

Barracuda Virtual Reactor Users' Conference 2024 Introductory Training Workshop

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Stelmach, CPFD Software

June 21, 2024

Agenda

9am : Introduction to Barracuda Virtual Reactor

Kuipers Example – Introduction

Cloud-based Linux VMs provided by  rescale

Kuipers Example – Project Setup

10:20 – 10:40 am : Break

Kuipers Example – Run Solver

Kuipers Example – Post-processing

Conclusion

Introduction to Barracuda Virtual Reactor

For today's session, we will walk through an abbreviated version of the Introduction presentation from our full New User Training course

The full presentation can be found on our website at:

<https://cpfd-software.com/introduction-to-barracuda-virtual-reactor/>

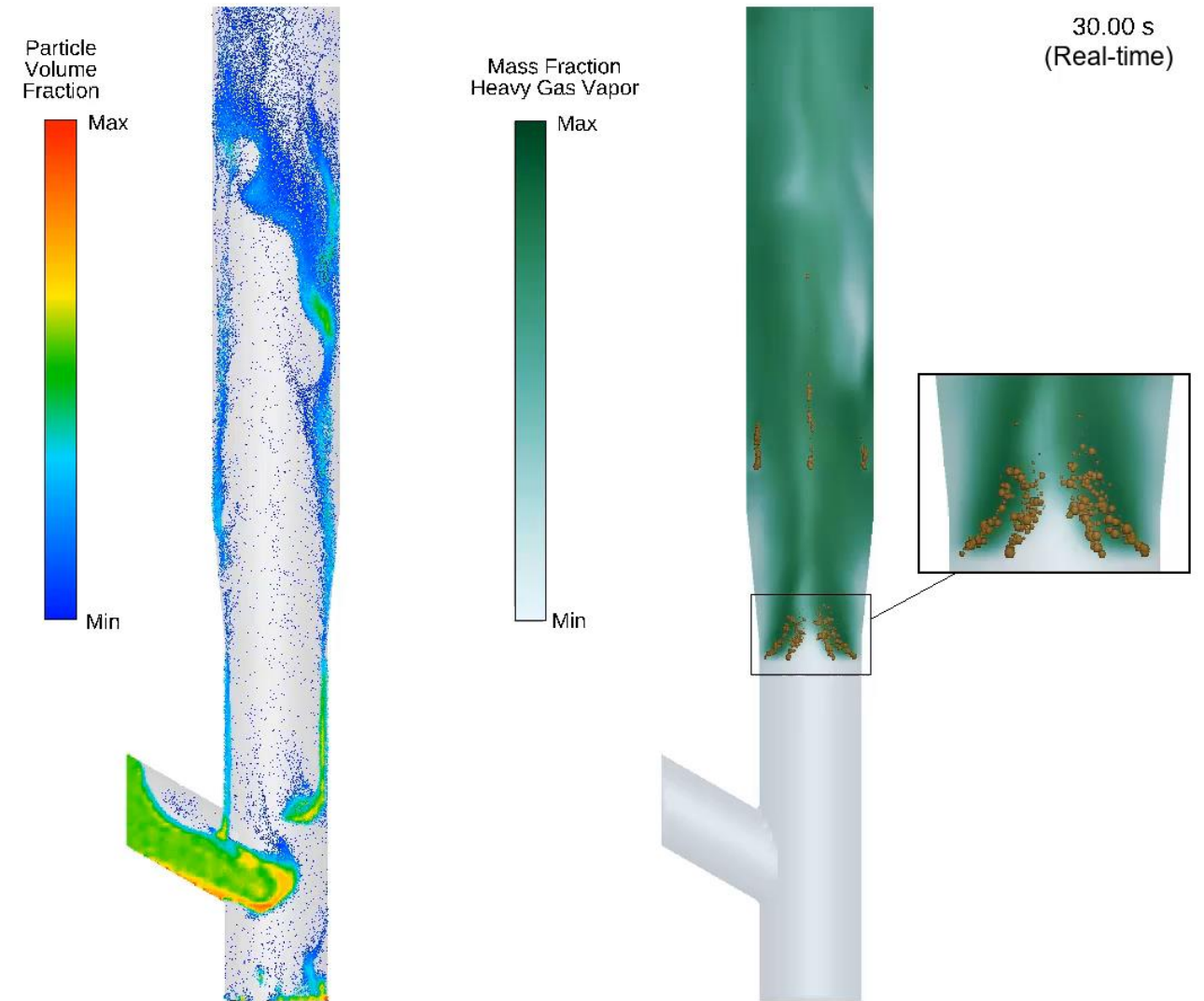
Introduction Outline

Introduction to CPFD Software and Barracuda Virtual Reactor

Industries & Applications

The CPFD[®] Modeling Approach

Deployment of Virtual Reactor



CPFD Software

Inventors of the CPFD technology and
Barracuda Virtual Reactor

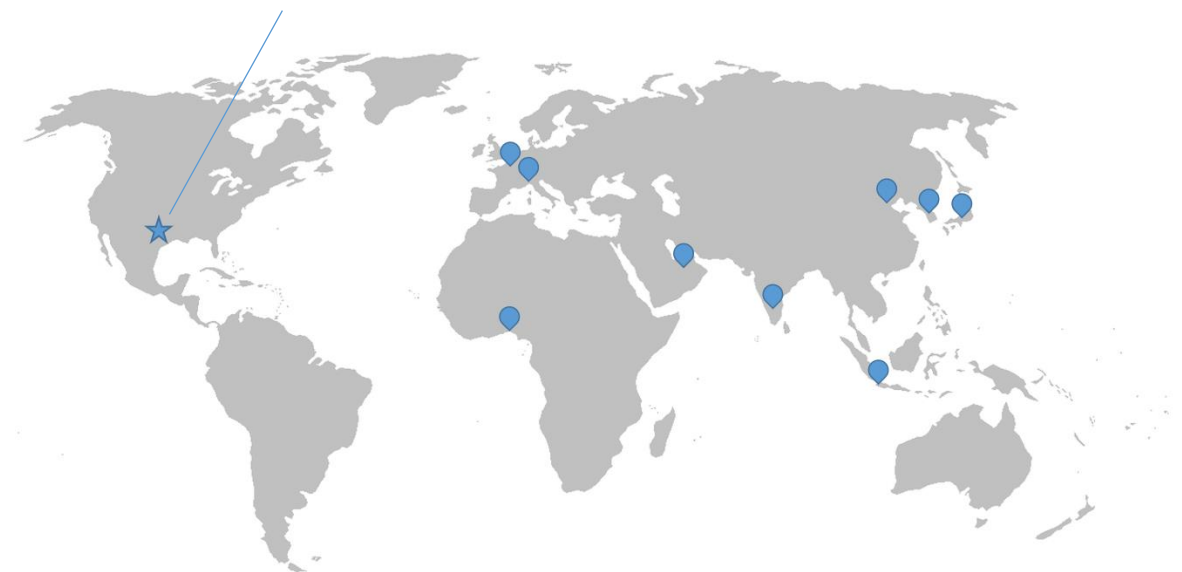
CPFD Software offers

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- Training
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Barracuda Virtual Reactor

Physics-based engineering software package

- Virtual Reactor is the only commercial software package focused specifically on chemically-reactive fluid-particle flow

Full software package:

- Graphical User Interface (GUI)
- Grid generator
- Solver
- Post-processor: Tecplot for Barracuda

