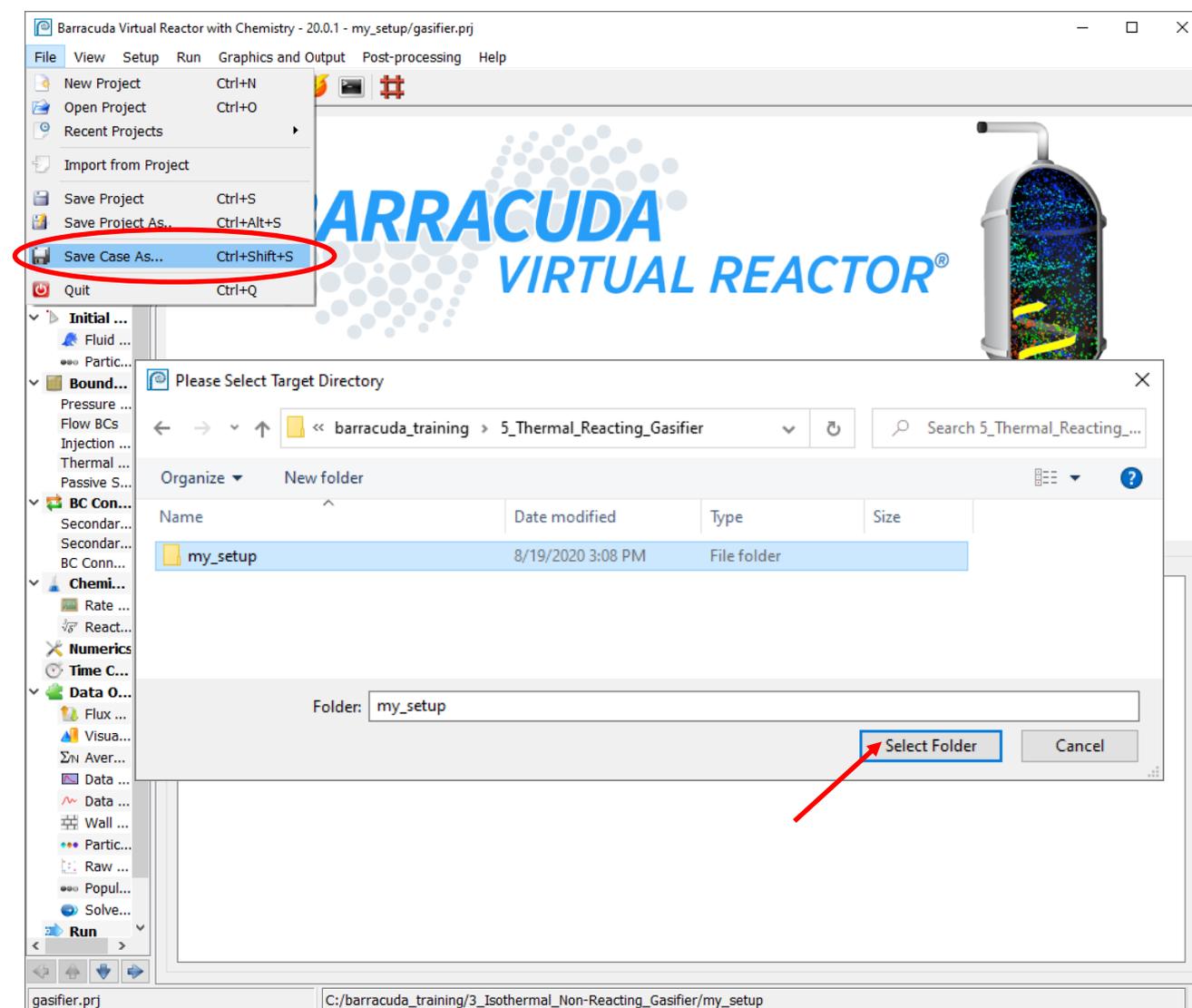
CPFD Software
1255 Enclave Parkway, Suite E
Houston, TX 77077 USA
+1 (713) 429-1252
www.cdfd-software.com

Save Case As...

Copy Gasifier project using "Save Case As..."

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

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



Selecting Files in the Save Case As... Dialog

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

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

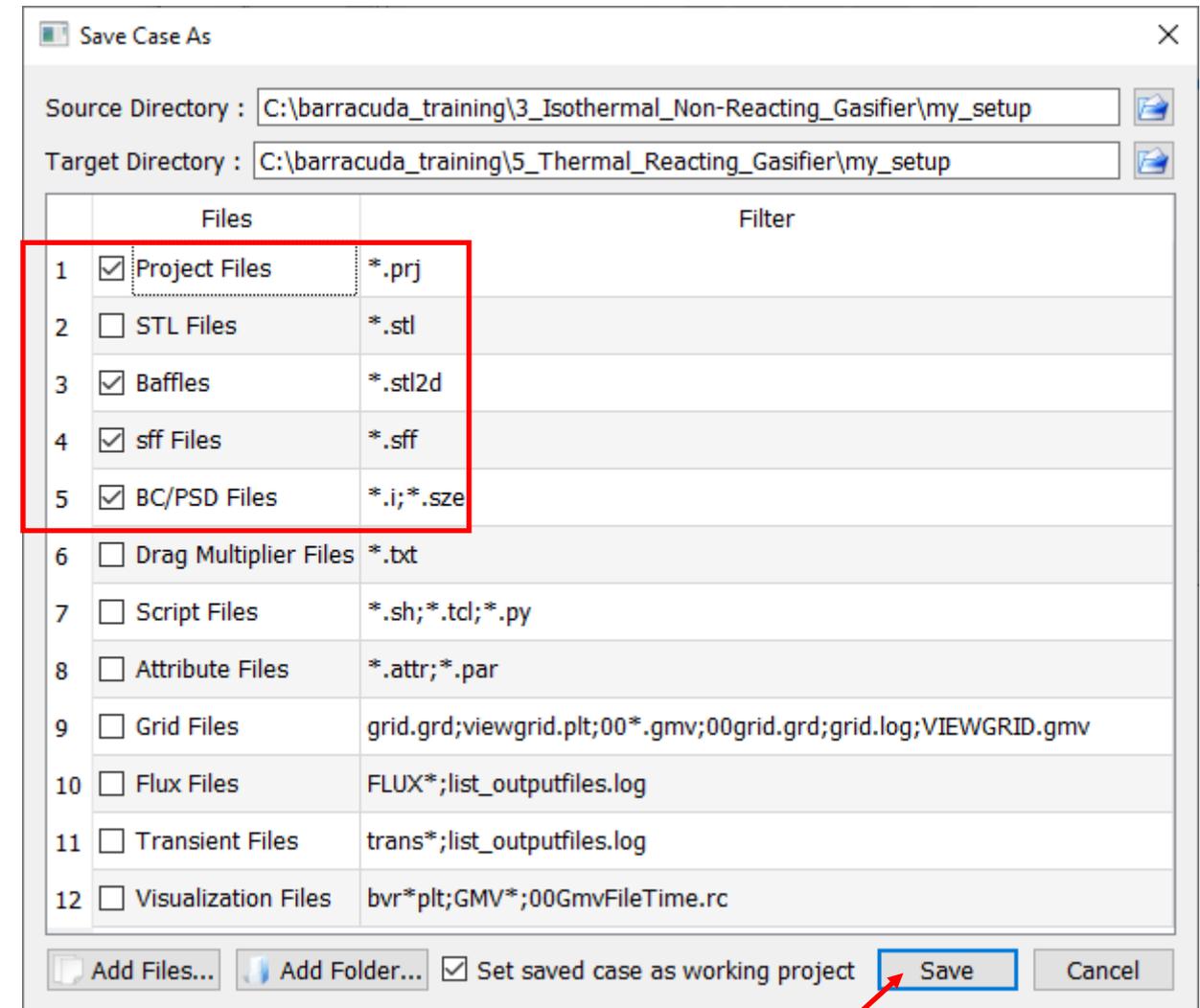
For the current case, keep:

- Project Files
- .sff, .i Files

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

- STL Files
- Grid Files

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



Gridding

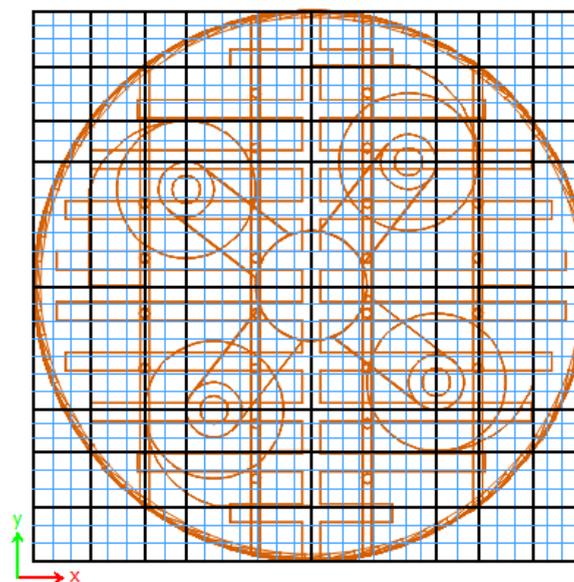
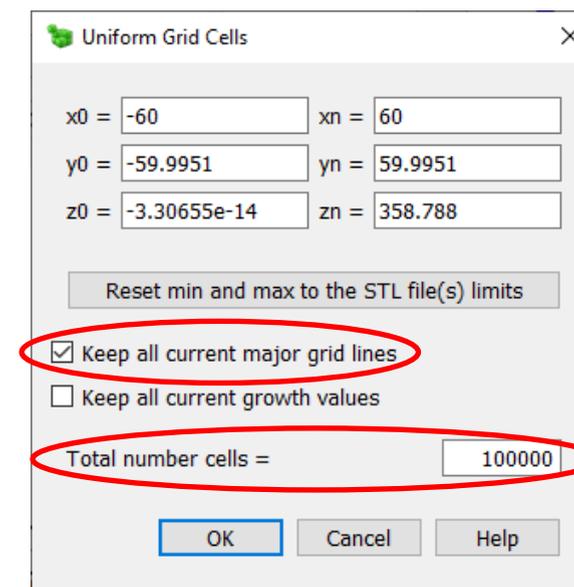
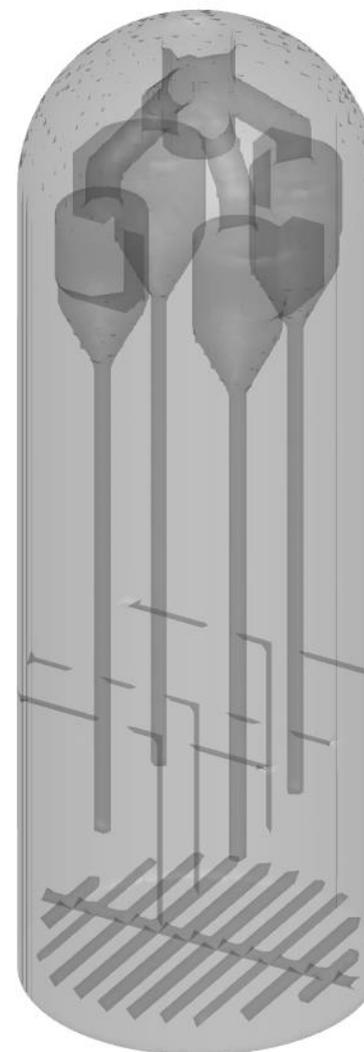
Gridding: Add the New STL File and set new Grid cells

In the Setup Grid section:

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

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

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



Modify the Grid to Capture Internal Structures

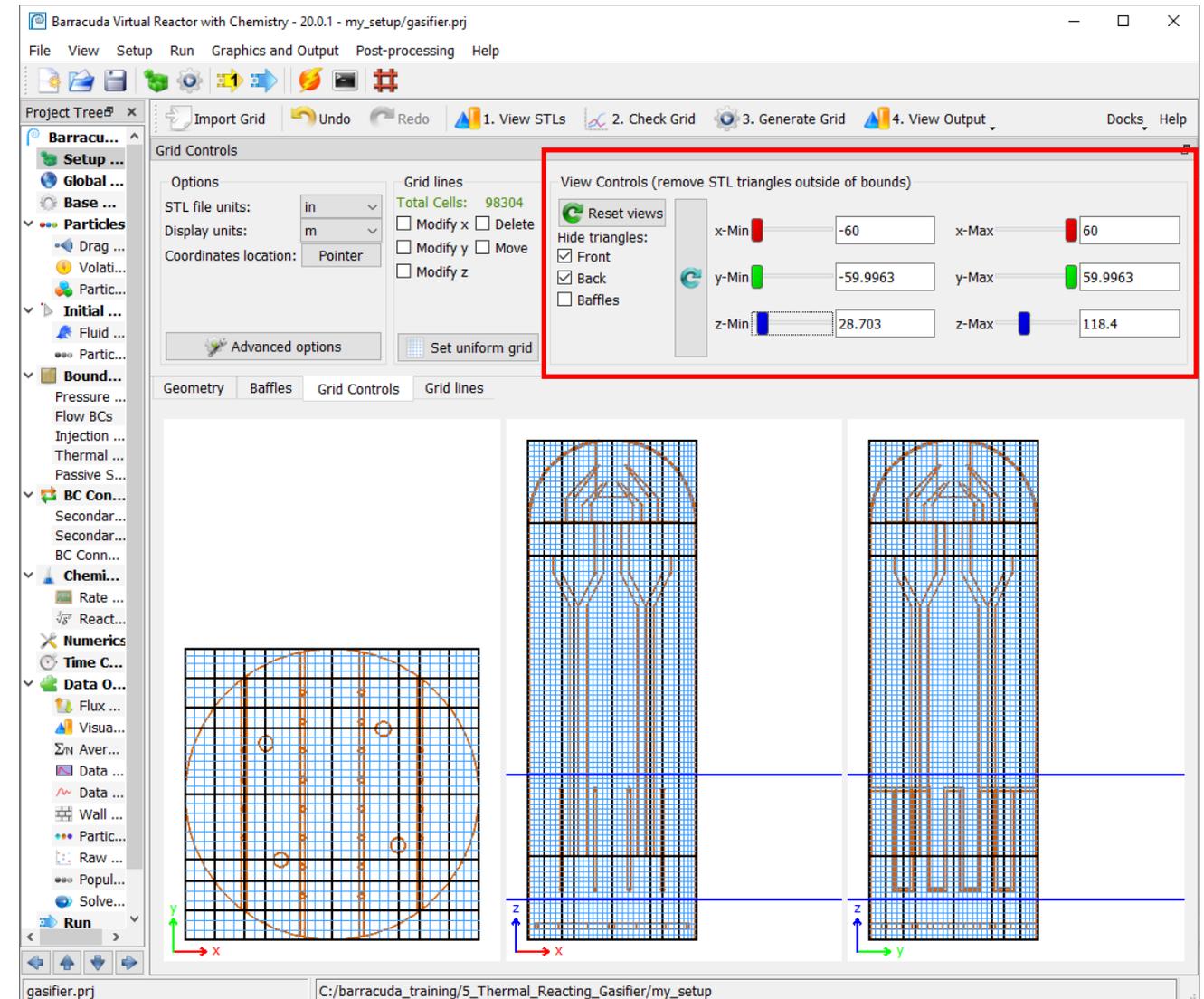
With this geometry, and with most real systems, you will not be able to capture everything perfectly.

