Wednesday Gasifier Training Problem
Part 1: Project Setup

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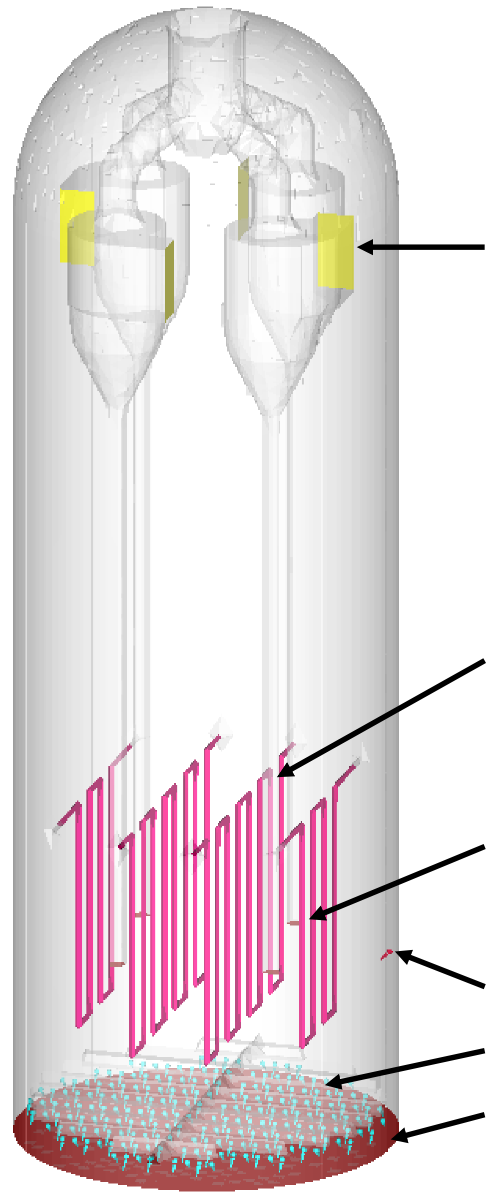
Training Objectives

- This training exercise adds more realism and complexity to the gasifier model defined yesterday.
  - More internal geometries are included: gas sparger and heating coils
  - Injection points are added to introduce fresh coal and steam into the system
  - Chemistry and thermal calculations are added
  - BC Connection filters are used for advanced post-processing
- Set up a complex model based on a previously defined simplified model.
  - Copy a project file to a new location using **Save Case As…**
  - Modify the grid as necessary
  - Adjust boundary condition definitions as necessary
  - Add chemistry and thermal definitions to project
- Use several newly introduced features of Barracuda.
  - Thermal calculations
  - Injection BCs
  - Chemical reactions

Process Sheet

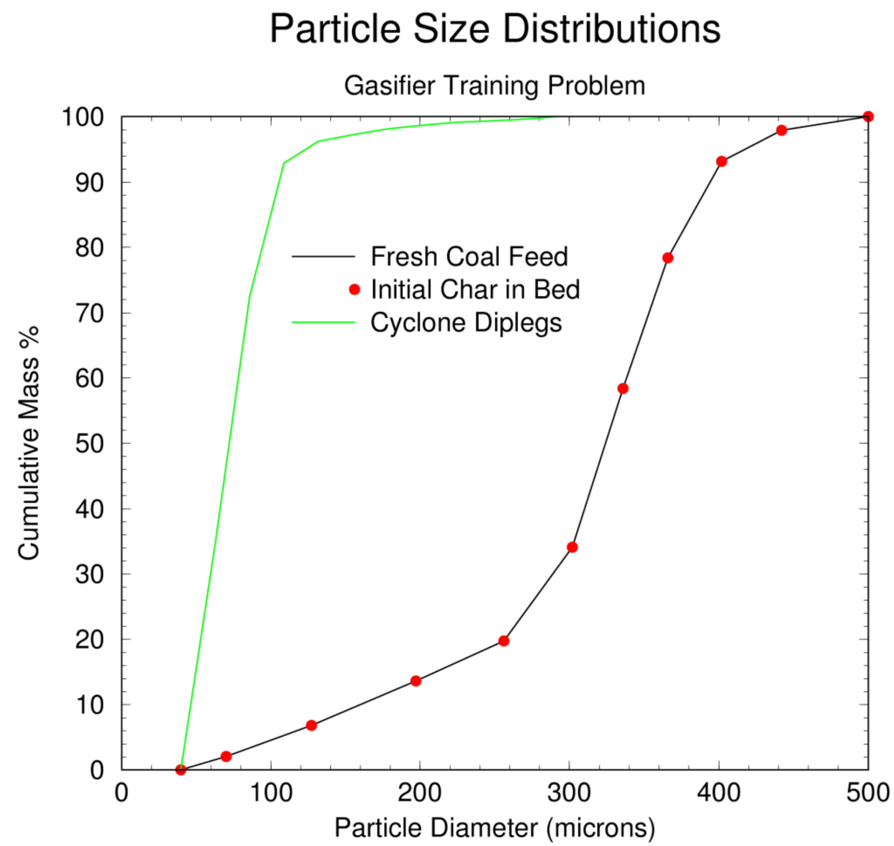
- Thermal calculations are enabled, initial temperature of particles and gas in bed set to 1300 K.
- Chemical reactions are included.

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_2O	None
Fresh Coal Feed	Mass flow rate = 5 g/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	Velocity = 0.5 m/s Temperature = 1300 K Gas: pure N_2	Cyclone dipleg particles with flow rate set to match elutriation into each cyclone.



Particle Properties

- Initial bed particles:
  - Assumed to be already devolatilized.
  - Particle composition (mass fractions):
    0.8999 Carbon (s), 0.1 Ash (s), and 0.0001 Volatiles (g)
  - PSD will be same as Tuesday Gasifier with name "psd_initial_char_in_bed.sff".
- Fresh coal particles:
  - Multi-material including volatiles which are released.
  - Particle composition (mass fractions):
    0.45 Carbon (s), 0.05 Ash (s), 0.5 Volatile
  - Volatile composition (mass fractions):
    0.4144 CH_4, 0.1702 CO, 0.0444 CO_2, 0.111 H_2, 0.26 H20
  - PSD will be same as Tuesday Gasifier with name "psd_fresh_coal_feed_particles.sff".
- Cyclone dipleg particles:
  - Composition, temperature, and PSD will be automatically determined by BC Connection.



For material properties, assume that the fresh coal particles have a density of 1450 kg/m^3 and that the initial bed and cyclone dipleg particles have a density of 725 kg/m^3

Chemical Reactions

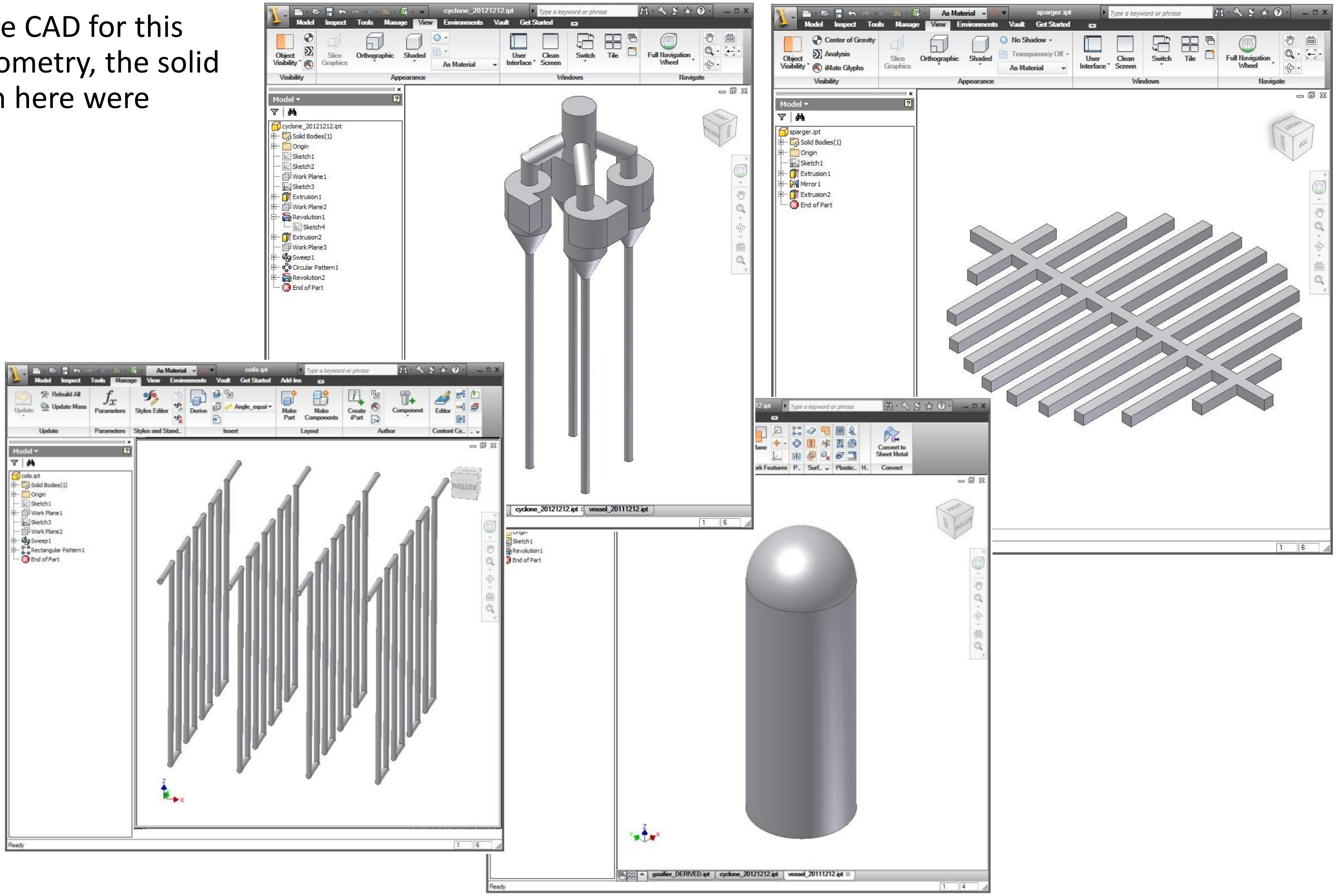
Reaction	Stoichiometric Equation	Reaction Rate Expression (mol m^{-3} s^{-1})	Source
Steam gasification	$C(s)+H_2O \rightarrow CO+H_2$	$r_{1,f} = 6.36 m_C T \exp\left(\frac{-22{,}645}{T}\right)[H_2O]$	Syamlal, 1992
	$CO+H_2 \rightarrow C(s)+H_2O$	$r_{1,r} = 5.218\times10^{-4} m_C T^2 \exp\left(\frac{-6{,}319}{T}-17.29\right)[H_2][CO]$	
CO_2 gasification	$C(s)+CO_2 \rightarrow 2CO$	$r_{2,f} = 6.36 m_C T \exp\left(\frac{-22{,}645}{T}\right)[CO_2]$	Syamlal, 1992
	$2CO \rightarrow C(s)+CO_2$	$r_{2,r} = 5.218\times10^{-4} m_C T^2 \exp\left(\frac{-2{,}363}{T}-20.92\right)[CO]^2$	
Methanation	$0.5C(s)+H_2 \rightarrow 0.5CH_4$	$r_{3,f} = 6.838\times10^{-3} m_C T \exp\left(\frac{-8{,}078}{T}-7.087\right)[H_2]$	Syamlal, 1992
	$0.5CH_4 \rightarrow 0.5C(s)+H_2$	$r_{3,r} = 0.755 m_C T^{0.5} \exp\left(\frac{-13{,}578}{T}-0.372\right)[CH_4]^{0.5}$	
Combustion	$2C(s)+O_2 \rightarrow 2CO$	$r_4 = 4.34\times10^{7} \theta_C T \exp\left(\frac{-13{,}590}{T}\right)[O_2]$	Yoon, 1978
Water gas- shift	$CO+H_2O \rightarrow CO_2+H_2$	$r_{5,f} = 7.68\times10^{10} \exp\left(\frac{-36{,}640}{T}\right)[CO]^{0.5}[H_2O]$	Bustamante, 2005
	$CO_2+H_2 \rightarrow CO+H_2O$	$r_{5,r} = 6.4\times10^{9} \exp\left(\frac{-39{,}260}{T}\right)[H_2]^{0.5}[CO_2]$	Bustamante, 2004

What do we want to learn from this model?

- Always keep in mind why you are running any model.
- For the previous, simplified gasifier training problem, we wanted to learn the following:
    - General fluidization characteristics
    - Entrainment rate of particles
- For this more complex model, we would like to additionally study:
    - Are there any hot-spots in the bed?
    - What is the gas composition leaving the cyclones?
    - Did the addition of thermal and chemistry affect the conclusions drawn based on studying results of the simplified model?