Parallelized using NVIDIA GPUs

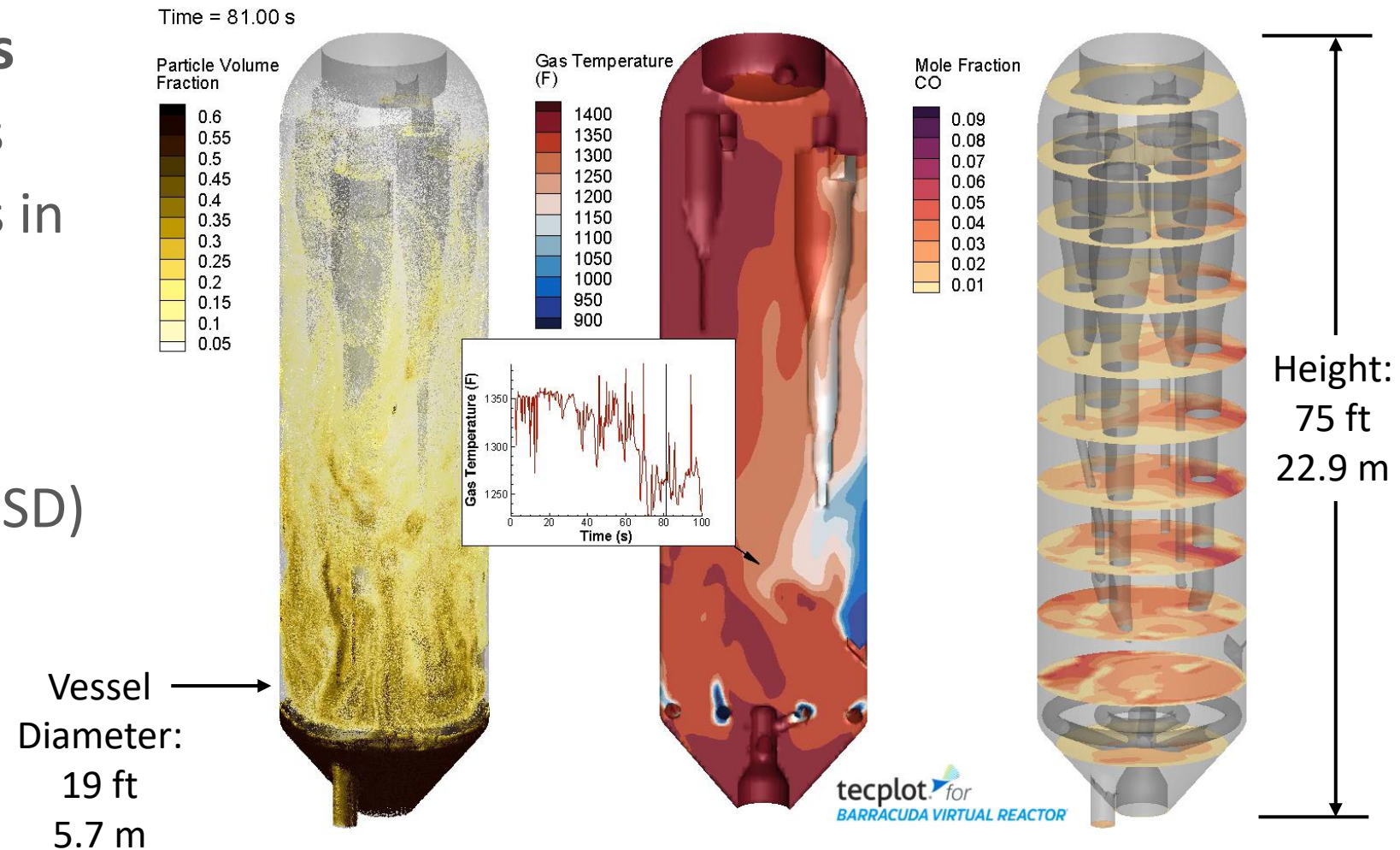
The screenshot displays the Barracuda Virtual Reactor software interface. The main window shows a 3D model of a reactor with a spiral internal structure. The Project Tree on the left lists various settings such as Setup Grid, Global Settings, Base Materials, Particles, Initial Conditions, Boundary Conditions, BC Connections, Chemistry, and Numerics. A data table window is open, showing simulation results for various parameters. The Tecplot post-processor window is also visible, displaying a 3D visualization of the reactor's internal structure with a color scale for particle volume fraction.

