Kuipers Bed Training Problem

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Training Goals

- This training example is designed to provide a quick introduction to the overall problem set-up process. Explanations are minimal. The Barracuda Graphical User Interface (GUI) will be explained in more detail later in this training class. The purpose of the assignments during the first day is to give the user an overall feel for the process and tools involved.

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Training Objectives

- Launch Barracuda

- Open project file with pre-setup grid

    - (Advanced gridding to be discussed during second day of training)

- Set up your calculation with the information provided

- Successfully run Kuipers Bed simulation

- Ask your instructor about any questions you may have

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The Kuipers Bed

- Kuipers et al. (1992) operated experimental "2D" fluidized bed

- The experimental setup consisted of
  - A thin rectangular bed (.57m x1.0m x 1.5 cm)
  - Fluidizing gas (0.25 m/s velocity) on bottom of reactor
  - Central gas jet (10 m/s)
  - Open to atmosphere at top

- During operation, Kuipers observed and measured
  - Bubbling behavior of bed
  - Bubble diameter
  - Particle volume fraction at various locations using IR sensor probe

- First training problem is to simulate the Kuipers bed with Barracuda
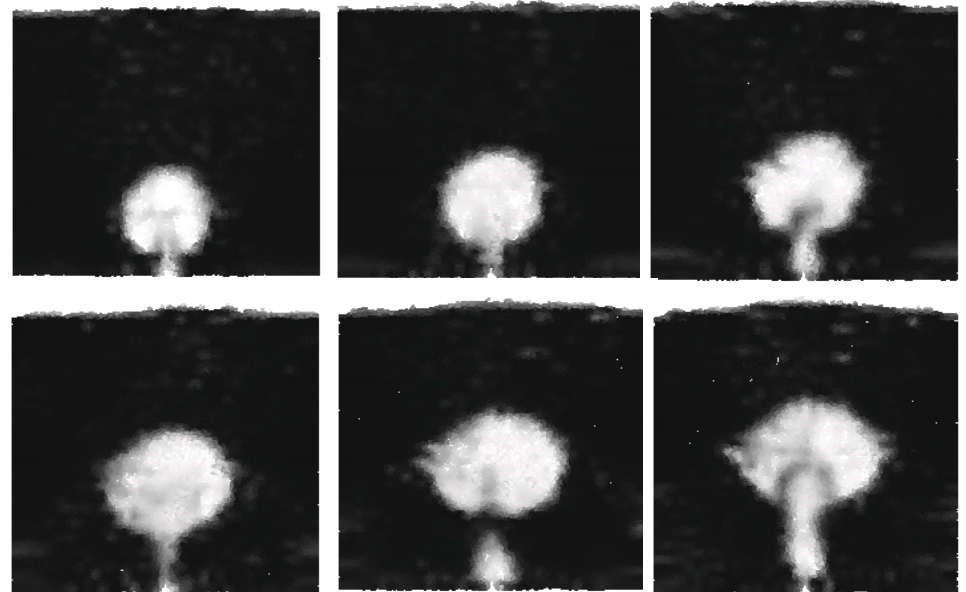
Kuipers, J, Tammes, Prins, and Swaaij (1992). Powder Technology 71: 87-99

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Simulation Objectives

- What can we learn from the simulation?
  - Fluidization behavior
  - Bubble diameters
  - Particle volume fraction
  - Particle mixing in time
  - Velocity data
    - Fluid
    - Particle
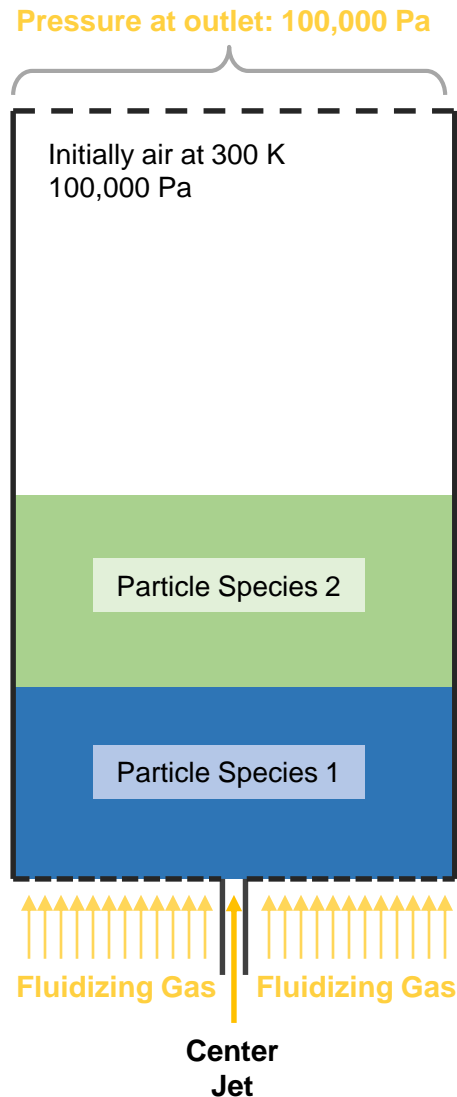 - Pressure profiles
  - Pressure gradients
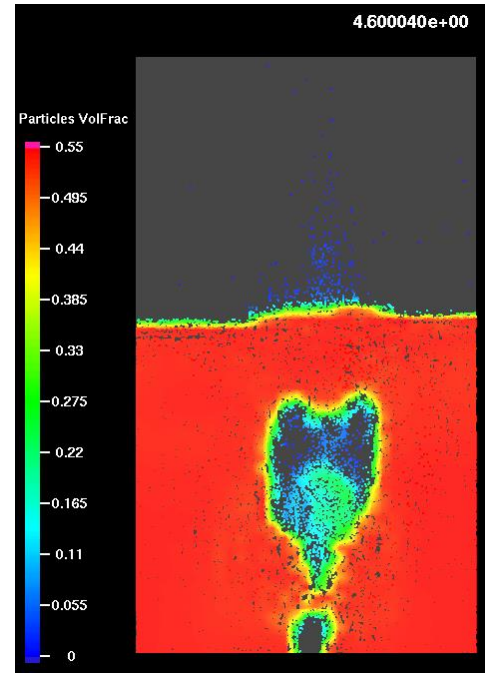
Instantaneous
particle volume fraction
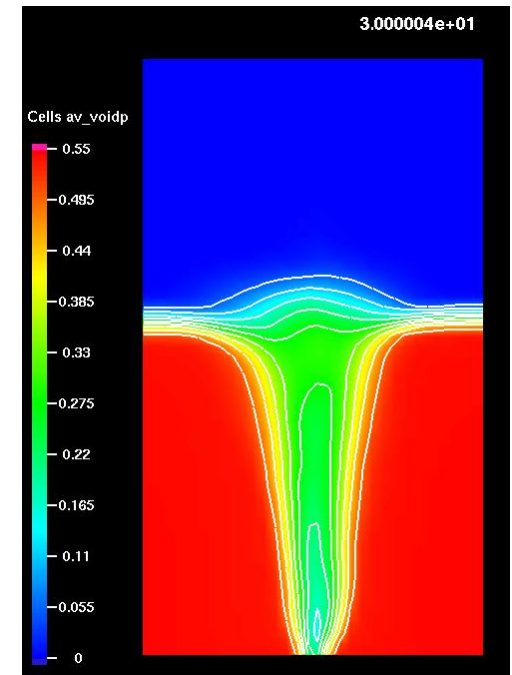

Time averaged
particle volume fraction

Process Sheet

Pressure at outlet: 100,000 Pa

Initially air at 300 K
100,000 Pa

Particle Species 2

Particle Species 1

Fluidizing Gas   Fluidizing Gas

Center
Jet

- Geometry
  - 57 cm wide
  - 1.5 cm deep
  - 100 cm total height
  - 50 cm initial bed height
  - 1.5 cm X 1.5 cm jet centered at bottom

- Particles
  - Use two identical particle species to view mixing behavior
  - Material density 2.66 g/cm3 (glass beads)
  - Diameter: 440μm - 560μm. This is 500 μm ±12%

- Initial conditions
  - Fluid phase: air at rest at atmospheric pressure
  - Solid phase: particles in bottom ½ of bed at close-pack (θcp = 0.55)

- Boundary conditions
  - Fluid
    - Grid velocity: 0.25 m/s
    - Center jet velocity: 10 m/s
    - Top open to atmosphere
  - Particles
    - Cannot enter or leave

Launching Barracuda

- Launch Barracuda. To do so you may click on the desktop icon or type "barracuda.17" at the command line
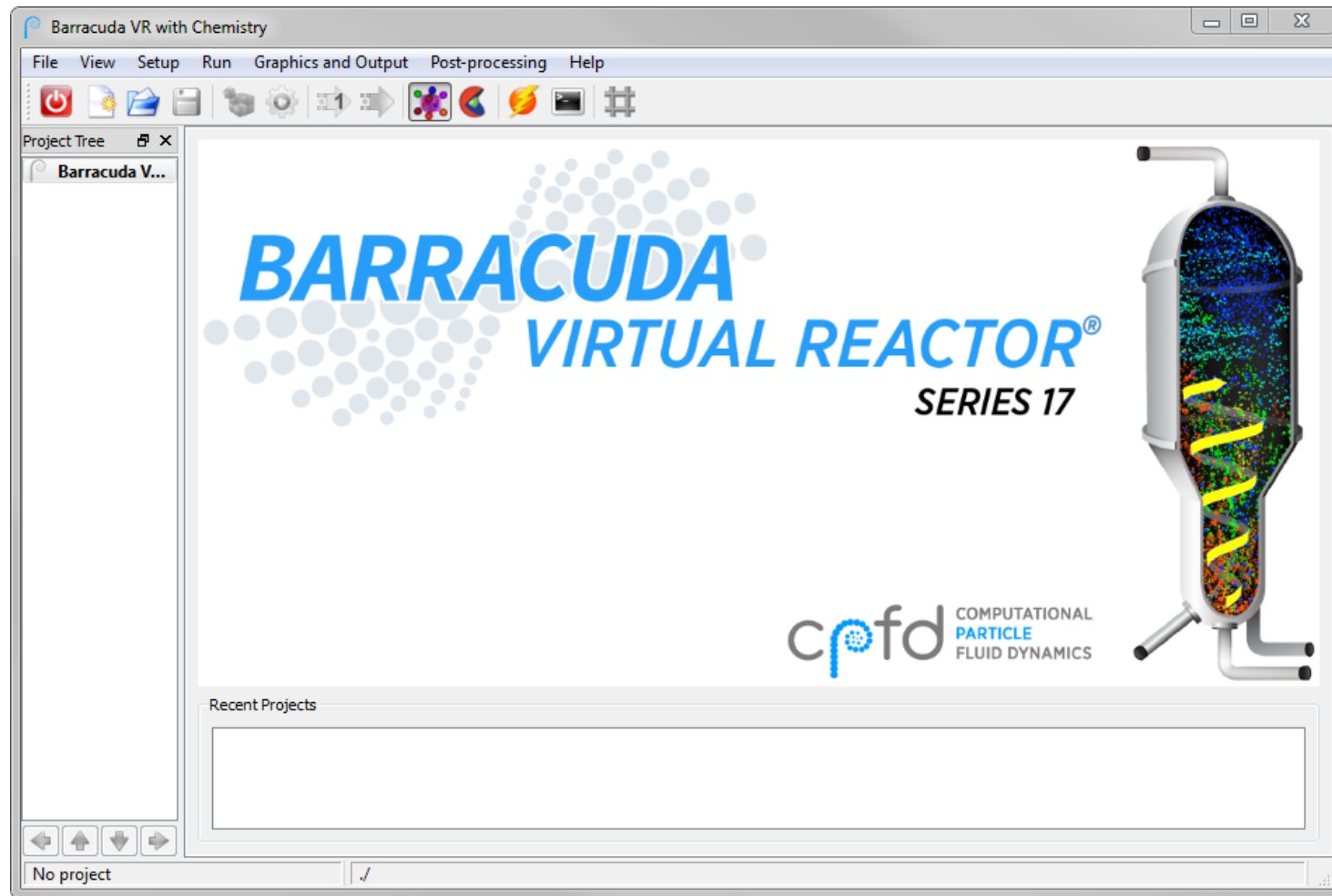
Opening a Project File

- Click on **File**, then **Open Project** to open an existing project.

- A project file window will pop up

- Navigate to:
  - On Linux: /home/training/barracuda_training/2_Kuipers/my_setup
  - On Windows: C:\training\2_Kuipers\my_setup

- Select **kuipers_mysetup.prj**

- Click **Open Project**

- The path to your training directory may be different than shown above. Use the appropriate path when navigating to your project.
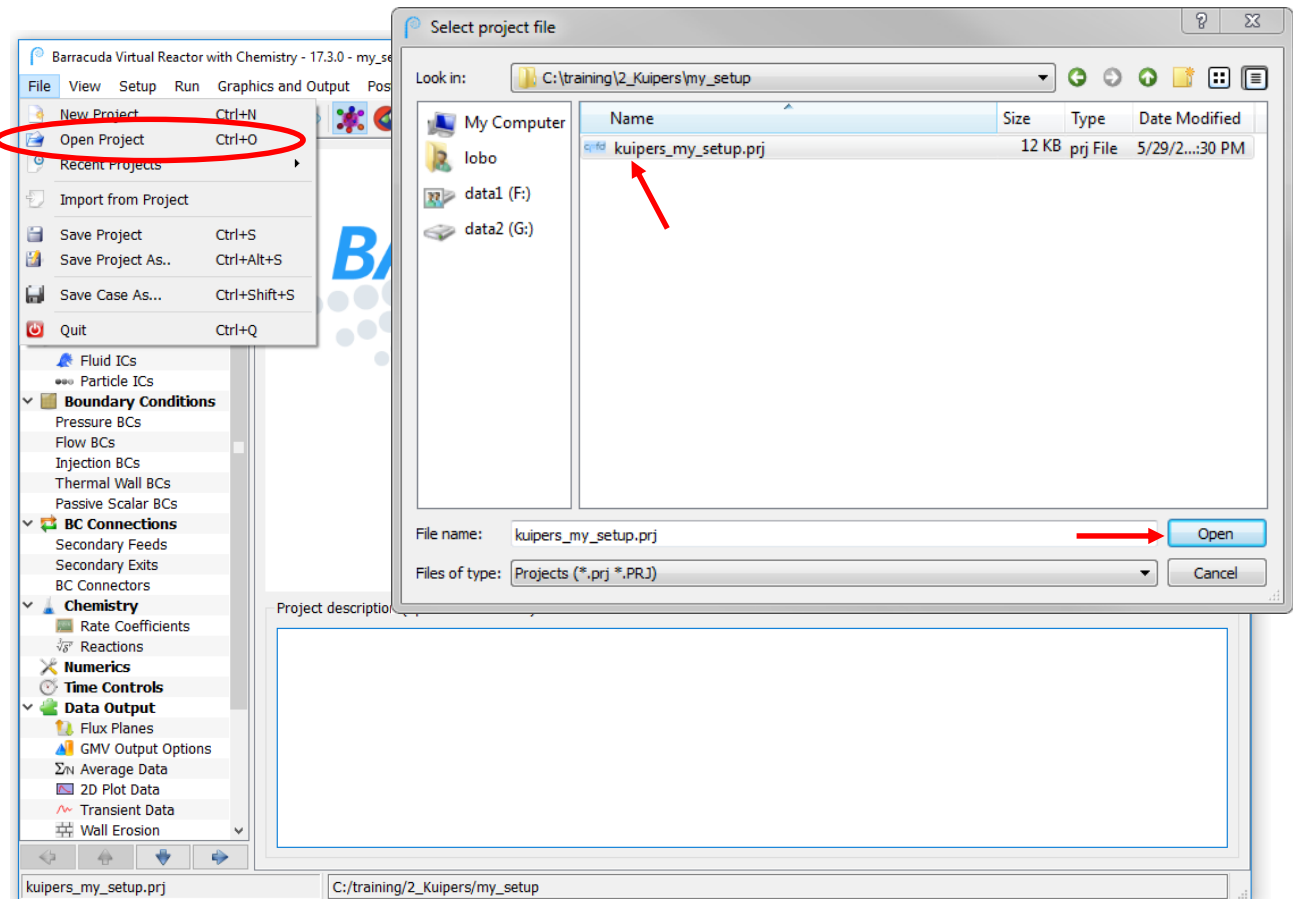
Navigating the Barracuda GUI

- Notice the project file and working directories are listed at the bottom of the main Barracuda GUI window
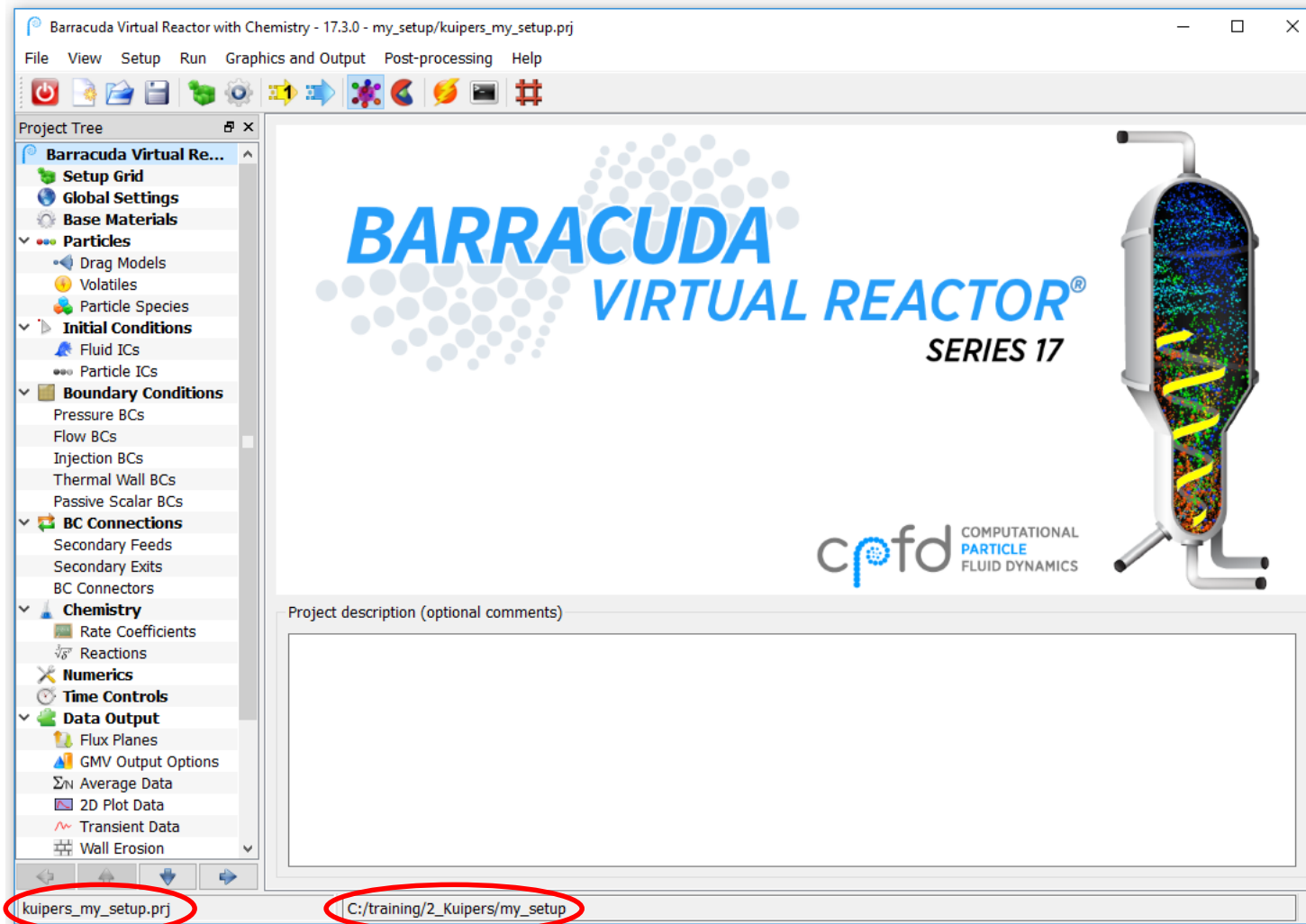
Setting up the Kuipers Bed Simulation
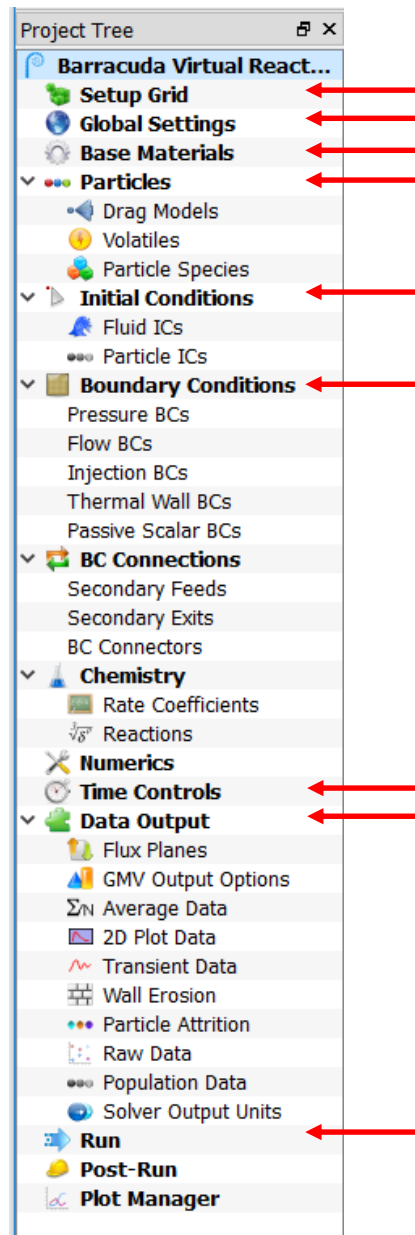
The Kuipers Bed simulation will be set up in 9 steps:

1. Setup Grid

Create the computational grid from a CAD file of the physical geometry

2. Global Settings

Set gravity and select isothermal calculation

3. Base Materials

Add materials to simulation and edit physical properties

4. Particles

Specify materials and particle size distributions for the particles in the model

5. Initial Conditions

Specify initial fluid and particle conditions. Specify initial particle locations

6. Boundary conditions

Specify fluid velocities and pressures at model boundaries

7. Time Controls

Specify simulation time, time step and restart interval

8. Data Output

Select data to be written during simulation for later analysis

9. Run

Check the model setup and run the simulation

Setup Grid

- Barracuda simulates fluid-particle behavior by dividing the physical domain into a 3D computational grid.