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

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

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

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



The Final Grid

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

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

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



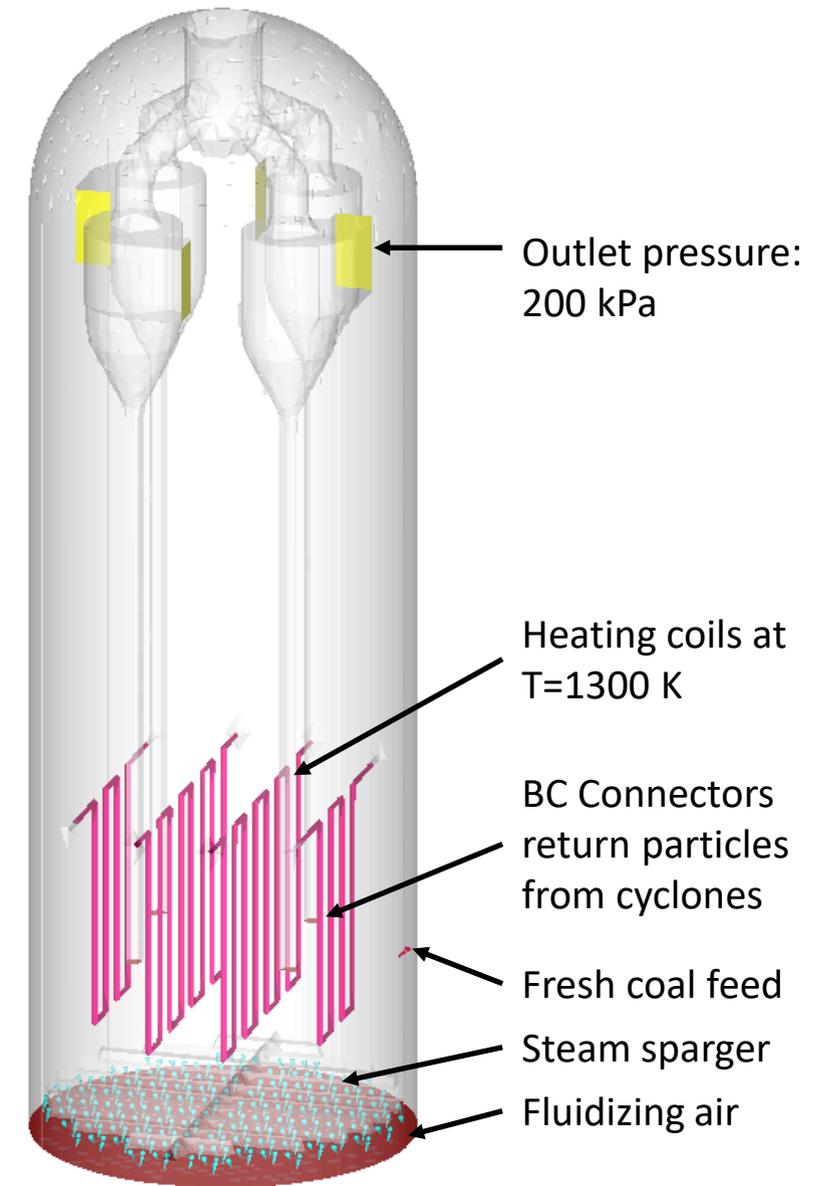
Setup

Process Sheet

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

Chemical reactions are included.

Boundary	Fluid Flow	Particle Flow
Fluidizing Air	Mass flow rate = 0.691 kg/s Temperature = 700 K Gas (mass fractions): 0.77 N ₂ , 0.23 O ₂	None
Steam Sparger through 204 injection nozzles	Mass flow rate = 0.296 kg/s Velocity = 10 m/s Temperature = 900 K Gas: pure H ₂ O	None
Fresh Coal Feed	Mass flow rate = 5e-3 kg/s Velocity = 5 m/s Temperature = 500 K Gas (mass fractions): 0.77 N ₂ , 0.23 O ₂	Fresh coal at 1 kg/s
Cyclone Diplegs	Controlled by BC Connector	Controlled by BC Connector



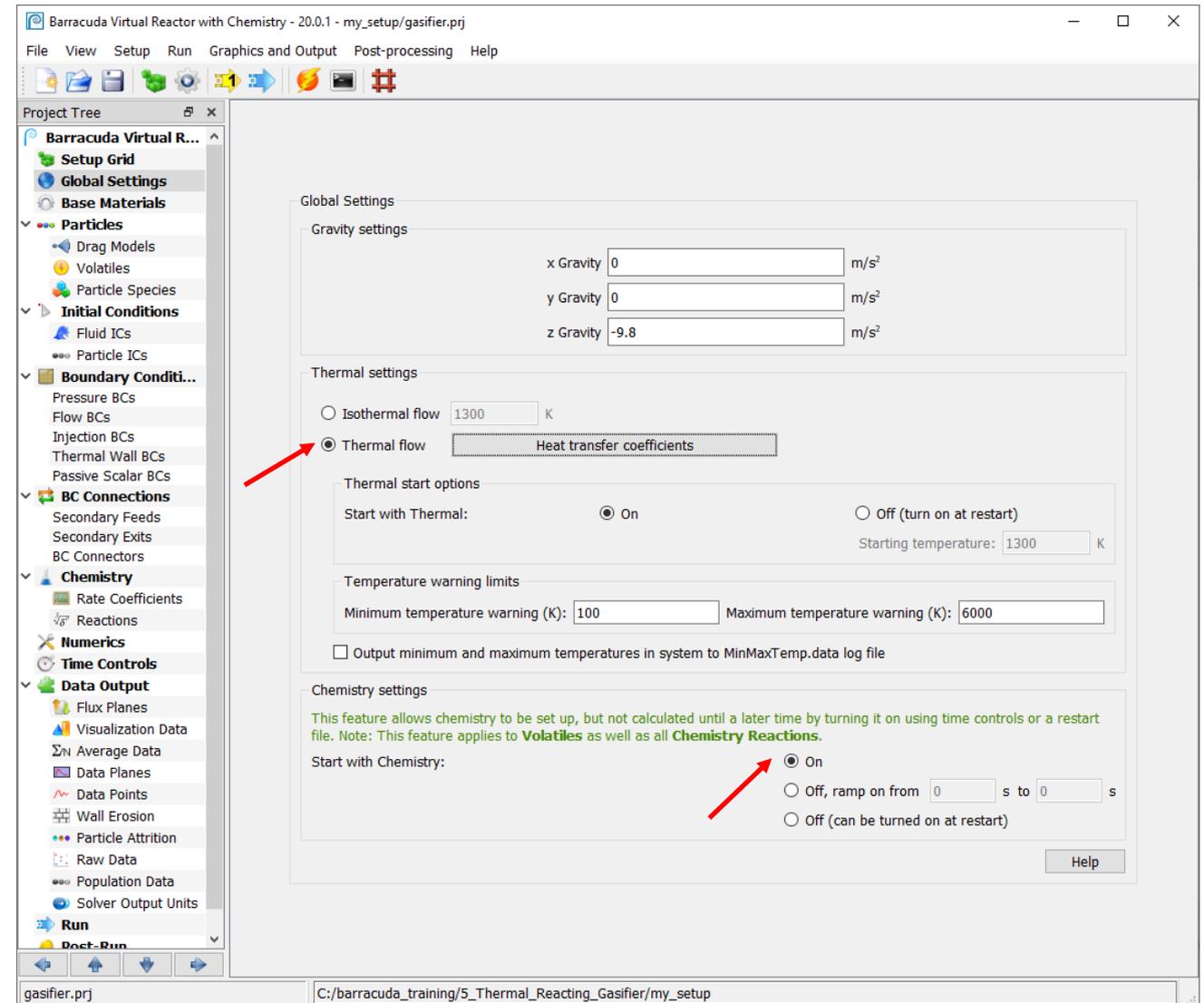
Enable Thermal Flow

In the Global Settings section

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

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

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



Automated Plotting of Polynomial Material Properties

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

You can visualize property data over a specified temperature range.

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

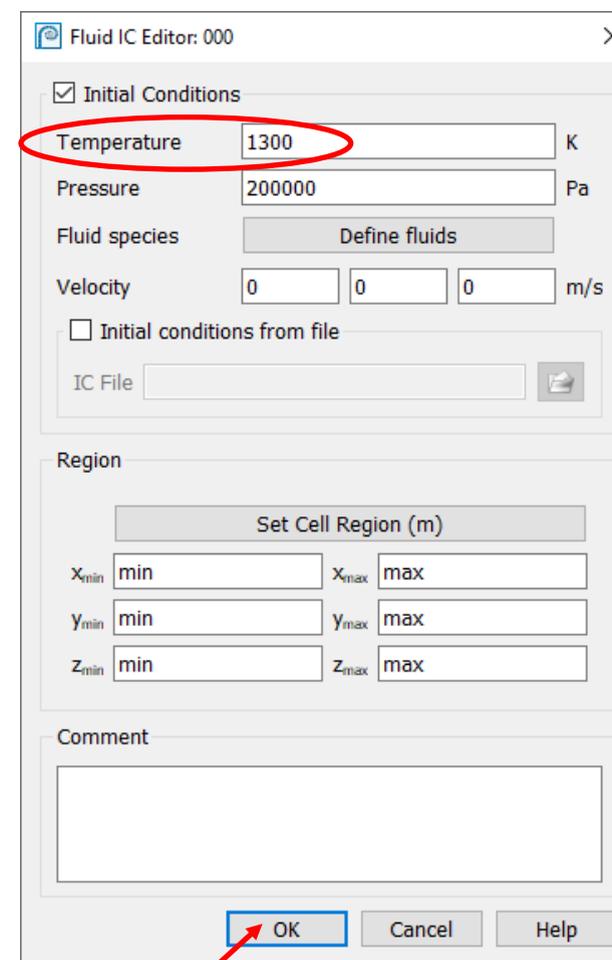
The screenshot displays the Barracuda Virtual Reactor software interface. The main window shows the Project Material List with columns for Chemical name, State, and Description. The Base Materials Editor is open, showing properties for Ash (Solid). The Thermal Conductivity property is selected, and the Material Property Editor dialog is open. In the Material Property Editor, the Expression field is set to a 4th-order polynomial: $168.9106 + -0.13343 \cdot T + 3.765e-05 \cdot T^2 + 0 \cdot T^3 + 0 \cdot T^4$. The Temperature Limits are set to Min. 200 K and Max. 2000 K. The Plot button is highlighted with a red arrow. A plot of Thermal conductivity (W/m/K) vs Temperature (K) is shown, with the y-axis ranging from 60 to 140 and the x-axis from 0 to 2000. The plot shows a decreasing trend of thermal conductivity with increasing temperature.

Temperatures of Initial and Boundary Conditions

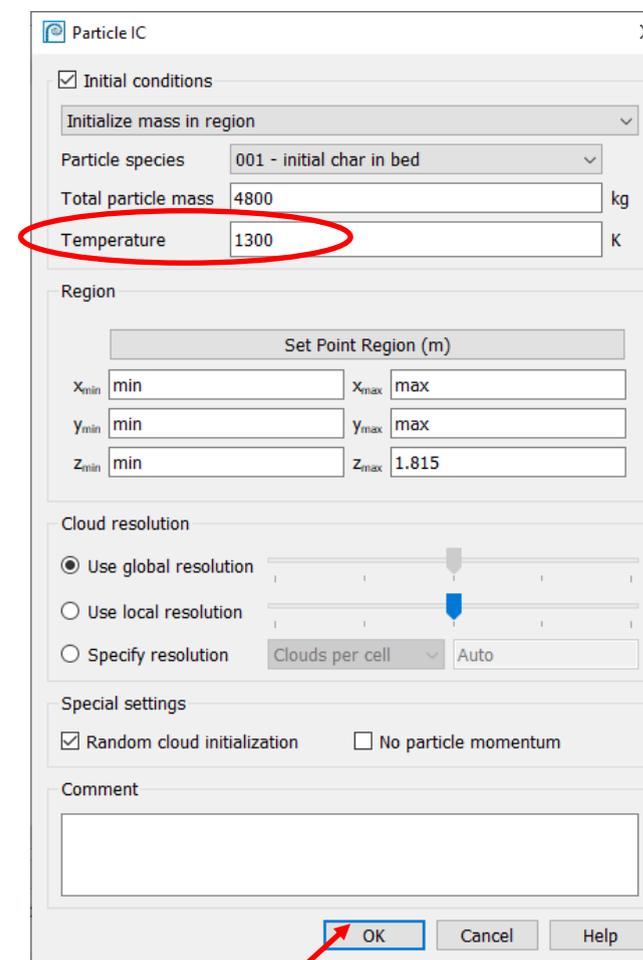
When the isothermal, non-reacting gasifier was set up, it was not important to consider the temperature specifications for initial and boundary conditions.

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

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



The screenshot shows the 'Fluid IC Editor: 000' dialog box. The 'Initial Conditions' section is checked, and the 'Temperature' field is set to 1300 K, circled in red. Other fields include Pressure (200000 Pa), Fluid species (Define fluids), and Velocity (0, 0, 0 m/s). The 'Region' section has 'Set Cell Region (m)' with x, y, and z min/max fields. A red arrow points to the 'OK' button at the bottom.