t	dt	Vol	Vol	u	u	v	v	w	w	p	p	CFL	Low	Med	Hi	R
s	s	itr	err	itr	err	itr	err	itr	err	itr	err					
3.93450e-01	2.541e-03	002	1.19e-08	004	1.78e-08	000	0.00e+00	004	1.84e-08	202	6.09e-07	1.37	13	0	0	0
3.95991e-01	2.541e-03	002	2.00e-08	004	2.50e-08	000	0.00e+00	004	2.57e-08	174	4.82e-07	1.37	14	0	0	0
3.98532e-01	2.541e-03	002	1.22e-08	004	3.39e-08	000	0.00e+00	004	2.65e-08	207	6.34e-07	1.37	14	0	0	0
4.01073e-01	2.541e-03	002	4.71e-08	004	4.33e-08	000	0.00e+00	004	3.06e-08	174	5.92e-07	1.37	15	0	0	0
4.03614e-01	2.541e-03	002	2.97e-08	004	4.93e-08	000	0.00e+00	004	1.09e-08	175	6.23e-07	1.37	15	0	0	0
4.06155e-01	2.541e-03	002	7.67e-08	004	3.11e-08	000	0.00e+00	004	4.77e-09	172	5.80e-07	1.37	16	0	0	0
4.08696e-01	2.541e-03	002	1.89e-08	004	2.59e-08	000	0.00e+00	004	2.13e-08	192	6.27e-07	1.37	14	0	0	0
4.11237e-01	2.541e-03	002	6.45e-08	004	2.33e-08	000	0.00e+00	004	2.04e-08	163	5.82e-07	1.38	12	0	0	0
4.13778e-01	2.541e-03	002	3.86e-08	004	1.67e-08	000	0.00e+00	004	2.53e-08	170	6.01e-07	1.38	9	0	0	0
4.16319e-01	2.541e-03	002	3.44e-08	004	1.37e-08	000	0.00e+00	004	3.80e-08	168	4.91e-07	1.38	9	0	0	0
4.18860e-01	2.541e-03	002	1.76e-08	004	1.45e-08	000	0.00e+00	004	6.16e-08	171	4.75e-07	1.38	10	0	0	0
4.21401e-01	2.541e-03	002	9.82e-08	004	3.58e-08	000	0.00e+00	005	2.16e-09	129	6.03e-07	1.38	8	0	0	0
4.23941e-01	2.541e-03	002	3.17e-08	005	6.02e-09	000	0.00e+00	004	1.23e-08	149	4.84e-07	1.38	7	0	0	0