- Each cell within the grid provides a location for the solver to calculate Eulerian values

  - Pressure

  - Temperature

  - Velocity

  - Composition, etc

- The grid also provides a framework for specifying boundary conditions within a simulation

- Adding cells to a simulation will increase the resolution and often accuracy of the solution

- Adding cells to a simulation will also increase the computational time required

- **For the Kuipers problem, gridline locations are already provided in the kuipers_mysetup.prj file**

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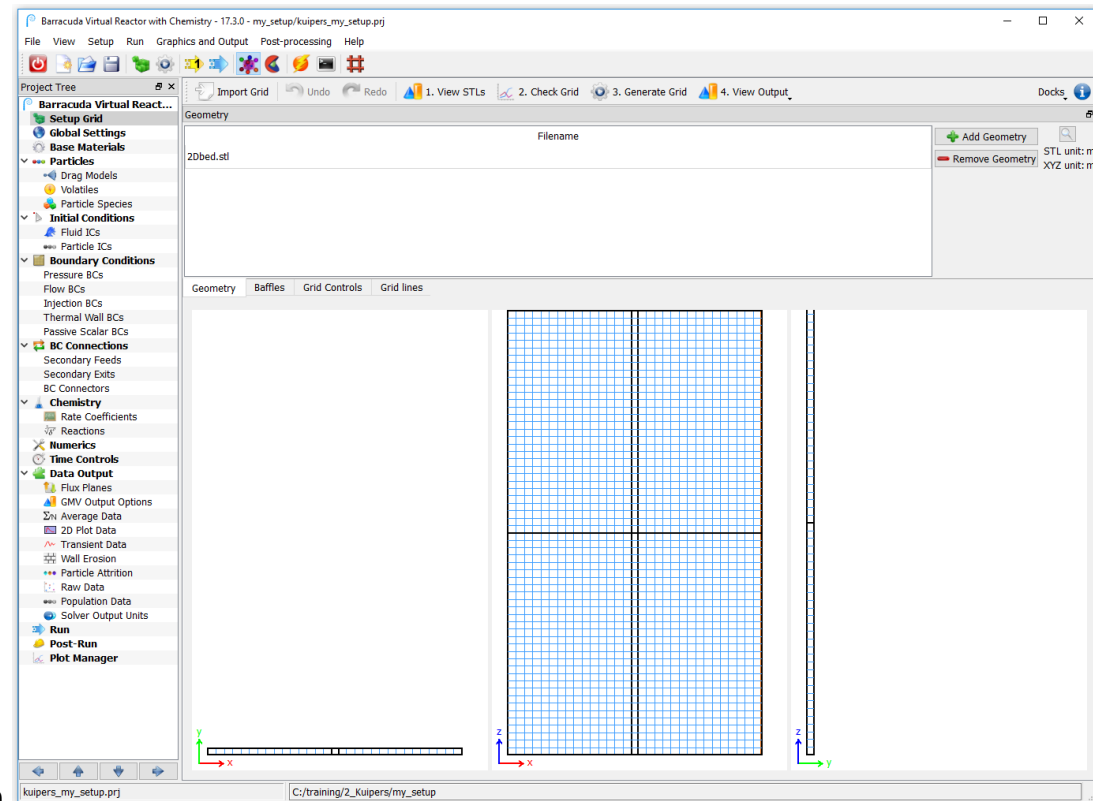
Setup Grid Window

- The setup grid window provides an interface for creating an appropriate grid for the model
- It contains the following tabs:
  - Geometry
  - Baffles
  - Grid Controls
  - Grid lines
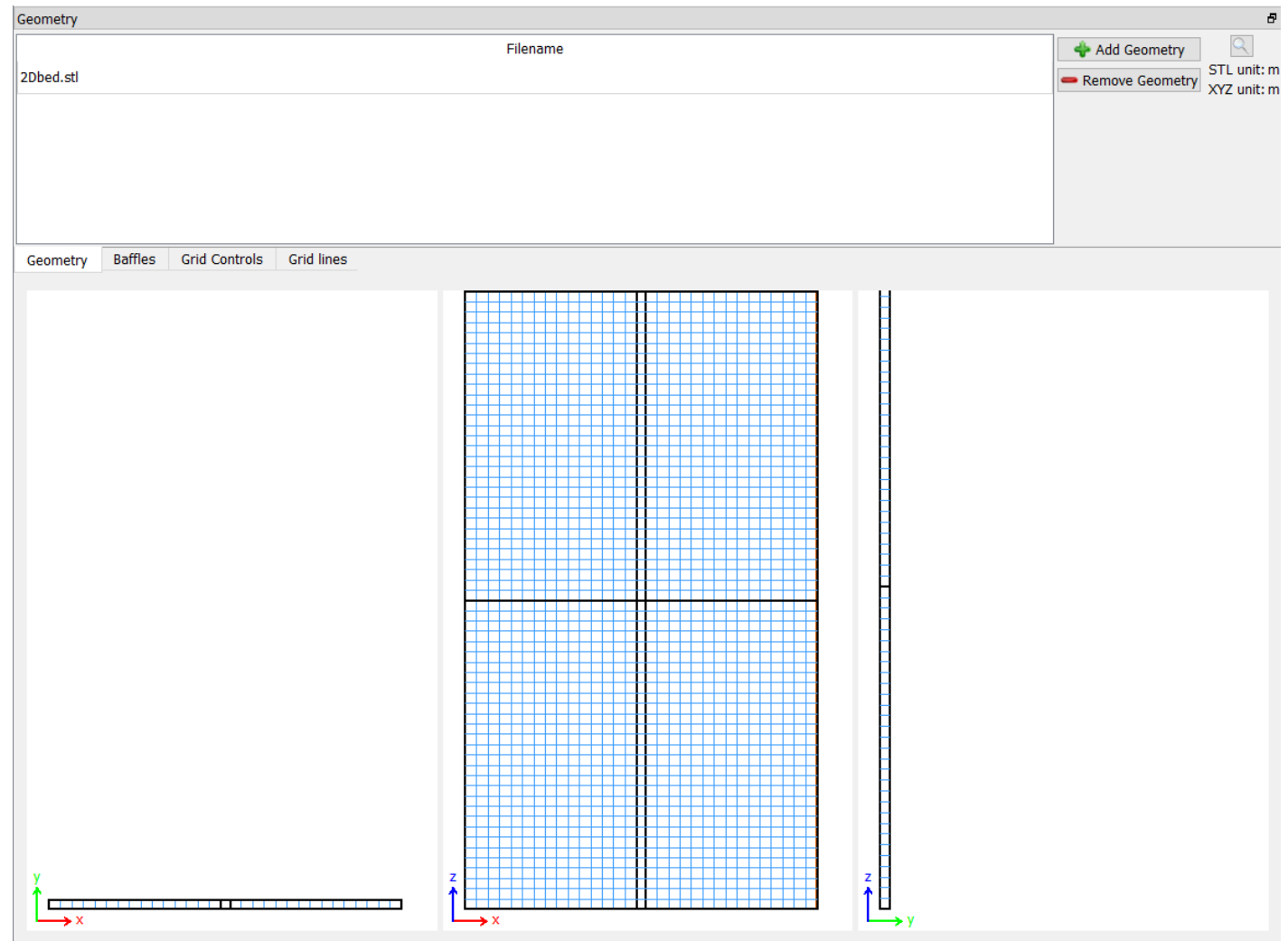
Grid Controls

- Using the mouse:

  - The grid may be translated using the center mouse button

  - Zoom in/out is accomplished holding the right mouse button and moving it up/down

  - Alternately, the scroll wheel can also be used for zoom (pending hardware and software configuration)

  - Note: each of the panel views can be panned and zoomed independently

- GUI button resets the grid view
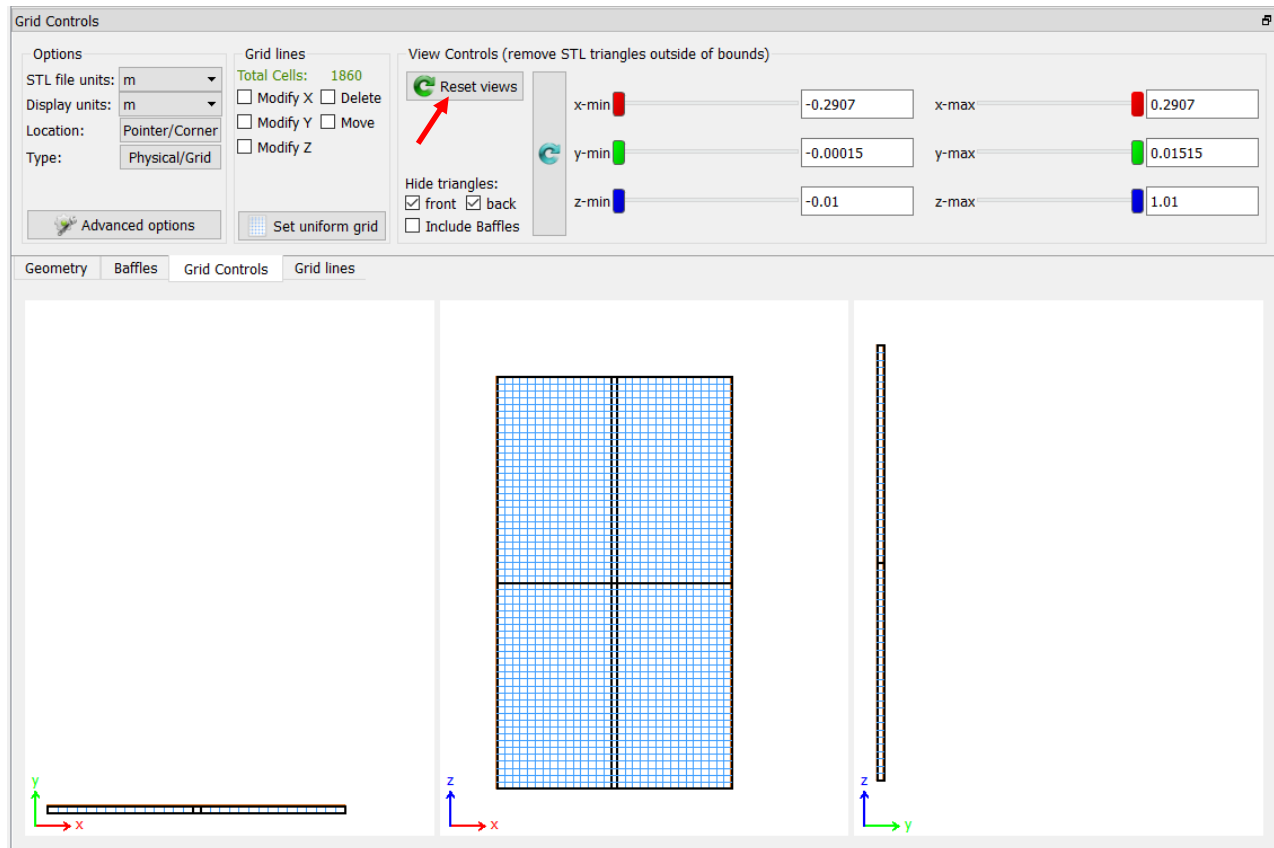
Generating and Viewing the Grid

- The computational grid will be generated based on the gridlines and STL file

- Click **Generate Grid**

- Once the grid generator runs, open the grid using the **View Output** button and selecting **View Grid**
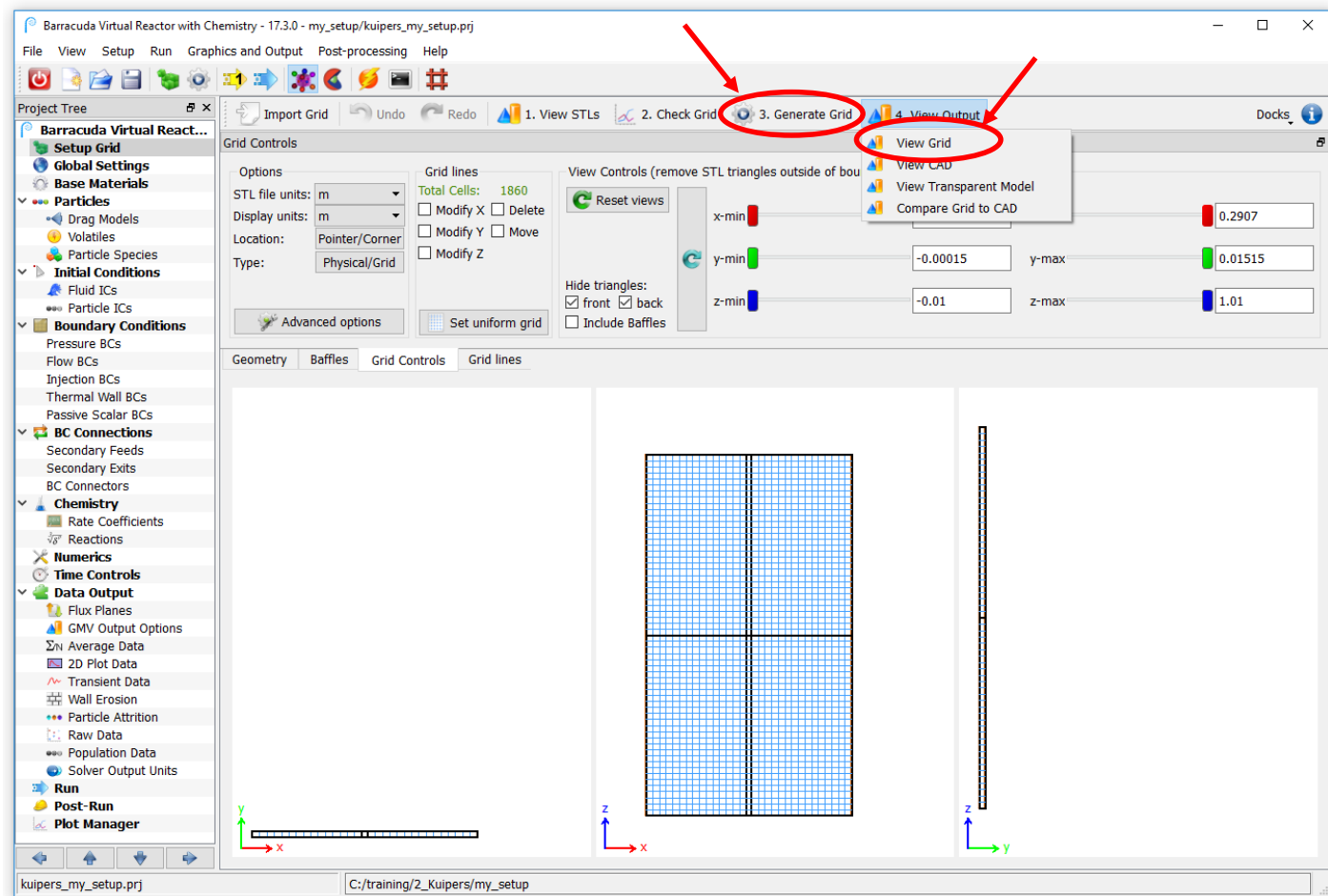
Viewing the Grid

- The grid may be rotated using the left mouse button

- To translate the grid, use the center mouse button

- Zooming is accomplished using the right mouse button

- **Note:** This is the coarsest grid possible for this problem (resolving the center jet with a single cell). This is not necessarily the recommended grid resolution, but rather intended to illustrate how the CPFD method obtains resolution from both the computational cells (grid) and computational particles (gridless).
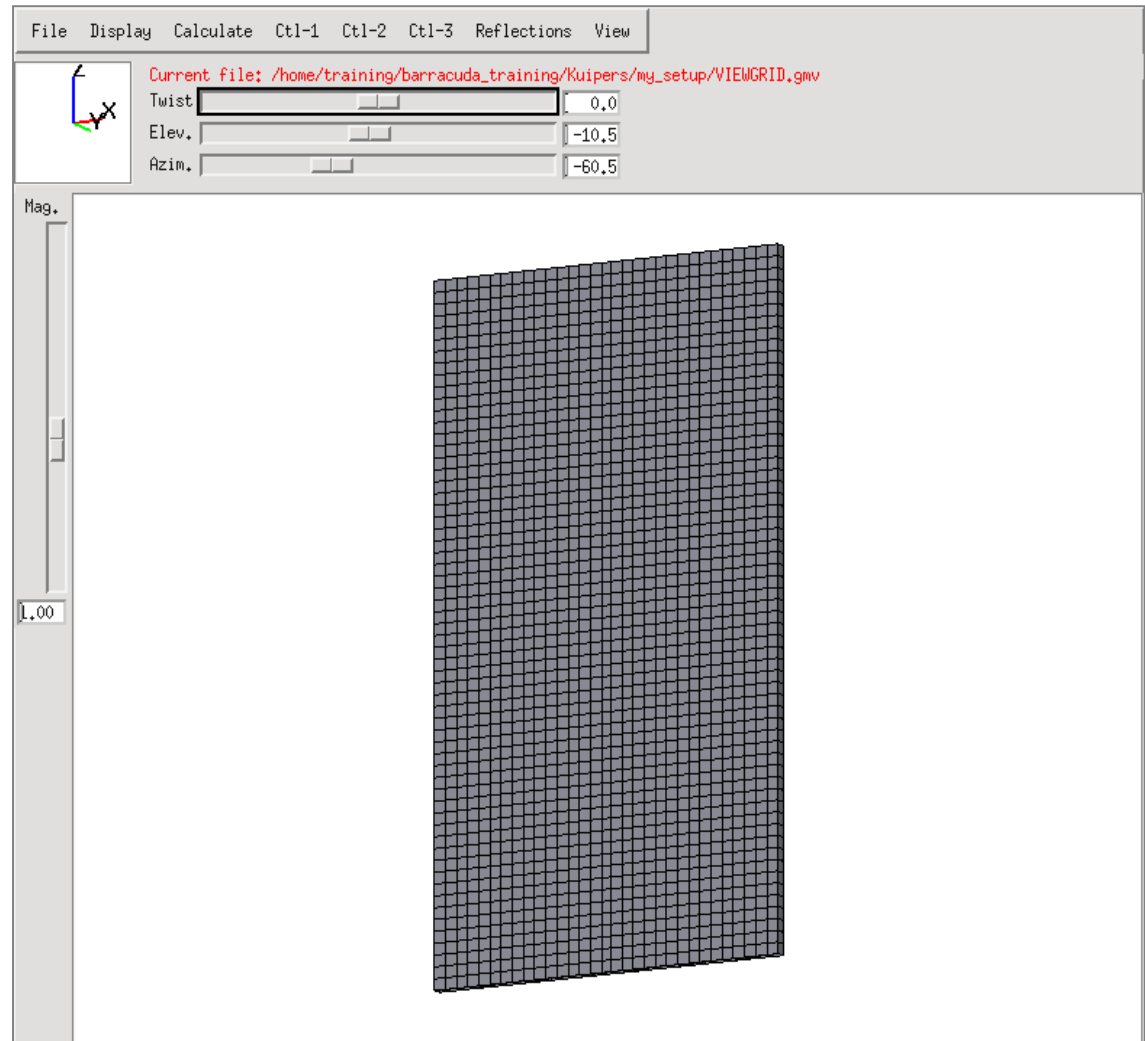
Overview of the Kuipers Bed Grid

Physical Setup

Pressure at outlet: 100,000 Pa

Initially air at 300 K
100,000 Pa

Particle Species 2

Particle Species 1

Fluidizing Gas   Fluidizing Gas

Center
Jet

Grid Setup

Center line to mark initial bed height

1.5 cm wide cell for center jet

Generated Grid

Top faces will become pressure boundary

Eulerian fluid calculations will be computed inside internal cells

Bottom faces will become flow boundary conditions

Grid is one cell thick to reflect 2D model

Grid Coordinates

- Initial and Boundary Conditions are located by x,y,z values

- **[** uses the minimum value, **]** uses the maximum value

Initial Particle Location:

Boundary	x		y		z	
Species 1	[	]	[	]	[	0.25
Species 2	[	]	[	]	0.25	0.5

Boundary Condition Location:

Boundary	x		y		z	
Fluidizing gas	[	-0.0075	[	max	[	[
Fluidizing gas	0.0075	]	[	max	[	[
Center jet	-0.0075	0.0075	[	max	[	[
Outlet Pressure	[	]	[	max	]	]

x values: -0.285 . . . . . . -0.0075 . . 0.0075 . . . . 0.285

z values: 1.0, 0.5, 0.25, 0

Particle Species 2
Particle Species 1
Fluidizing Gas   Fluidizing Gas
Center Jet
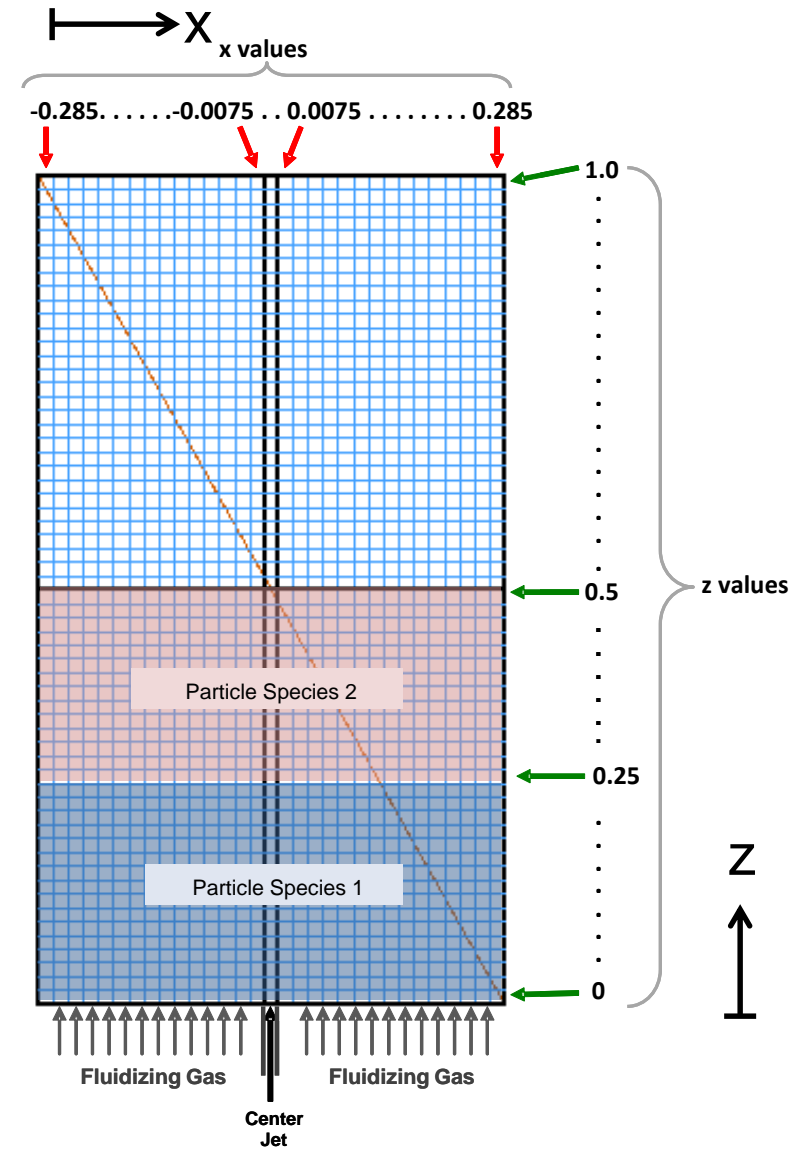
Global Settings

- Click on **Global Settings**

- Set your **Gravity** vector

  - In this example, gravity is in the negative z-direction

  - Notice the vector magnitude is "9.8" m/s^2

  - Note: All units in Barracuda are SI unless otherwise noted

- Isothermal flow should be selected.