The screenshot shows the 'Particle IC' dialog box. The 'Initial conditions' section is checked, and the 'Temperature' field is set to 1300 K, circled in red. Other fields include Particle species (001 - initial char in bed) and Total particle mass (4800 kg). The 'Region' section has 'Set Point Region (m)' with x, y, and z min/max fields. A red arrow points to the 'OK' button at the bottom.

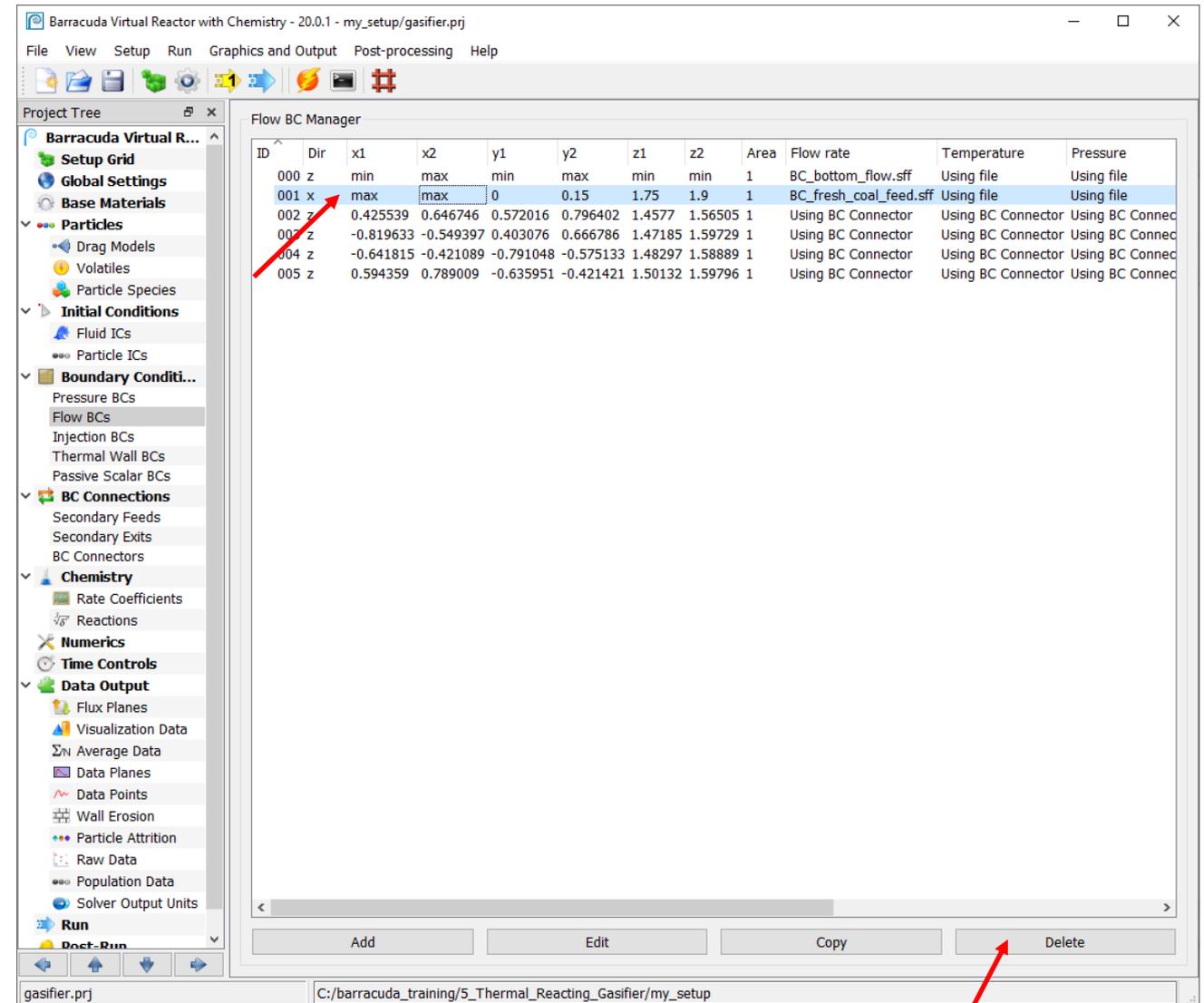
Fresh Coal Feed Injection

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

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

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

- Select the flow BC
- Click on Delete



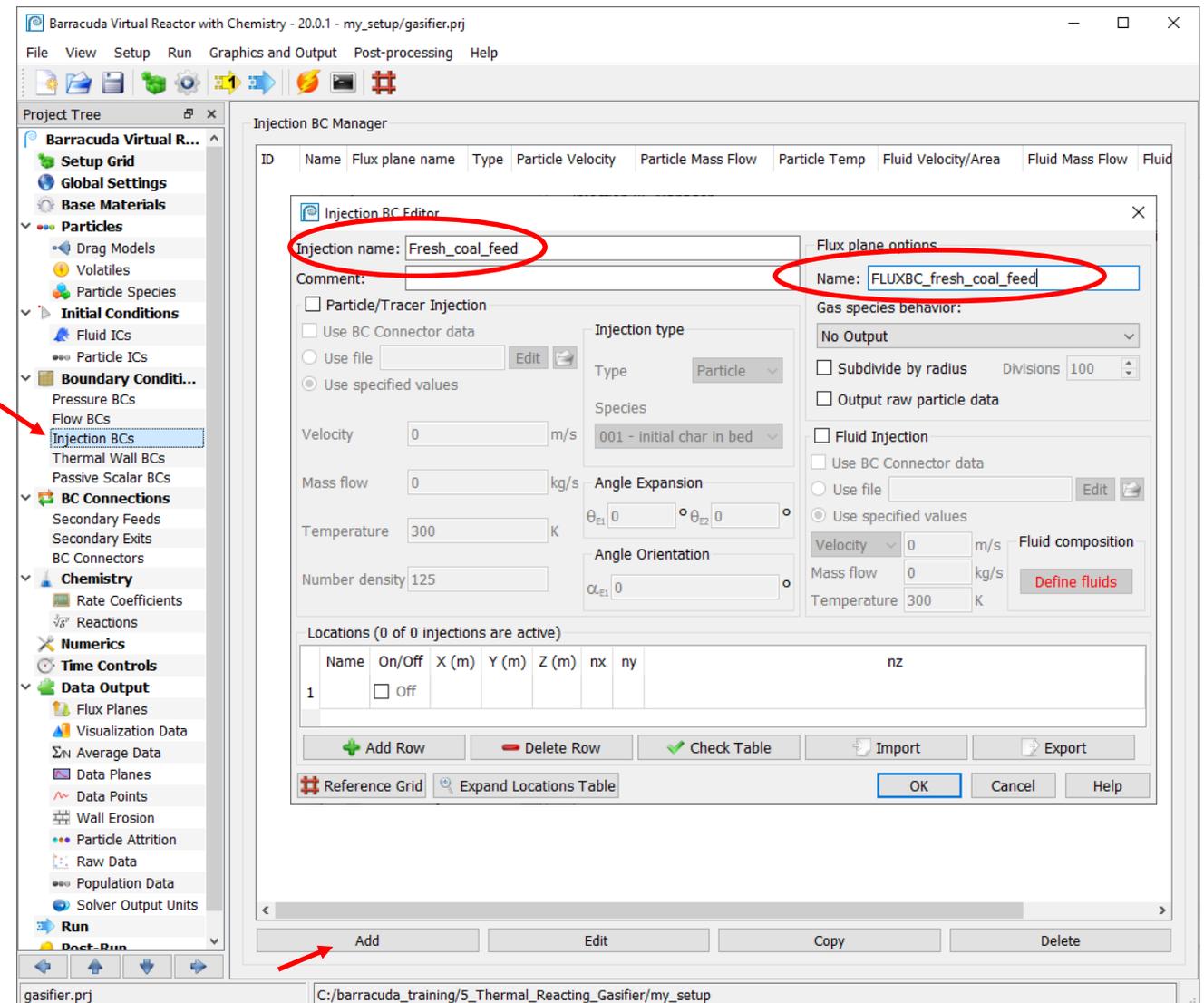
Fresh Coal Feed Injection

Click on Injection BC:

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

Click on Add

Start by entering an Injection Name and Flux Plane Name



Fresh Coal Feed Injection

Select Particle/tracer Injection

Select Use file to specify the particle mass flow rate:

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

Select Particle for Type

Select Fresh coal feed for Species

Set the Angle Expansion to 15

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

Injection BC Editor:

- Injection name: Fresh_coal_feed
- Comment: (empty)
- Particle/Tracer Injection
- Use BC Connector data
- Use file: particle_injection.sff **Edit**
- Use specified values
- Velocity: 0 m/s
- Mass flow: 0 kg/s
- Temperature: 300 K
- Number density: 125
- Injection type: Type: Particle
- Species: 002 - fresh coal feed
- Angle Expansion: θ_{E1} 15 θ_{E2} 15
- Angle Orientation: α_{E1} 0
- Flux plane options: Name: FLUXBC_fresh_coal_feed
- Gas species behavior: No Output
- Subdivide by radius Divisions: 100
- Output raw particle data
- Fluid Injection
- Use BC Connector data
- Use file (empty) **Edit**
- Use specified values
- Velocity: 0 m/s
- Mass flow: 0 kg/s
- Temperature: 300 K
- Fluid composition: **Define fluids**

Locations (0 of 0 injections are active):

Name	On/Off	X (m)	Y (m)	Z (m)	nx	ny	nz	Particle Mass Weight	Particle Temp Multiplier
1	<input type="checkbox"/> Off								

Particle Injection Boundary Conditions Editor:

Time (s)	On/Off	Temperature (K)	Velocity (m/s)	Mass Flow Rate (kg/s)	Number Density Manual
1	0 <input checked="" type="radio"/> On	500	5	1	1000
2	<input checked="" type="radio"/> On				

File: fresh_coal_feed_particle_injection.sff **Save** Save As Close Help

Fresh Coal Feed Injection

Select Fluid Injection

Select Use file to specify the fluid mass flow rate:

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

Specify the Fluid Composition

- 0.77 N₂
- 0.23 O₂

Injection BC Editor

Injection name: Fresh_coal_feed
Comment:
 Particle/Tracer Injection
 Use BC Connector data
 Use file [particle_injection.sff] Edit
 Use specified values
Velocity: 0 m/s
Injection type: Type: Particle, Species: 002 - fresh coal feed

Fluid Injection Boundary Conditions Editor

Time (s)	On/Off	Temperature (K)	Velocity (m/s)	Mass Flow Rate (kg/s)
1 0	<input checked="" type="radio"/> On	500	5	5e-3
2	<input checked="" type="radio"/> On			

File: fresh_coal_feed_fluid_injection.sff Save Save As Close Help

Mixture

Component	Fraction
N2 (G)	0.77
O2 (G)	0.23

Specify mixture by: Mass fraction Sum of fractions: 1

Flux plane options

Name: FLUXBC_fresh_coal_feed
Gas species behavior: No Output
 Subdivide by radius Divisions: 100
 Output raw particle data
 Fluid Injection
 Use BC Connector data
 Use file [coal_feed_fluid_injection.sff] Edit
 Use specified values
Velocity: 0 m/s Fluid composition
Mass flow: 0 kg/s
Temperature: 300 K **Define fluids**

Fresh Coal Feed Injection

Specify the location of the fresh coal feed nozzle:

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

Injection BC Editor

Injection name: Fresh_coal_feed

Comment:

Particle/Tracer Injection

Use BC Connector data

Use file `particle_injection.sff` Edit

Use specified values

Injection type

Type: Particle

Species: 002 - fresh coal feed

Velocity: 0 m/s

Mass flow: 0 kg/s

Temperature: 300 K

Number density: 125

Angle Expansion: θ_{E1} 15 θ_{E2} 15

Angle Orientation: α_{E1} 0

Flux plane options

Name: FLUXBC_fresh_coal_feed

Gas species behavior: No Output

Subdivide by radius Divisions: 100

Output raw particle data

Fluid Injection

Use BC Connector data

Use file `coal_feed_fluid_injection.sff` Edit

Use specified values

Velocity: 0 m/s

Mass flow: 0 kg/s

Temperature: 300 K

Fluid composition: Define fluids

Locations (1 of 1 injections are active)

Name	On/Off	X (m)	Y (m)	Z (m)	nx	ny	nz	Particle Mass Weight	Particle Temp Multiplier	Fluid Mass Weight
1 Feed	<input checked="" type="checkbox"/> On	1.5	0	1.75	-1	0	-1	1	1	1
2	<input type="checkbox"/> Off									

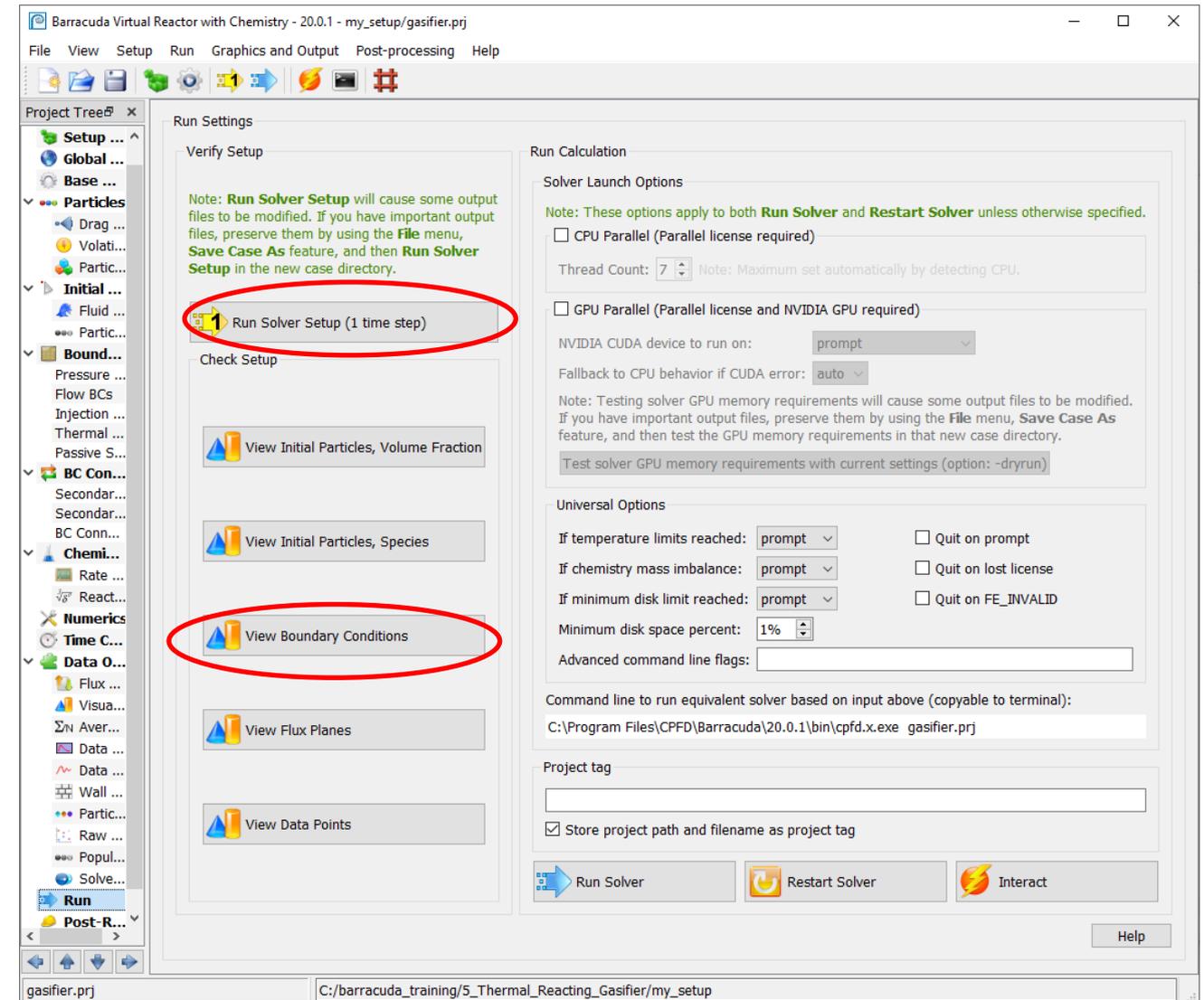
Add Row Delete Row Check Table Import Export Particle weight sum 1 Fluid weight sum 1