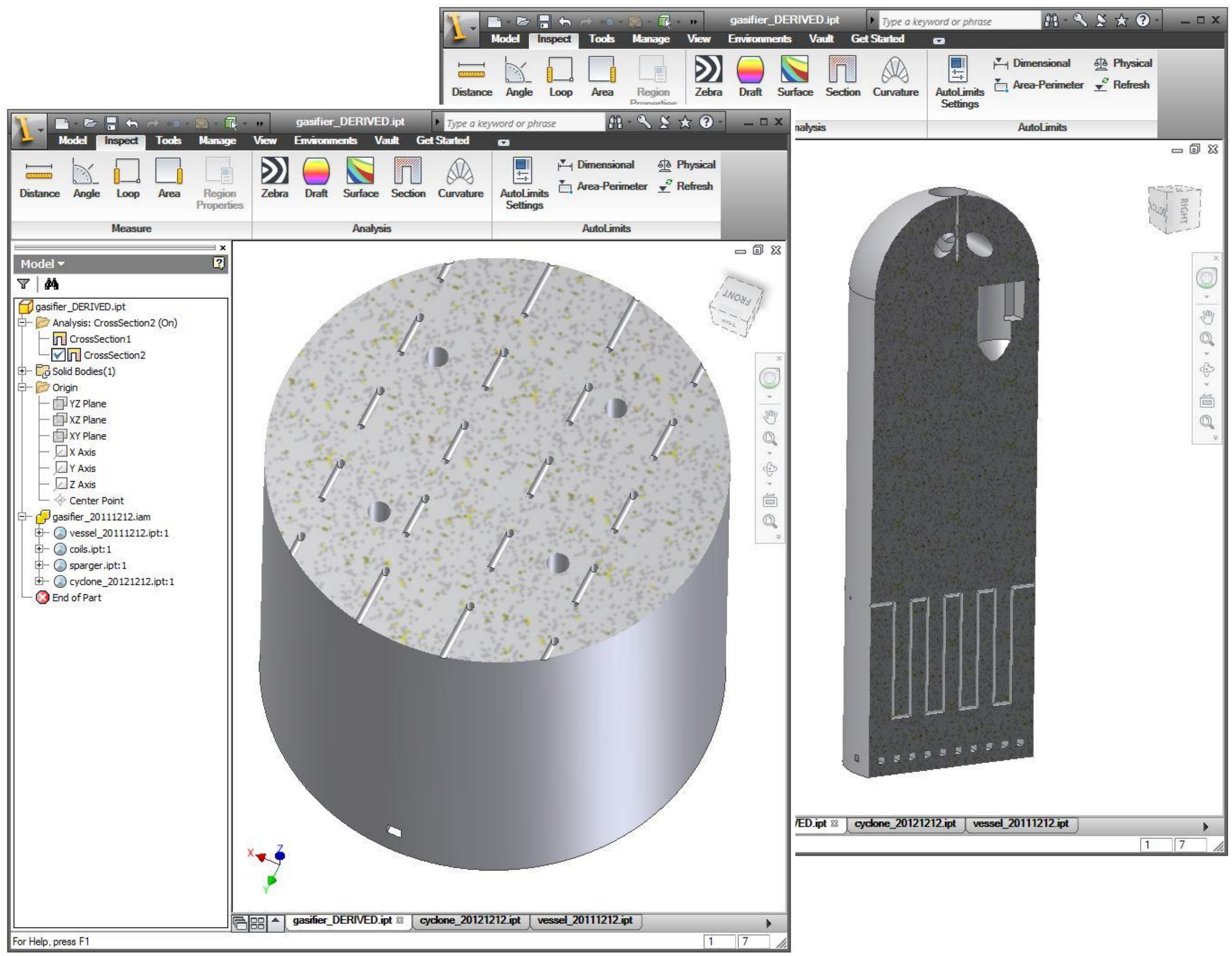
More Complex Geometry

- To create the CAD for this complex geometry, the solid parts shown here were created.



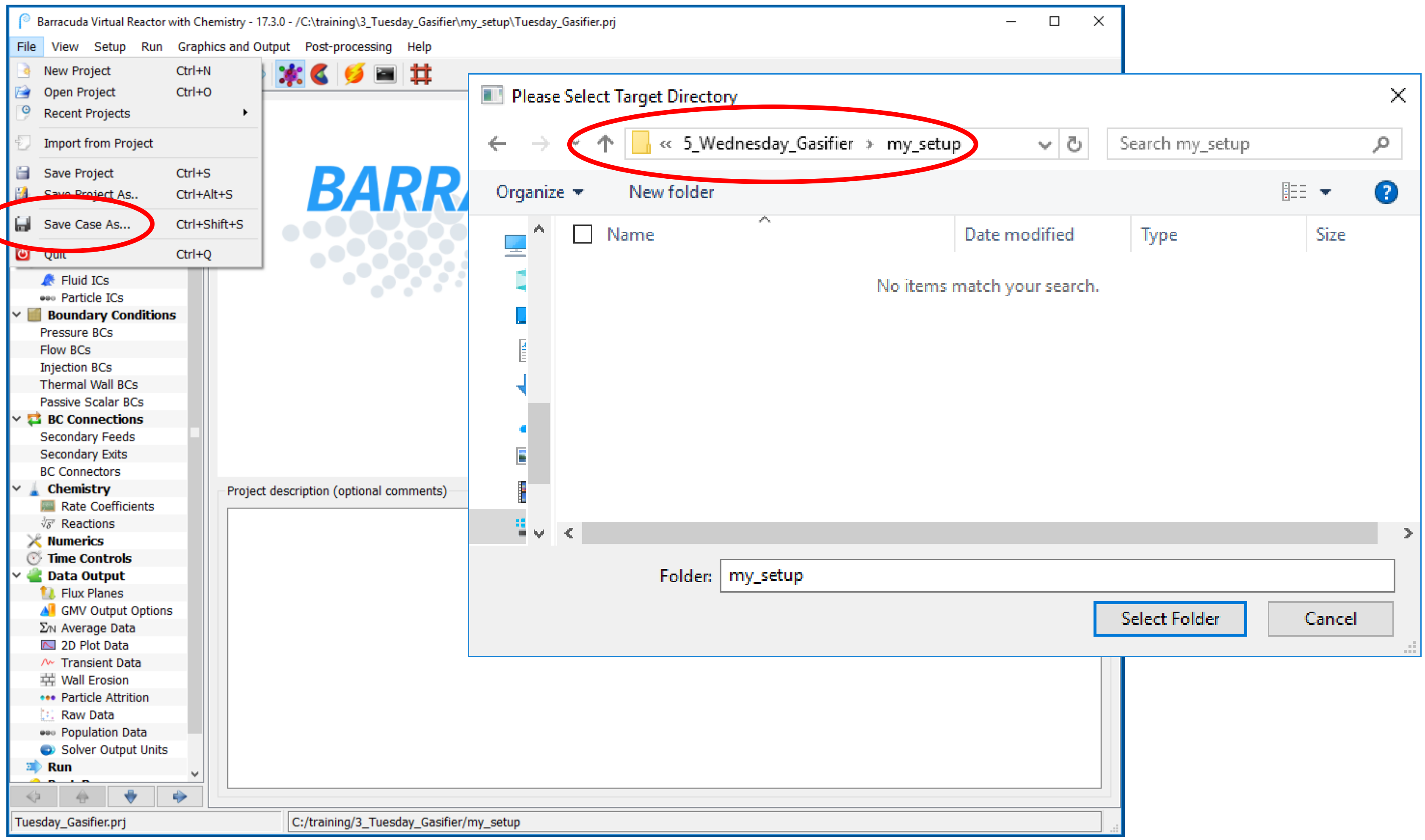
Final STL File with Internal Structures Subtracted

- The cyclones, gas sparger, and heating coils were subtracted from the vessel.
- The example here was made with AutoDesk Inventor, using a "Derived Part" based on an assembly of the individual parts.
- This resulted in a solid model of the internal flow volume in which particles and fluid can travel.
- Remember: we need a model of the interior flow volume. We do not want a "thin-walled" geometry.



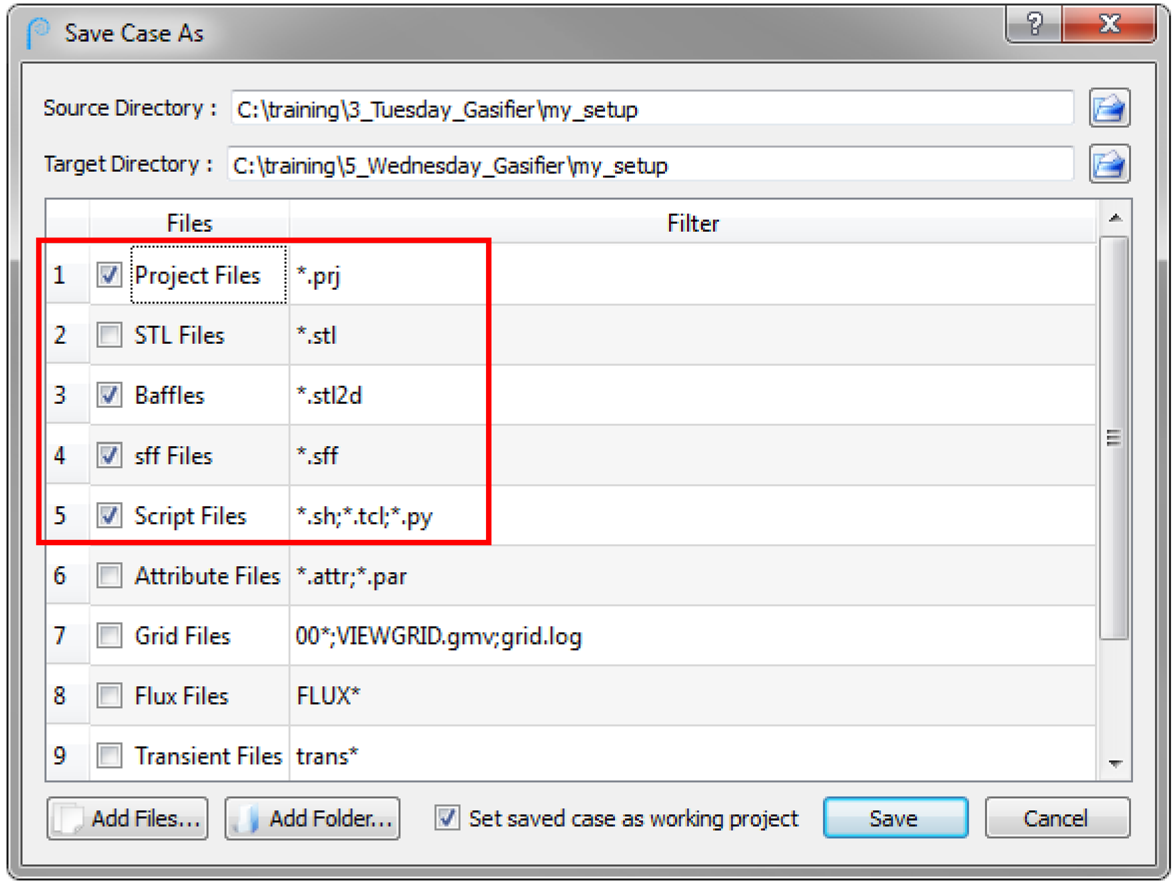
Copy Tuesday Gasifier project using “Save Case As…”

- Open the Tuesday gasifier project with Barracuda VR.
- Use the Barracuda GUI menu **File →Save Case As…**
- For the Target Directory, navigate to and select **5_Wednesday_Gasifier/my_setup**



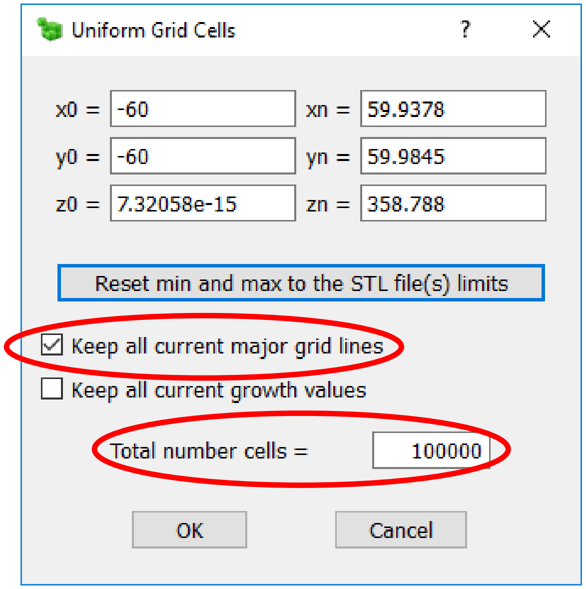
Selecting Files in the **Save Case As…** Dialog

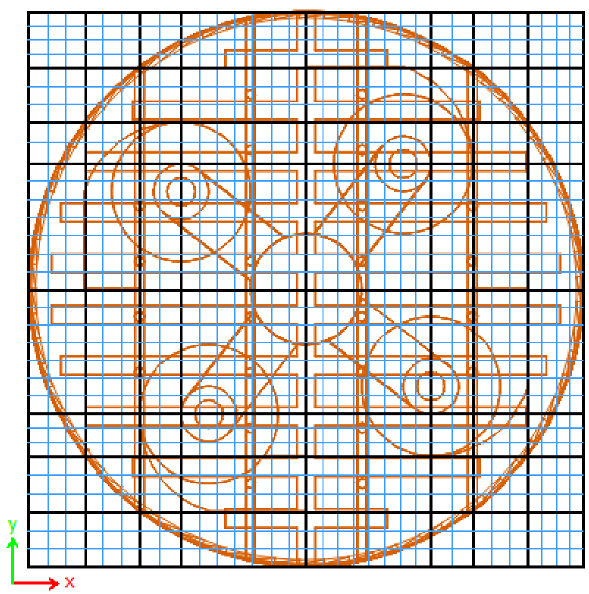
- A full Barracuda VR project setup includes the base project file (*prj), the geometry (*stl), transient boundary condition files (*sff), particle size distribution files (*sff), and potentially other files as well.
- The **Save Case As…** dialog allows you to select exactly which files you want to include or exclude during the copy operation.
- For the current case, keep:
  - Project Files
  - sff Files
  - Script Files
- Because the Wednesday Gasifier geometry is different, do not keep:
  - STL Files
  - Grid Files
- Also, we don't want to copy over any results files (Flux, Transient, or GMV).