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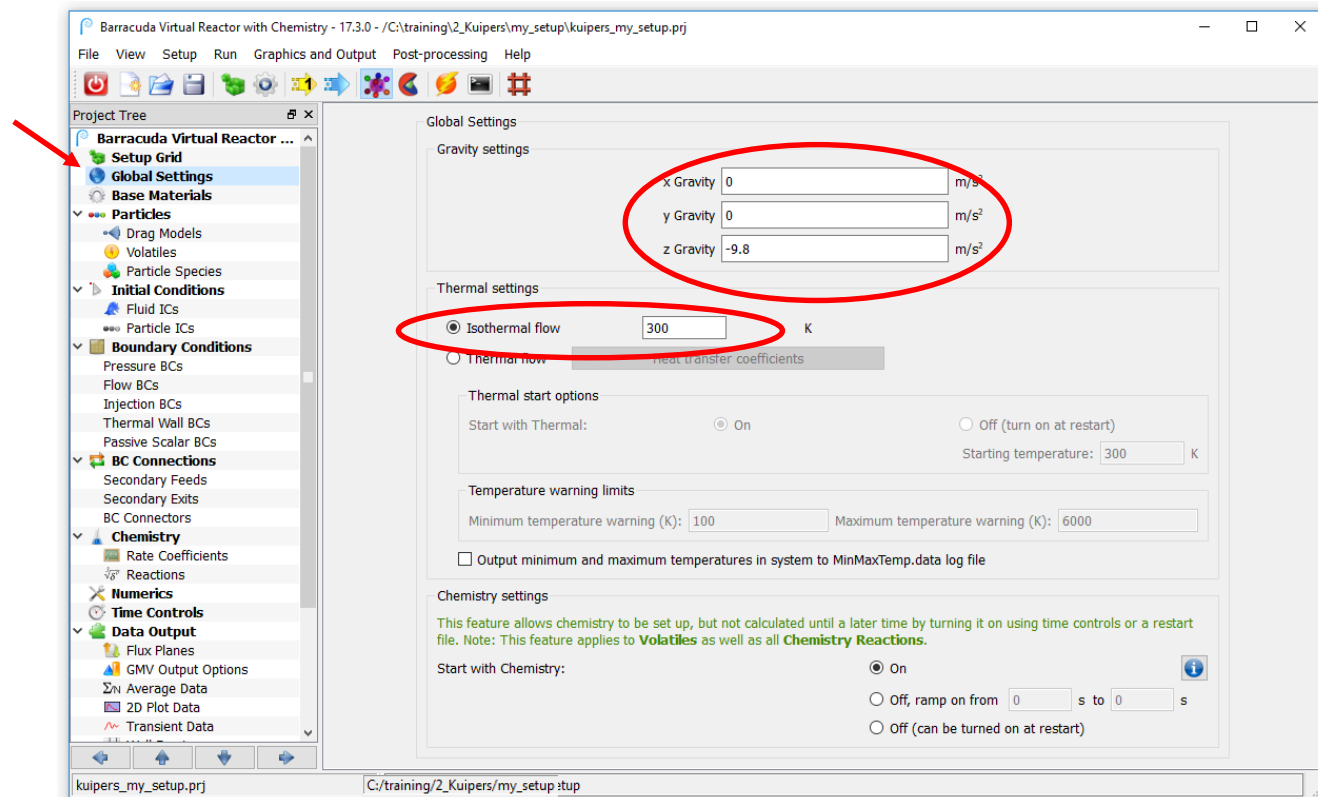
Base Materials

- Click on **Base Materials**

- All project materials, fluids and solids, must be defined here

- Project materials can be imported from the **Material library** OR new materials can be created with the **Add** button

- All material properties can be edited in the **Base Materials** window

- Flow can be set as compressible (default) or incompressible

SIMULATE > UNDERSTAND > OPTIMIZE
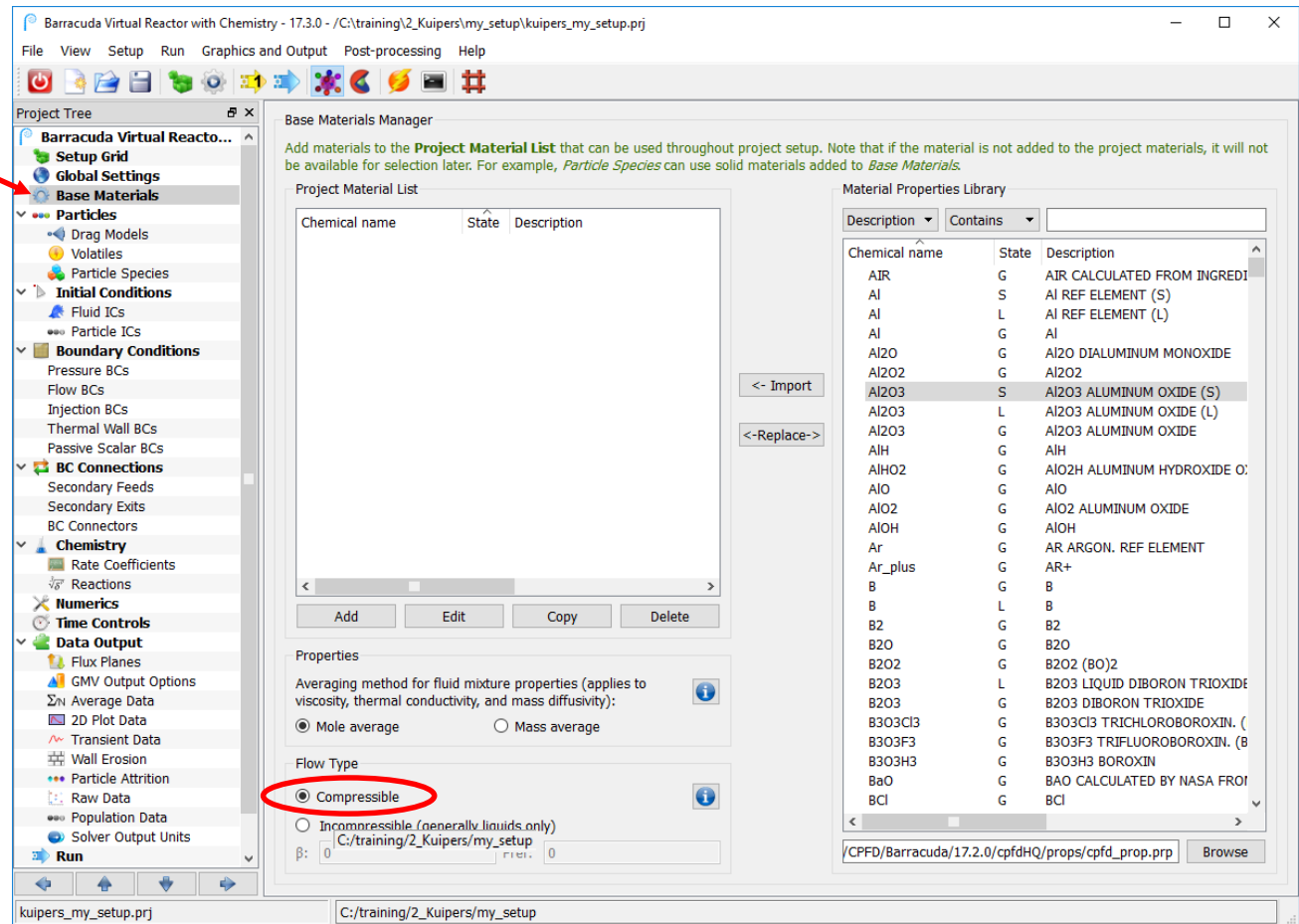
Base Materials

For the Kuipers setup:

- Verify **Compressible flow** is selected, since the fluid is a gas

- Air and glass need to be added

- Select AIR from the **Material Library**

- Click **Import**

- AIR now appears in the **Project Material List** at the left
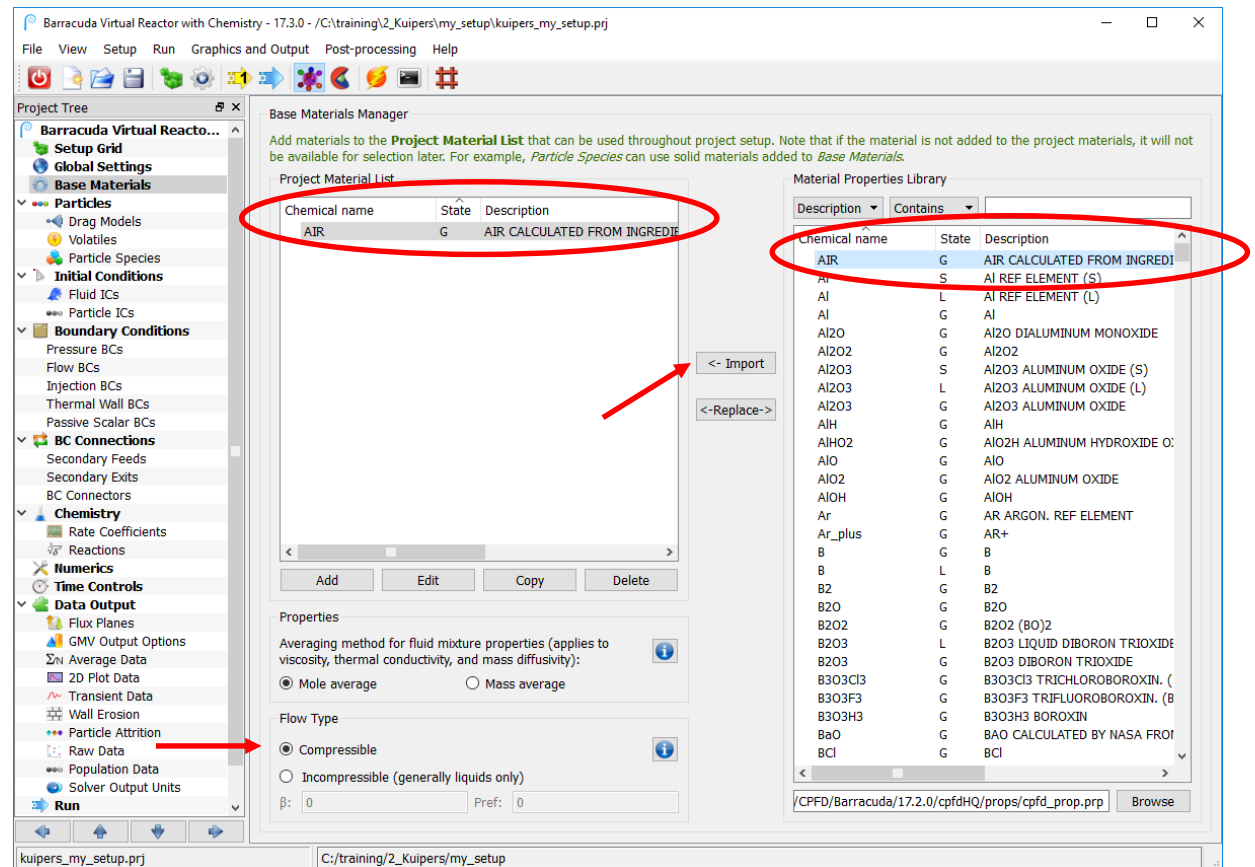
Base Materials

- To define the solid material, click on **Add**

- In the **Material Properties** window, enter the **Chemical name** as "GLASS". Enter an appropriate description

- Set the **State (Gas, Liquid, Solid)** to solid

- Set the **Density** to 2660 kg/m³

- Set the **Molecular weight** to 60 g/mol

- Click **OK**

- GLASS now appears in the **Project Material List** at the left
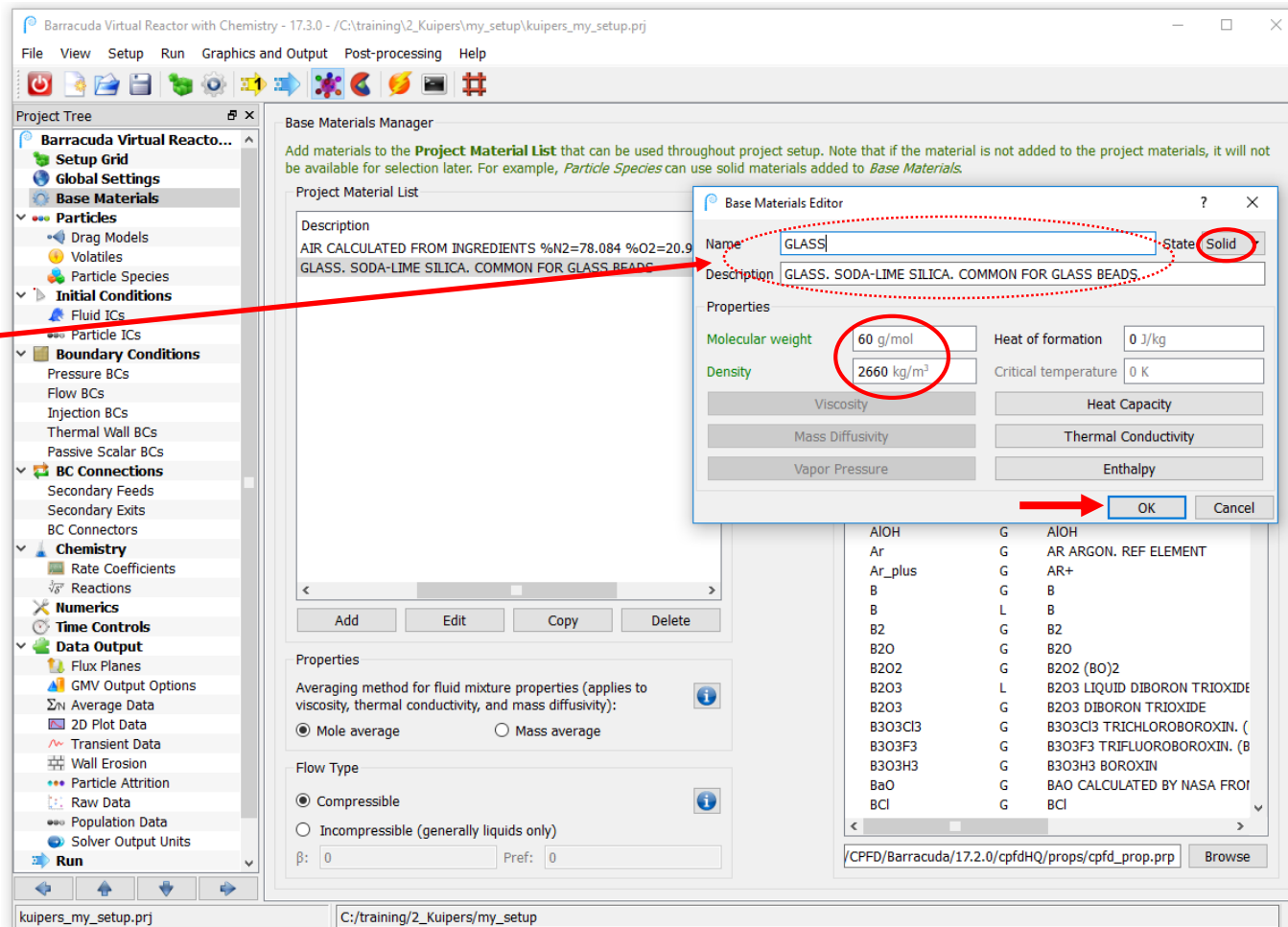
- NOTE: Other material property data such as thermal conductivity, heat capacity, and heat of formation would have to be specified <u>if</u> this were a thermal or reacting problem. Viscosity is required if the new material is a fluid

- NOTE: **Red** writing means that data needs to be input, **green** writing means that the property is ready, **black** writing means that the property is not needed for the calculation

Particles

- Click on the **Particles** page

- Enter a **Close pack volume fraction** of "0.55"

- This is the maximum amount of solids packing permitted in a region

- 0.55 means that up to 55% of a reasonably-sized control volume can be occupied by particles. Conversely, at least 45% of the same volume must be occupied by the fluid
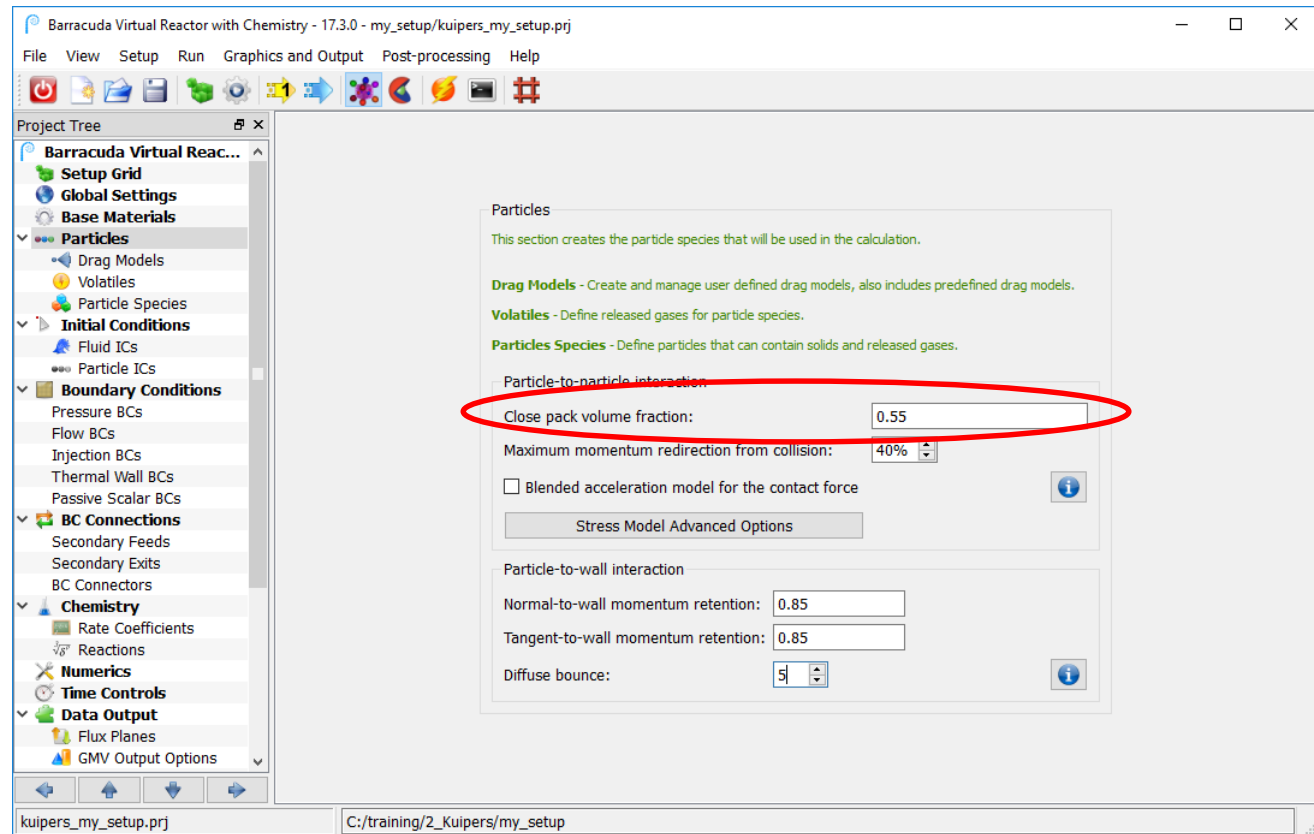
Particles

- Set **Particle-to-wall interaction** properties

- A **Normal-to-wall momentum retention** coefficient is the maximum normal component of particle momentum which can be retained after the particle "bounces" off a wall.

  - Set this to "0.85"

- A **Tangent-to-wall momentum retention** coefficient is the maximum tangential component of particle momentum which can be retained after the particle "bounces" off a wall.