Reference Grid Expand Locations Table OK Cancel Help

Fresh Coal Feed Injection

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

- Run Solver Setup
- View Boundary Conditions

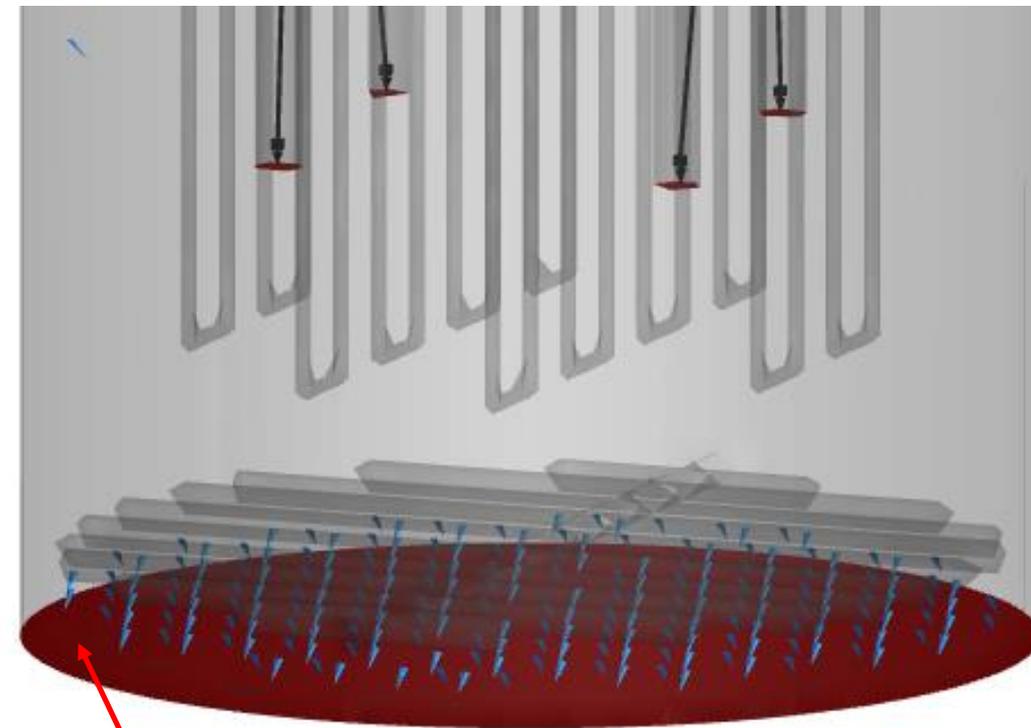


Separate the Air and Steam BCs

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

Now that we are including the sparger, it is necessary to separate the fluidizing air (N_2+O_2) from the steam:

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



Steam introduced through 204 injection points located on the sparger

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

Flow BC as Uniform Air Distributor

Navigate to Flow BCs window

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

The screenshot displays the Barracuda Virtual Reactor interface with several windows open:

- Flow BC Manager:** A table listing boundary conditions. The selected entry is:

ID	Dir	x1	x2	y1	y2	z1	z2	Area	Flow rate	Temperature	Pressure	Particle
000	z	min	max	min	max	min	min	1	BC_bottom_flow.sff	Using file	Using file	No exit
- Flow BC Editor:** Shows configuration for the selected boundary condition. The 'z-direction flow' radio button is selected. The 'Fluid composition' section has 'Define fluids' selected. The 'Transient fluid and particle flow file' section shows 'SFF file: BC_bottom_flow.sff' and an 'Edit' button.
- Mixture:** Shows the composition of the fluid. The 'Mixture' table is:

Component	Fraction
N2 (G)	0.77
O2 (G)	0.23
- Flow Boundary Conditions Editor:** Shows a table for transient conditions. The 'Mass Flow Rate (kg/s)' header is circled in red, with a red arrow pointing to it and the text 'Double-click to change header'. The table data is:

Time (s)	Mass Flow Rate (kg/s)	Temperature (K)	Pressure (Pa)
1 0	0.691	700	2e5
2			

Steam Injection BC

Create a new injection BC for the steam sparger:

- Navigate to Injection BCs window
- Click on Add
- Enter an Injection Name
- Enter a Flux Plane name
- Select Fluid Injection
- Use file to specify the fluid mass flow rate:
 - Click on Edit
 - Enter the appropriate values
 - Save the file using a descriptive name
- Click on Define fluids
 - 100% H2O

The screenshot shows two overlapping windows from the software. The top window is the 'Injection BC Editor' for an injection named 'Steam_sparger'. It has several tabs: 'Particle/Tracer Injection', 'Use BC Connector data', 'Use file', and 'Use specified values'. The 'Use file' tab is selected, and the 'Injection type' is set to 'Particle'. The 'Species' is '001 - initial char in bed'. The 'Use file' option is selected, and the file 'BC_sparger_injection.sff' is specified. The 'Edit' button next to the file name is circled in red. The 'Flux plane options' section shows 'Name: FLUXBC_steam_sparger' and 'Gas species behavior: No Output'. The 'Fluid Injection' checkbox is checked. The 'Define fluids' button is also visible. The bottom window is the 'Fluid Injection Boundary Conditions Editor', which contains a table with columns for Time (s), On/Off, Temperature (K), Velocity (m/s), and Mass Flow Rate (kg/s). The table has three rows, all with 'On' in the On/Off column. The 'Save' button at the bottom of this window is also circled in red.

Time (s)	On/Off	Temperature (K)	Velocity (m/s)	Mass Flow Rate (kg/s)
1 0	On	900	0	0
2 0.1	On	900	10	0.296
3	On			

Steam Injection BC

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

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

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

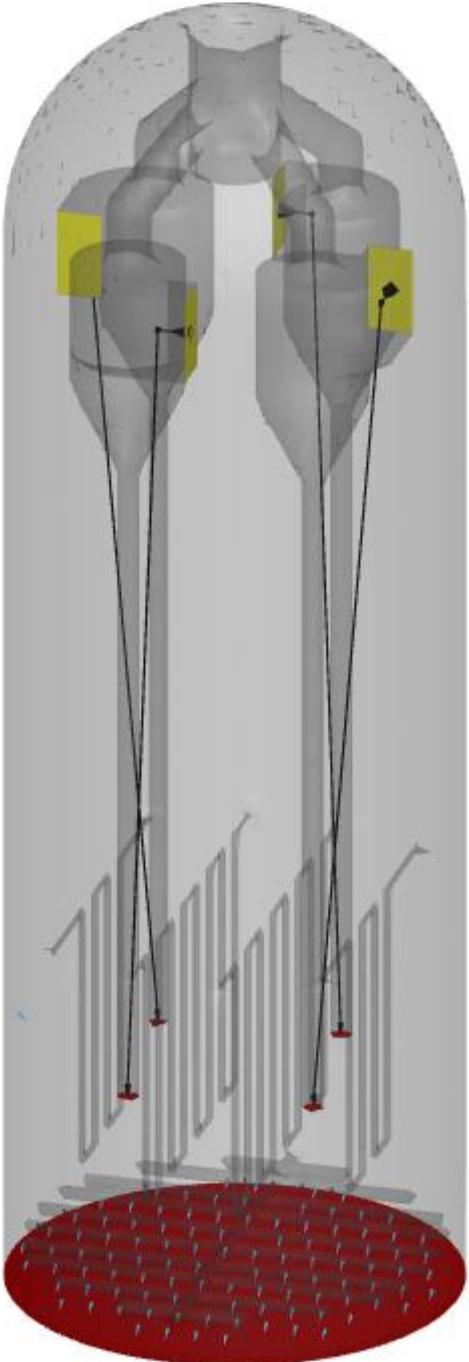
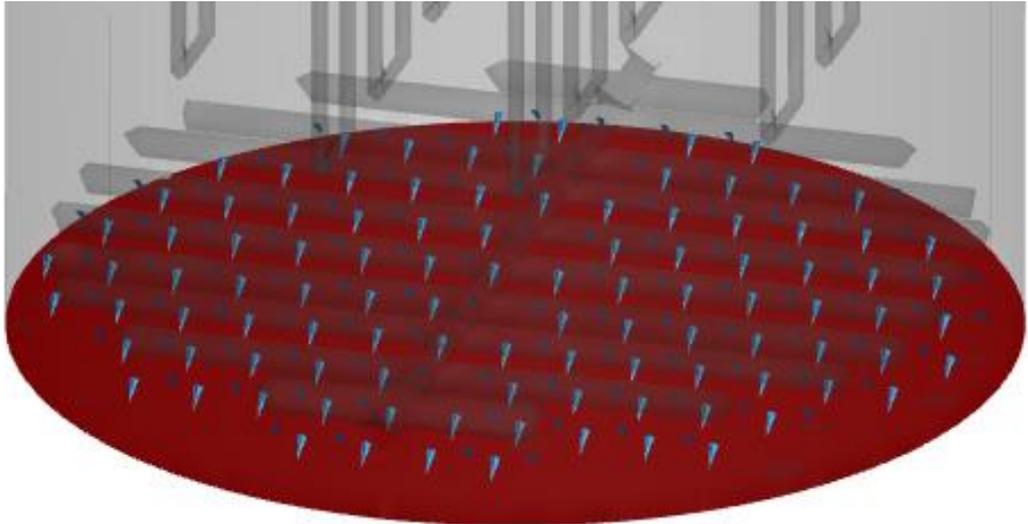
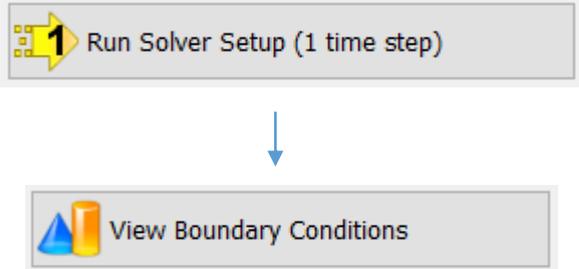
- Click on Import
- Select the file sparger_injection_bc_locations.csv
- Click on Open
- Click OK in the import dialog
- Click OK in the Injection BC Editor

The screenshot displays the Barracuda VR GUI interface for configuring injection boundary conditions. It includes several overlapping windows:

- Injection BC Editor:** Shows the 'Injection name' set to 'Steam_s', 'Injection type' set to 'Particle', and 'Use file' selected. A 'Separator Selection' dialog is open, showing 'Comma' as the selected separator.
- Open File:** A file explorer window showing the file 'sparger_injection_bc_locations.csv' selected in the file list. The file name and type are shown in the bottom bar.
- Locations Table:** A table with columns: Name, On/Off, X (m), Y (m), Z (m), nx, ny, nz, Fluid Mass Weight, and Fluid Temp Multiplier. The first row is labeled '1' and has 'Off' checked in the On/Off column.
- Buttons:** 'Add Row', 'Delete Row', 'Check Table', 'Import', 'Export', 'Reference Grid', 'Expand Locations Table', 'OK', 'Cancel', and 'Help' are visible at the bottom of the main window.