Gridding: Add the New STL File

- In the **Setup Grid** section, highlight “gasifier_tuesday.stl” and click **Remove**.
- Click **Add** and select the new geometry, “gasifier_wednesday.stl”.
- There are more internals in the current STL file than in the Tuesday Gasifier.
- Use **Set uniform grid**, and change the total number of cells to 100,000. Be sure to click on **Keep all current major grid lines**, so that grid lines for the cyclone horns and diplegs are not lost
- If you generate the grid now, you can inspect the STL geometry using **View Ouptut → View CAD**.
- Using **View Output → View Transparent Model**, you can see the regions that need attention during gridding.

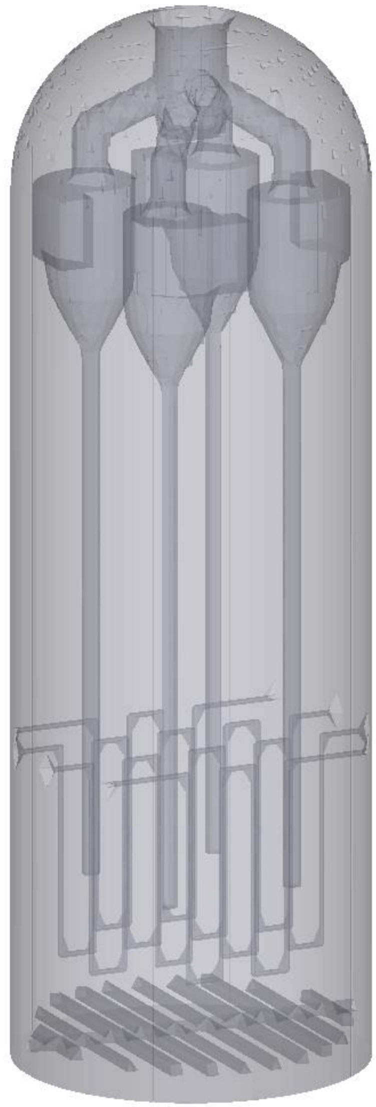




Modify the Grid to Capture Internal Structures

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

  Tuesday: 28,556
  Wednesday: 119,658



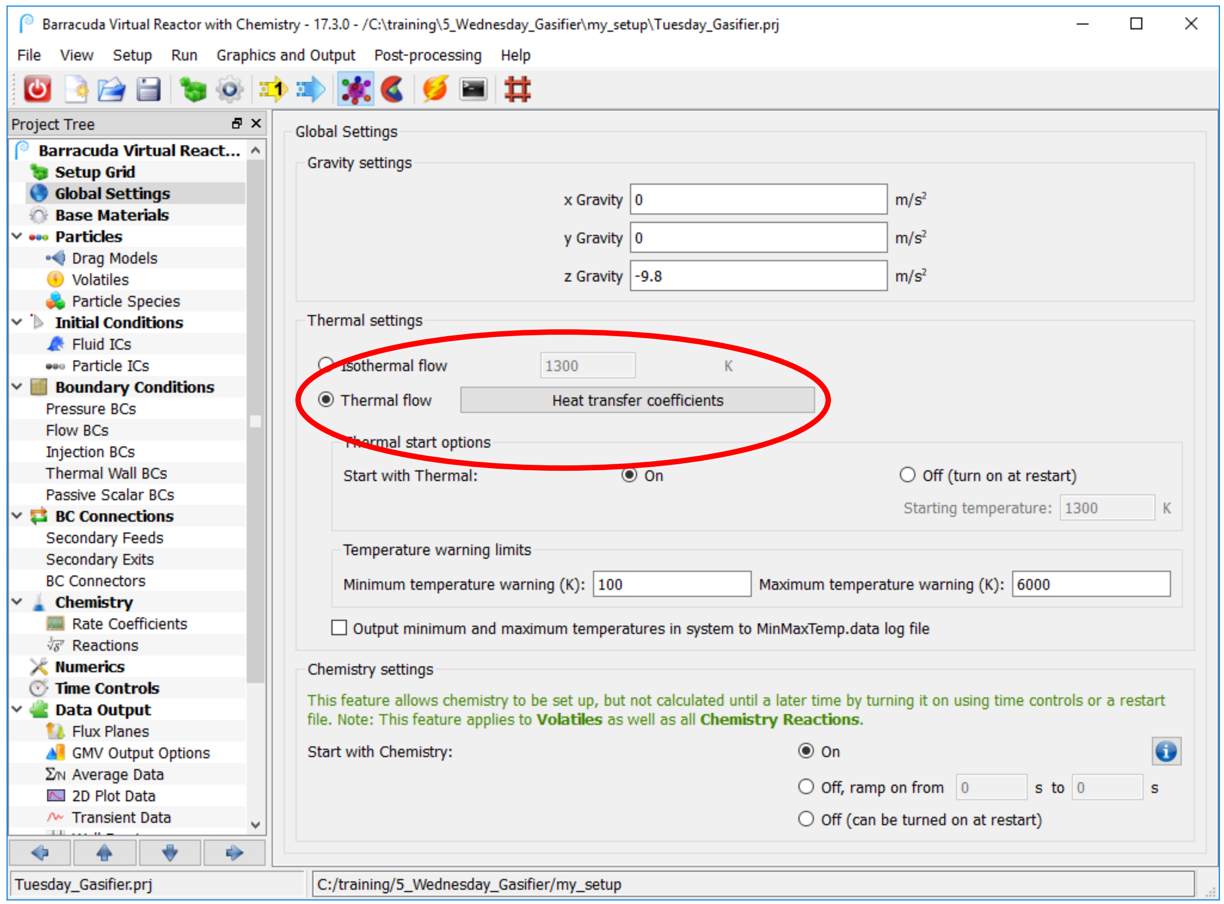
At left is a view of the pre-setup grid, using the built-in shortcut **View Output, View Transparent Model**. Notice that not all of the geometry is perfectly captured. But, it is possible to not completely miss any of the internal structures.

Tip: To facilitate checking the transparent model during gridding, save the attribute file by clicking on **File → Put attributes**.

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

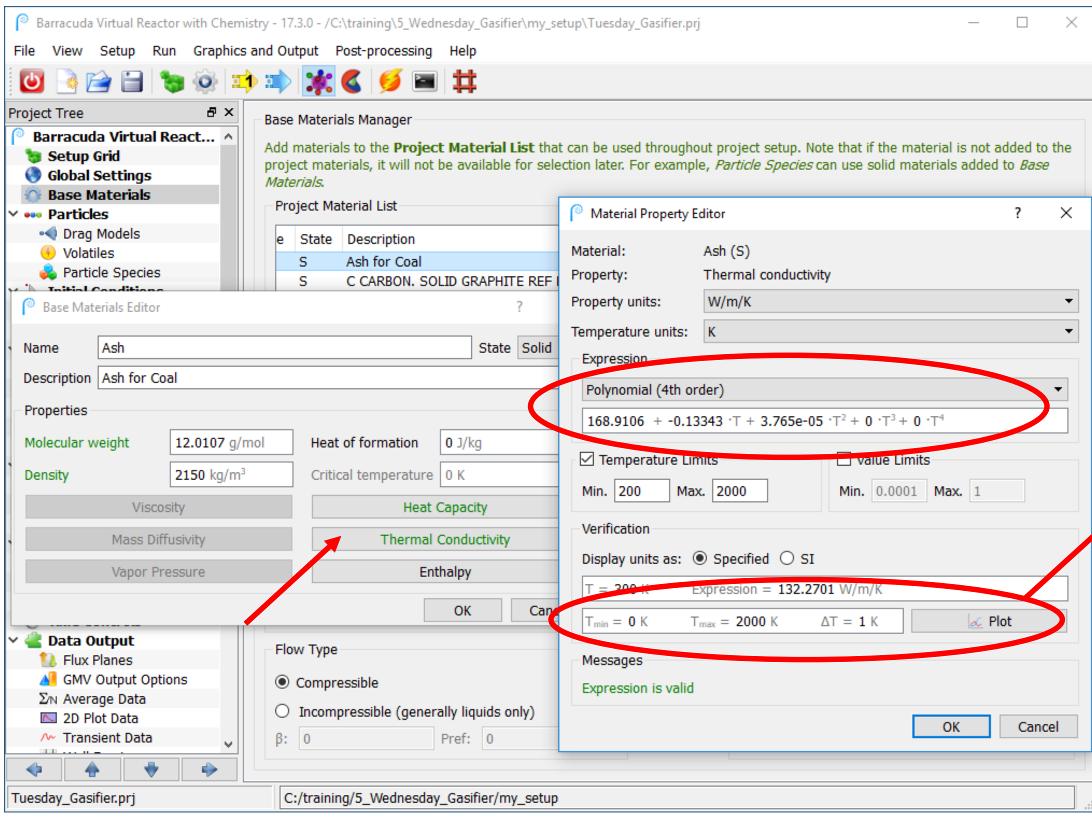
Enable Thermal Flow

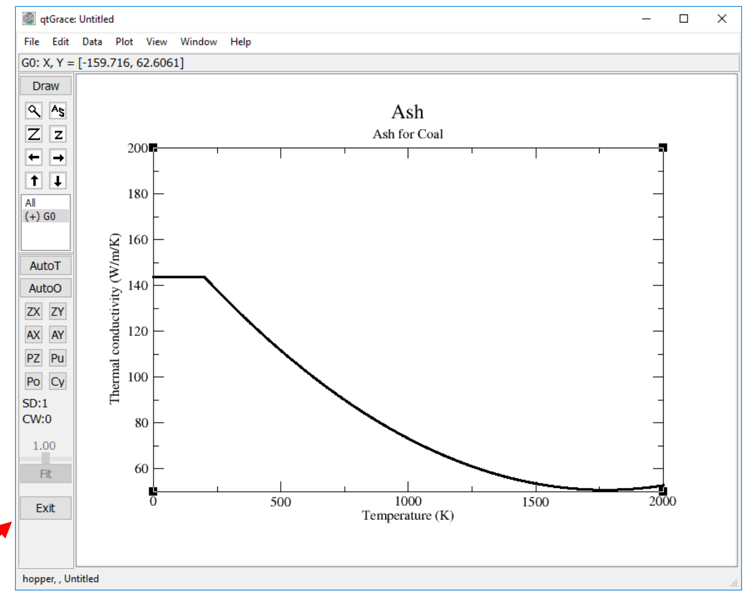
- In the **Global Settings** section, choose the **Thermal Flow** radio button to enable thermal calculations.
- It is possible to delay the start of thermal calculations by using the **Start with Thermal: Off** option. However, for this training exercise, we will **Start with thermal: On**.
- The **Heat transfer coefficients** button can be used to adjust the heat transfer coefficients between wall-and-fluid and particles-and-fluid (defaults used here).
- 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.
- Start with chemistry “On”.



Automated Plotting of Polynomial Material Properties

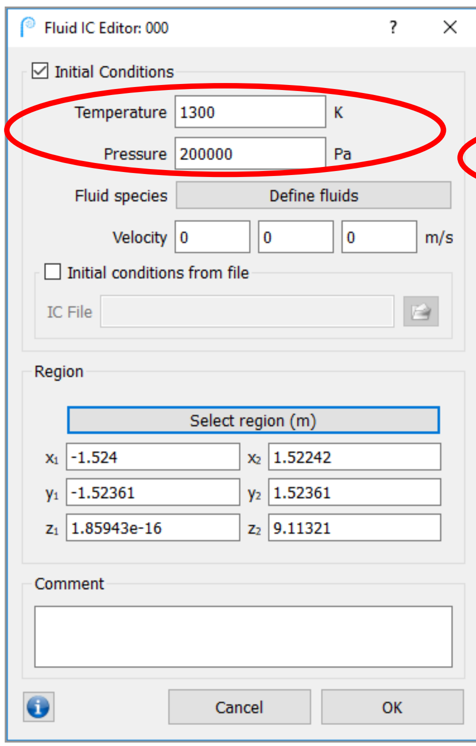
- This feature allows users to plot the expressions (Polynomial (4th order), Double Polynomial, Interpolated from SFF File) for property data in **Base Materials**.
- Users can visualize property data over a range of temperatures present within a simulation.
- To view the plot for the polynomial, click on the **Plot** button in the GUI.