  - Set this to "0.85"

- A **Diffuse bounce** coefficient is the amount of particle scatter after the particle "bounces" off a wall

  - Set this to "5" which is the maximum value

SIMULATE > UNDERSTAND > OPTIMIZE
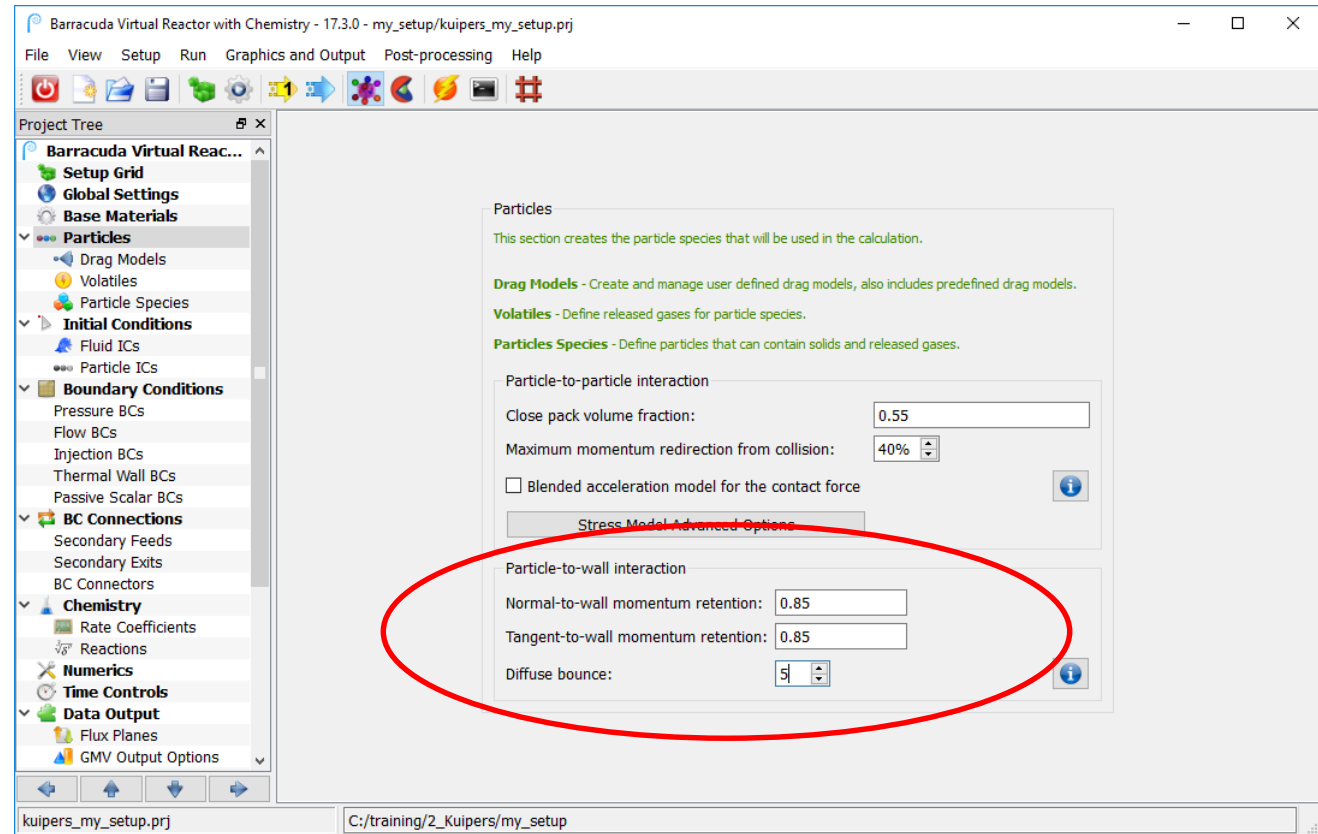
Particle Species

- Click on **Particle Species**

- We are now ready to define the particle species in the system

For the Kuipers setup:

- We have only one type of solid particle (GLASS)

- However, we want to use two colors (one in bottom half of bed, another in top half) to view mixing

- To accomplish this, we must define two separate species of the same material (GLASS)
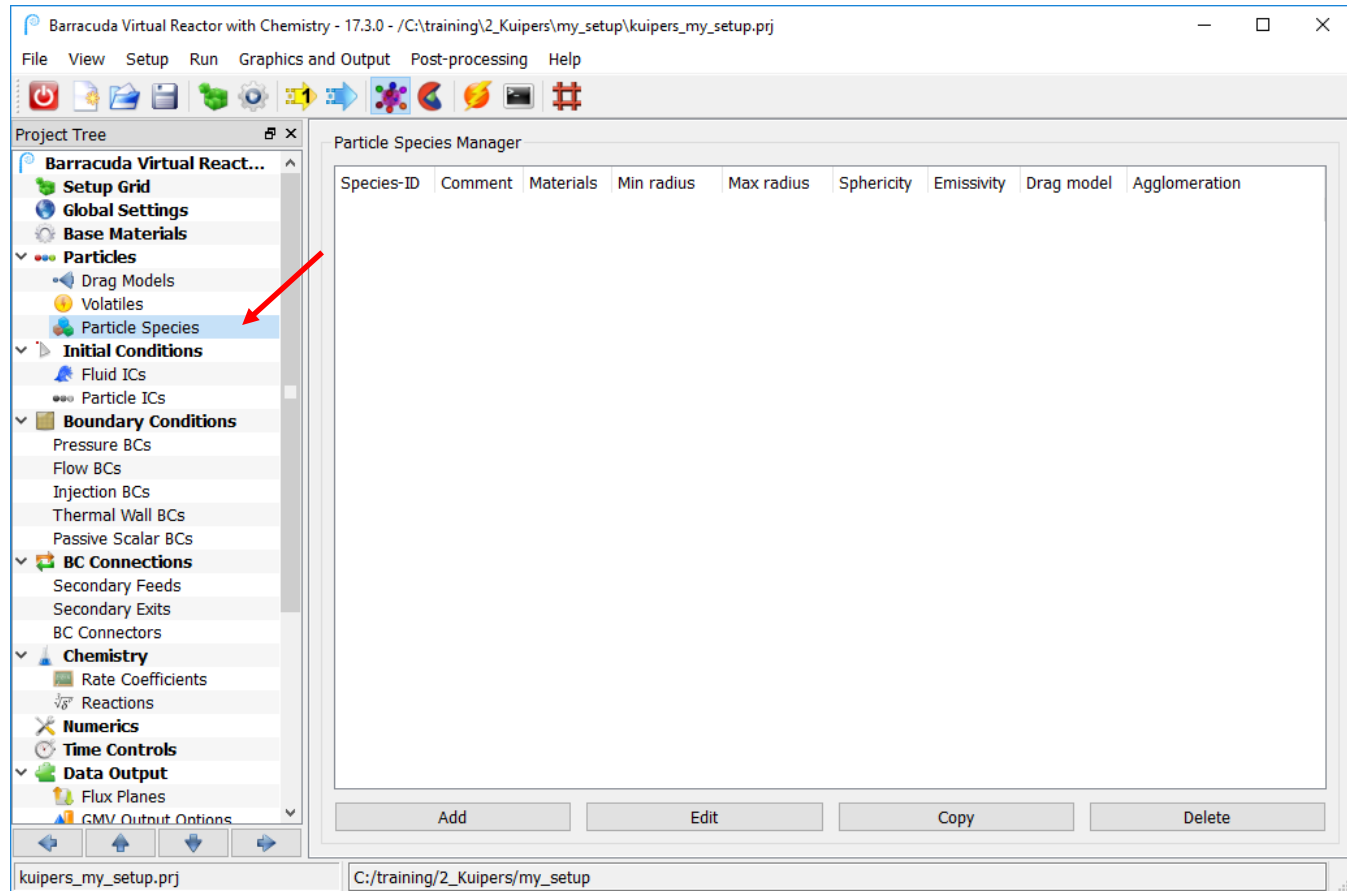
Particle Species

- Click on **Add**

- The **Particle Species Editor** window will pop up, click on **Applied Materials**

- **Applied Materials Manager** window will pop up, click on **Add**

- In the **Applied material** window, select GLASS

- Set the **Mass fraction amount** to "1"

- Click **OK**

- Click **OK** in **Applied Materials Manager** window.
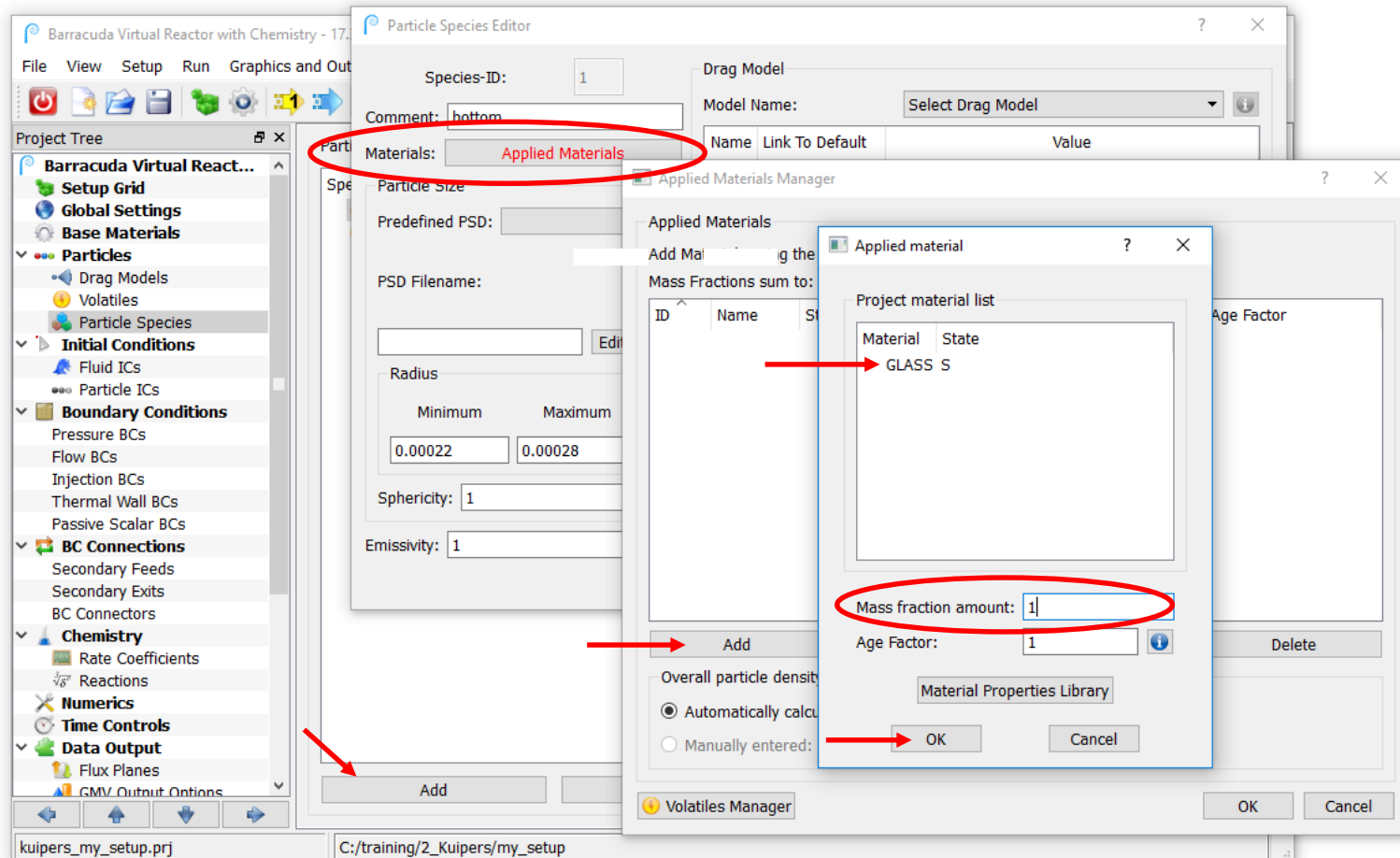
Particle Species

- We are now ready to define the particle radius

- For the Kuipers setup, the particle diameters are between 440 and 560 μm

- Set the particle **Radius** to "2.2e-4 to 2.8e-4" meters

- Since we have two identical particle species, add a descriptive **Comment** for species 1

- Select Wen-Yu as **Drag model** in the drop down menu

- Click **OK**
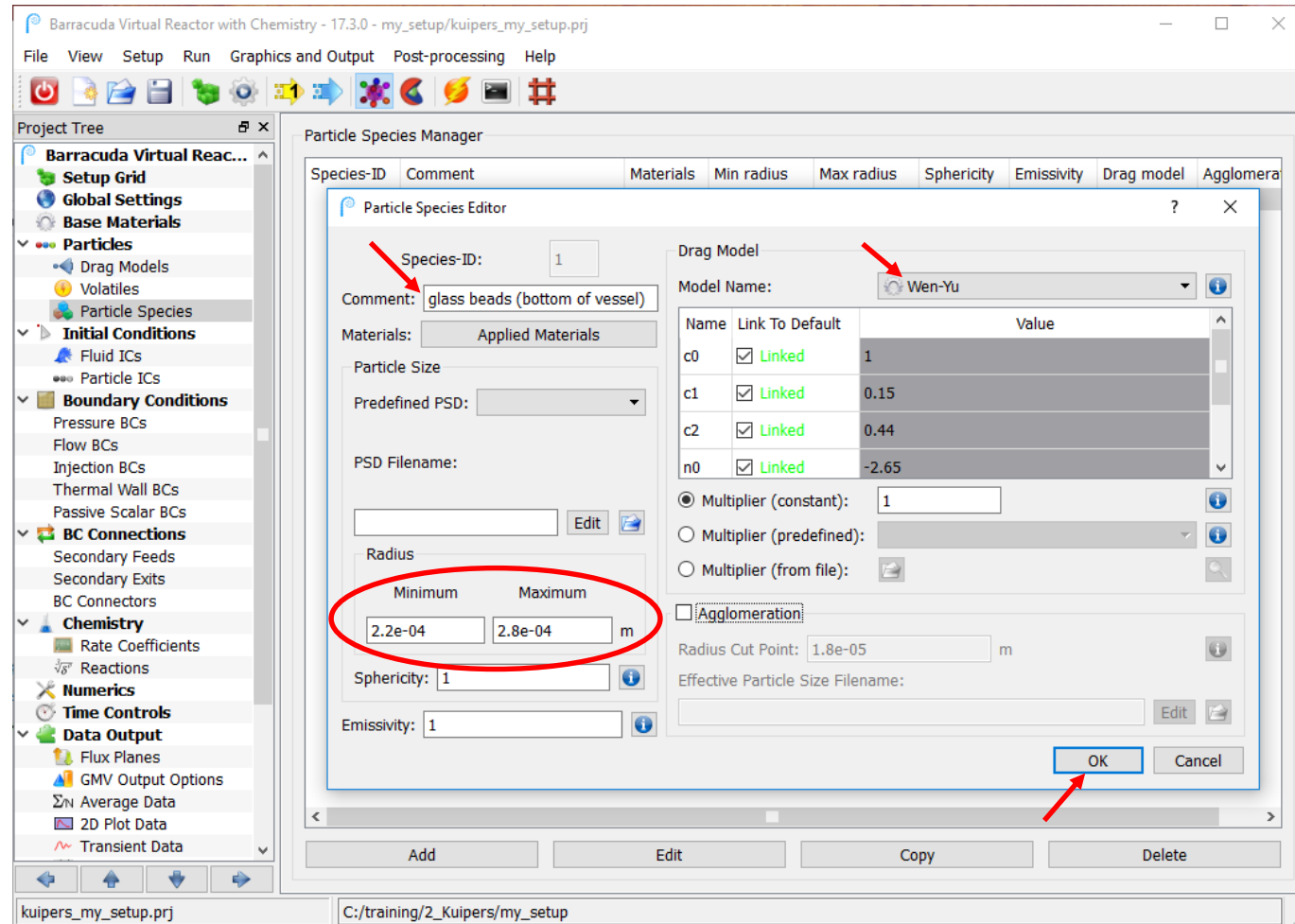
Particle Species

- To define a second, identical particle species, simply copy the first

- Select species **001**, then click **Copy**

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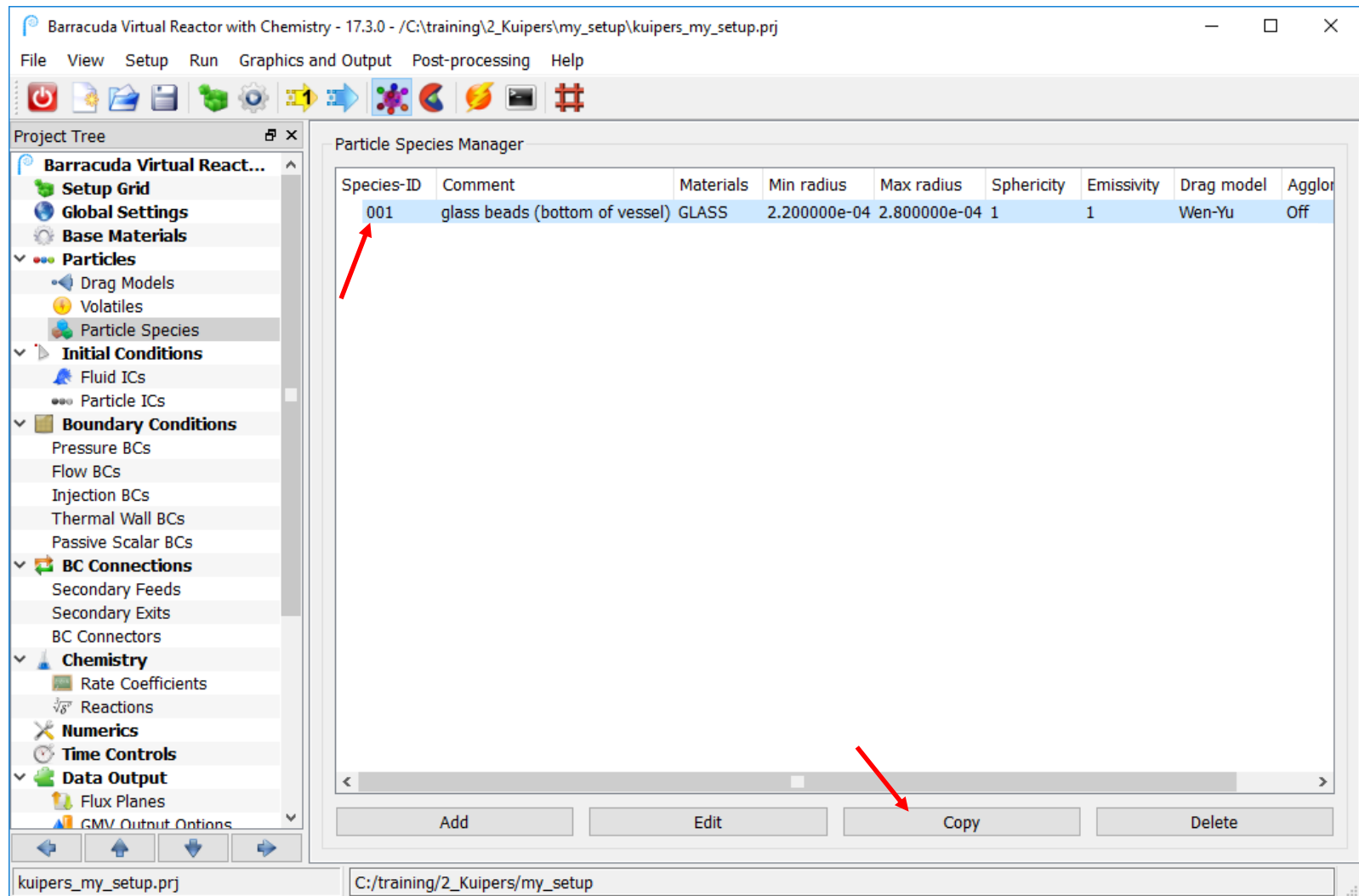
Particle Species

- To change the comment describing the second particle, select species **002**

- Click **Edit**

- Change the Comment

- Click **OK**
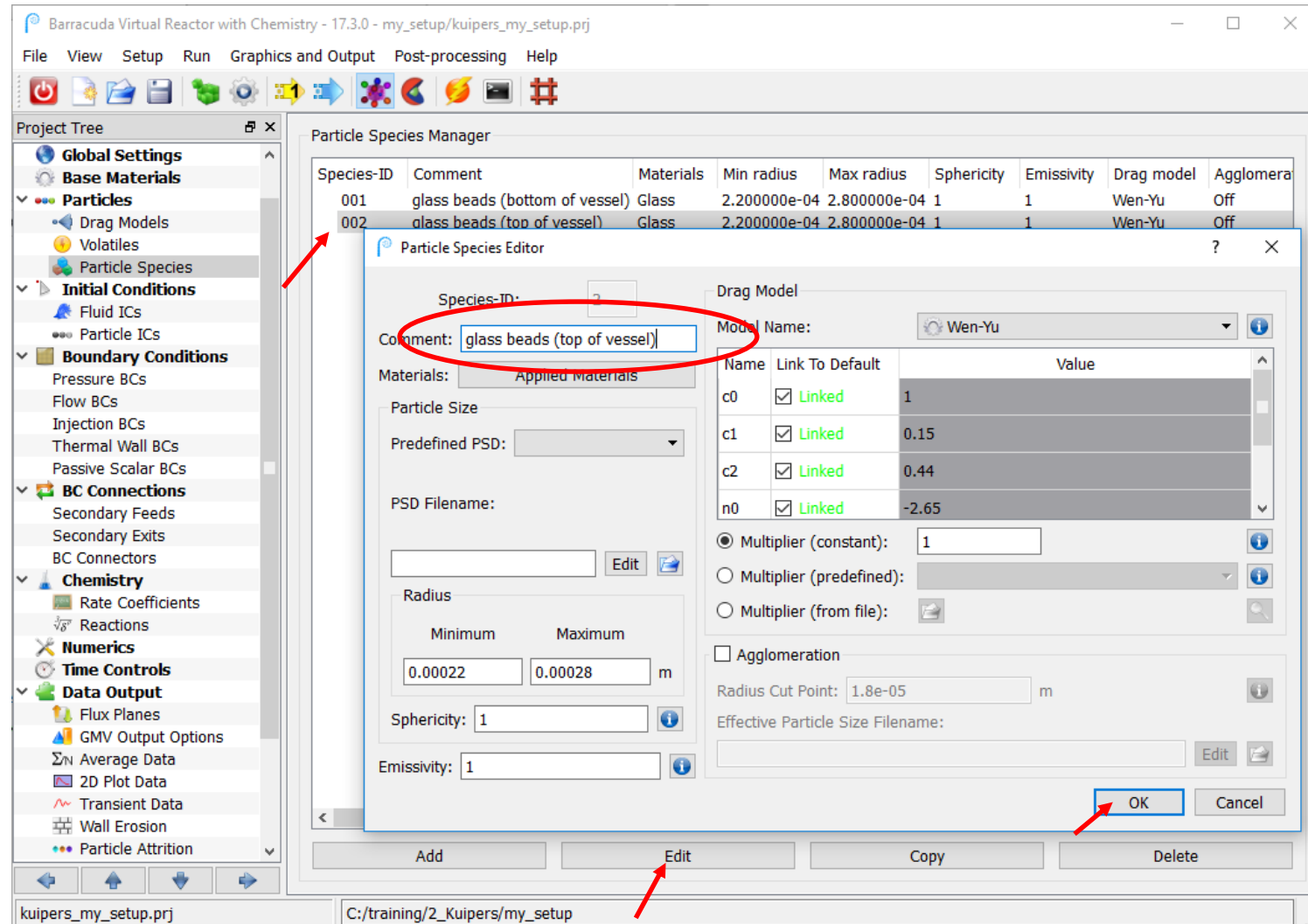
Fluid Initial Conditions

- Click on **Fluid ICs**

- Select the default fluid species

- Click on **Edit**

- Click on **Define fluids**
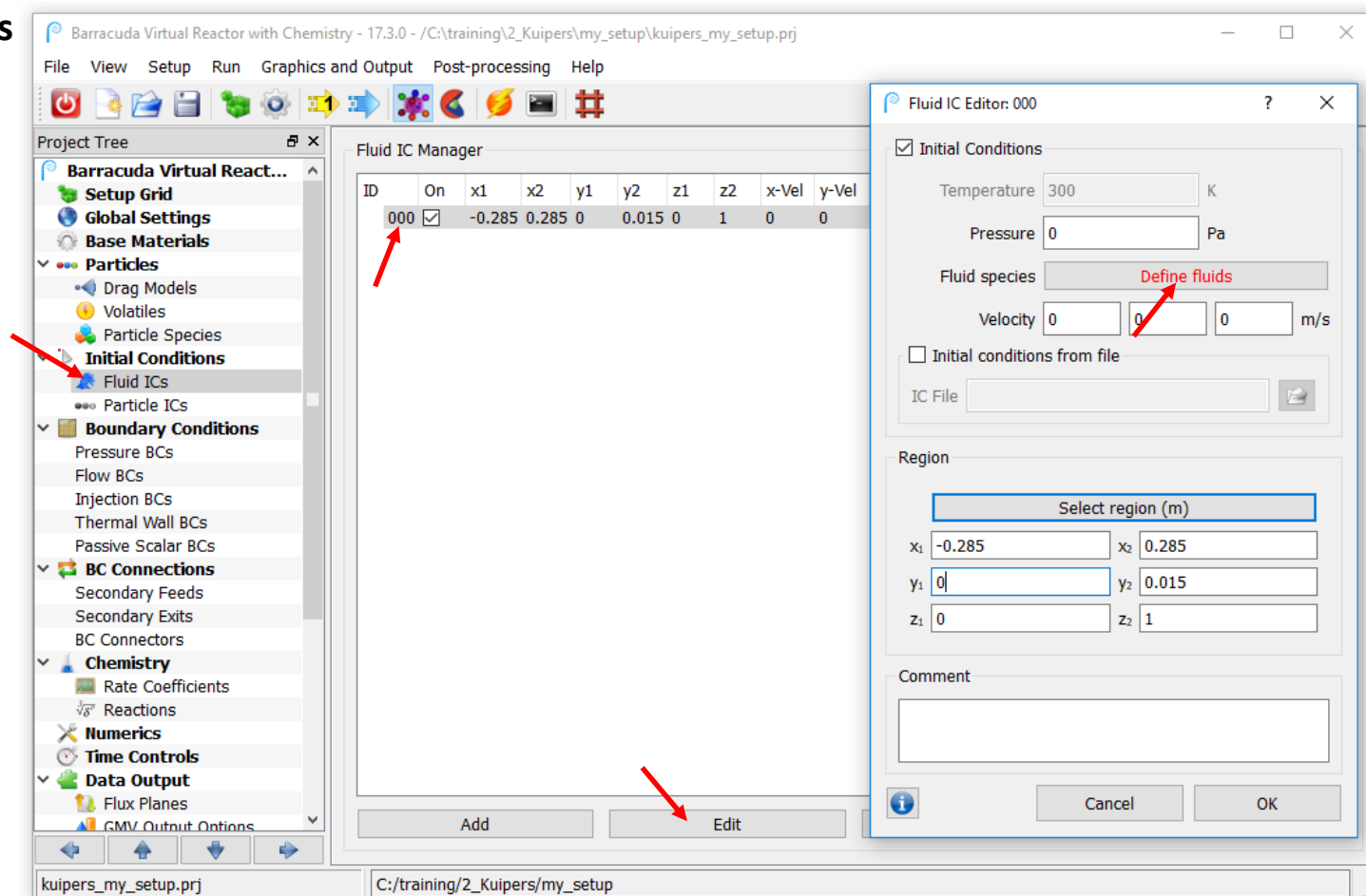
Fluid Initial Conditions