Steam Injection BC

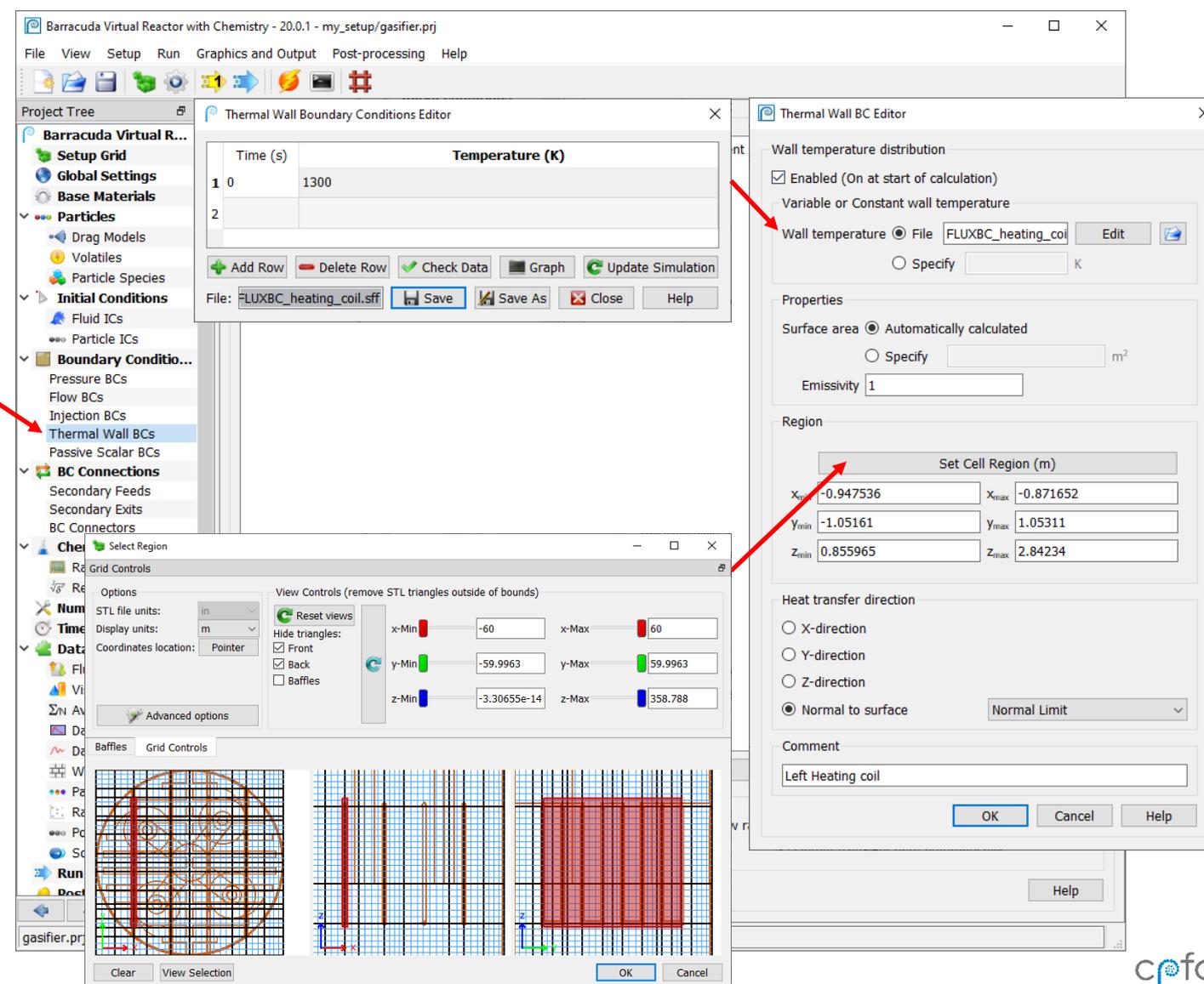
Once the steam injections have been created, run the simulation for a single time step and check the boundary conditions.



Thermal Wall BCs: Heating Coils

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

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



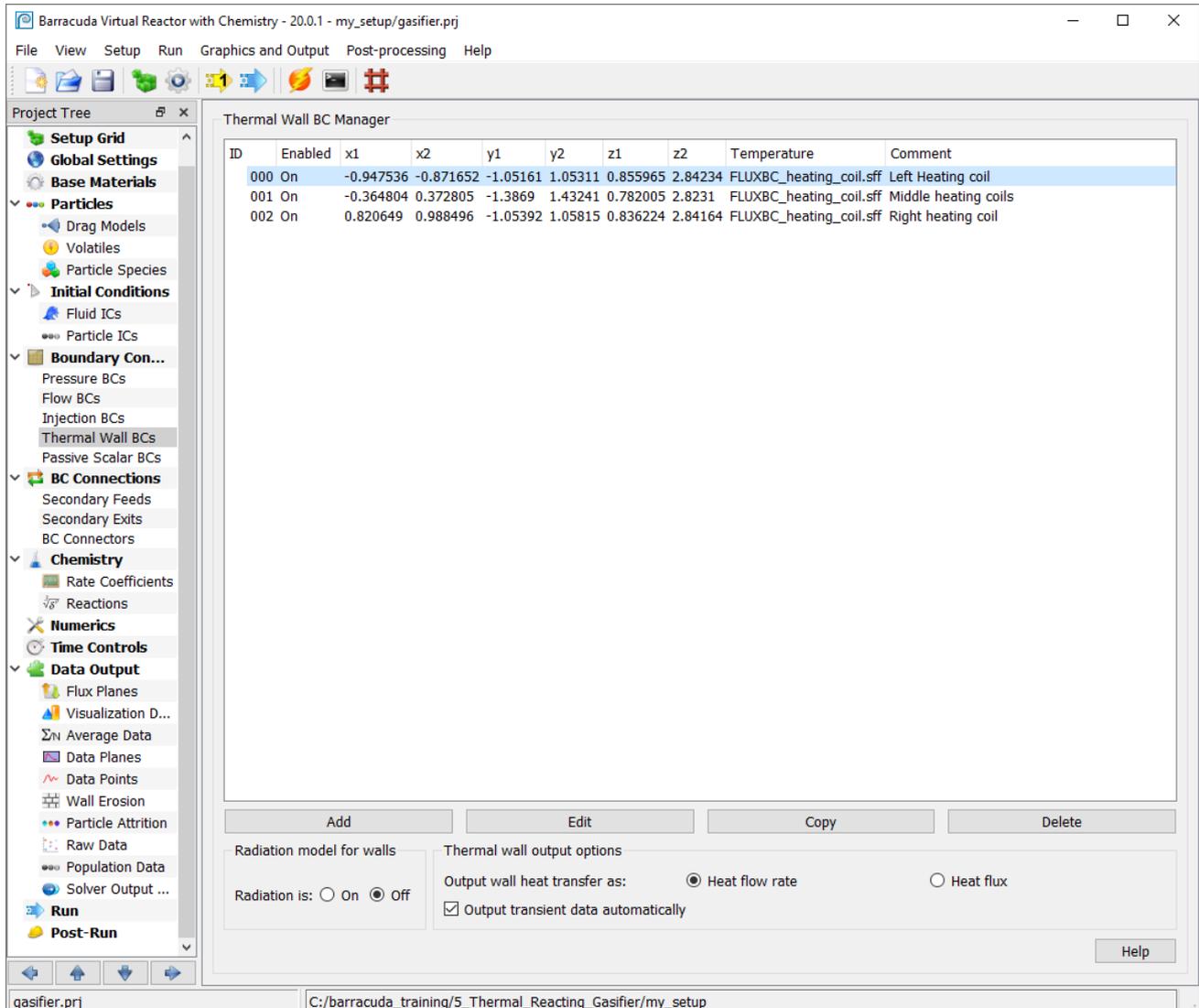
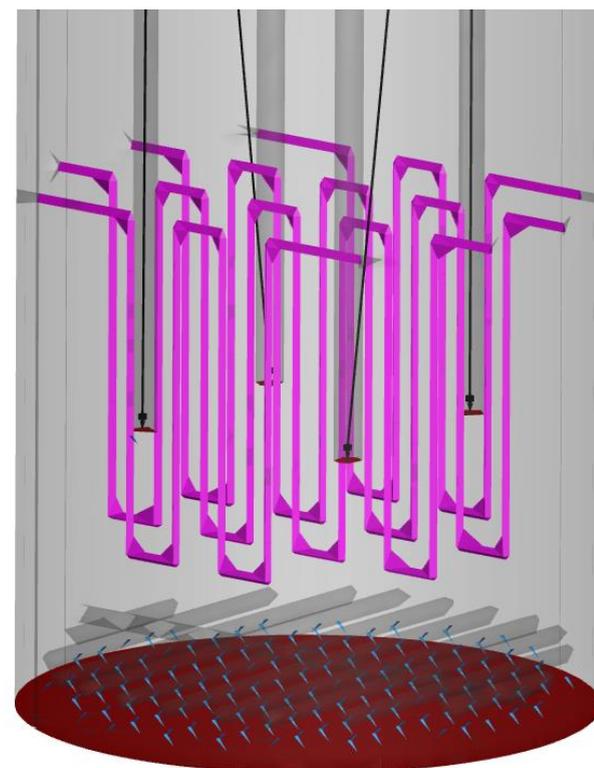
Thermal Wall BCs: Heating Coils

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

 Run Solver Setup (1 time step)



 View Boundary Conditions



The screenshot shows the 'Thermal Wall BC Manager' window in the Barracuda Virtual Reactor software. The window contains a table of boundary conditions and several control options.

ID	Enabled	x1	x2	y1	y2	z1	z2	Temperature	Comment
000	On	-0.947536	-0.871652	-1.05161	1.05311	0.855965	2.84234	FLUXBC_heating_coil.sff	Left Heating coil
001	On	-0.364804	0.372805	-1.3869	1.43241	0.782005	2.8231	FLUXBC_heating_coil.sff	Middle heating coils
002	On	0.820649	0.988496	-1.05392	1.05815	0.836224	2.84164	FLUXBC_heating_coil.sff	Right heating coil

Buttons: Add, Edit, Copy, Delete

Radiation model for walls: Radiation is: On Off

Thermal wall output options: Output wall heat transfer as: Heat flow rate Heat flux

Output transient data automatically

Help

Chemistry

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

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

The top screenshot shows the 'Chemistry Rate Coefficients Manager' window. It contains a table with 8 rows of reaction data:

ID	Name	Reaction Type	Coefficient Type	Expression	Comment
00 k0	Volume-Average	Arrhenius Chem Rate	Arrhenius Chem Rate	$6.36 T^{*1} e^{(-22645 / T)}$	Steam gasification (forward)
01 k1	Volume-Average	Arrhenius Chem Rate	Arrhenius Chem Rate	$0.0005218 T^{*2} e^{(-6319 / T + -17.29)}$	Steam gasification (reverse)
02 k2	Volume-Average	Arrhenius Chem Rate	Arrhenius Chem Rate	$6.36 T^{*1} e^{(-22645 / T)}$	CO2 gasification (forward)
03 k3	Volume-Average	Arrhenius Chem Rate	Arrhenius Chem Rate	$0.0005218 T^{*2} e^{(-2363 / T + -20.92)}$	CO2 gasification (reverse)
04 k4	Volume-Average	Arrhenius Chem Rate	Arrhenius Chem Rate	$0.006838 T^{*1} e^{(-8078 / T + -7.087)}$	Methanation (forward)
05 k5	Volume-Average	Arrhenius Chem Rate	Arrhenius Chem Rate	$0.755 T^{*0.5} e^{(-13578 / T + -0.372)}$	Methanation (reverse)
06 k6	Volume-Average	Arrhenius Chem Rate	Arrhenius Chem Rate	$4.34e+07 T^{*1} e^{(-13590 / T)}$	Combustion
07 k7	Volume-Average	Arrhenius Chem Rate	Arrhenius Chem Rate	$7.68e+10 e^{(-36640 / T)}$	WGS (forward)
08 k8	Volume-Average	Arrhenius Chem Rate	Arrhenius Chem Rate	$6.4e+09 e^{(-39260 / T)}$	WGS (reverse)

The bottom screenshot shows the 'Chemistry Reactions Manager' window. It contains a table with 8 rows of reaction data:

ID	Reaction Type	Rate	Equation	Comment
00 VA:	Stoichiometric	Equation: $C(S) + H2O \Rightarrow CO + H2$ R00 = $(k0[H2O])$		
01 VA:	Stoichiometric	Equation: $CO + H2 \Rightarrow C(S) + H2O$ R01 = $(k1[H2][CO])$		
02 VA:	Stoichiometric	Equation: $C(S) + CO2 \Rightarrow 2 CO$ R02 = $(k2[CO2])$		
03 VA:	Stoichiometric	Equation: $2 CO \Rightarrow C(S) + CO2$ R03 = $(k3[CO]^2)$		
04 VA:	Stoichiometric	Equation: $0.5 C(S) + H2 \Rightarrow 0.5 CH4$ R04 = $(k4[H2])$		
05 VA:	Stoichiometric	Equation: $0.5 CH4 \Rightarrow 0.5 C(S) + H2$ R05 = $(k5[CH4]^0.5)$		
06 VA:	Stoichiometric	Equation: $2 C(S) + O2 \Rightarrow 2 CO$ R06 = $(k6[O2])$		
07 VA:	Stoichiometric	Equation: $CO + H2O \Rightarrow CO2 + H2$ R07 = $(k7[CO]^0.5[H2O])$		
08 VA:	Stoichiometric	Equation: $CO2 + H2 \Rightarrow CO + H2O$ R08 = $(k8[H2]^0.5[CO2])$		

Chemical Reactions

Definitions and units:

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

Reaction	Stoichiometric Equation	Reaction Rate Expression ($\text{mol m}^{-3} \text{s}^{-1}$)	Source
Steam gasification	$\text{C(s)} + \text{H}_2\text{O} \rightarrow \text{CO} + \text{H}_2$	$r_{1,f} = 6.36m_C T \exp\left(\frac{-22,645}{T}\right) [\text{H}_2\text{O}]$	Syamlal, 1992
	$\text{CO} + \text{H}_2 \rightarrow \text{C(s)} + \text{H}_2\text{O}$	$r_{1,r} = 5.218 \times 10^{-4} m_C T^2 \exp\left(\frac{-6,319}{T} - 17.29\right) [\text{H}_2][\text{CO}]$	
CO ₂ gasification	$\text{C(s)} + \text{CO}_2 \rightarrow 2\text{CO}$	$r_{2,f} = 6.36m_C T \exp\left(\frac{-22,645}{T}\right) [\text{CO}_2]$	Syamlal, 1992
	$2\text{CO} \rightarrow \text{C(s)} + \text{CO}_2$	$r_{2,r} = 5.218 \times 10^{-4} m_C T^2 \exp\left(\frac{-2,363}{T} - 20.92\right) [\text{CO}]^2$	
Methanation	$0.5\text{C(s)} + \text{H}_2 \rightarrow 0.5\text{CH}_4$	$r_{3,f} = 6.838 \times 10^{-3} m_C T \exp\left(\frac{-8,078}{T} - 7.087\right) [\text{H}_2]$	Syamlal, 1992
	$0.5\text{CH}_4 \rightarrow 0.5\text{C(s)} + \text{H}_2$	$r_{3,r} = 0.755m_C T^{0.5} \exp\left(\frac{-13,578}{T} - 0.372\right) [\text{CH}_4]^{0.5}$	
Combustion	$2\text{C(s)} + \text{O}_2 \rightarrow 2\text{CO}$	$r_4 = 4.34 \times 10^7 \theta_C T \exp\left(\frac{-13,590}{T}\right) [\text{O}_2]$	Yoon, 1978
Water gas- shift	$\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$	$r_{5,f} = 7.68 \times 10^{10} \exp\left(\frac{-36,640}{T}\right) [\text{CO}]^{0.5} [\text{H}_2\text{O}]$	Bustamante, 2005
	$\text{CO}_2 + \text{H}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$	$r_{5,r} = 6.4 \times 10^9 \exp\left(\frac{-39,260}{T}\right) [\text{H}_2]^{0.5} [\text{CO}_2]$	Bustamante, 2004