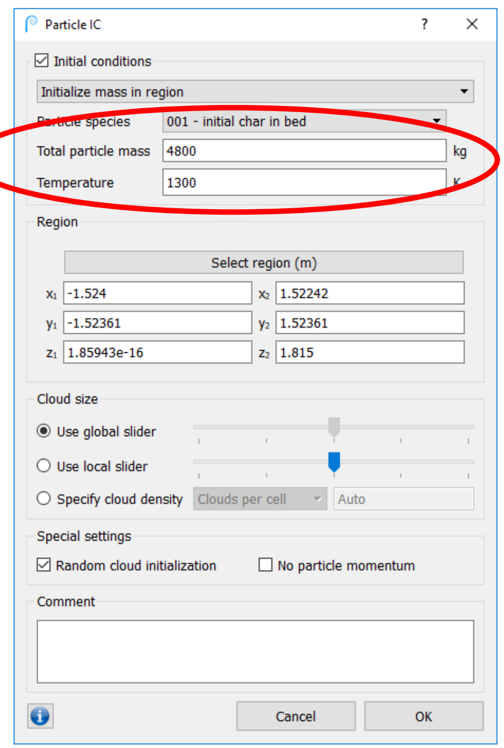




Temperatures of Initial and Boundary Conditions

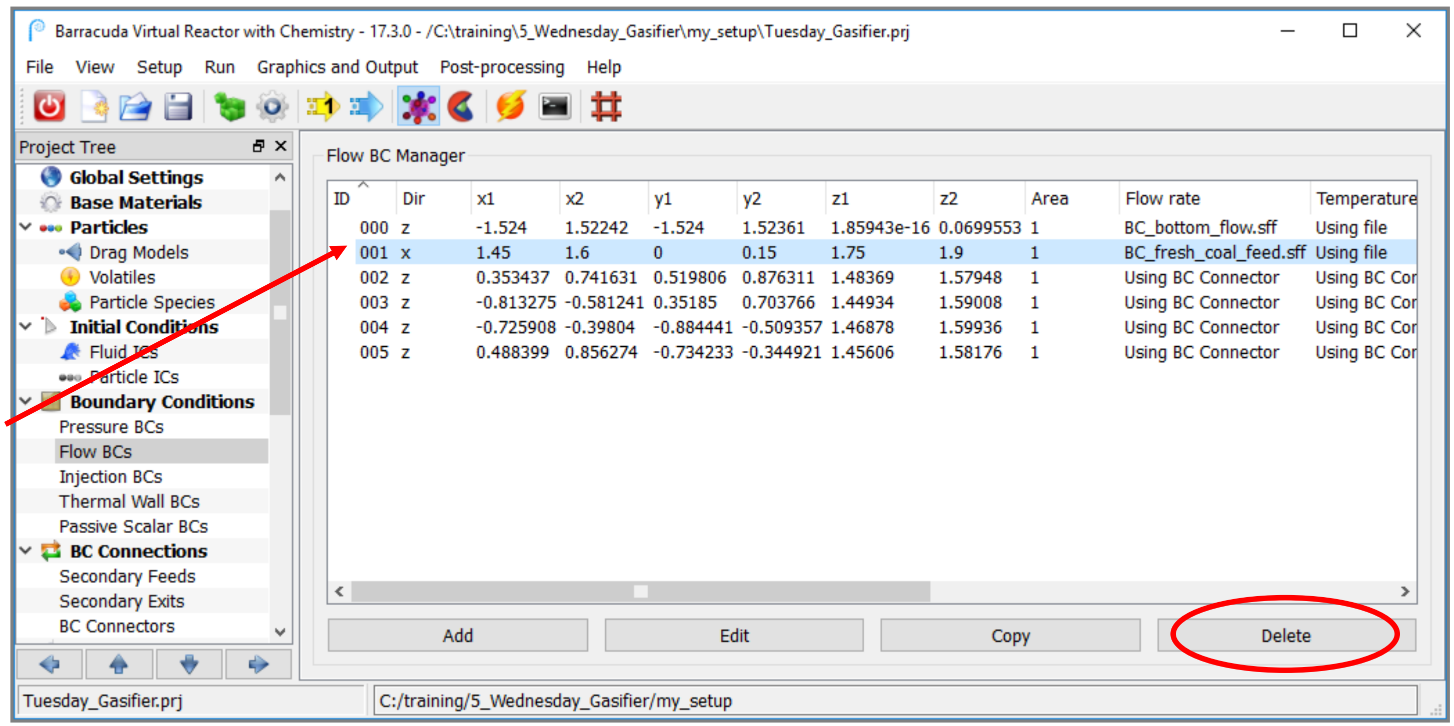
- When the Tuesday gasifier was set up as isothermal, it was not important to consider the temperature specifications for initial and boundary conditions.
- However, when turning on thermal calculations, it is important to review the settings (some of them may have been initialized to default values by Barracuda VR), and apply correct temperatures to all initial and boundary conditions.
- One particular item to check is the initial condition temperature of the fluid and particles. Barracuda VR initializes this to 300 K by default, which will cause extreme heat transfer difficulties during start-up of this hot gasifier if it is not corrected.
- Initialize the system to a **Temperature** of “1300” K.





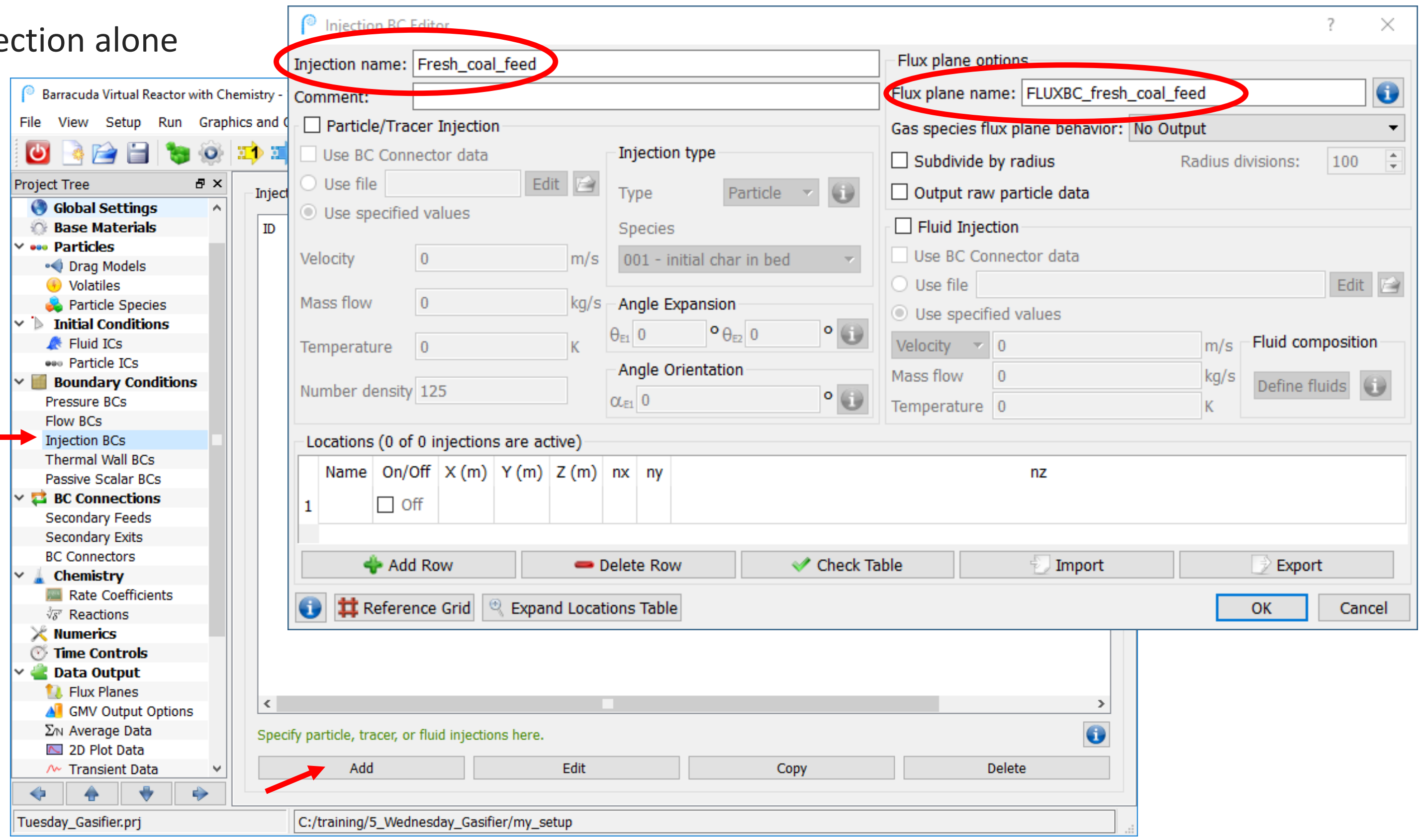
Fresh Coal Feed Injection

- Instead of using a flow boundary on a face 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 from the project.



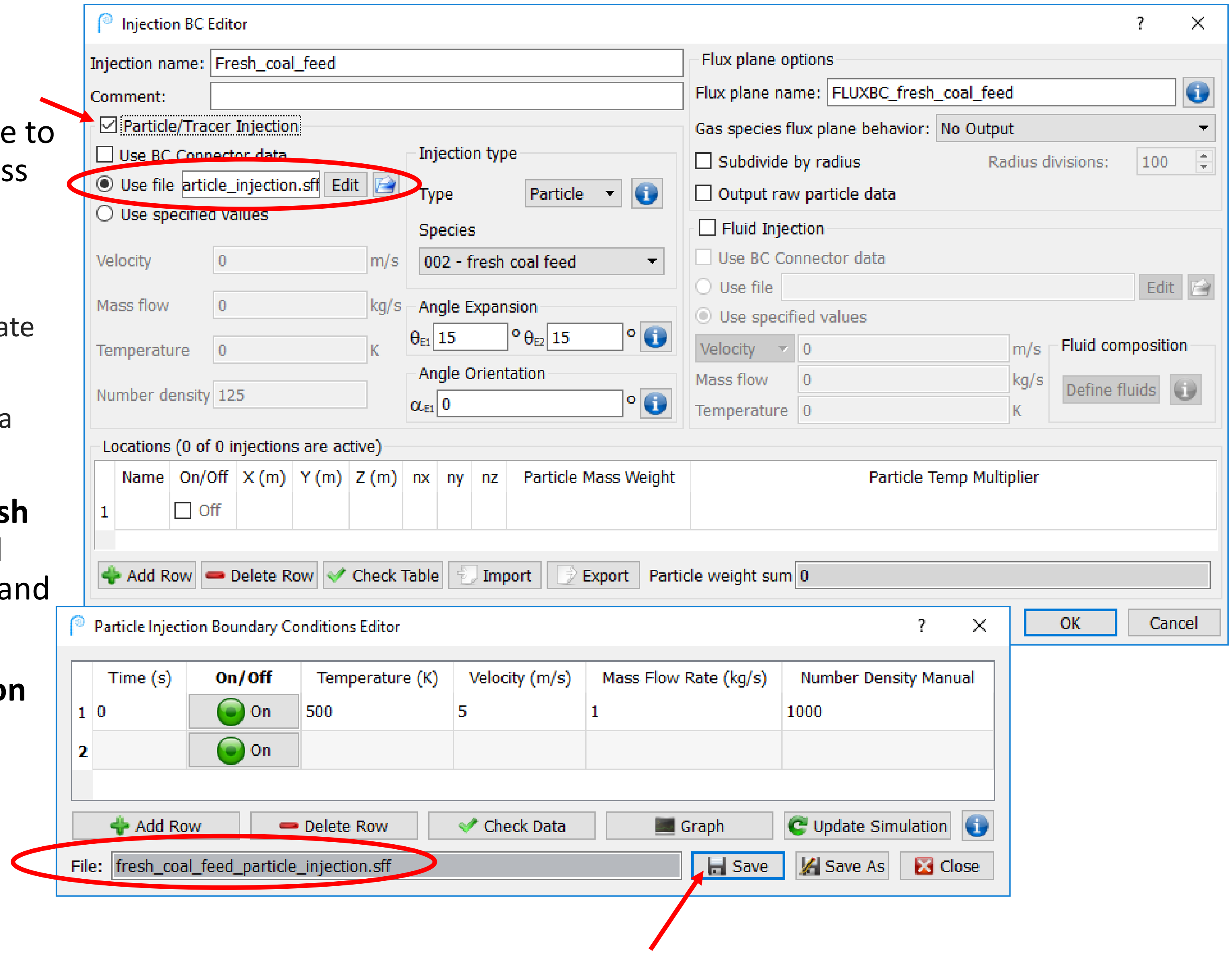
Fresh Coal Feed Injection

- 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**.



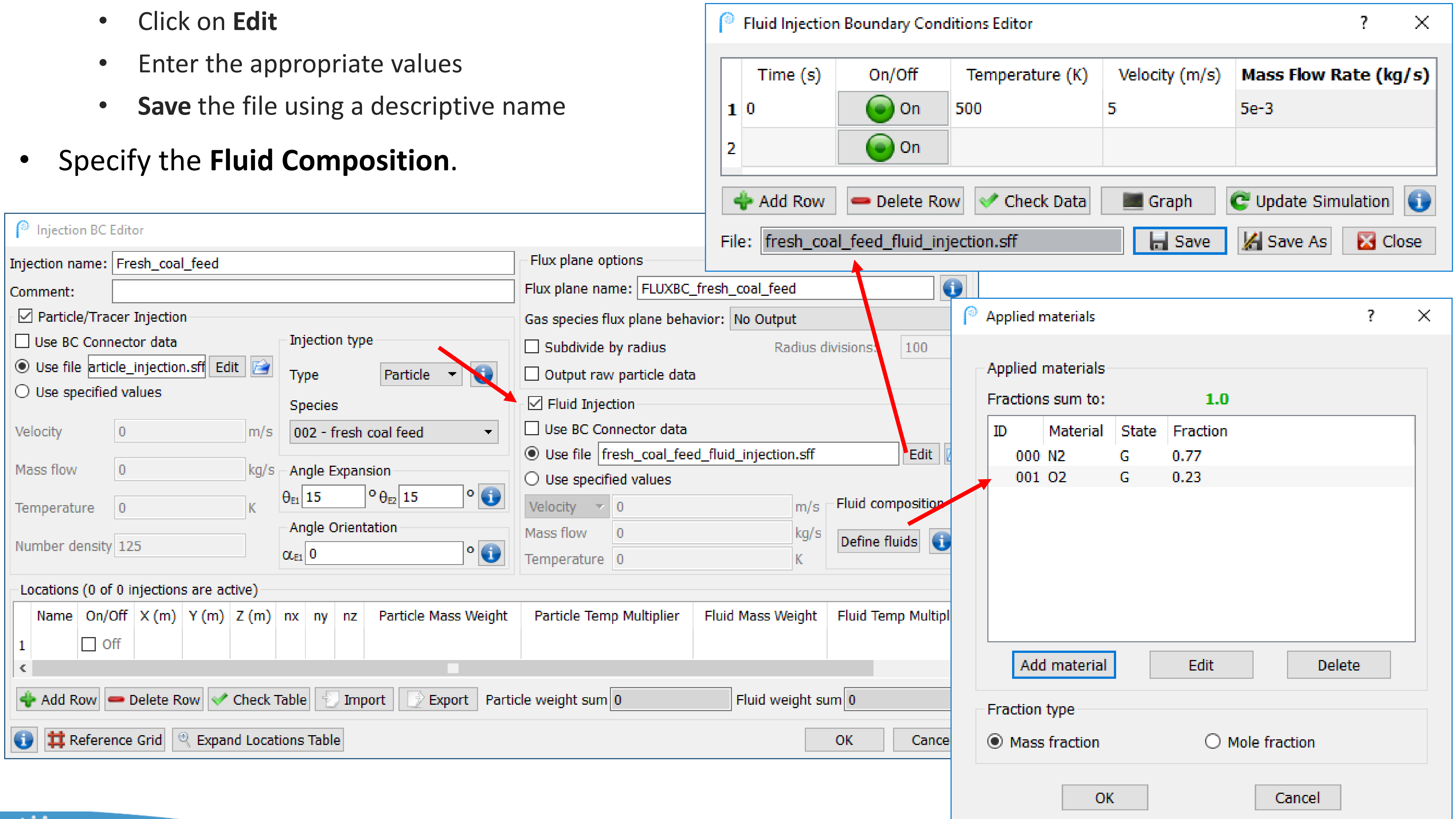
Fresh Coal Feed Injection

- Select **Particle/tracer Injection**.
- Use a transient (.sff) file to specify the particle mass flow rate:
  - Click on **Edit**
  - Enter the appropriate values
  - **Save** the file using a descriptive name
- Select **Particle** and **Fresh coal feed** from the pull down menus for **Type** and **Species**.
- Set the **Angle Expansion** to “15”.