- The **Applied Materials** window will pop up. Click on **Add Material**

- Select **AIR** and set the **Mass fraction amount** to "1"

- Click **OK**
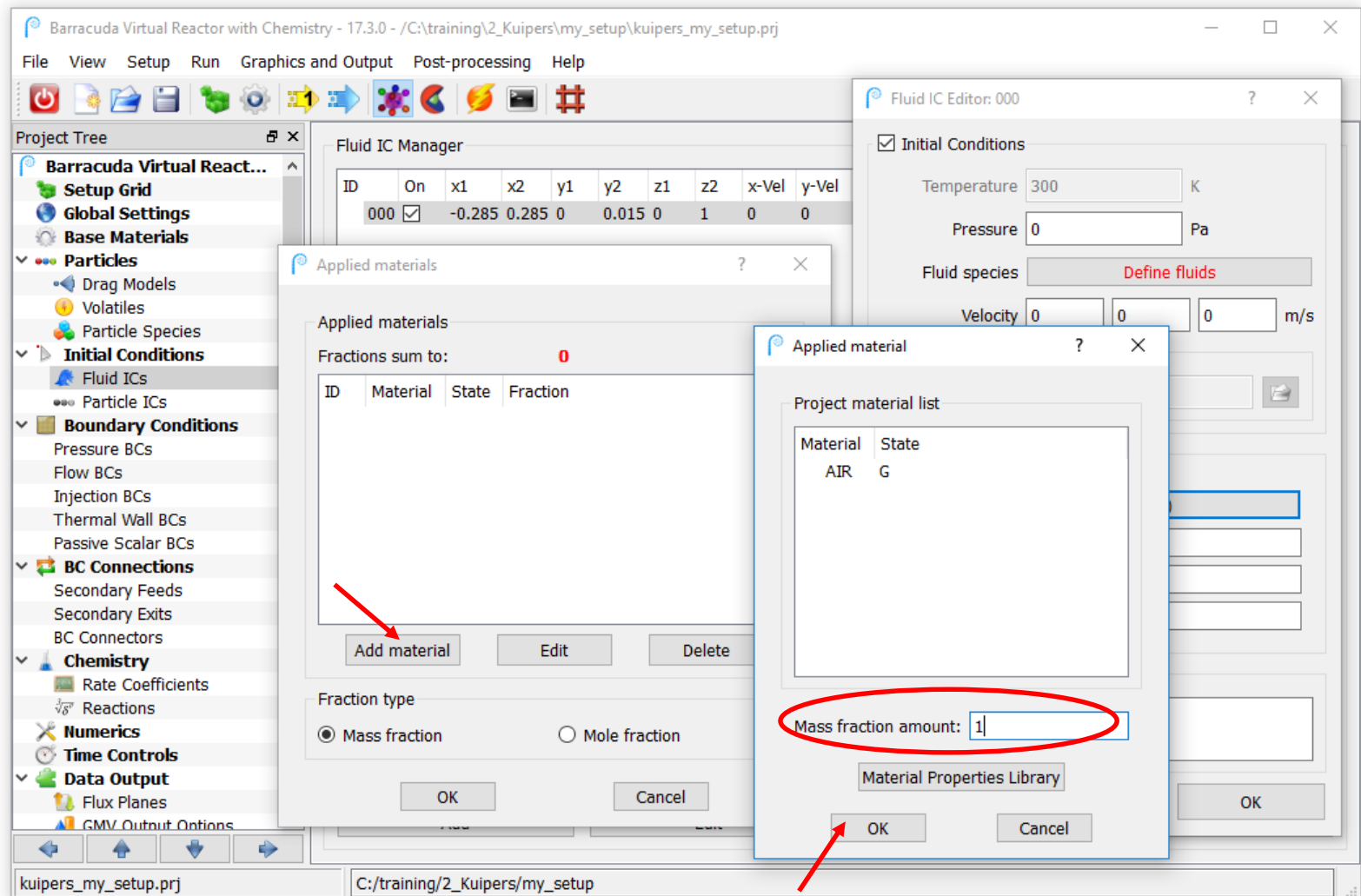
Fluid Initial Conditions

- Once the fluid is defined, specify the velocity, pressure, and location of the fluid

- In this example problem, air is initially at rest at atmospheric pressure

- Leave the x, y, and z fluid velocities at zero

- Set the **Pressure** to "1e5" Pa

- Since the air initially occupies the entire bed (area above and in between quartz particles), use [and] to input the minimum and maximum values

- Click **OK**

Particle Initial Conditions

- Click on **Particle ICs**

- Click **Add**
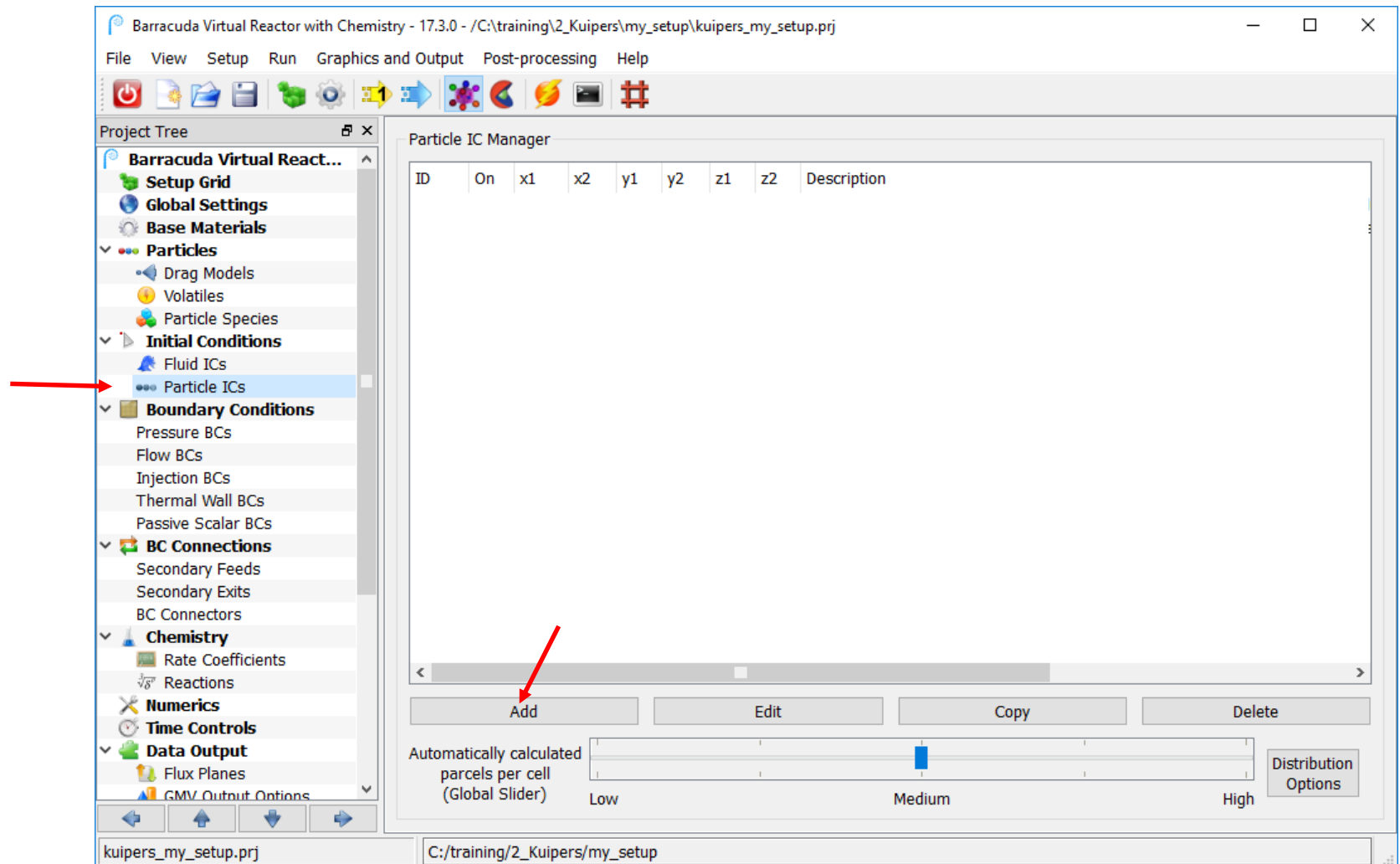
Particle Initial Conditions

- A **Particle initialization** window will pop up

- On the Initialize tab select **Initialize volume fraction in region**

- On the **Particle species** tab select **001- glass beads (bottom of vessel)**

- Set the **Particle volume fraction** to "0.55"

- Specify the **Computational particle location** at the start of the calculation:
  - Since we want these particles to be on the bottom half of the bed, we set z1 to "[" (giving a 0) and z2 to "0.25"

- Remember to add a descriptive **Comment**

- Click **OK**

Particle Initial Conditions

- Next, define the initial conditions for the second particle species

- Click **Add**

- On the Initialize tab select **Initialize volume fraction in region**

- On the **Particle species** tab select **002-glass beads (top of vessel)**

- Set the **Particle volume fraction** to "0.55"

- Specify the **Computational particle location**
  - Since we want these particles to be on the top half of the bed, we set z1 to "0.25" and z2 to "0.5"

- Remember to add a descriptive **Comment**
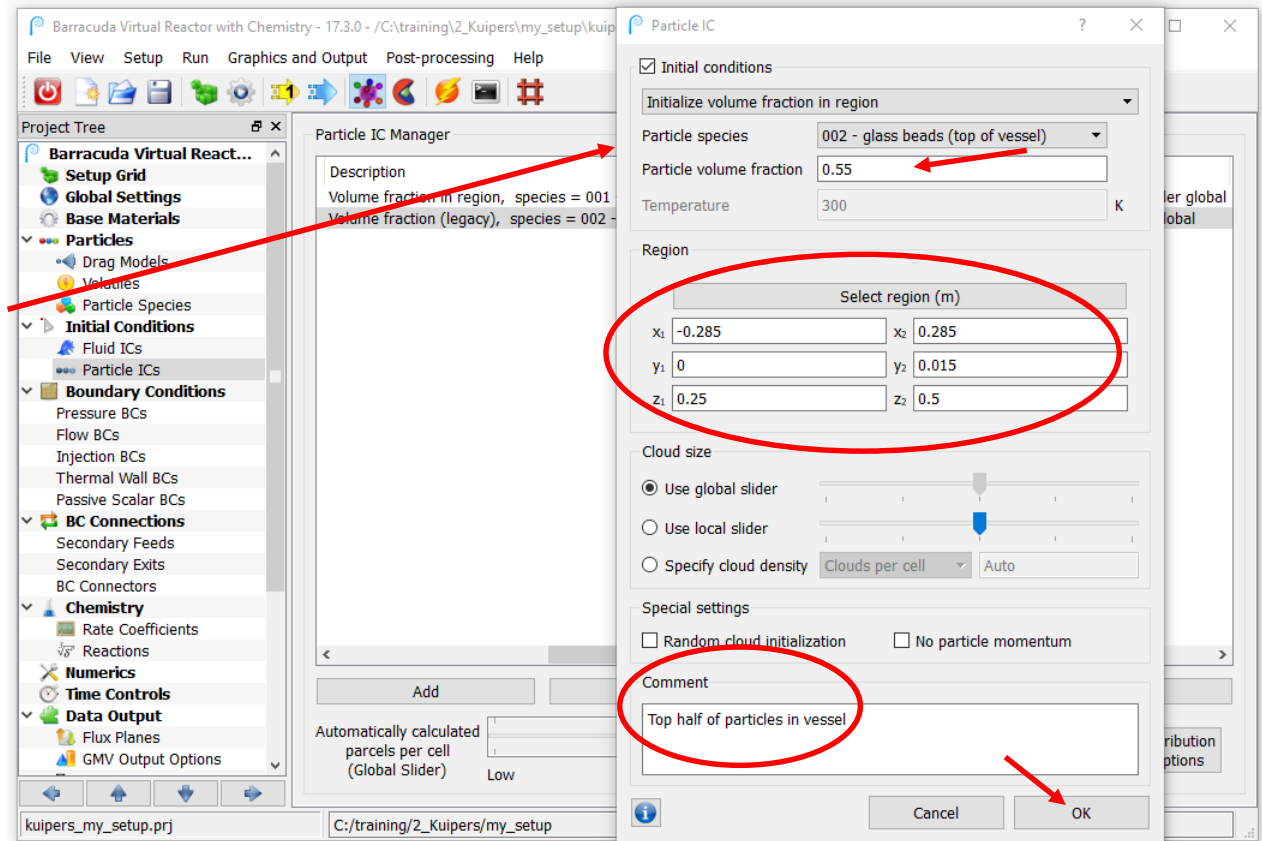
- Click **OK**

Pressure Boundary Conditions

- Click on **Pressure BCs**

- Click **Add**
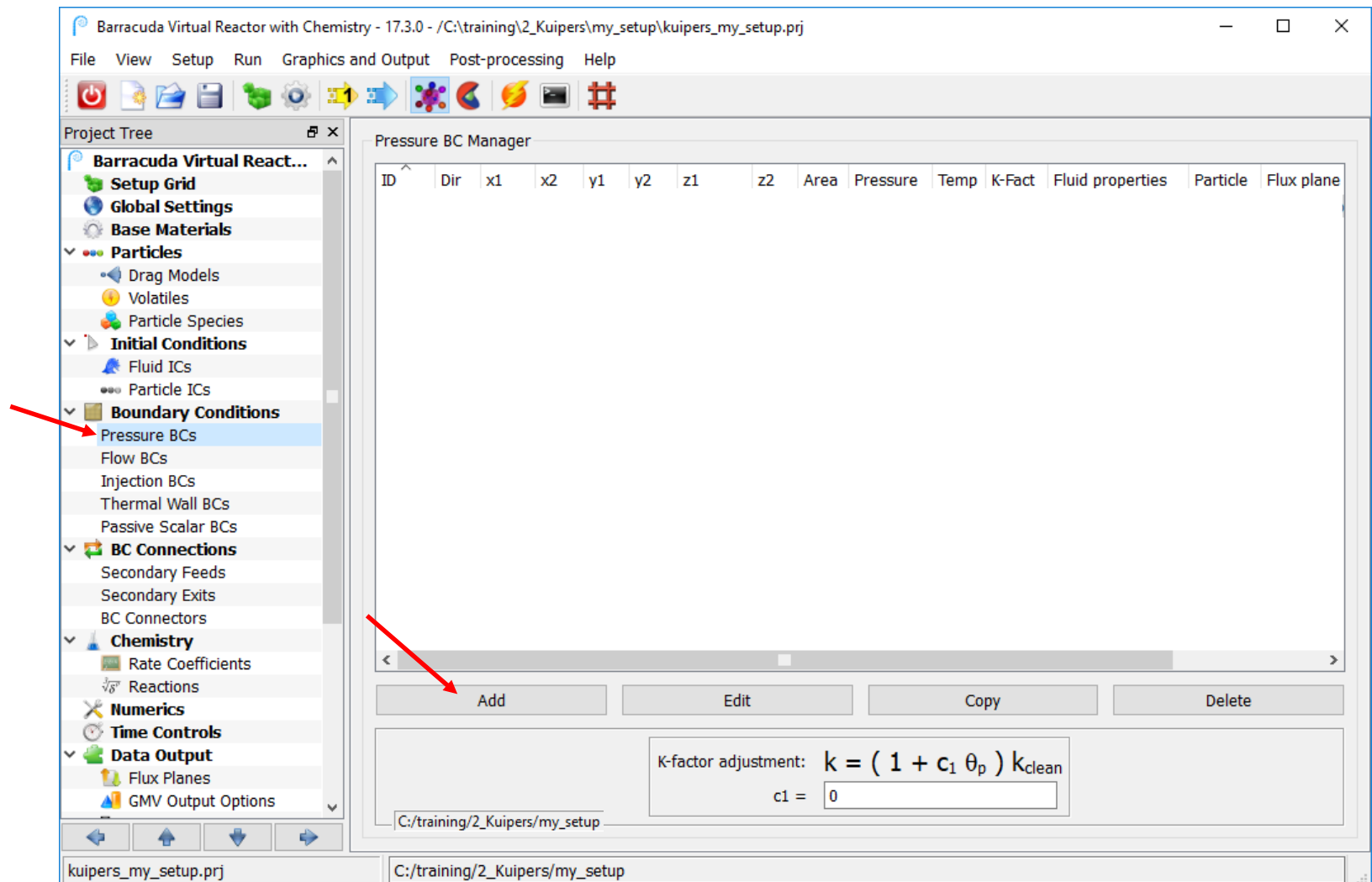
Pressure Boundary Conditions

- Define the fluid by clicking on **Define fluid species**

- The **Applied materials** window will pop up

- Click on **Add material**

- Select **AIR** and set the **Mass fraction amount** to "1"

- Click **OK**
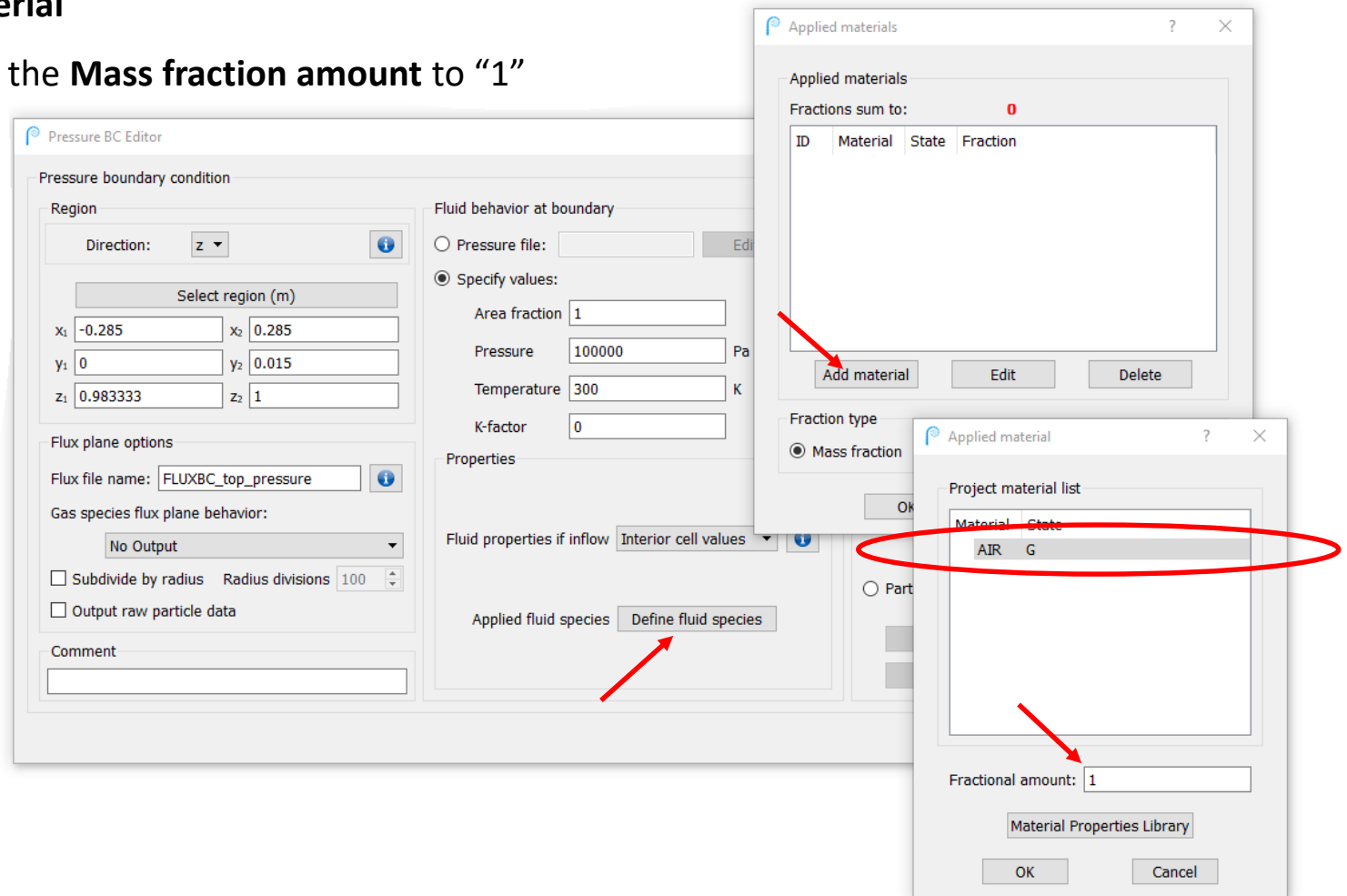
Pressure Boundary Conditions

- Once the fluid is defined, specify the pressure

- Set the **Pressure** to "1e5" Pa

- Provide a **Flux file name** for the boundary

- Flux planes track the transient flow of fluids and solids crossing pre-defined planes and model boundaries. Use a descriptive name

  - Tip: Starting a Flux file name with "Flux_" or "FLUX_" will facilitate post-processing later on. This is recommended.