Barracuda Virtual Reactor for Gas-Particle Systems

Gas-phase domains with particles

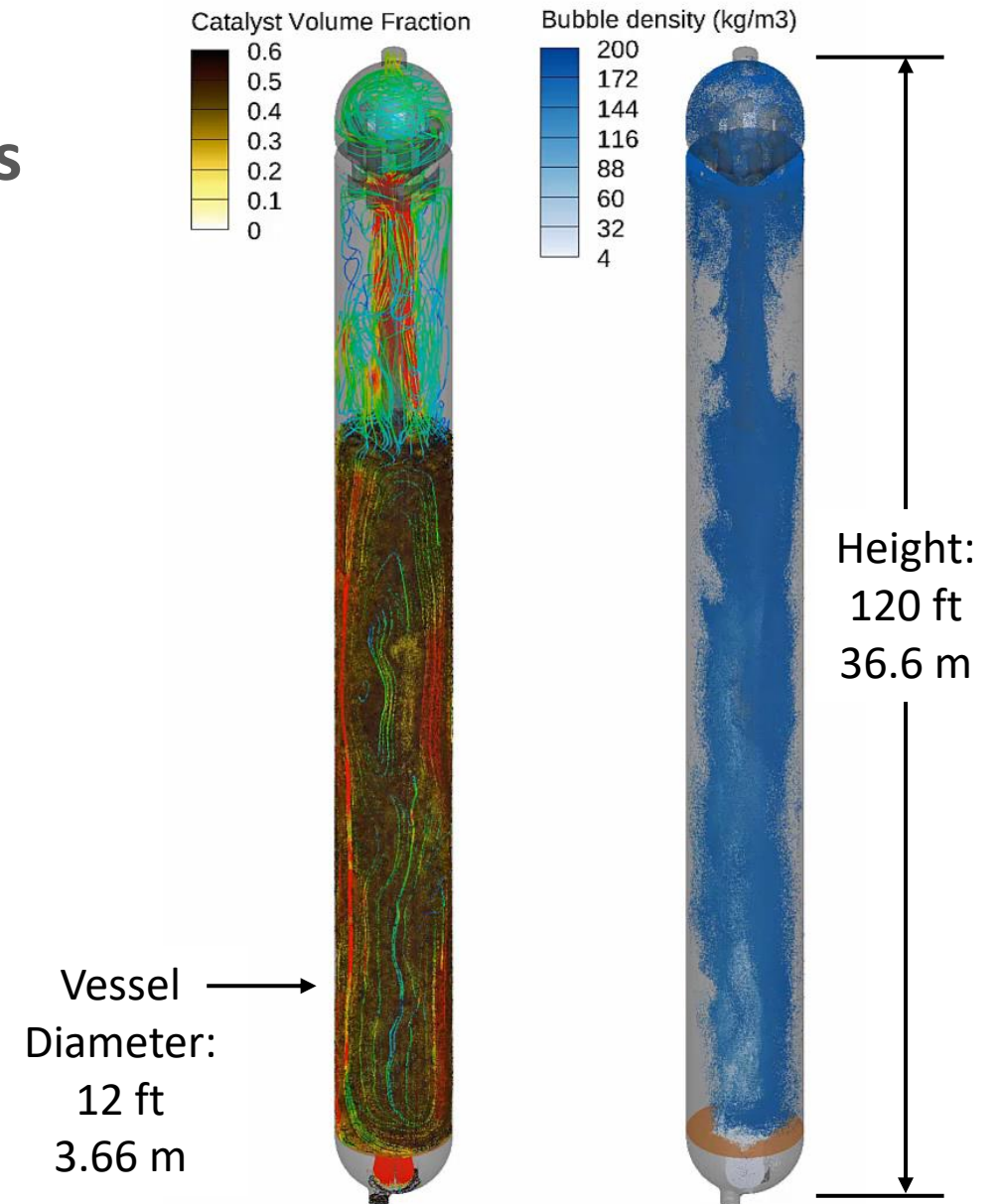
- Compressible flow calculations
- Unlimited number of materials in the gas and particle phases
- Unlimited number of particle species
- Full particle size distribution (PSD)
- Thermal calculations
- Chemical reactions



Barracuda Virtual Reactor for Vapor-Liquid-Solid Systems

Liquid-phase domains with particles and bubbles

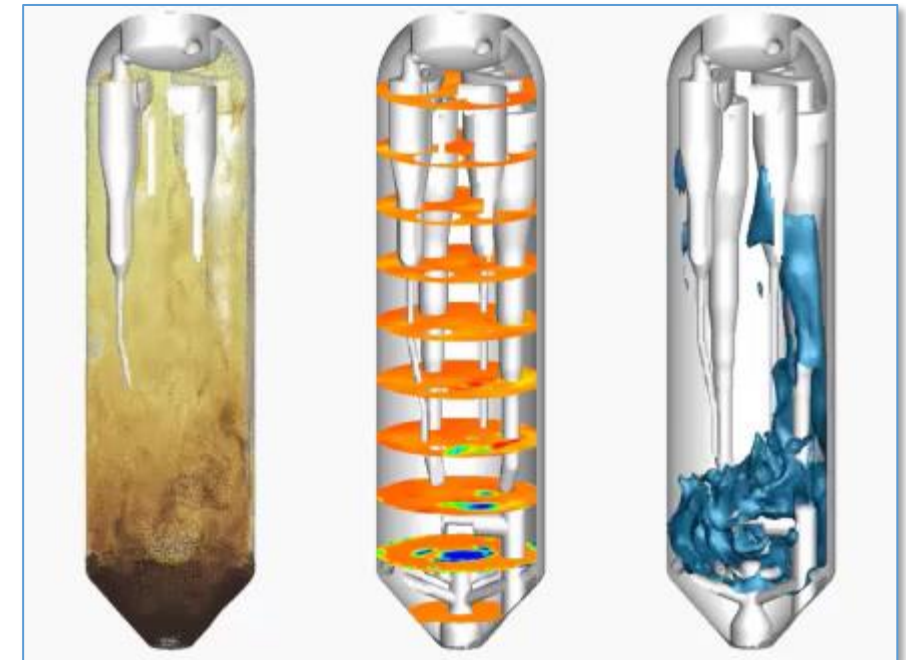
- Incompressible flow calculations
- Vapor-Liquid-Solid (VLS) systems
- Unlimited number of materials in the fluid and particle phases
- Unlimited number of particle species
- Unlimited number of bubble species
- Full size distributions for particles and bubbles
- Thermal calculations
- Chemical reactions