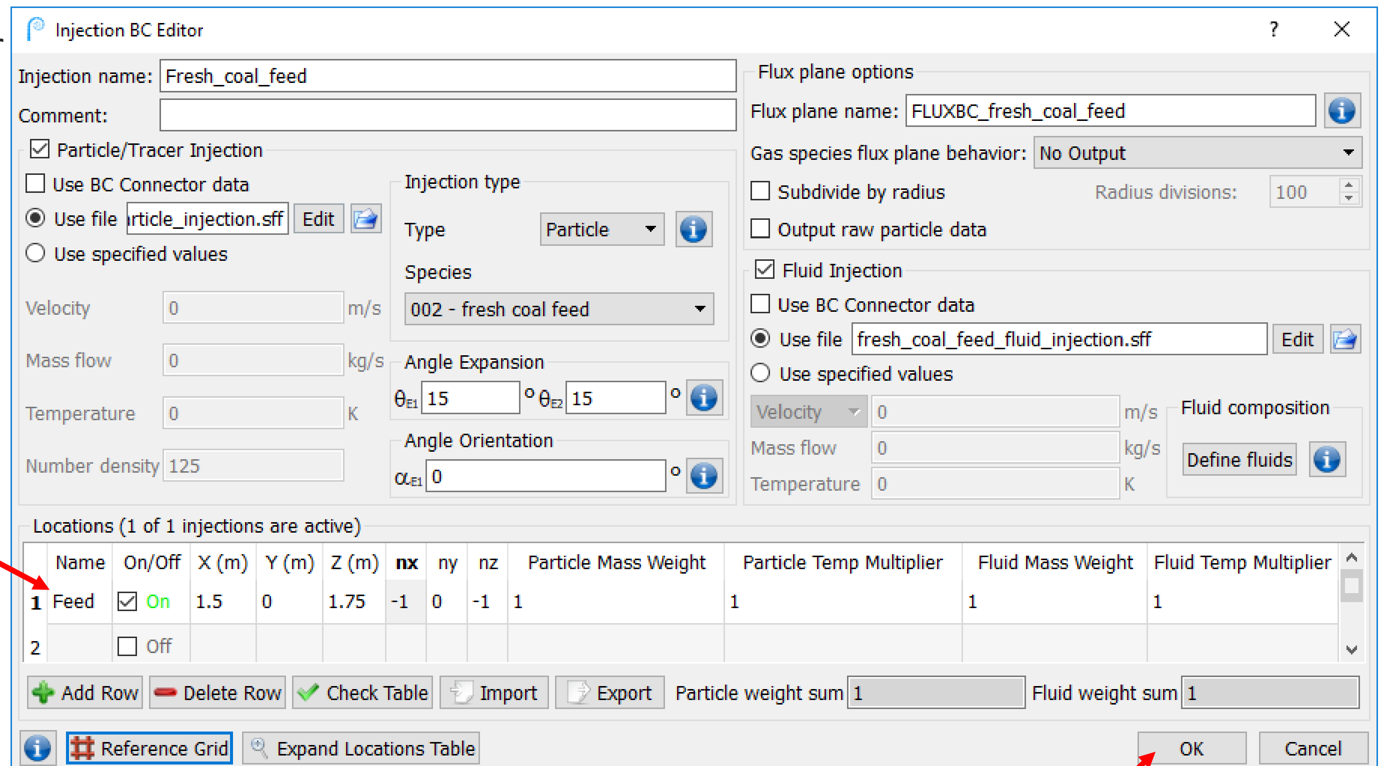
Fresh Coal Feed Injection

- Select **Fluid Injection**.
- Use a transient (.sff) 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**.



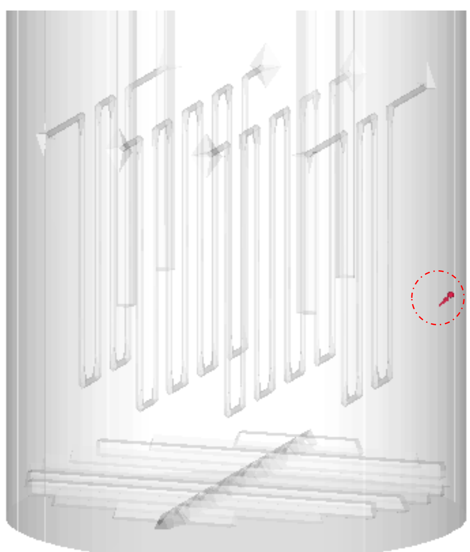
Fresh Coal Feed Injection

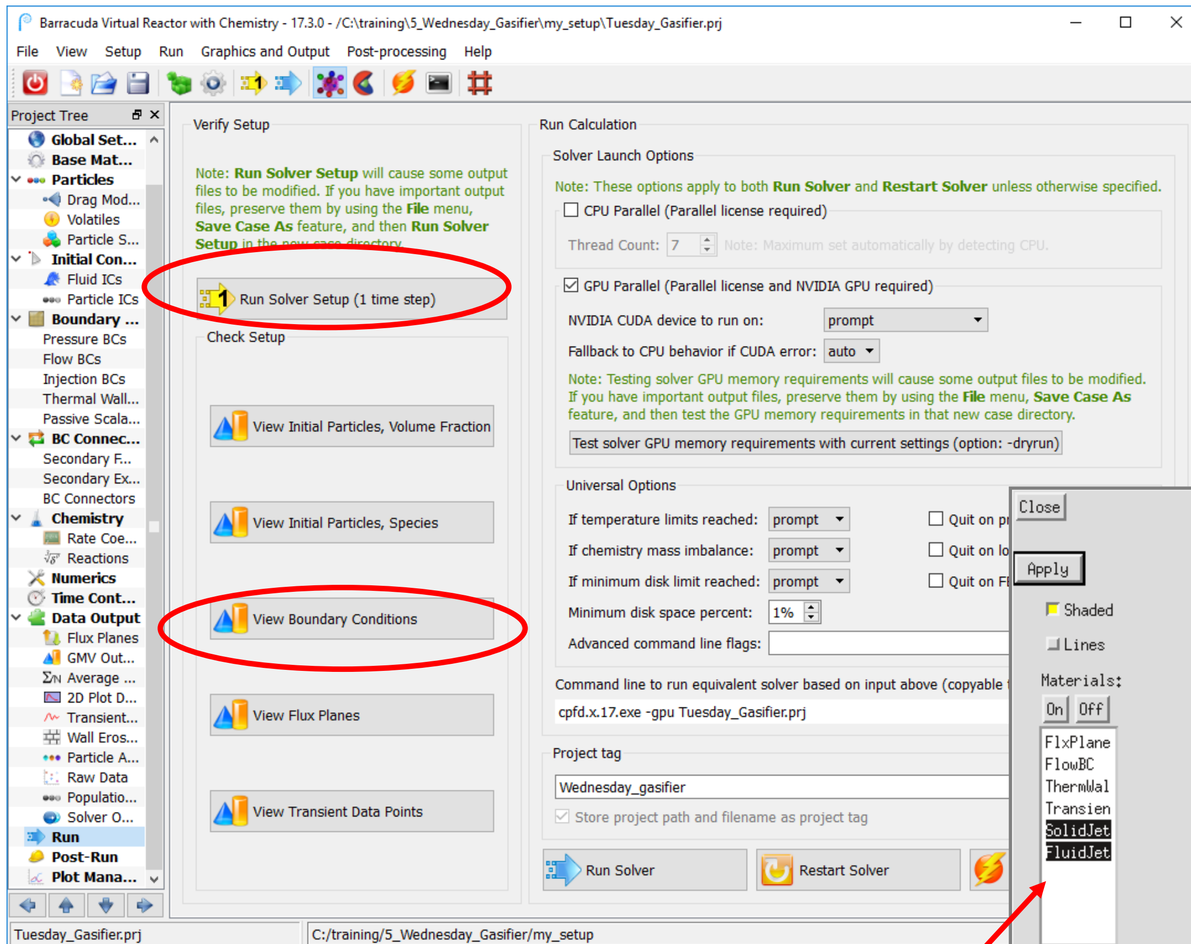
- Specify the location of the fresh coal feed nozzle.
- Enter an appropriate **Name** for the injection point.
- Select “**On**”.
- Enter the x,y,z location and the directional vector for the nozzle.
- Enter a value of “1” for:
  - Particle Mass Weight
  - Particle Temp Multiplier
  - Fluid Mass Weight
  - Fluid Temp Multiplier
- Click **OK**.

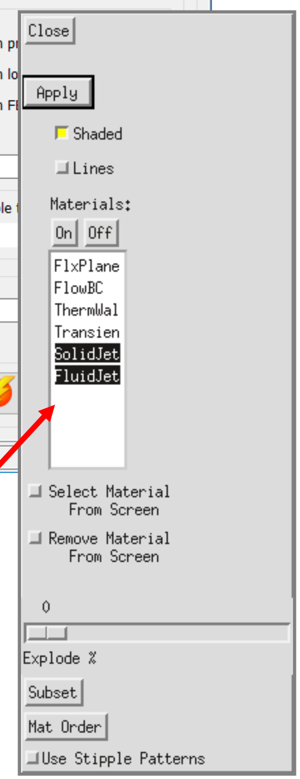


Fresh Coal Feed Injection

- Before continuing with the project setup, check the location of the nozzle by running the simulation for a single time step.
- Under **Run**, click **View Boundary Conditions**.



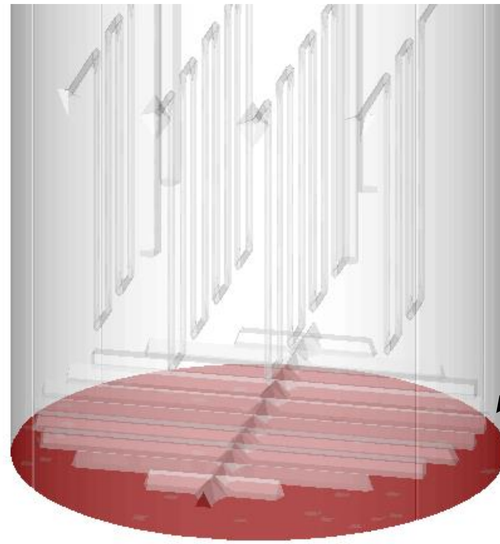




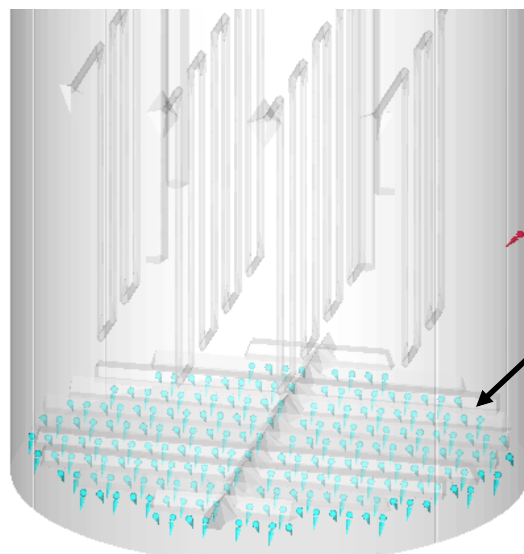
Tip: To view only the nozzle, click on **Display → Polygons** in the Gmv window, select **SolidJet** and **FluidJet** only, and click **Apply**.

Separate the Air and Steam BCs

- One simplification that was made in the Tuesday gasifier was the exclusion of the gas sparger geometry.
- 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.
    - **Review the Process Sheet** (slide 3) for air mass flow rate and temperature.
- Create an injection BC on the bottom surface of the sparger, and introduce 100% steam at this location through 204 nozzles.
    - See next slide for details.
- **NOTE**: An injection BC requires that the user input both the mass flow rate and a velocity. Often, the mass flow information only is given and velocity must be calculated based on nozzle diameter.