- Enter the plane **Location** (maximum index in z with **]**). Why these values?

- Enter a **Comment** (if desired)

- Click **OK**

Flow Boundary Conditions

- Click on **Flow BCs**
  - The Flow BC page is used to define fluid boundary conditions where flow rate (mass or velocity) is known
  - Flow rate can either be constant (using the Specify values option) OR entered as a transient value in a separate data file

- Click on **Add**

- Start by defining the fluid. Click on **Define fluids** and follow the same steps as before:
  - Click **Add material**
  - Select **AIR**
  - Set the **Mass fraction amount** to "1"
  - Click **OK**

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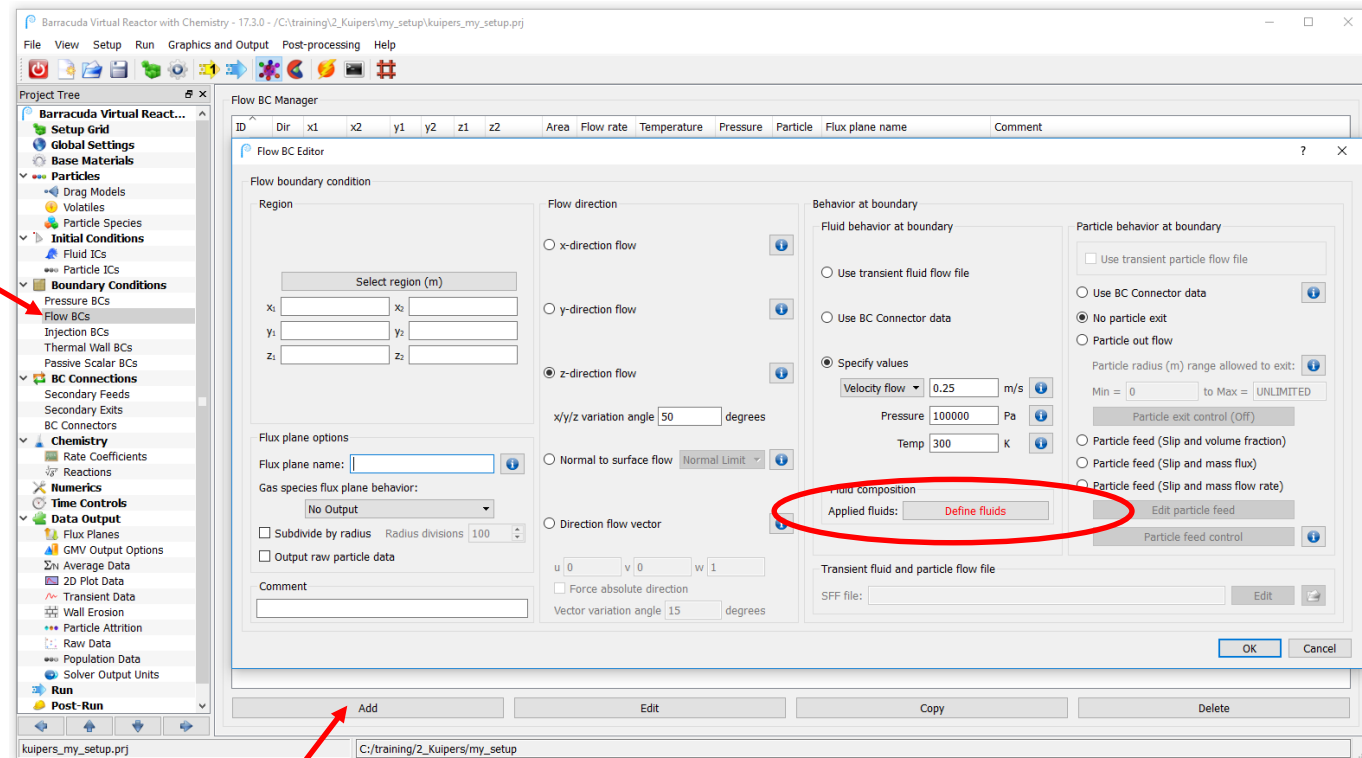
Flow Boundary Conditions

- Once the fluid is defined, specify the Velocity values
  - A positive velocity means flow is directed into the model space (negative means out-flow)
  - The velocity is a "superficial velocity" (through an open area, in the absence of particles)
- Set up the project to bring in fluidizing air at a **Velocity Flow** of "0.25" m/s
- Set the **Pressure** to "1e5" Pa
- Leave the **Flow direction** setting at z-direction

Flow Boundary Conditions

- In the Kuipers setup, fluidizing air enters the system across the bottom of the bed on either side of the center jet
  - This requires that flow boundaries on either side of the jet be specified separately
  - Begin by defining the boundary for the fluidizing air entering at low indices in the x-direction

- Specify the plane **Region** as follows:
  - Set x1 to "**[**" and x2 to "-0.0075"
  - Set y1 to "**[**" and y2 to "**]**"
  - Set z1 to "**[**" and z2 to "**[**"

- Next, provide a **Flux plane name** for the boundary

- Enter a **Comment** (if desired)

- Click **OK**

Flow Boundary Conditions

- The boundary for the fluidizing air entering at high indices in the x-direction is a duplicate of the previously created boundary

- **Copy** the existing boundary condition then click on **Edit** and enter the plane **Location** as follows:
  - Set x1 to "0.0075" and x2 to "**]**"
  - Set y1 to "**[**" and y2 to "**]**"
  - Set z1 to "**[**" and z2 to "**[**"

- Next, provide a **Flux plane name** for the boundary

- Enter a **Comment** (if desired)

- Click **OK**
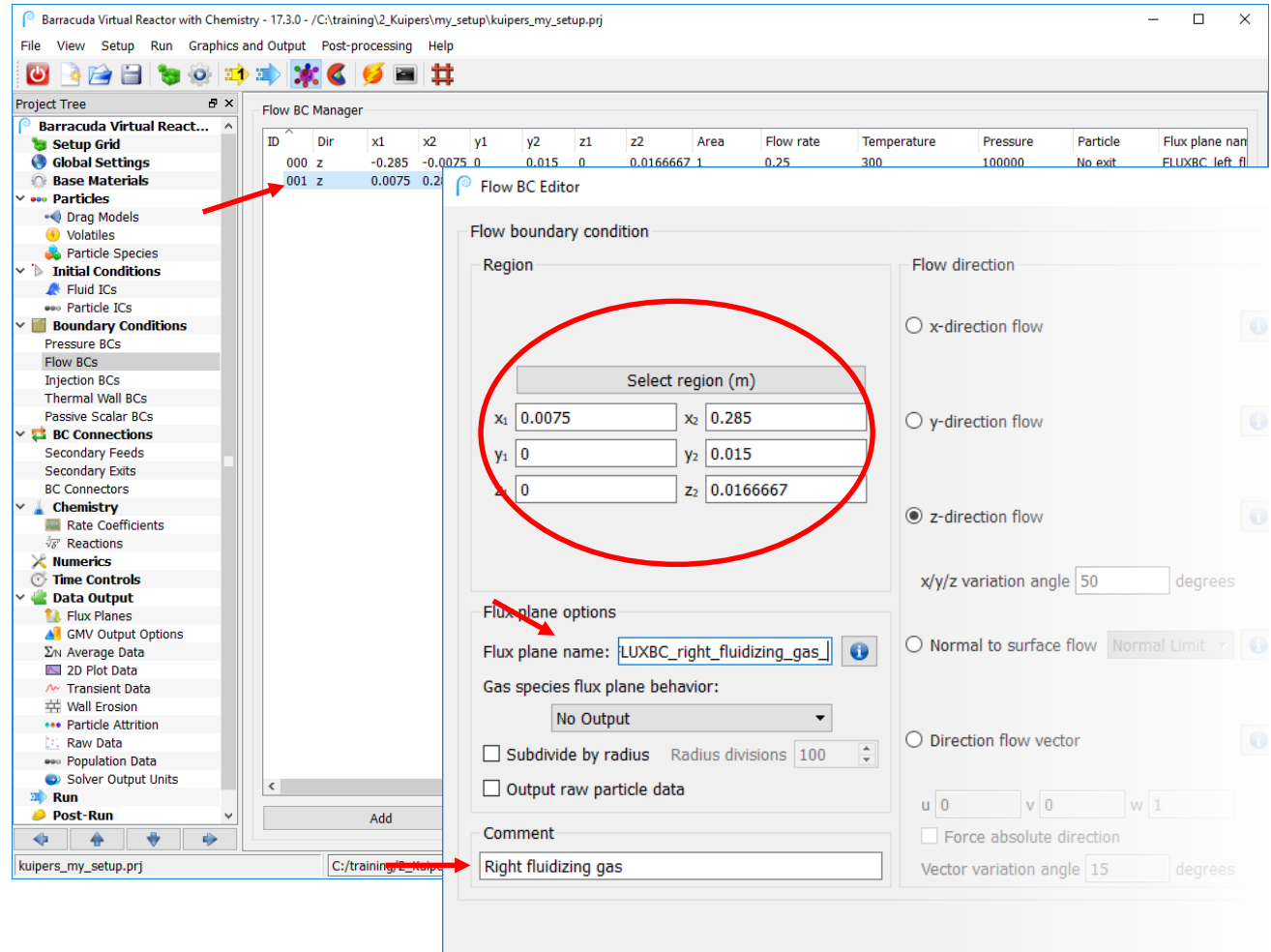
Flow Boundary Conditions

- Next create a boundary for the air entering through the central jet. Enter the plane **Location** as follows:
    - Set x1 to "-0.0075" and x2 to "0.0075"
    - Set y1 to " [" and y2 to "] "
    - Set z1 to " [" and z2 to " ["

- Set **Velocity flow** to "10" m/s

- Remember to provide a **Flux plane name** for the boundary and to add a **Comment**

- Click **OK**

Time Controls

- Click on **Time Controls**

- Leave the **Time step** as 0.0001 s

- Set the **End time** to "20" s

- Barracuda can restart an existing simulation from an IC file. Two types of IC files are automatically written during a simulation:

  - Restart file: a restart IC file is written once at every specified interval of simulation time

  - Backtrack file: a backtrack IC file is written once at every specified interval of clock time

- Leave the restart file intervals at the default values
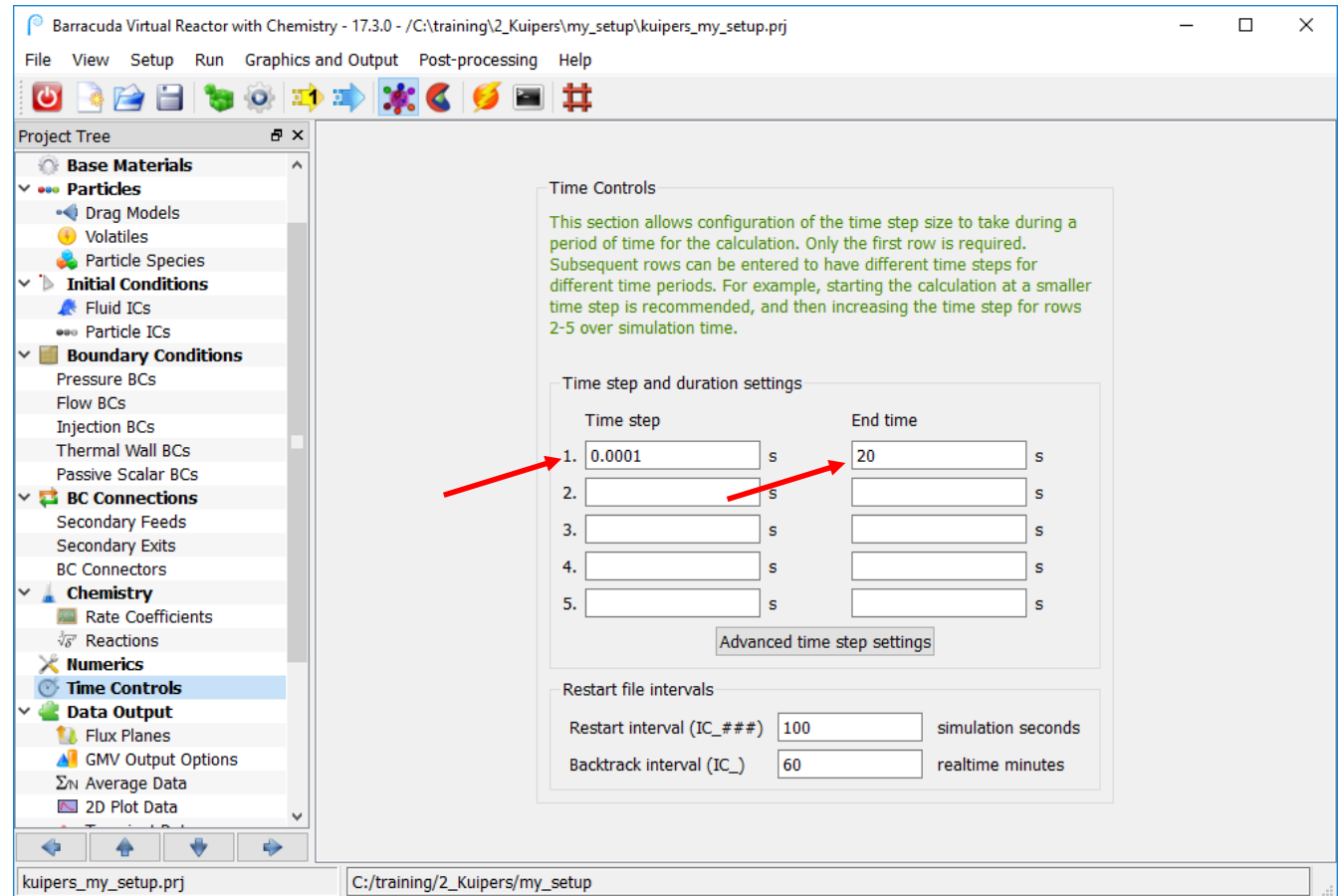
Data Output Options

- Click on **Data Output**

- For the Kuipers problem, the following types of data will be output
  - Flux planes – Track the transport of fluid and solids through a defined plane in the model
  - GMV output data – Select variables for visualization of fluid and solid states in GMV
  - Average Data – Select some Gmv output data to be averaged as the simulation runs
  - Transient Data – High frequency tracking of data at a specified location in a model
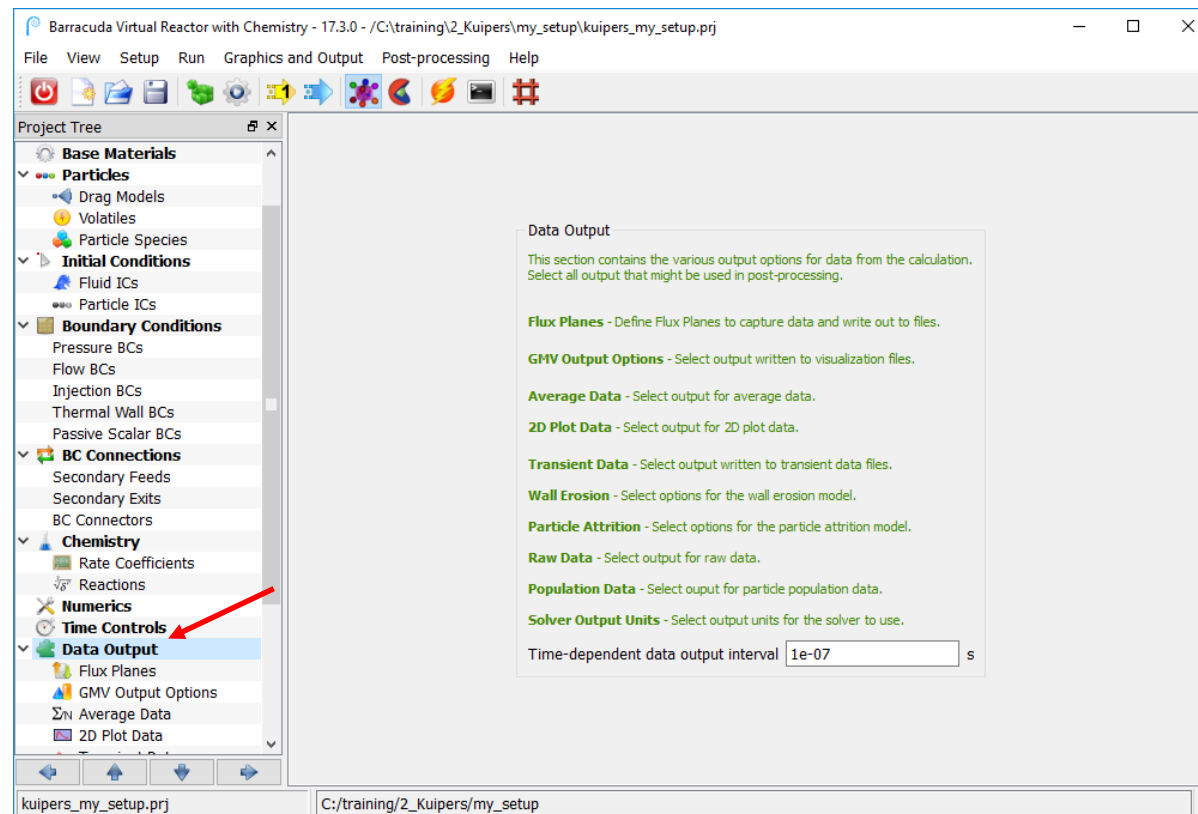
Grid Coordinates

- Cells indices are an alternative way to reference locations in a Barracuda model. Each computational cell is identified by a unique i-j-k coordinate.

- The i-, j-, and k-indices reference cells in the x-, y- and z-directions, respectively.

- Several Data Output options use either cell indices exclusively, or allow a choice between i-j-k and x-y-z:

  - Flux Planes

  - 2D Plot Data

  - Transient Data
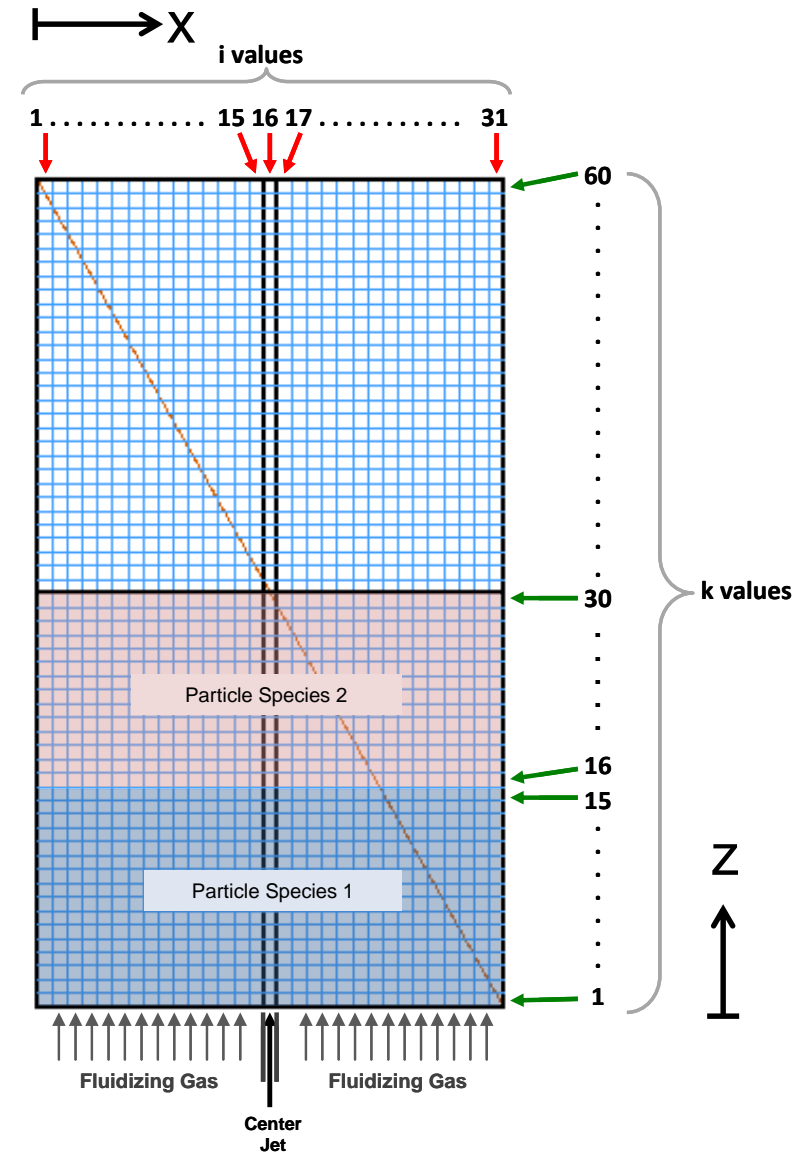
Data Output: Flux Planes

- Click on **Flux Planes**

- Click **Add**

- Provide a descriptive **File name** for the flux plane

- Select **Directional flux**

- Enter the **Plane Location** values as shown, using i-j-k values (also called "Node")