Virtual Reactor Industries and Application Areas

Barracuda Virtual Reactor is used in a wide variety of industries:

- FCCU/Refining
- Petrochemicals
- Gasification
- Materials & Chemicals
- Power Generation
- Clean Technologies & Renewables
- Research & General Fluidization



<https://cpfd-software.com/resources/webinar/>

Improving Performance Through Simulation

Barracuda Virtual Reactor is used to:

- Determine root cause of phenomena
- Reduce risk of changes through virtual testing
- Identify additional optimization opportunities
- Accelerated R&D, commercialization and scale-up

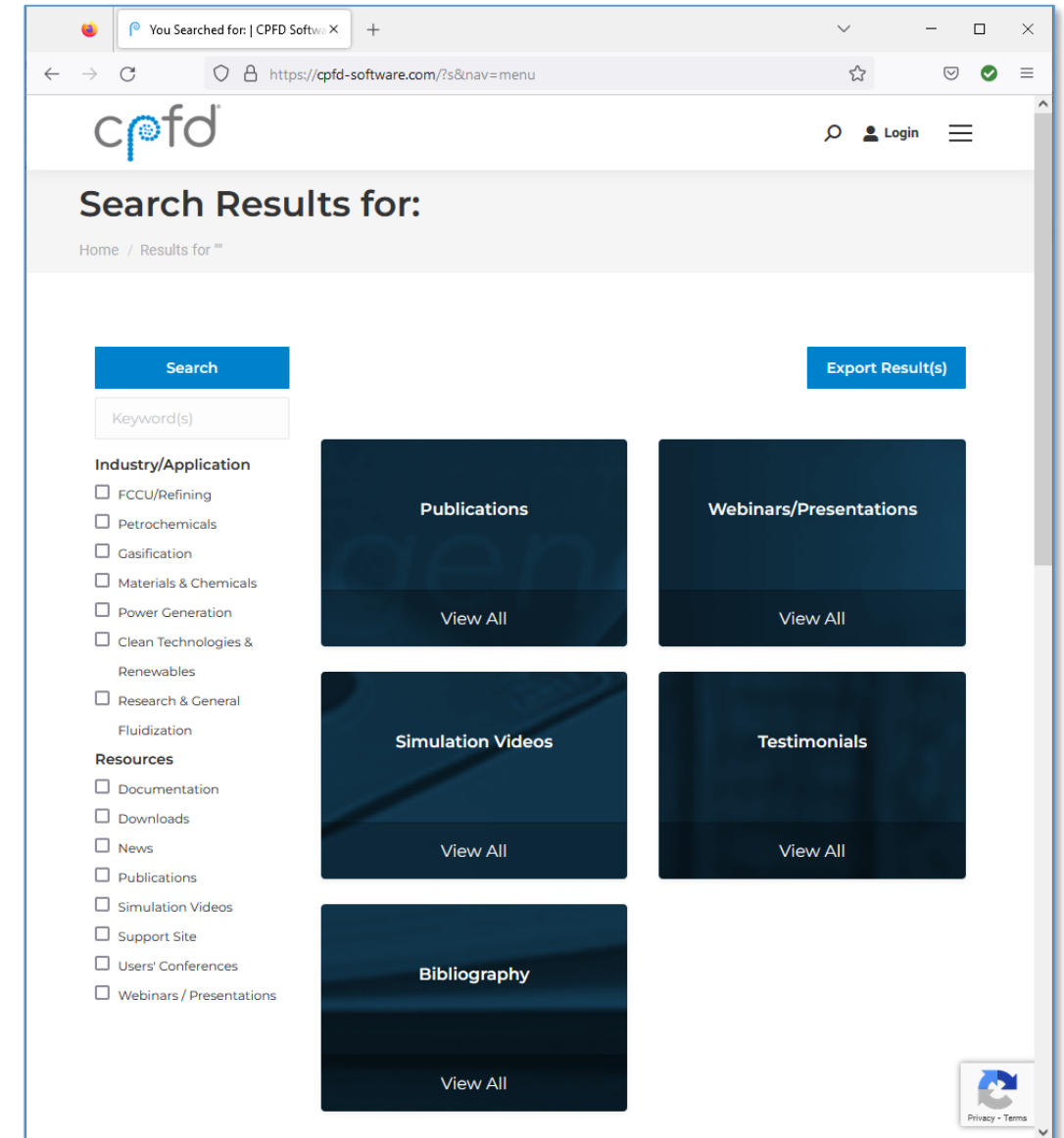