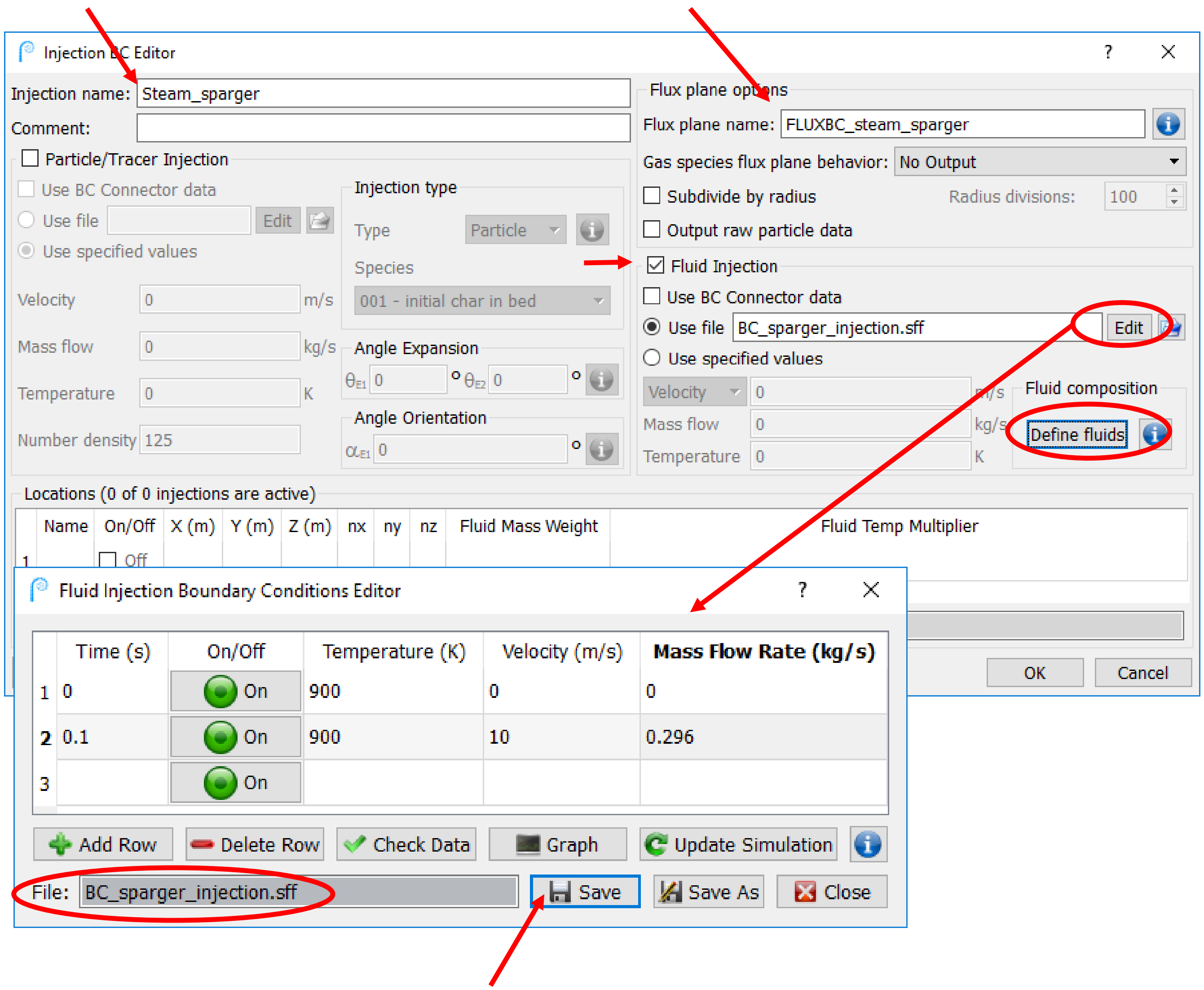
Air (N_2 + O_2) introduced through flow BC on bottom surface of vessel



Steam introduced through 204 injection points located on the sparger

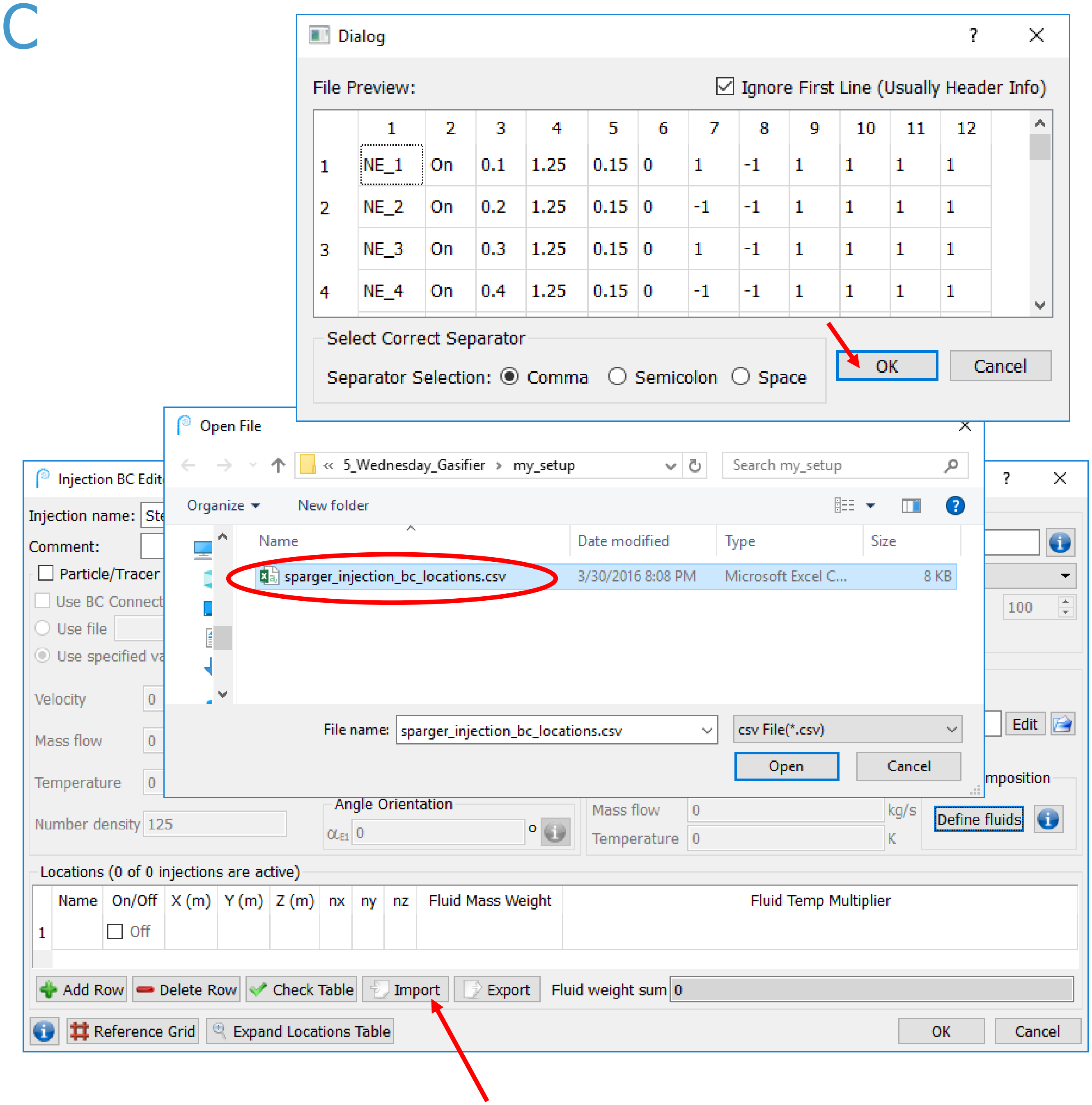
Steam Injection BC

- Create a new injection BC for the steam sparger by clicking on **Add** on the **Injection BC** page.
- Enter an **Injection Name** and **Flux Plane** name.
- Select **Fluid Injection**.
- Use a transient (.sff) 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 as 100% steam.



Steam Injection BC

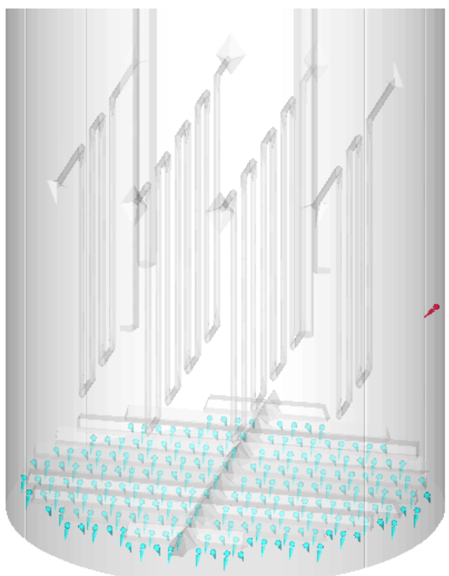
- Creating and editing large sets of location and direction data is most conveniently done in Excel, Open Office, or other spreadsheet application:
  - Data from the **Locations** table can be exported as a comma-separated value (CSV) file by clicking on the **Export** button in the Barracuda VR GUI
  - Once the file has been edited, it can be easily imported into the locations table
- To save time, a CSV file containing the locations and directions of the 204 nozzles has already been created for this problem.
- Click on **Import** and select the file sparger_injection_bc_locations.csv, which is located in the "my_setup" folder.
- Click **OK** in the import dialog.

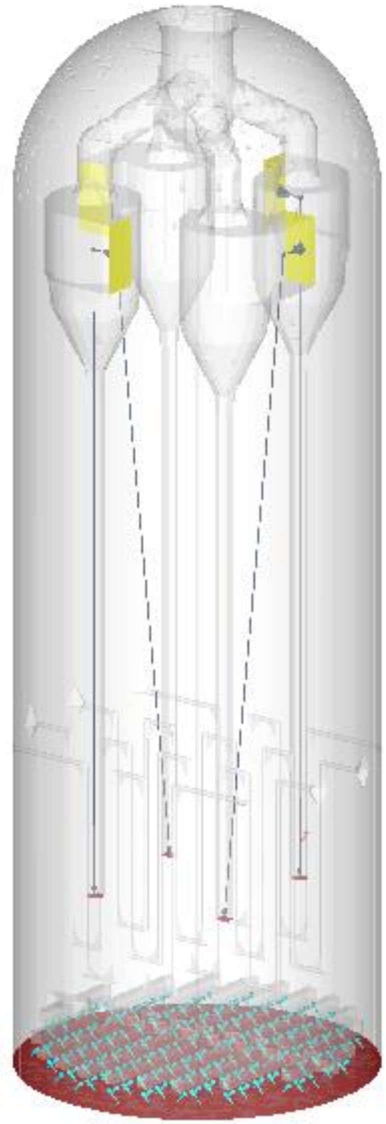


Steam Injection BC

- Once the locations table has been imported, click **OK** and run the simulation for a single time step to check the location of the nozzles.

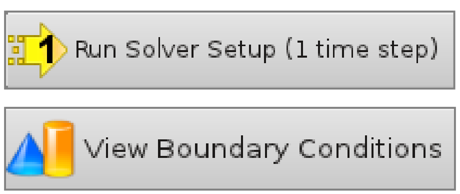
- **Tip**: To view only the nozzle, click on **Display → Polygons** in the Gmv window, select **SolidJet** and **FluidJet** only, and click **Apply**.