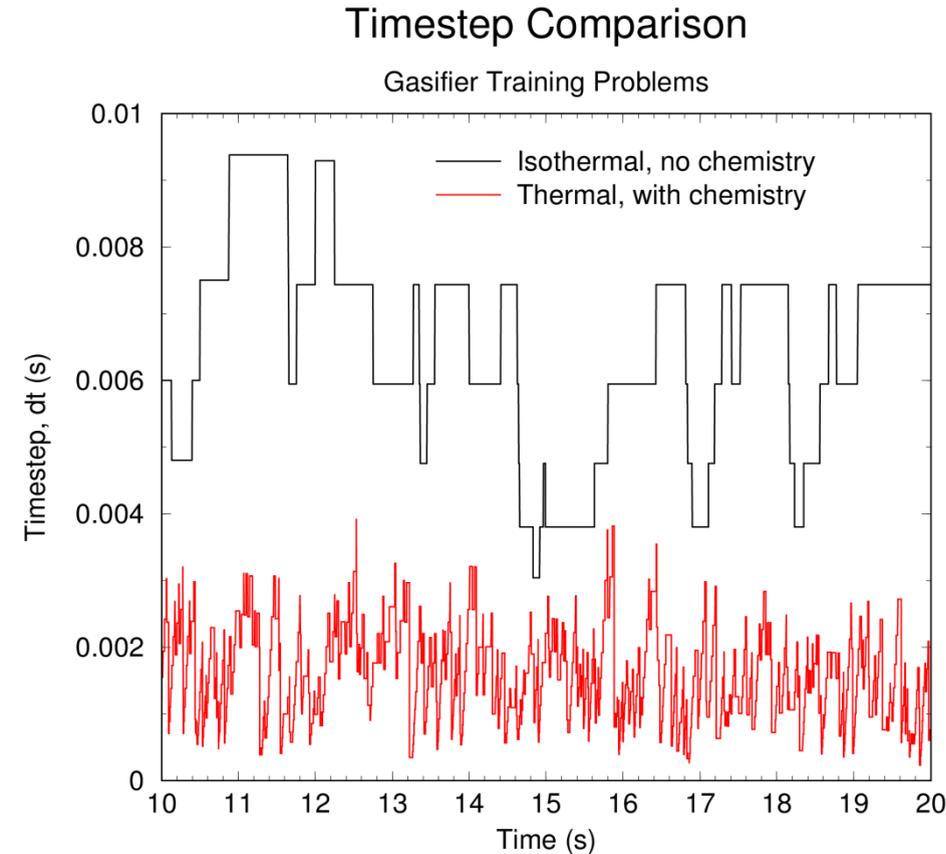
Time Controls

Leave the end-time at 100 s.

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

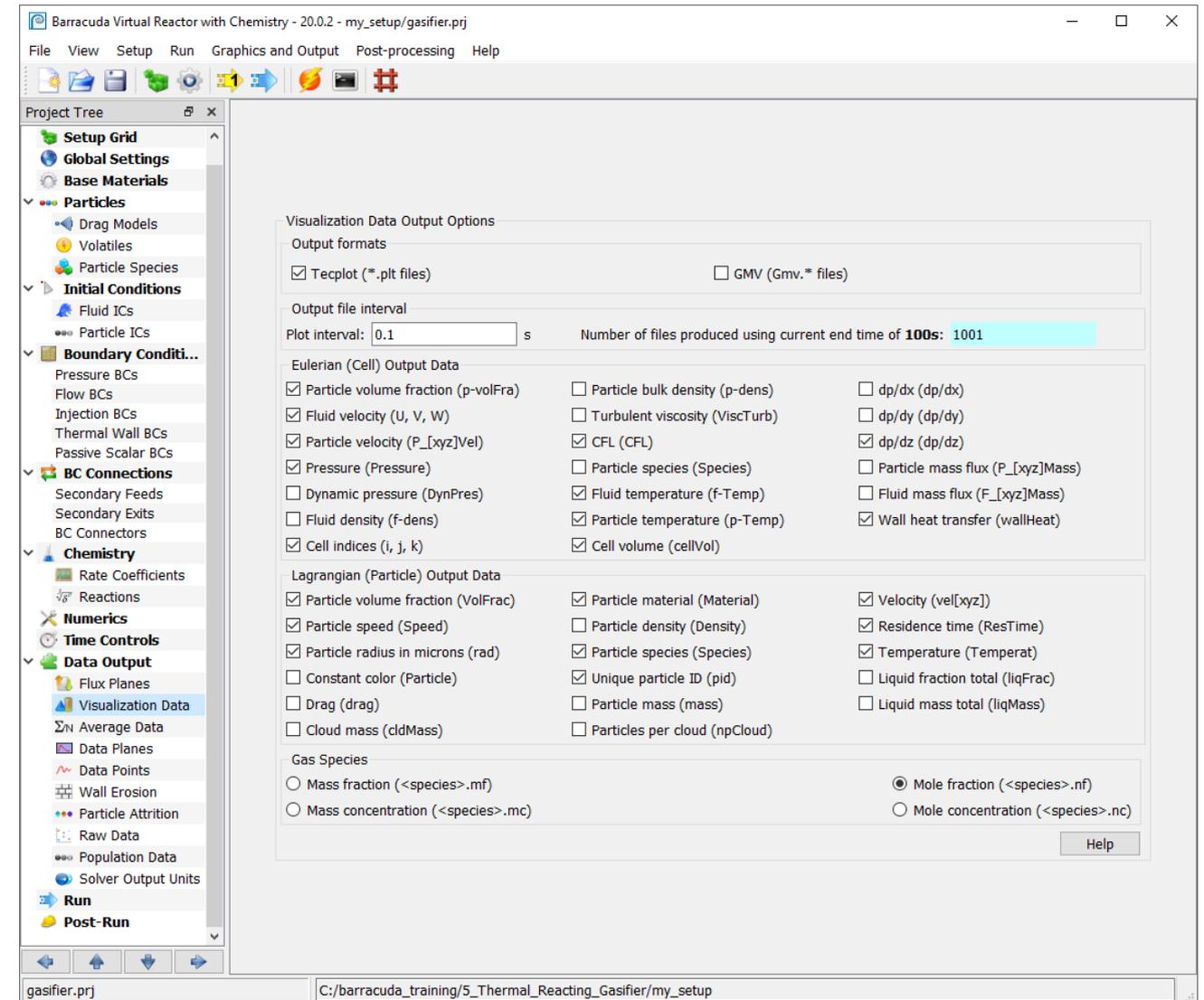
Leave the time-step at 0.01 s.

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



Tecplot Output Options

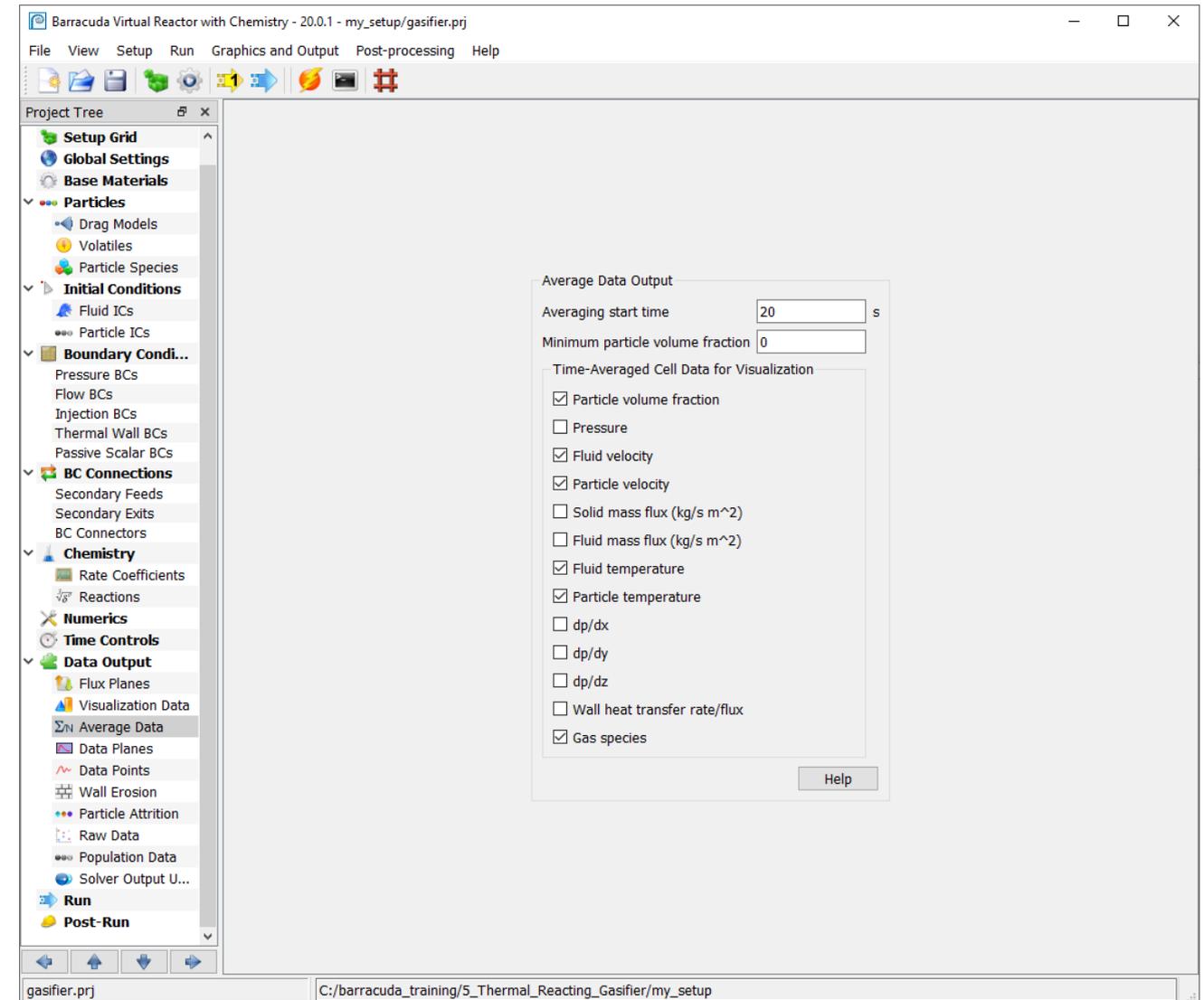
Since thermal and chemistry are now being incorporated into the model, it is important to review the data output settings. Make sure that all necessary output data is selected.



Average Data

Leave averaging start time at 20 s

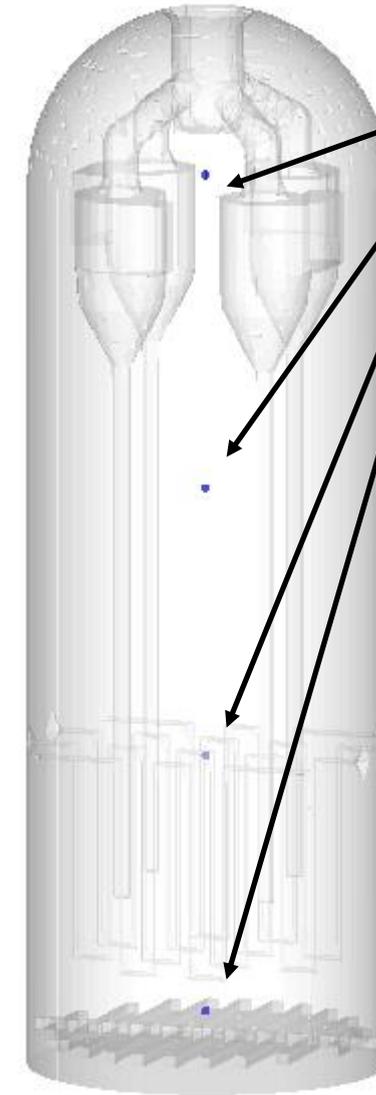
Since we have now turned on thermal and chemistry, be sure to check the boxes for Fluid and Particle temperature.



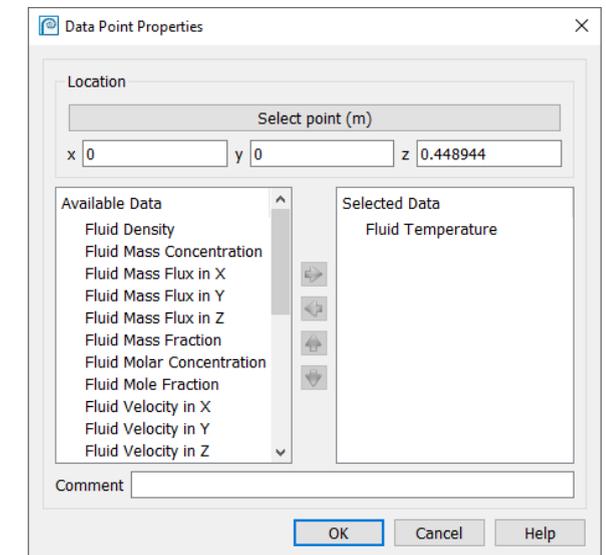
Data Points

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

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



4 data points along the central axis



Check Model Setup

Run the simulation for a single time-step.

Check the Boundary Conditions:

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

Check the Initial Conditions:

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

Check Data Output:

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

Review the project setup with your instructor and then Run Solver

The screenshot displays the Barracuda Virtual Reactor software interface. The main window shows the 'Run Solver Setup' dialog box, which is used to configure the simulation. The dialog box is divided into several sections: 'Verify Setup', 'Run Calculation', and 'Universal Options'. The 'Verify Setup' section includes a 'Run Solver Setup (1 time step)' button and several 'View' buttons for initial particles, species, boundary conditions, flux planes, and data points. The 'Run Calculation' section includes 'Solver Launch Options' with checkboxes for 'CPU Parallel' and 'GPU Parallel', and a 'Test solver GPU memory requirements' button. The 'Universal Options' section includes settings for 'If temperature limits reached', 'If chemistry mass imbalance', and 'If minimum disk limit reached'. The 3D visualization on the right shows a gasifier reactor with a bed of particles at the bottom, colored by Particle Volume Fraction from 0 (blue) to 0.6 (red). The reactor has two vertical tubes in the center and several horizontal tubes at the bottom. The top of the reactor is a dome shape.