- Enter a **Comment** (if desired)
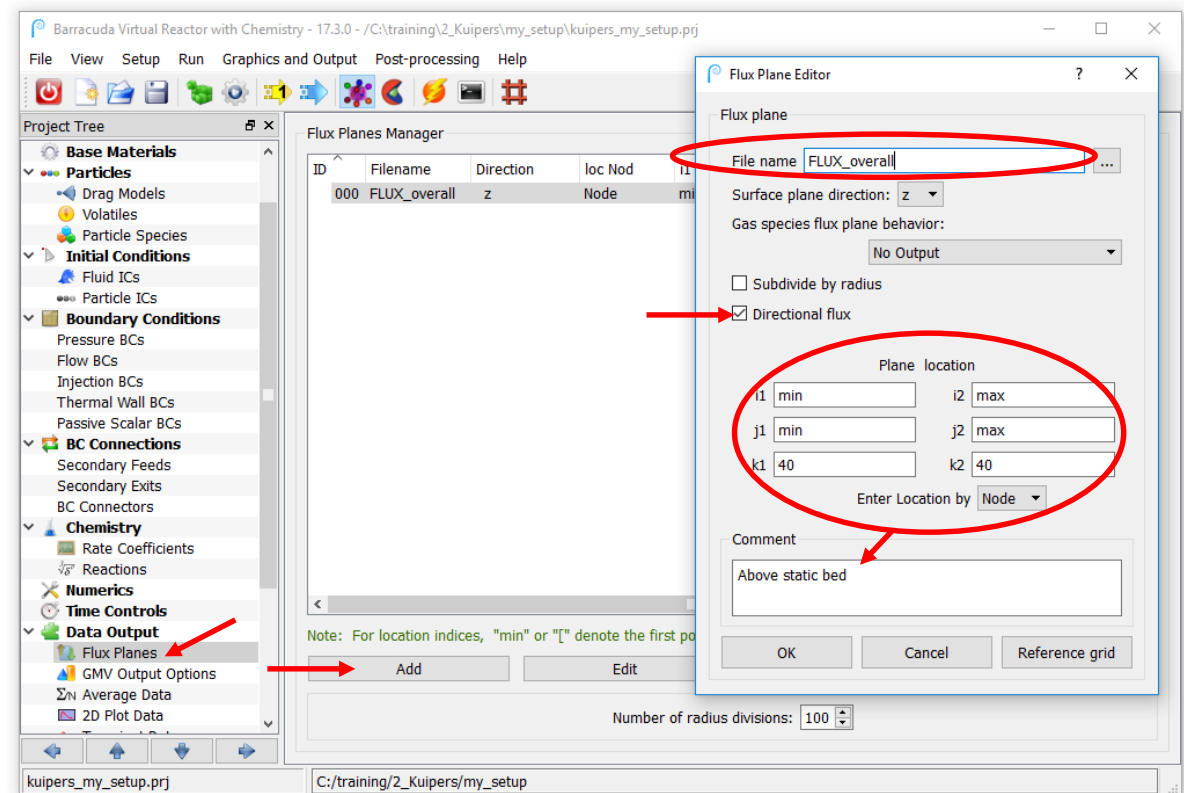
- Click **OK**

Data Output: GMV Output Options

- Click on **GMV Output Options**

- The information selected here will be written to your Gmv output files

- The **Eulerian Output Data** is mapped to the grid

- The **Lagrangian Output Data** is mapped to particle locations

- Ensure these entities are selected since they will be required for a post-processing assignment. Show your instructor this window before proceeding
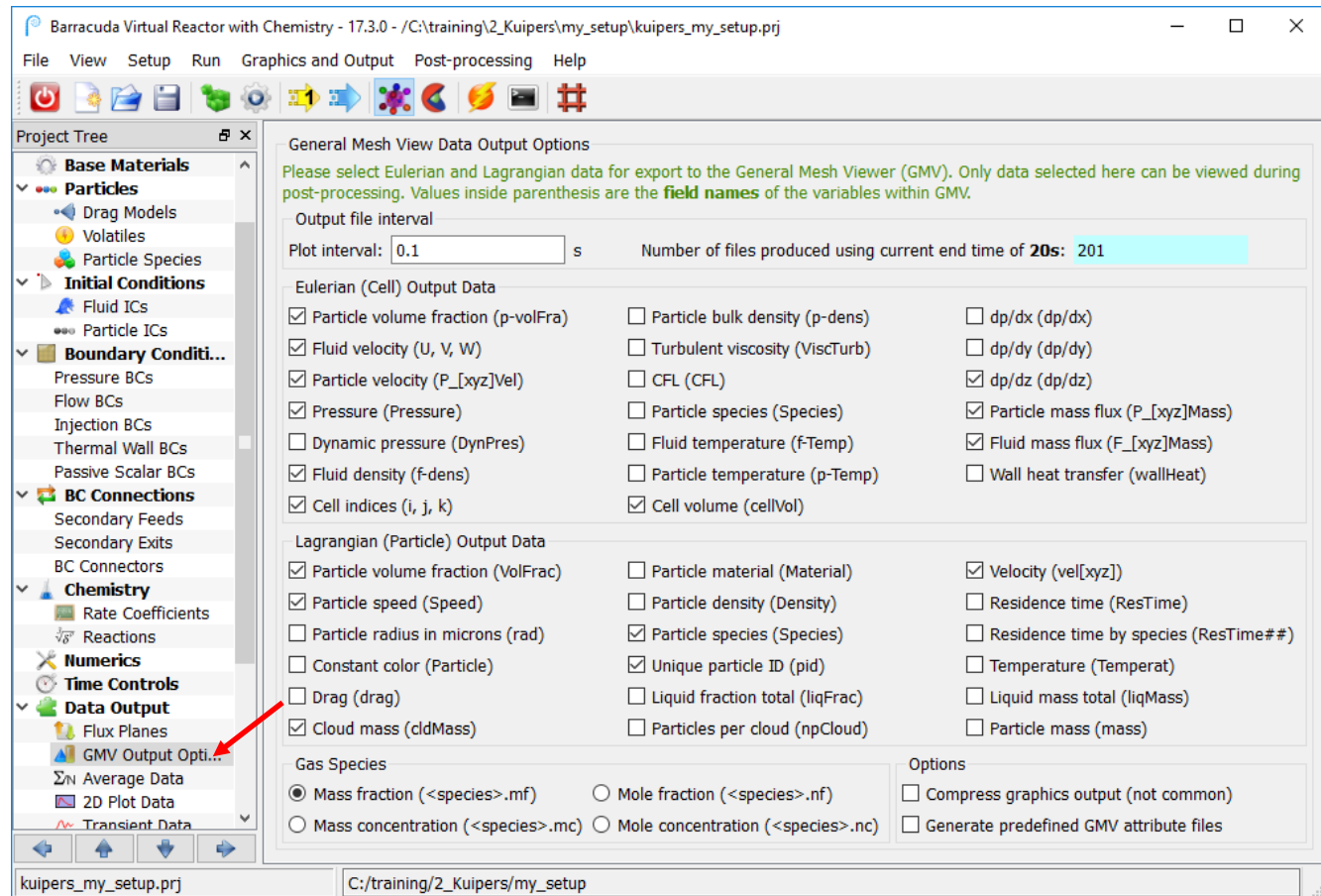
Data Output: Average Data

- Click on **Average Data**

- Often time-averaged data gives more insight into quasi-steady behavior than instantaneous data

- Select a **Start time for average** once you think quasi-steady behavior will have begun

- Select the data you wish to average
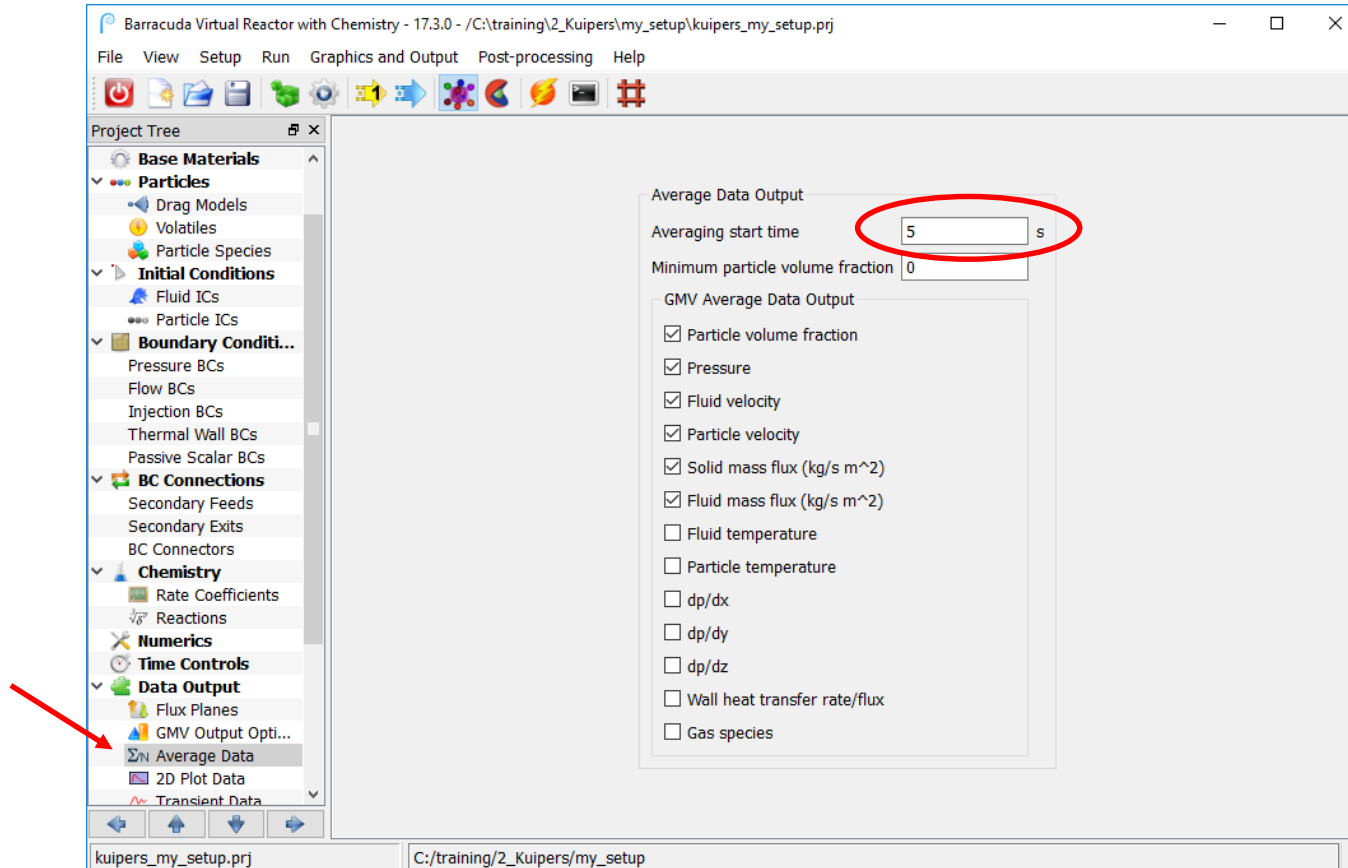
Data Output: Transient Data

- Click on **Transient Data**

- Barracuda can monitor transient data at locations in the computational domain

- Data will be written to a file

- Select the data type and location(s) in either grid (i,j,k) or absolute (x,y,z) coordinates

- For the Kuipers problem, change the coordinates from x,y,z to Node

- Enter the coordinates shown on the right
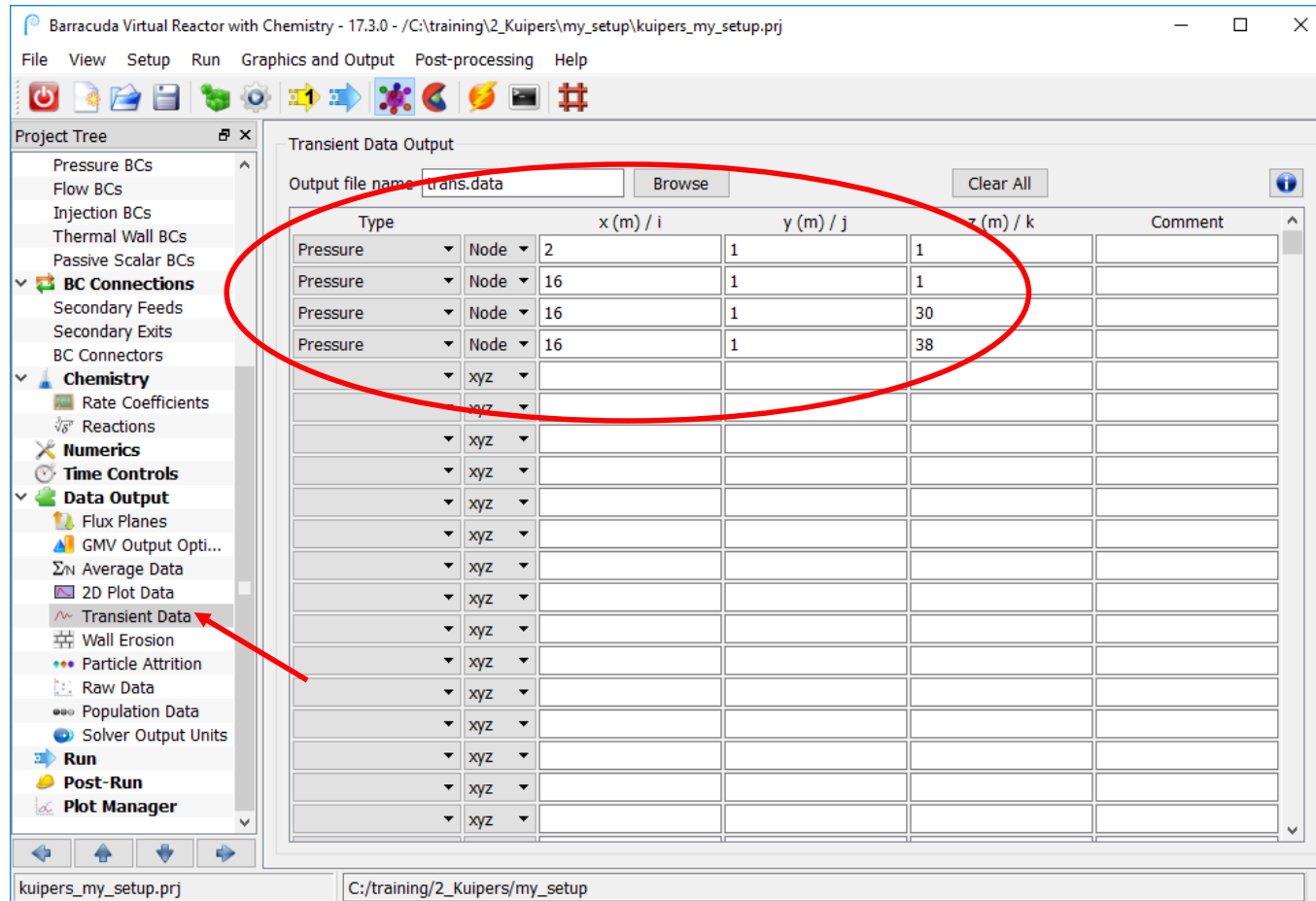
Run Solver Setup

- **Save** the project file

- Click on **Run**

- Click on **Run Solver Setup**
  - This will run the simulation for one time step and write a single Gmv file
  - All boundary and initial conditions are stored in the Gmv file
  - This first Gmv file is needed to check the problem setup
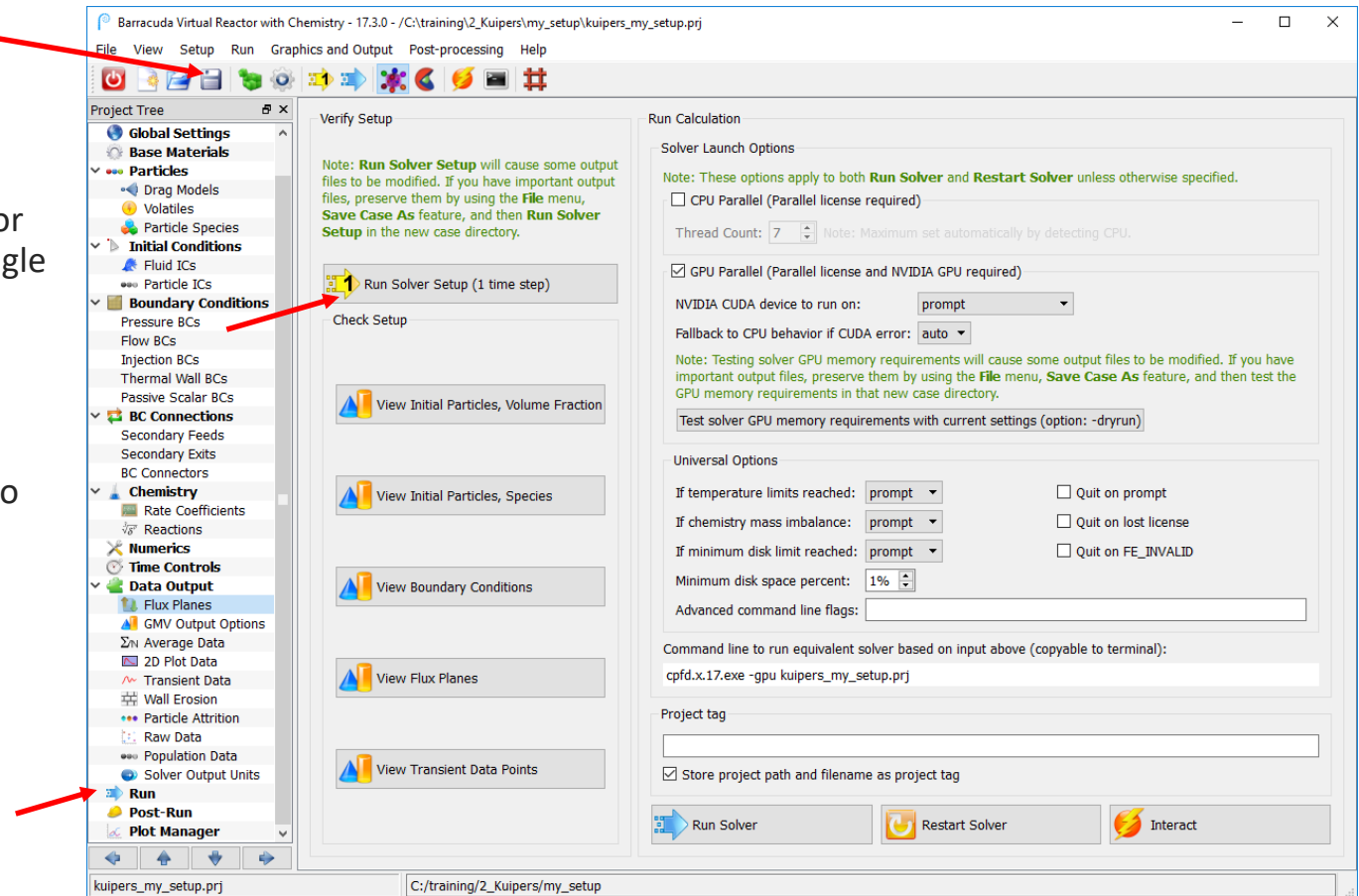
Run Solver Setup

- Solver information will be output to the run window

- Tip: Leave the window open while a calculation is running. If it is closed, the calculation will stop!

- The calculation is complete when the date/time stamp is displayed at the bottom of the solver window

Checking your Setup

- Before letting your calculation run, check the following:
  - are your particles defined correctly and located where you want them?
  - are your boundary conditions in the right place?
  - are your transient data points located where you want them?
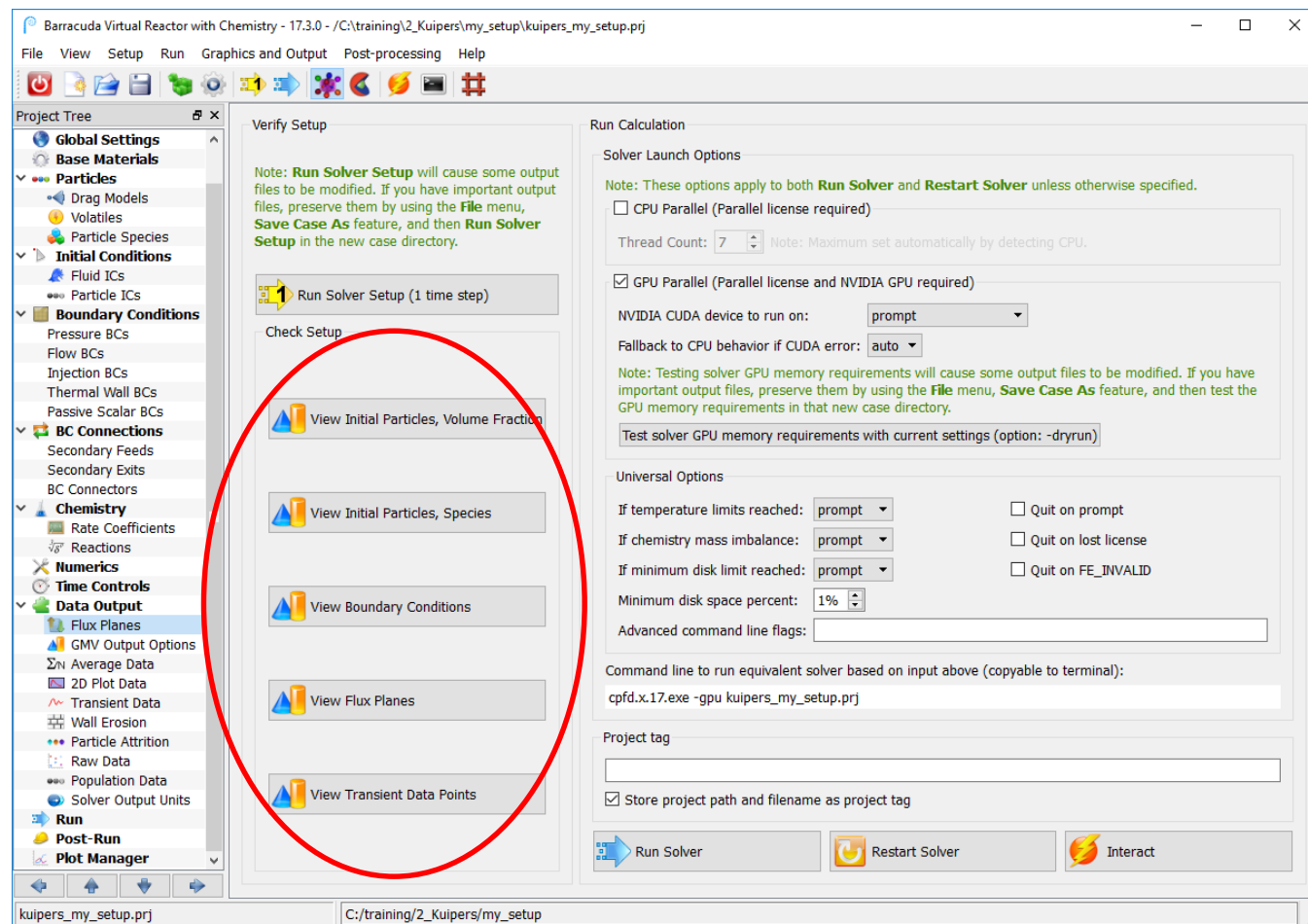
Checking your Setup - Particles