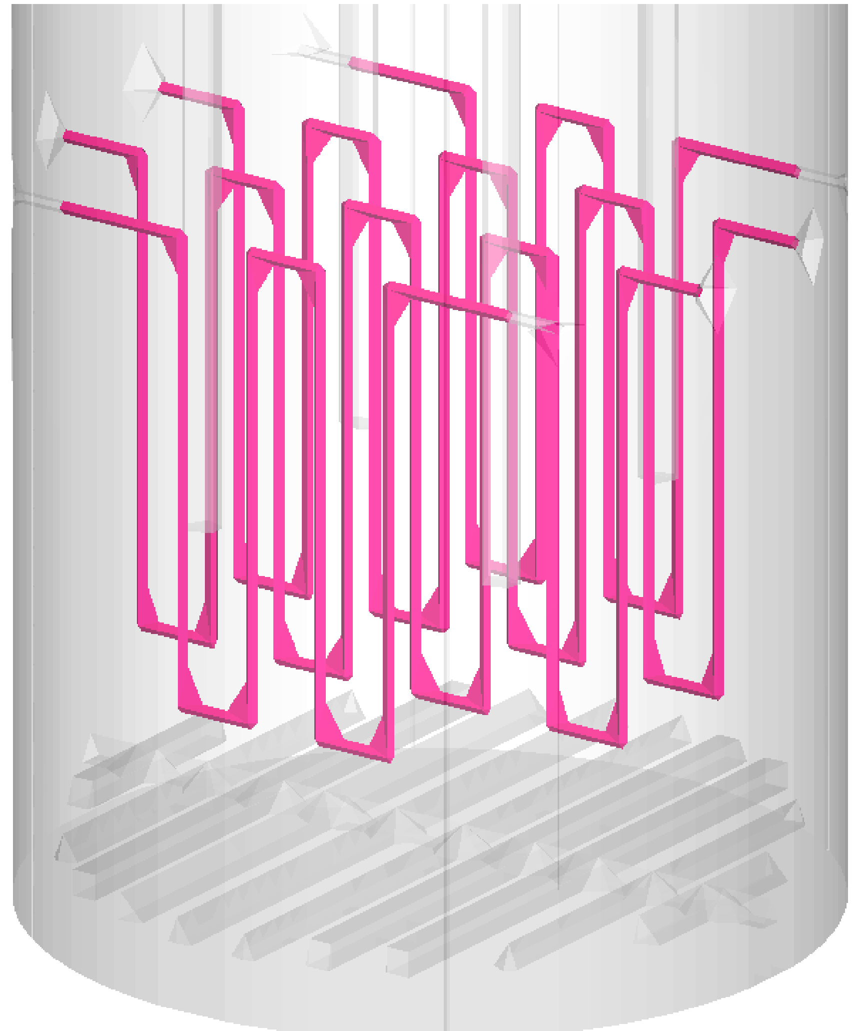




Thermal Wall BCs: Heating Coils

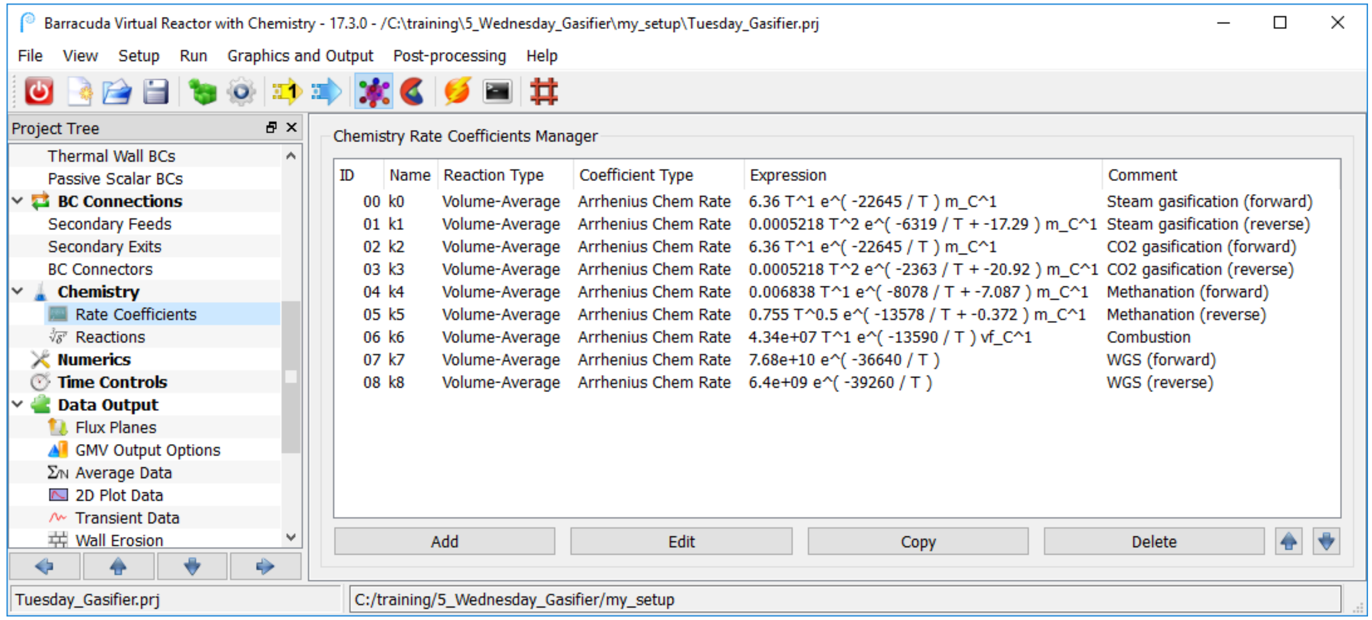
- The gasification process requires input of heat. We will define thermal wall BCs on the heating coils, setting the temperature in a transient input (.sff) file.
- Specifying the locations of thermal walls is very similar to that of flow BCs.
- Use **Normal to surface** and avoid placing any thermal wall BCs on the outer vessel wall or cyclone diplegs. **Hint**: you will have to define at least three separate thermal wall BC blocks.
- Keep the default option of outputting thermal wall heat transfer information to a transient data file. This will allow us to see how much heat is being provided by the heating coils.
- **Run Solver Setup (for 1 time-step)**, and verify that the thermal wall BCs are applied correctly.

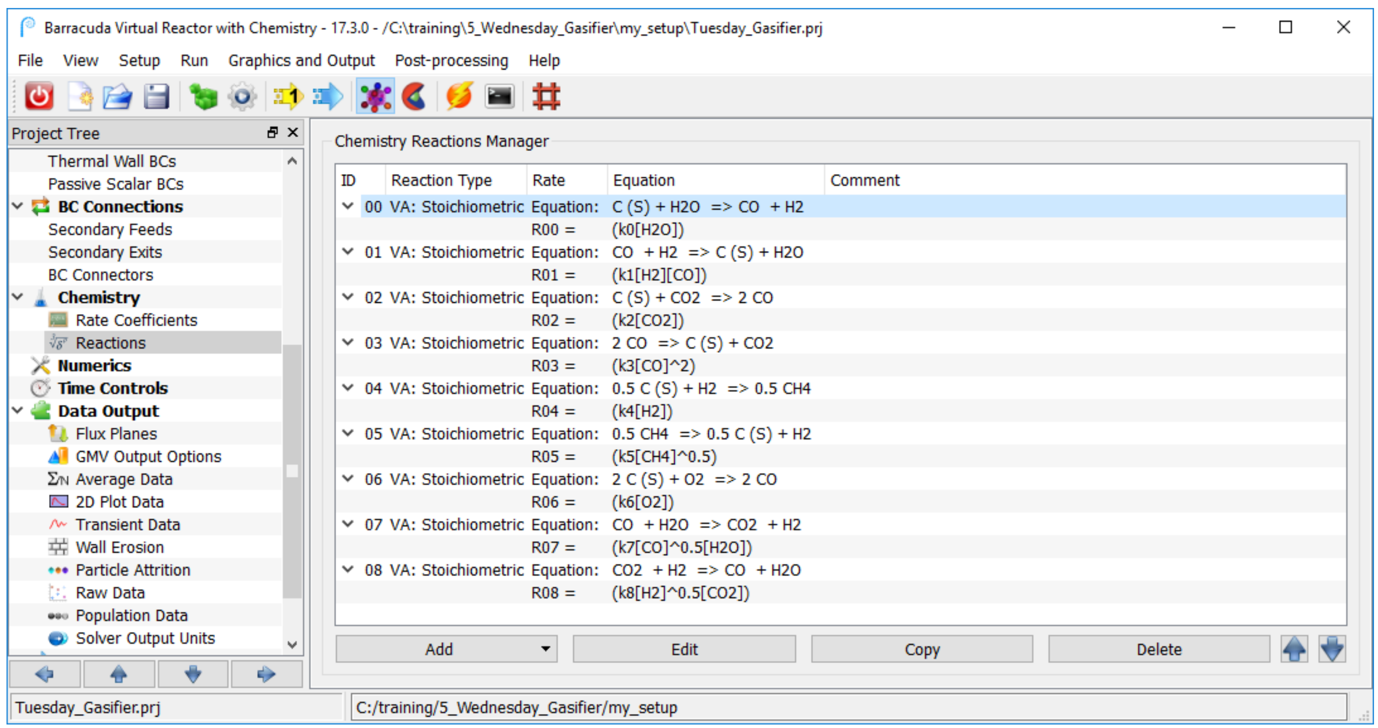




Chemistry

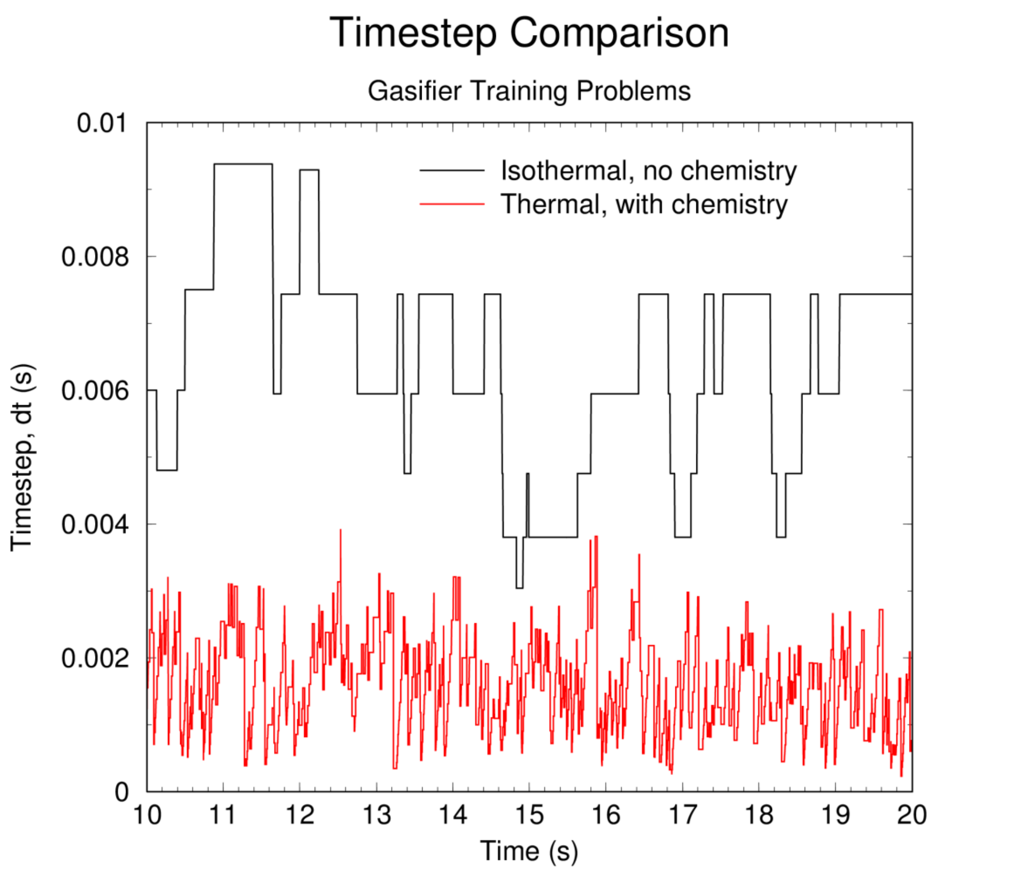
- The gasification reactions listed on Slide 5 need to be input to the chemistry section.
- For this training problem, we will use stoichiometric, volume-average chemistry.
- Definitions and units for the terms used on Slide 5 are:
    - m_C = mass concentration of carbon (kg/m^3)
    - T = fluid temperature (K)
    - θ_C = carbon volume fraction
    - [X] = mole concentration of species X (mol X / m^3 gas volume)





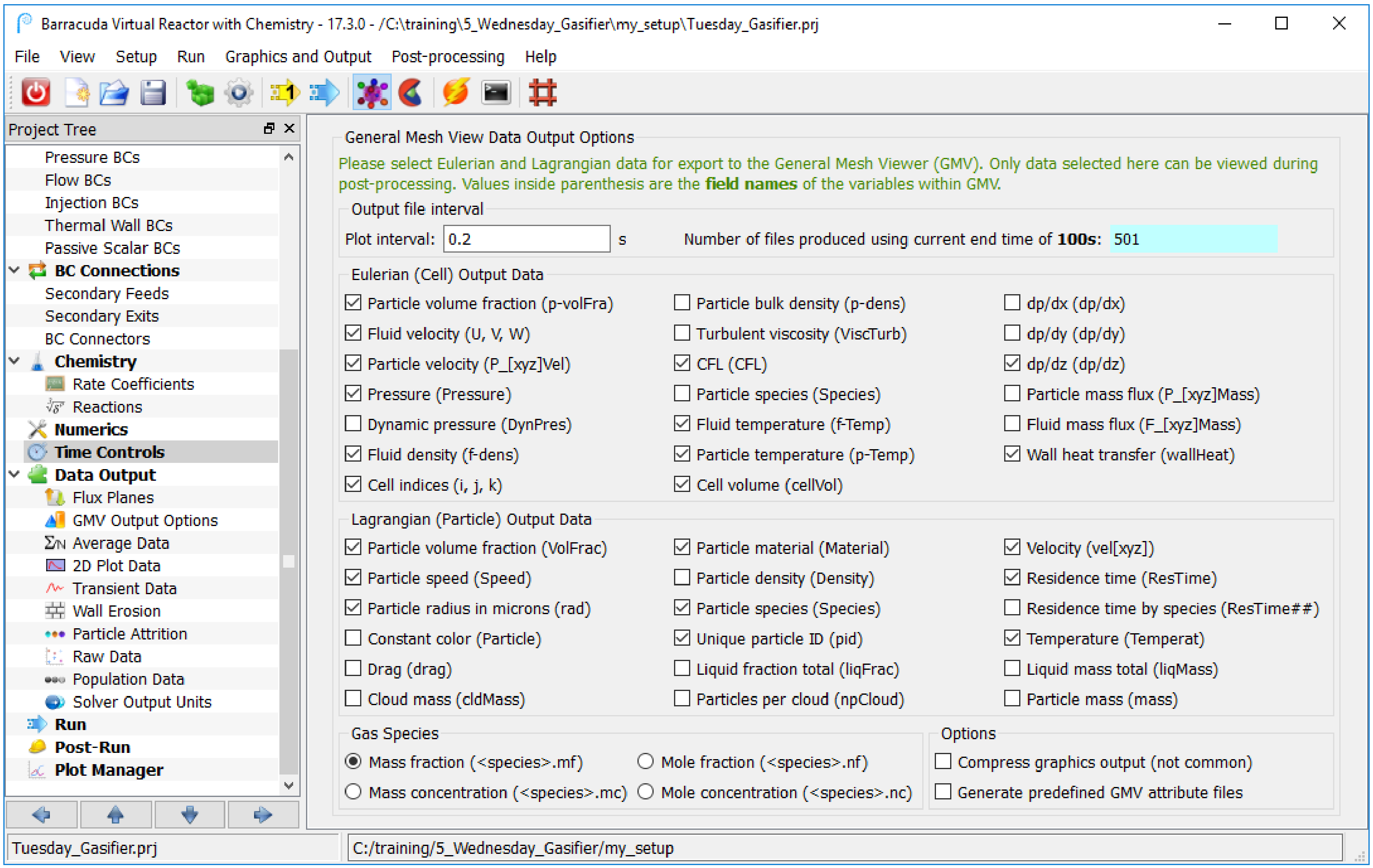
Time Controls

- 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 Tuesday gasifier.