Post processing

Training Objectives

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

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

Copy Layout files

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

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

Time-Integrated Particle Entrainment

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

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

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

The screenshot shows the Tecplot 360 EX 2019 R1 interface. The main plot displays three curves representing Cyclone 1 (blue), Cyclone 2 (red), and Cyclone 3 (green). The Y-axis ranges from -50 to 50. A 'Mapping Style' dialog box is open, showing a table of mappings. A 'Create Mappings' sub-dialog is also open, showing the configuration for 'Cyclone 4' with X-Axis: 1: Time (s) and Y-Axis: 8: Time integrated particle mass of all s. A red arrow points to the 'Mapping Style' button in the main interface, and another red arrow points to the 'Create Map...' button in the Mapping Style dialog.

Map Number	Map Name	Show Map	Zone
1	Fluid mass flow rate (kg/s)	<input type="checkbox"/>	1: Time (s)
2	Fluid volume flow rate (m ³ /s)	<input type="checkbox"/>	1: Time (s)
3	Fluid mass flux (kg/s*m ²)	<input type="checkbox"/>	1: Time (s)
4	Time integrated fluid mass crossing flux plane...	<input type="checkbox"/>	1: Time (s)
5	Particle mass flow rate of all species (5 time st...	<input type="checkbox"/>	1: Time (s)
6	Particle mass flux of all species (5 time step av...	<input type="checkbox"/>	1: Time (s)
7	Cyclone 1	<input checked="" type="checkbox"/>	1: Time (s)
8	Time integrated particle mass of species 1 (kg)	<input type="checkbox"/>	1: Time (s)
9	Time integrated particle mass of species 2 (kg)	<input type="checkbox"/>	1: Time (s)
10	Time integrated fluid energy crossing flux pla...	<input type="checkbox"/>	1: Time (s)
11	Time integrated particle energy crossing flux ...	<input type="checkbox"/>	1: Time (s)
12	Average residence time for all particle species ...	<input type="checkbox"/>	1: Time (s)
13	Average residence time for particle species 1 (s)	<input type="checkbox"/>	1: Time (s)
14	Average residence time for particle species 2 (s)	<input type="checkbox"/>	1: Time (s)
15	Cyclone 2	<input checked="" type="checkbox"/>	1: Time (s)
16	Cyclone 3	<input checked="" type="checkbox"/>	1: Time (s)

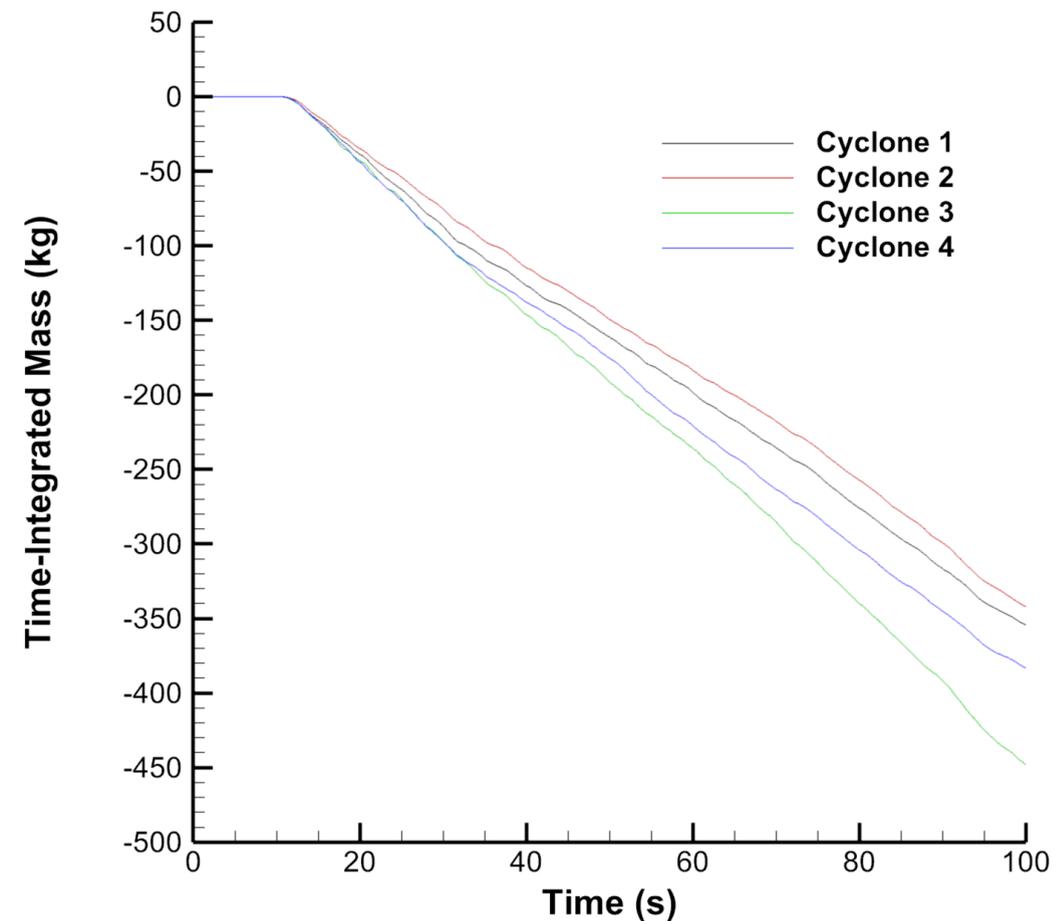
Interpreting Time-Integrated Data

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

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

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

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



Outlet Gas Composition

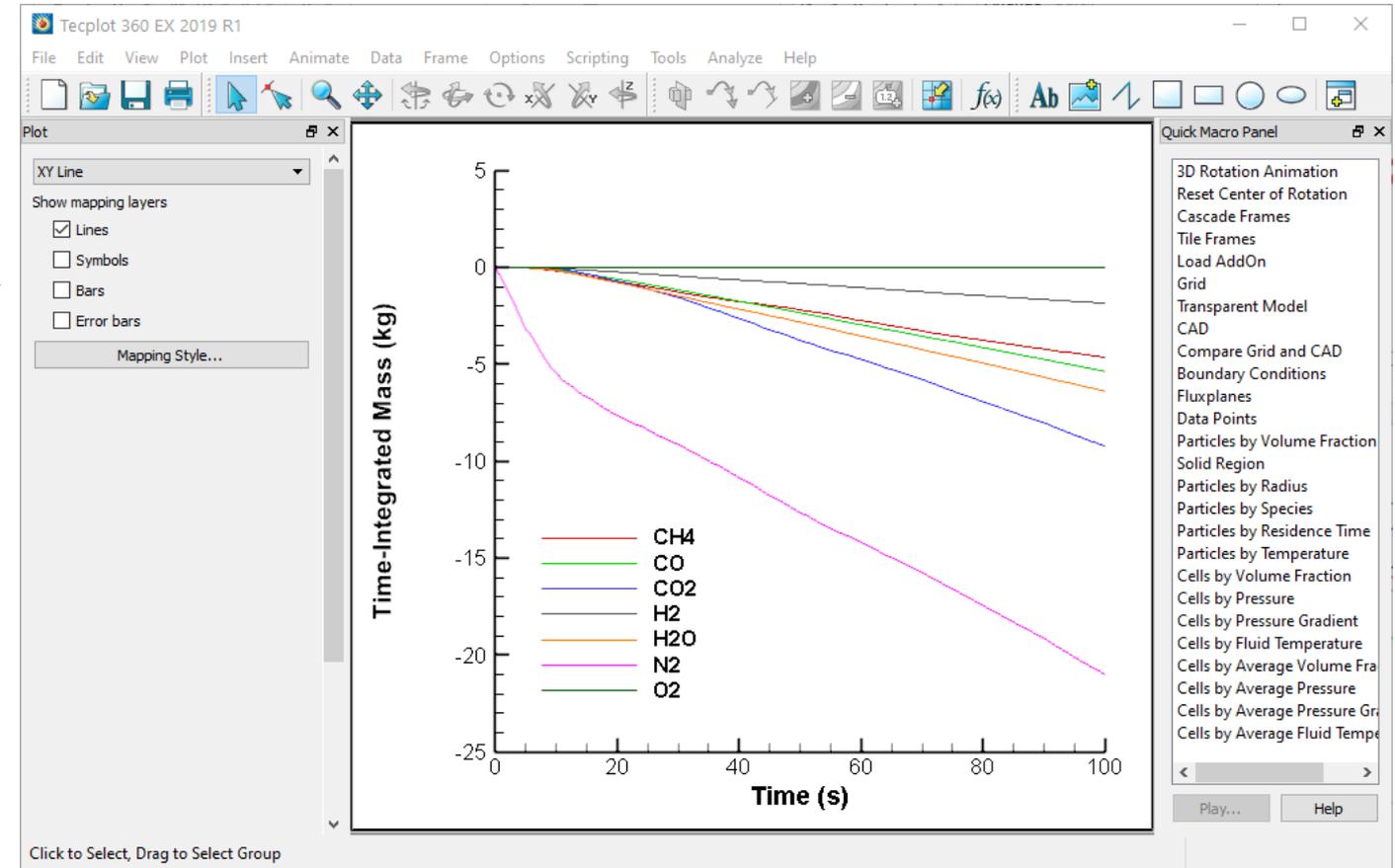
For chemically reacting systems, the gas composition at system outlets is often of interest.

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

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

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

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



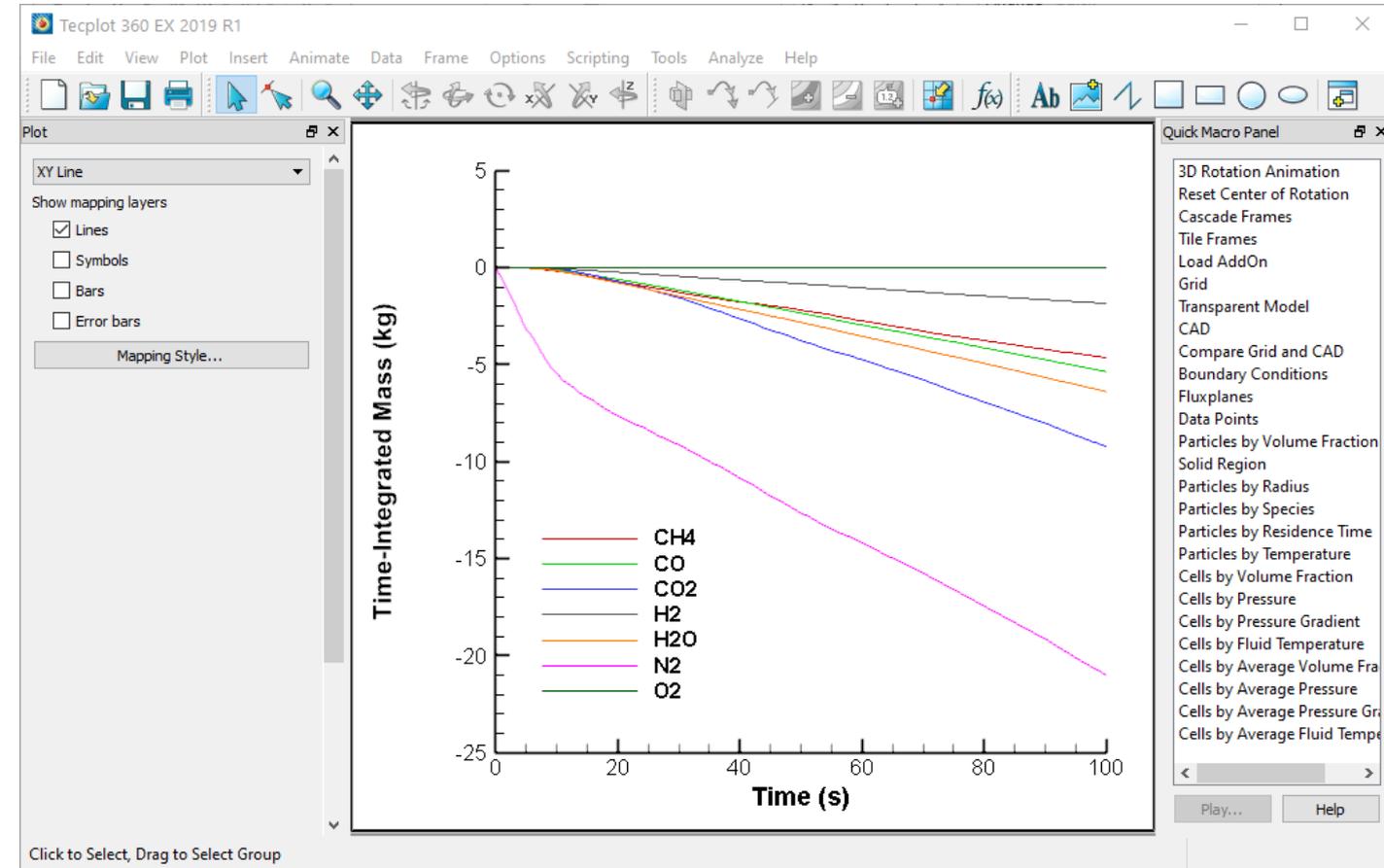
Interpretation of Gas Composition Plot

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

The sign convention at Boundary Condition flux planes is:

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

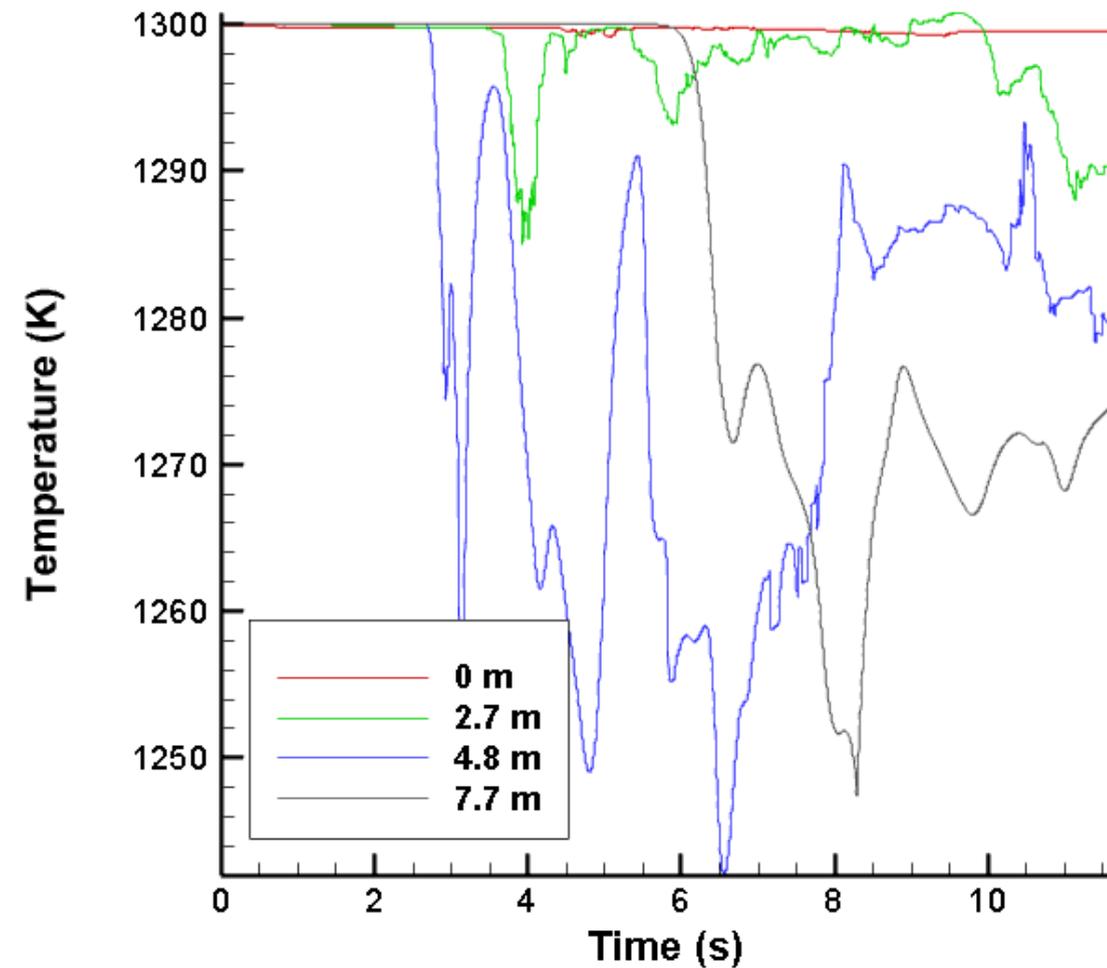
The gas composition plot can be used to help judge when the system reaches pseudo-steady state. Once the time-integrated lines achieve constant slope, the gas composition at the outlet is no longer changing.



Plotting Fluid Temperature from Data Points

Create an xy plot from trans.data00 file

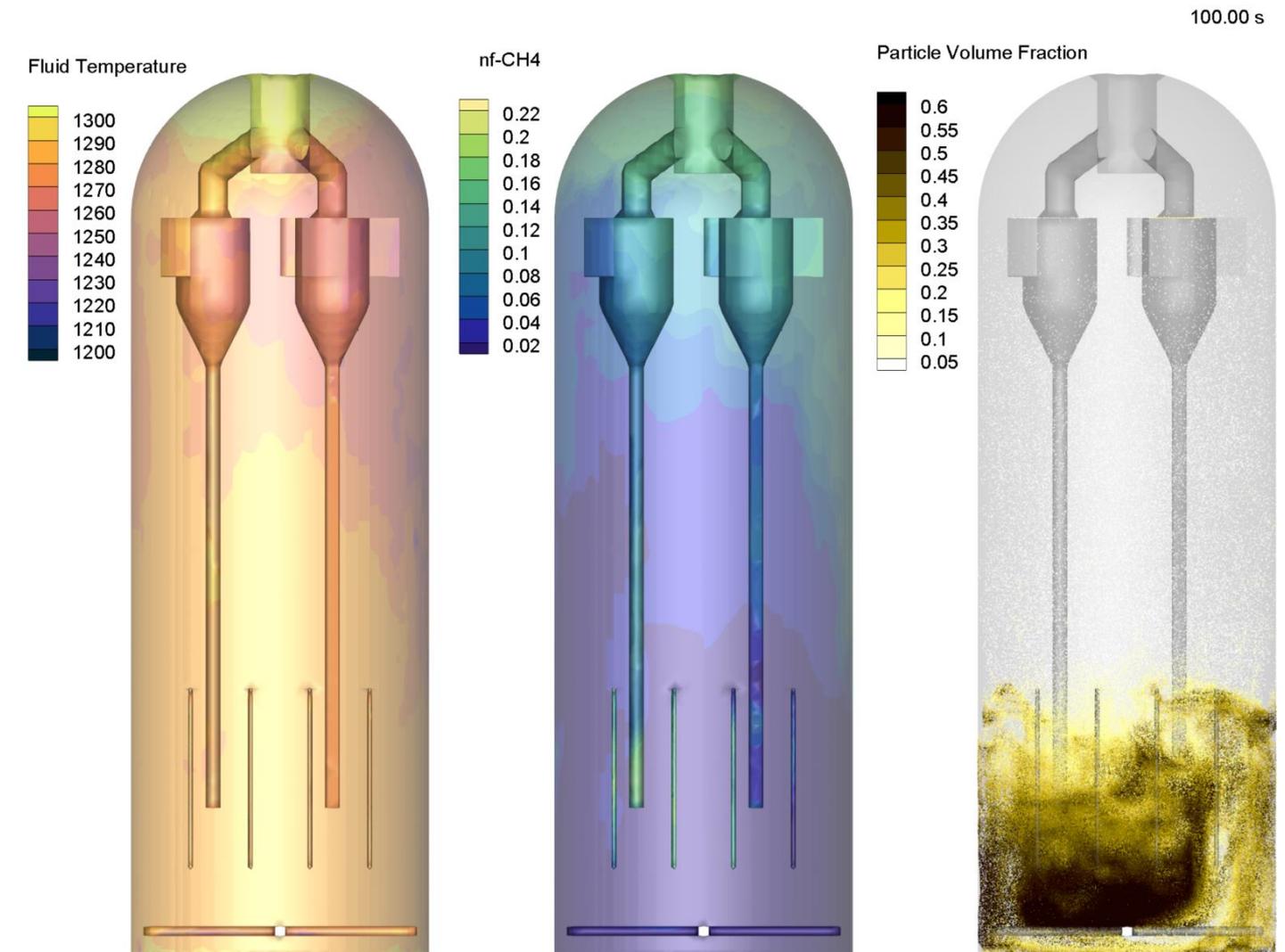
Plot data from all 4 data points



Combining Animations

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

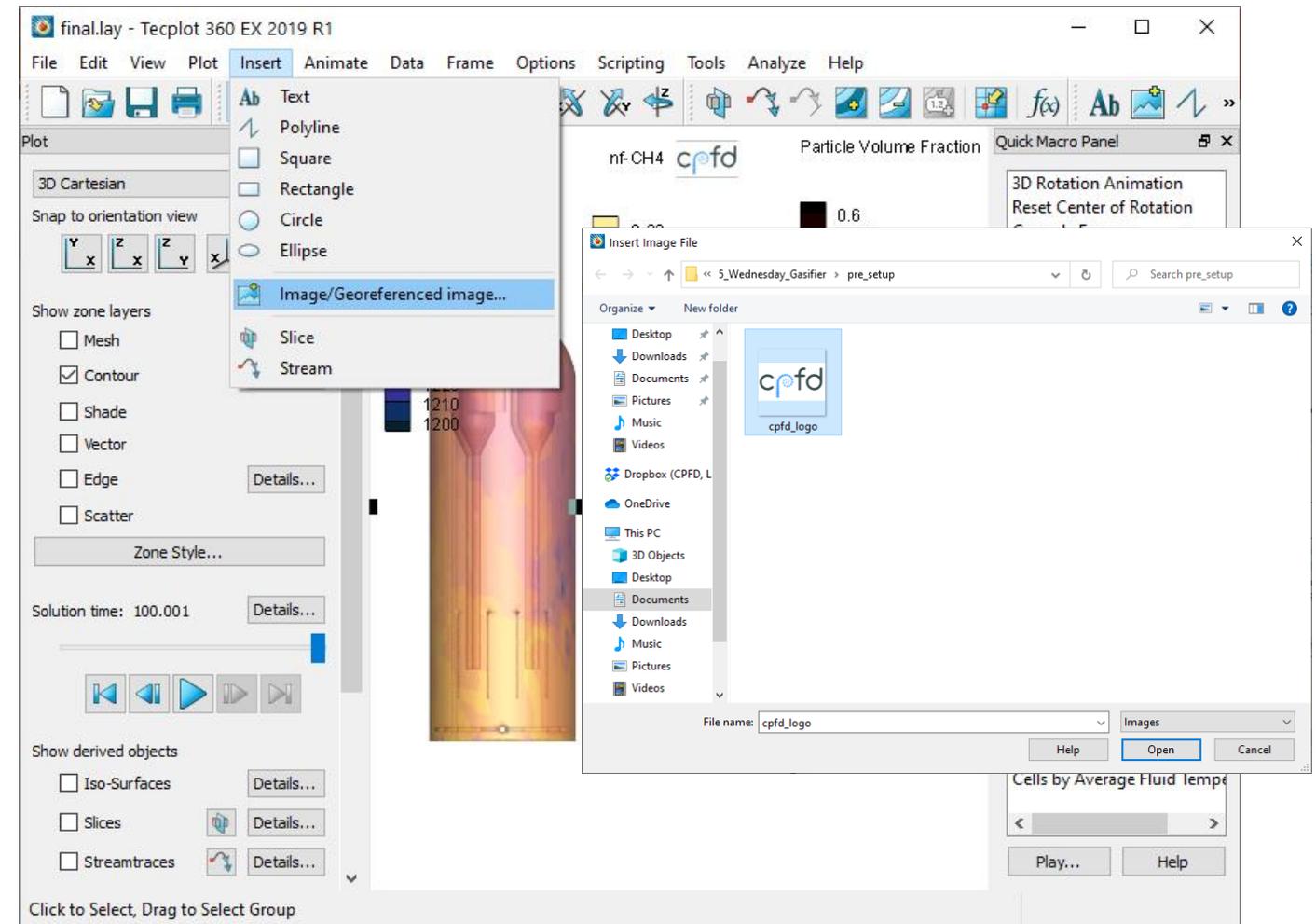
Watch this [video](#) and then create an image like the one to the right



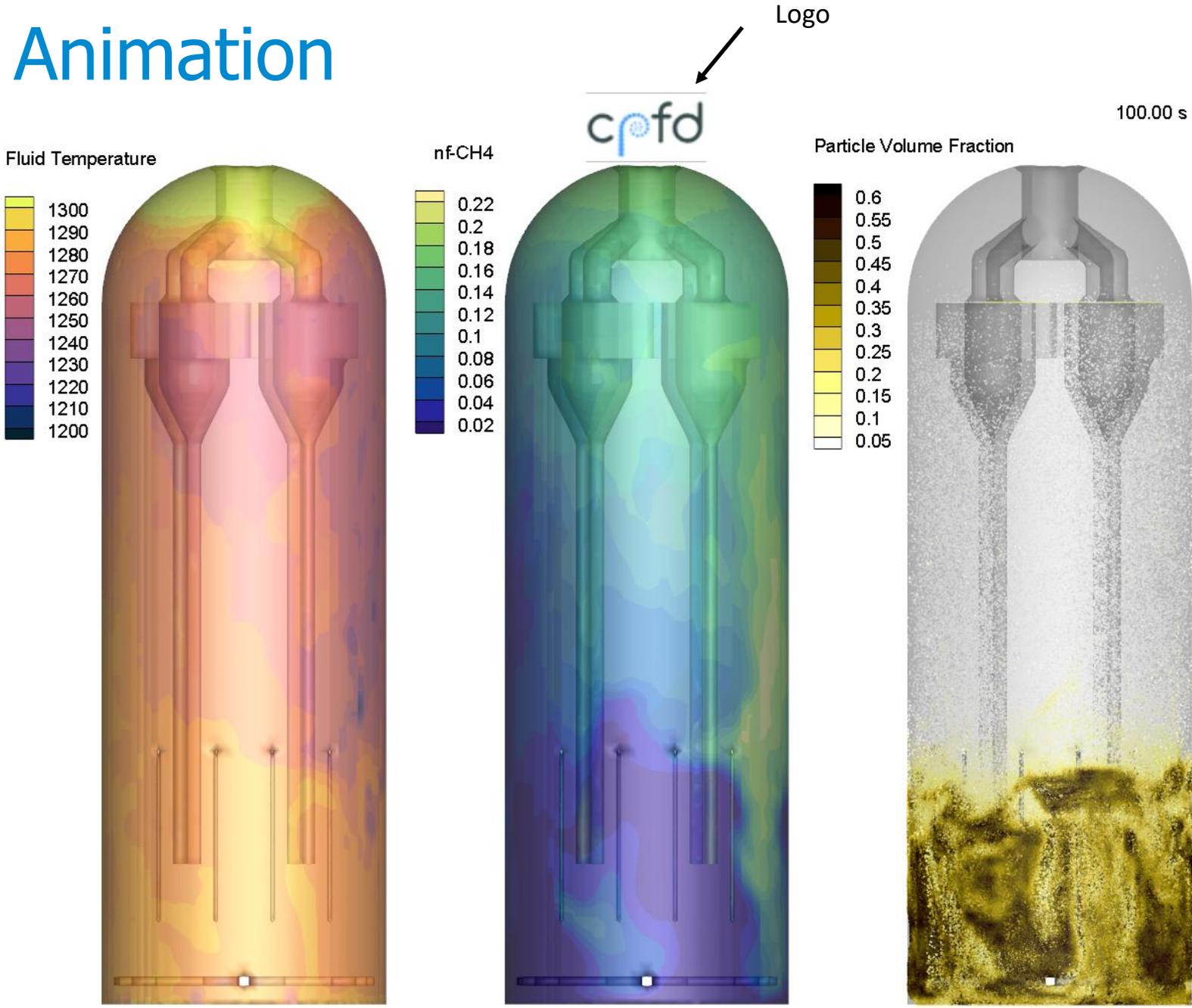
Adding Logos to Animations

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

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



The Final Animation



Additional Post-Processing

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

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