- Click on **View Initial Particles, Volume Fraction**

- Verify the initial location of the particles in the bed

- To change the view:
  - Use the mouse buttons: left button rotates, center button translates, and right button zooms OR
  - Use the sliders at the top in the GUI
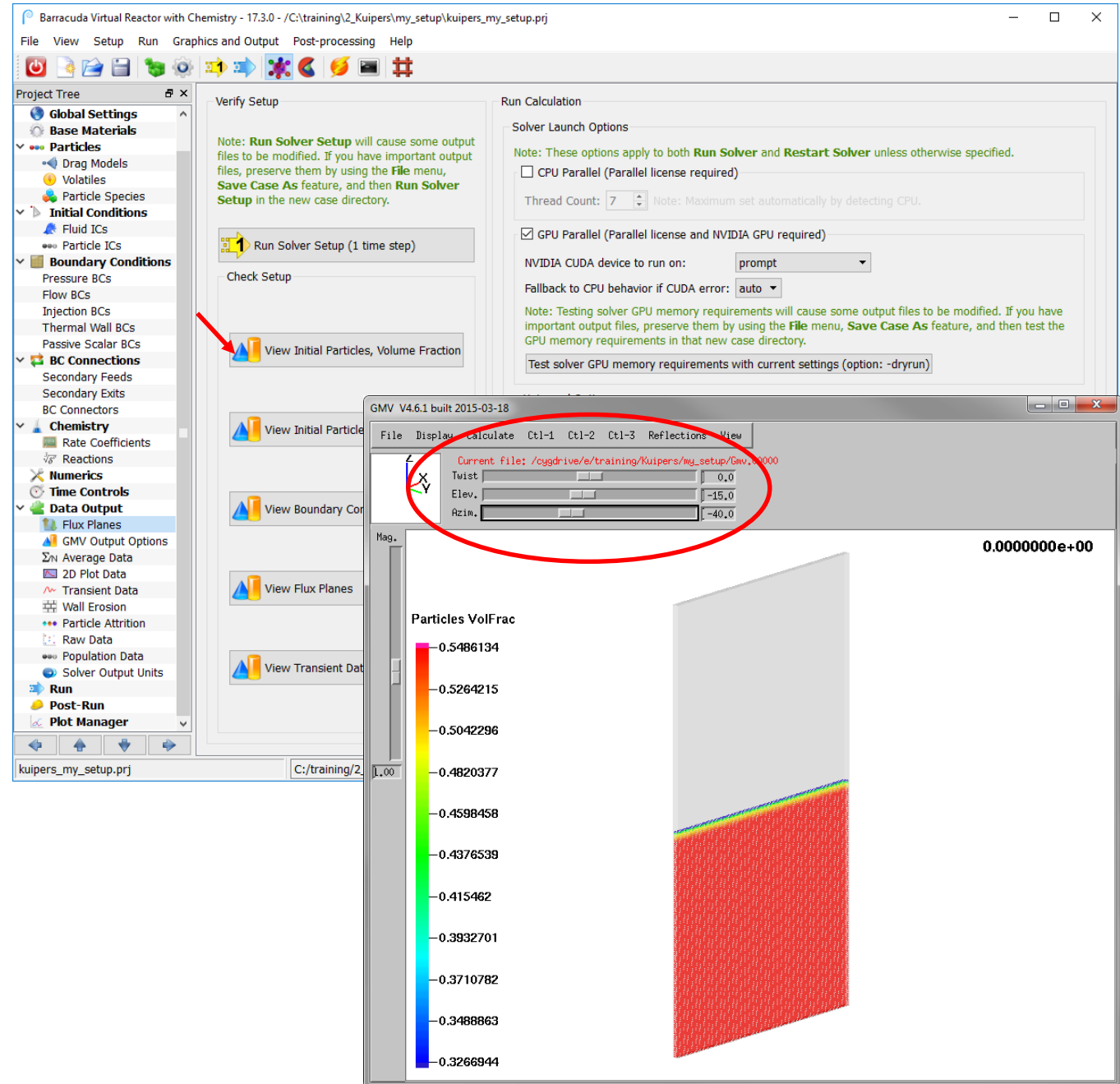
Checking your Setup – Particle Species

- Click on **View Initial Particles, Species**

- Verify the initial location of the two particle species in the bed
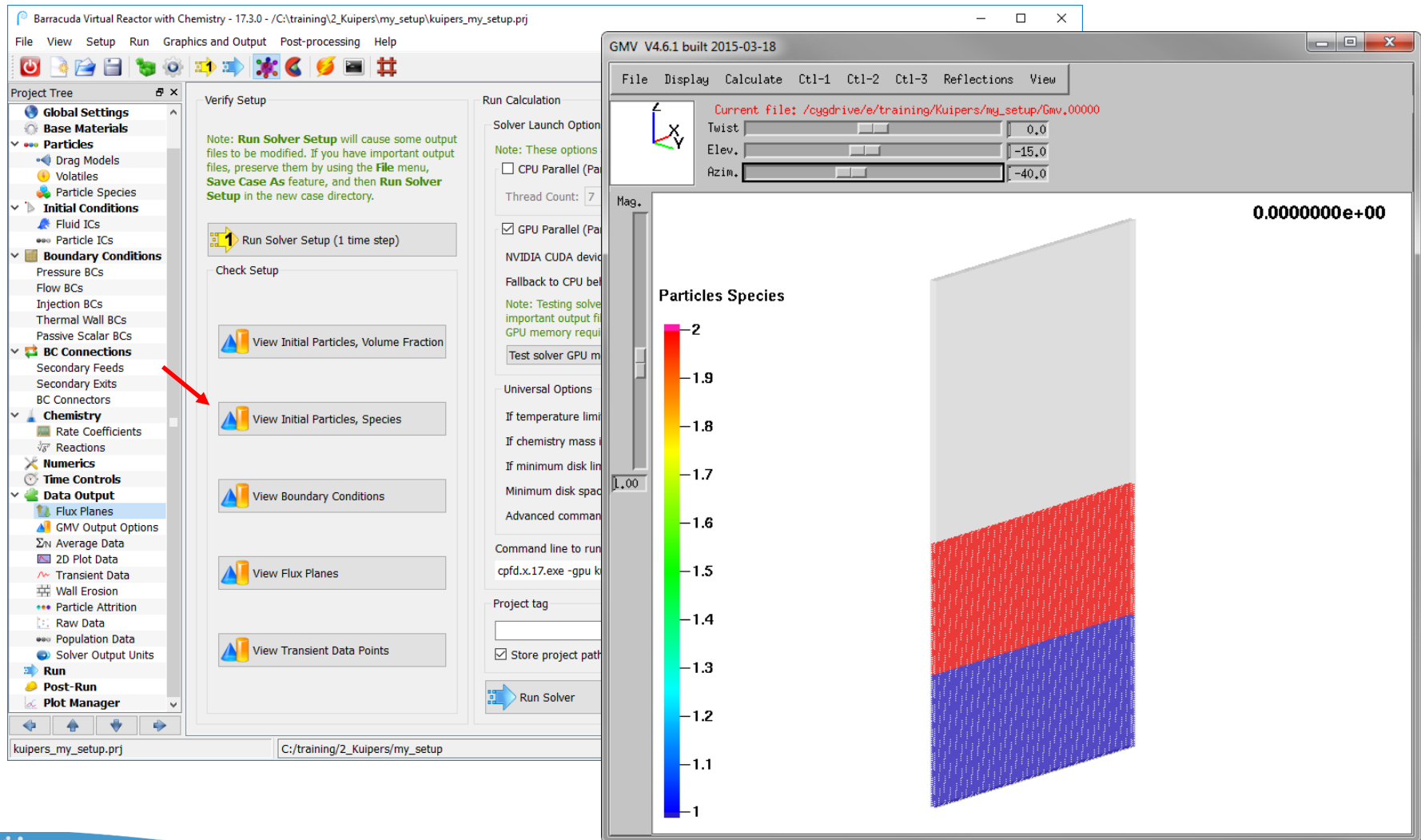
Checking your Setup – Boundary Conditions

- Click on **View Boundary Conditions**

- Verify that the boundary conditions are in the right place
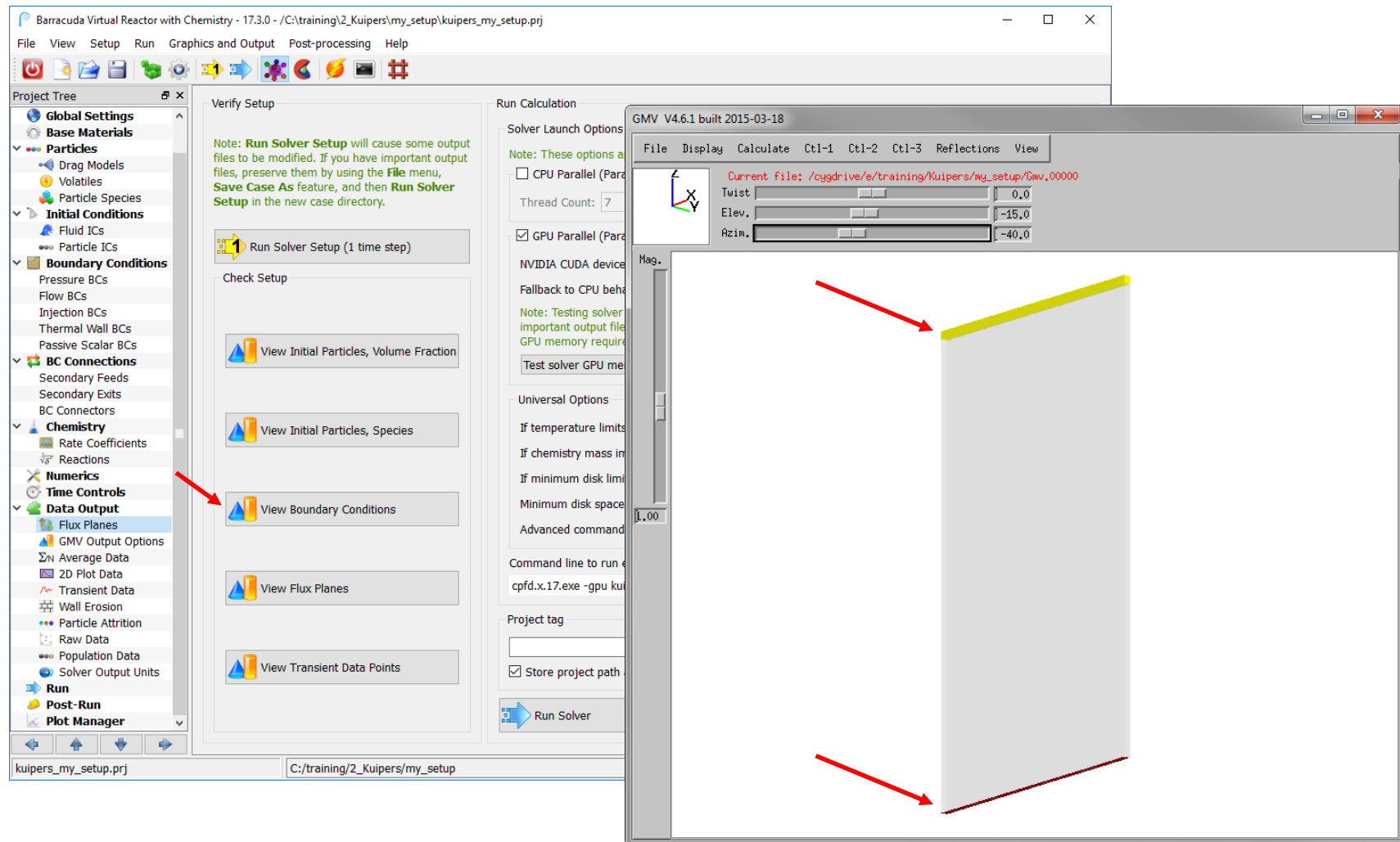
Checking your Setup – Flux Plane Location

- Click on **View Flux Planes**

- Verify that the flux planes are in the right place
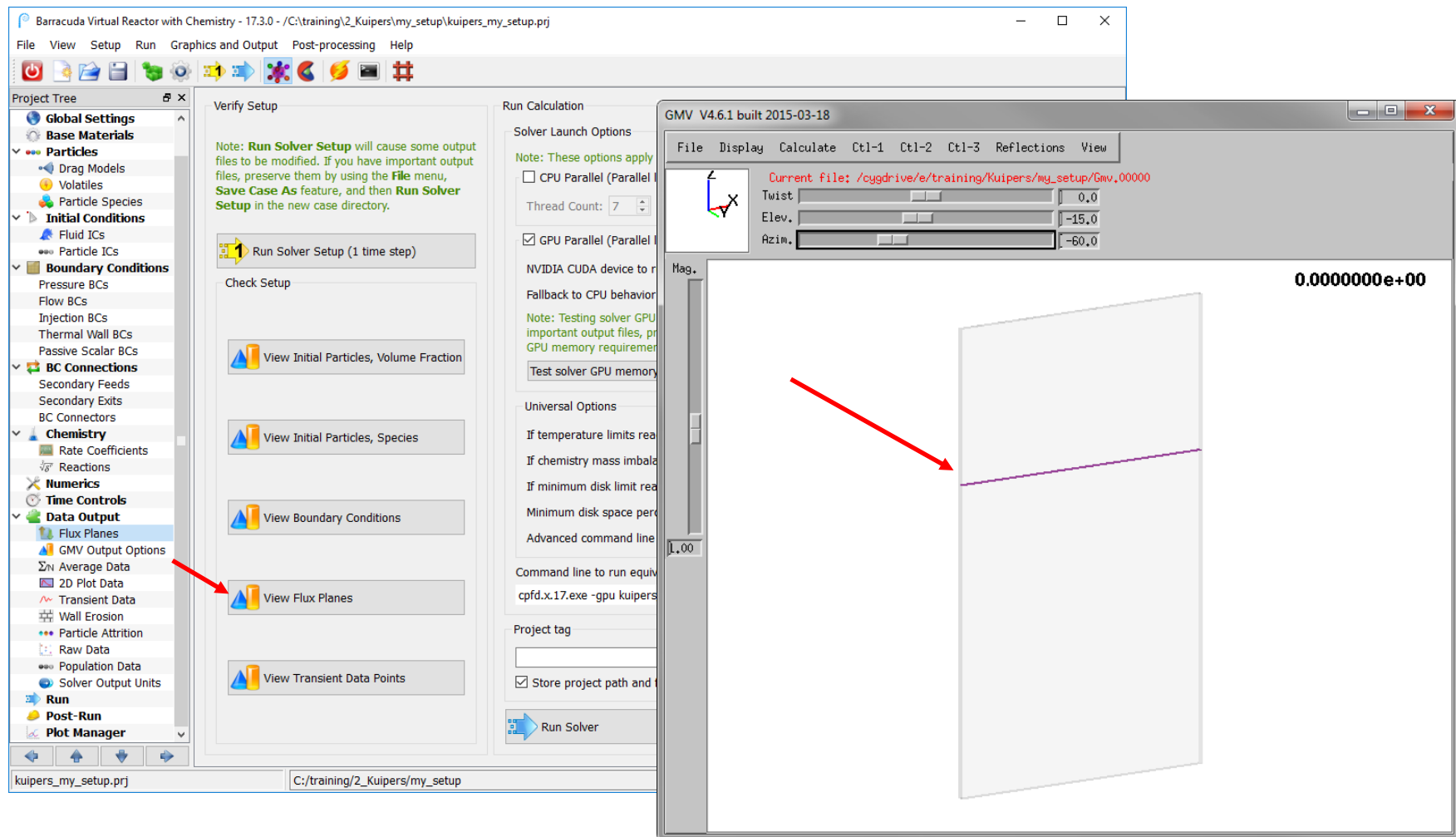
Checking your Setup – Transient Data Point Location

- Click on **View Transient Data Points**

- Verify that the transient data points are in the right place

- Show your instructor your initial particle locations and boundary conditions before proceeding
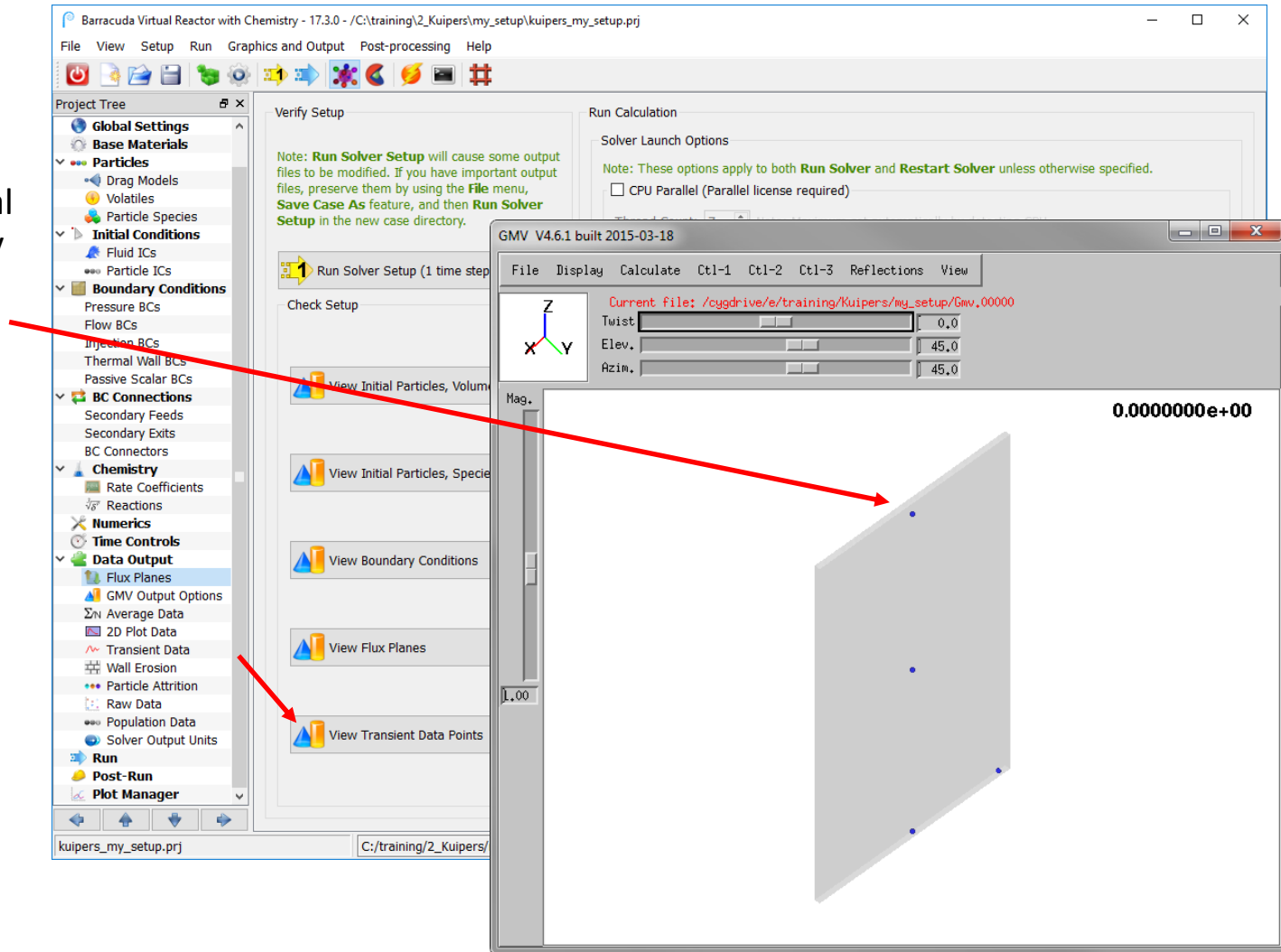
Executing the Simulation

- To begin running your calculation, click on **Run Solver**
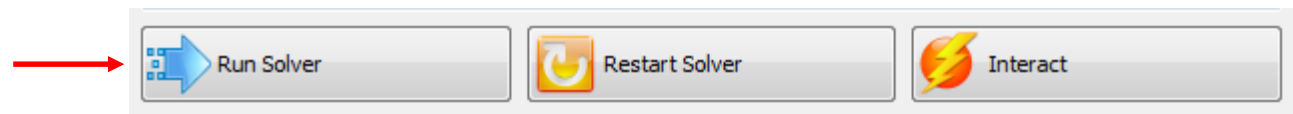
- Examine the solver window

Solver Output Window

Current Simulation Time **Current Time step** **Solver Convergence Data** **CFL number:** Typically safe to run between 0.7 – 1.5


```
Select "Barracuda Virtual Reactor - 17.3.0 - /C:\training\2_Kuipers\my_setup\kuipers_my_setup.prj"  - cpfd.x.17.exe  -gpu kuipers_my_setup.prj    —  □  ×

   Global memory:      4096 MB
   Clock rate:         1.49 GHz
   CUDA cores:         960
   HstToDev Bandwidth: 3737 MB
Reprise environment variable: cpfd_LICENSE=27015@127.0.0.1


Reprise Project tag: path:C:\training\2_Kuipers\my_setup/kuipers_my_setup.prj

-----------------------------------------------------------------------------------
      t          dt    Vol    Vol      u      u      v      v      w      w      p      p
      s           s    itr    err    itr    err    itr    err    itr    err    itr    err      CFL  Low Med  Hi  R
-----------  --------- --- -------- --- -------- --- -------- --- -------- ---- -------- ----- --- --- --- --
0.00000e+00  1.000e-04 000  0.00e+00 000  0.00e+00 000  0.00e+00 000  0.00e+00    0  0.00e+00  0.00  96   0   0  0
Dumping Gmv.00000
1.00000e-04  1.000e-04 002  2.07e-08 001  0.00e+00 000  0.00e+00 002  1.19e-12   26  8.59e-07  0.04  95   0   0  0
2.00000e-04  1.000e-04 002  3.76e-08 003  2.06e-09 000  0.00e+00 003  3.89e-09   22  7.00e-07  0.04  95   0   0  0
3.00000e-04  1.000e-04 002  6.99e-08 003  1.81e-09 000  0.00e+00 003  2.97e-09   19  6.95e-07  0.04  95   0   0  0
4.00000e-04  1.000e-04 002  8.21e-08 003  9.70e-10 000  0.00e+00 003  1.32e-09   18  5.78e-07  0.04  96   0   0  0
```

If CFL number is significantly below 0.7: Increase the time step!

Dynamic Solver Interaction

- It is possible to dynamically interact with the Barracuda solver while the calculation is running

- Click on **Interact**

- Only enter information you wish to change

- Here, we can increase the **Time step** to "1e-3" seconds. Enter the new time and click **Submit**

SIMULATE > UNDERSTAND > OPTIMIZE

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Dynamic Solver Interaction

- Notice the solver begins running at the new time step

- Tip: It is Generally recommended to slowly raise the time step. It is also advisable to request a restart file before changing calculation parameters

Let it Run

- If everything is as expected, let the solver run

- Next we'll work through a post-processing assignment

SIMULATE > UNDERSTAND > OPTIMIZE