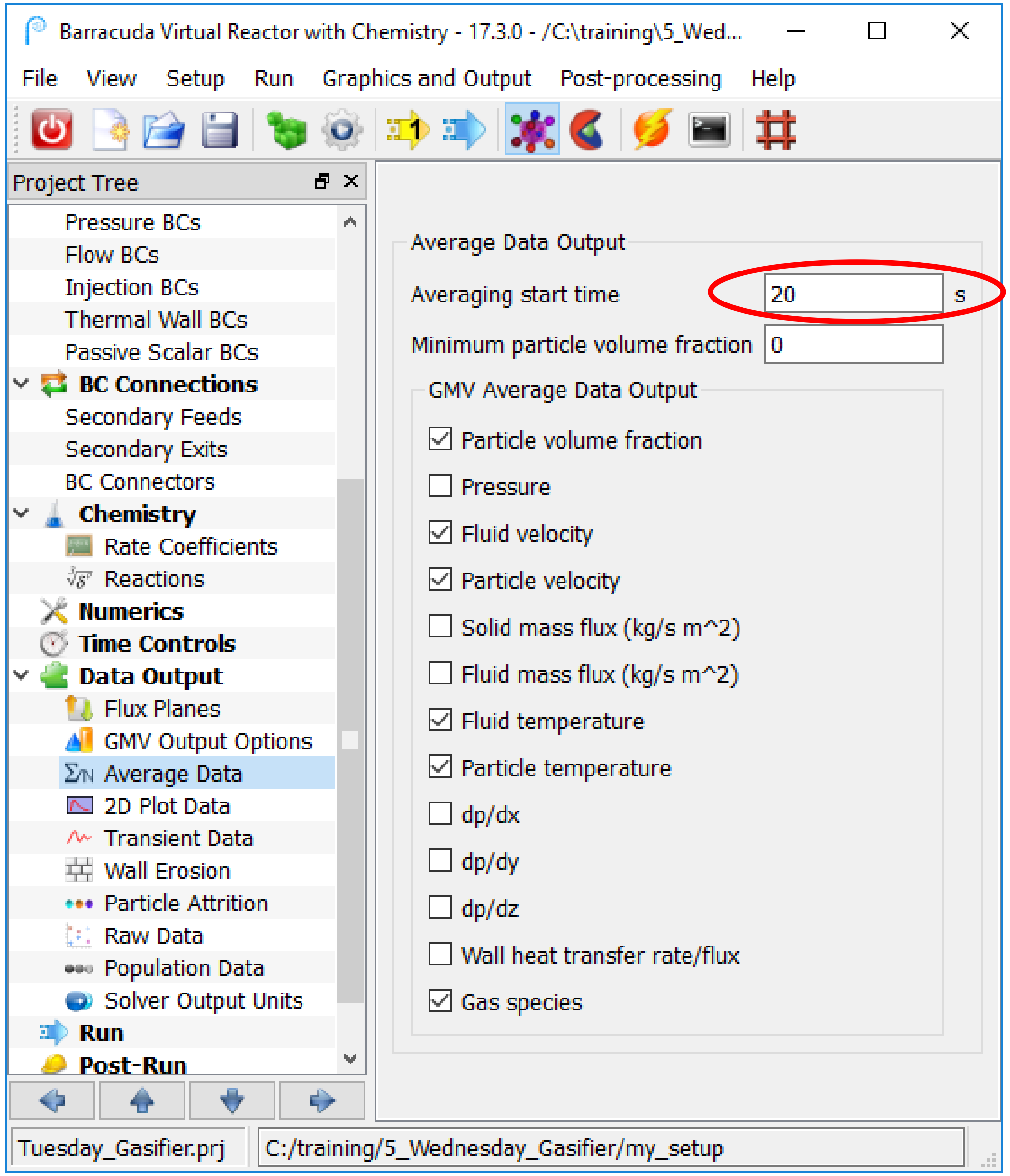
GMV Output Options

- 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.



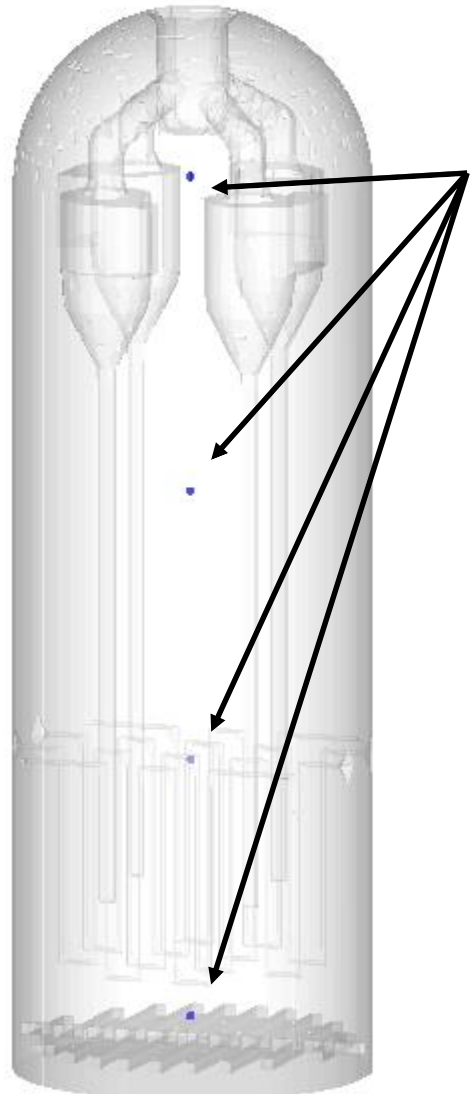
Average Data

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



Transient Data

- Transient data points can be defined to monitor many different variables during the course of a simulation.
- For this model, define several transient data points to monitor the fluid temperature (**Fluid temp**) at different elevations in the bed.
- Note that transient data points can be specified using either **xyz** or **Node** locations. If you choose to use xyz, the locations must be specified in units of meters. Use reference grid if needed.

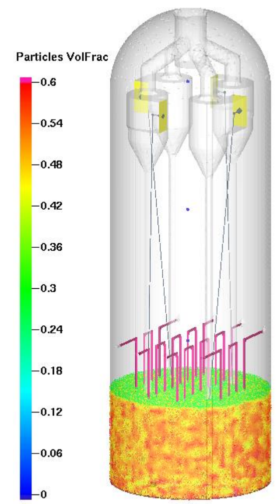


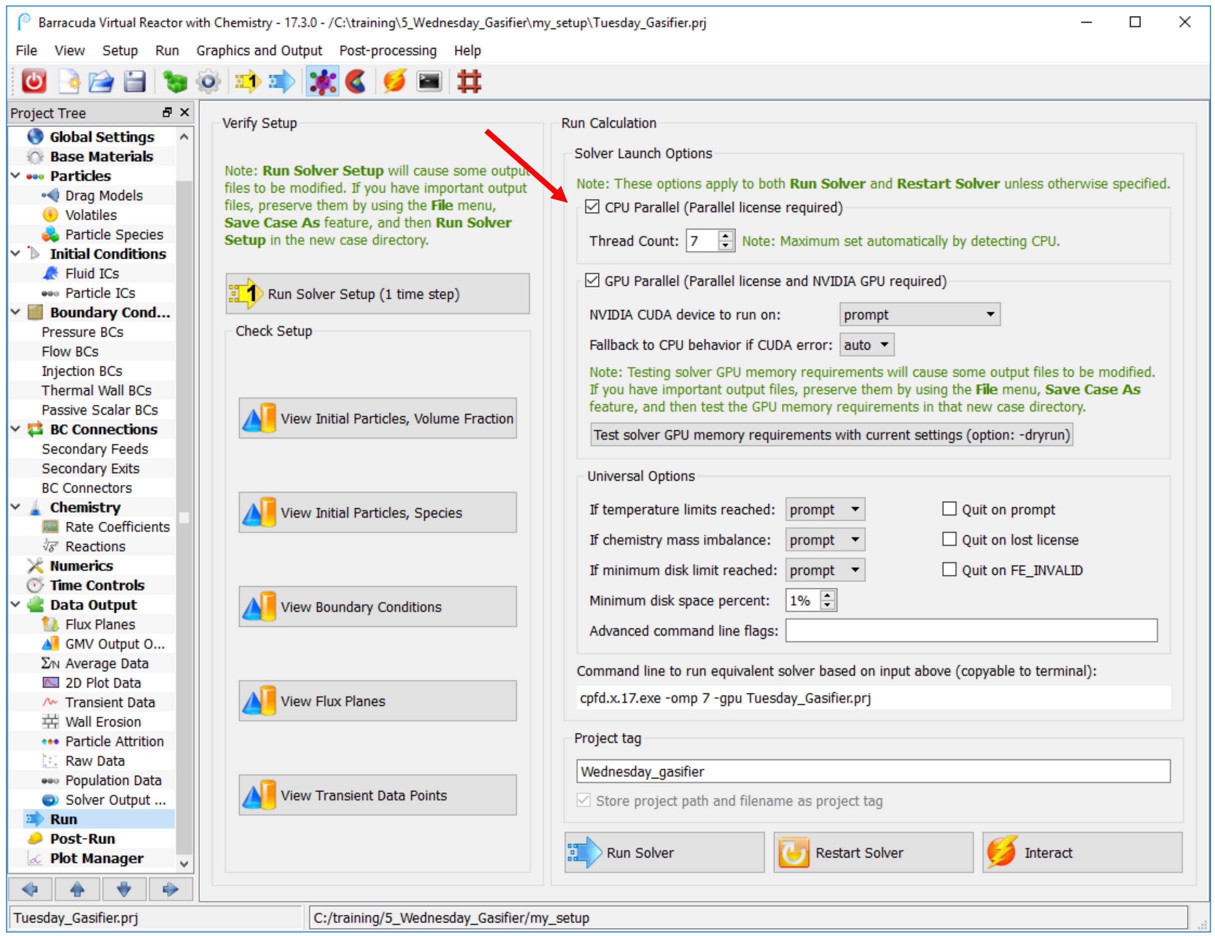
Define 4 transient data points along the central axis of the bed to monitor fluid temperature.

Check that the transient data points are at the desired locations.

Check Model Setup

- **Save** your project.
- 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?
- 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!
- Review the project setup with the instructor, and start the project running when you are confident it is set up correctly.





"Particle Feed Deficit" Warning

- Early in the simulation, a warning will be written to the solver run window

```
"Barracuda Virtual Reactor - 17.3.0 - pre_setup/Wednesday_Gasifier.prj" - cpfd.x.17.exe -omp 7 -gpu Wednesday_Gasifier.prj
# Decrease dt from CFL. Old =  1.000e-02 New =  8.000e-03 (10 30 4)
 2.50000e-01  8.000e-03 003  2.86e-08 008  1.60e-08 008  1.49e-08 008  2.18e-08 009  1.25e-06  856  9.98e-08  1.53   0.00 107   0   0  2
 2.58000e-01  8.000e-03 003  1.87e-08 007  6.78e-08 007  9.99e-08 007  6.47e-08 009  9.70e-08  684  9.75e-08  1.28   0.00 108   0   0  2
 2.66000e-01  8.000e-03 003  1.84e-08 007  2.65e-08 007  3.41e-08 007  8.00e-08 008  5.90e-07  777  9.88e-08  1.22   0.00 120   0   0  2
 2.74000e-01  8.000e-03 003  1.85e-08 007  8.10e-08 008  7.49e-09 007  4.90e-08 010  1.14e-06  729  9.97e-08  1.17   0.00 132   0   0  2
 2.82000e-01  8.000e-03 003  3.07e-08 007  8.94e-08 007  5.20e-08 007  9.97e-08 010  7.81e-07  760  9.84e-08  1.08   0.00 129   0   0  2
Injection [FLUXBC_fresh_coal_feed]:[Feed] @ ( 1.500e+00, 0.000e+00, 1.750e+00) has particle feed deficit.
    A mass of  1.997e-01 kg needs at least 1.911e-01 seconds to be recovered,
    given the specified [1.000000e+00 kg/s] and current [1.003408e+00 kg/s] rates of feed.

 2.90000e-01  8.000e-03 003  3.75e-08 007  4.85e-08 007  4.14e-08 007  2.81e-08 010  5.08e-07  716  9.93e-08  0.97   0.00 122   0   0  2
 2.98000e-01  8.000e-03 003  2.17e-08 007  2.95e-08 007  2.42e-08 007  2.98e-08 009  2.62e-06  686  9.86e-08  1.19   0.00 117   0   0  2
 3.06000e-01  8.000e-03 003  2.54e-08 007  2.61e-08 007  1.69e-08 007  1.50e-08 008  1.57e-06  666  8.94e-08  1.00   0.00  77   0   0  2

      t           dt    Vol     Vol    u       u     v       v     w       w     h       h     p       p
      s            s    itr     err   itr     err   itr     err   itr     err   itr     err   itr     err     CFL   dT/dt Low Med  Hi  R
 ------------ --------- --- --------- --- --------- --- --------- --- --------- --- --------- ---- --------- ----- ------ --- --- --- --
 3.14000e-01  8.000e-03 003  3.77e-08 007  2.54e-08 007  1.78e-08 007  2.29e-08 009  1.21e-07  651  9.96e-08  1.06   0.00  39   0   0  2
```

- This type of warning indicates that a particle feed BC cannot meet the specified mass flow rate. This can happen when:
  - Trying to feed into a cell that already has a high concentration of particles (such as the initial packed bed in the Wednesday Gasifier setup)
  - Trying to feed a particle mass flow rate that is physically too high
- Barracuda always honors the close-pack volume fraction, and will not feed particles if the cell is too full of particles

Recovering from Particle Feed Deficit

- The solver keeps track of the mass deficit, and tries to recover the mass at a later time if possible
- In the Wednesday Gasifier, the particle mass feed deficit is able to recover by about t = 0.5 s