Barracuda Virtual Reactor Publications and Resources

Searchable database of publications about Virtual Reactor:

- Hundreds of peer-reviewed journal articles authored by Virtual Reactor users from around the world
- Topics range from general fluidization research to industrial-scale applications

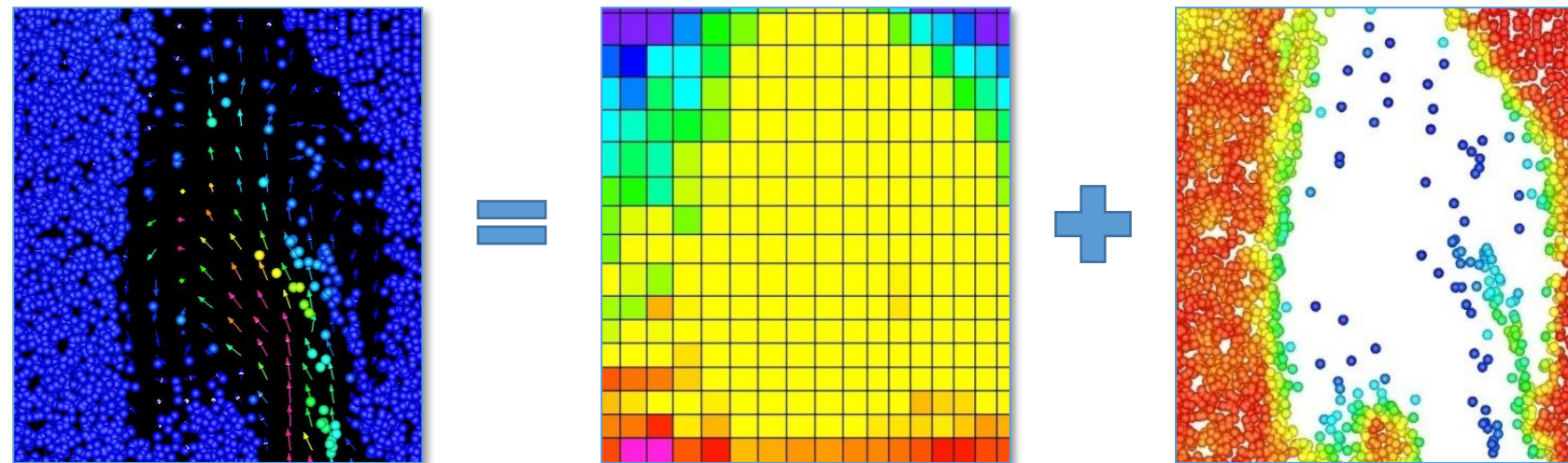
<https://cpfd-software.com/resources/>



The CPFDF Approach to Modeling Fluid-Particle Flow

Eulerian-Lagrangian method of modeling multiphase fluid-particle flow

- Based on Multiphase Particle-in-Cell (MP-PIC)
- Fluid phase is modeled on a computational grid, like traditional CFD
- Particles and bubbles are discrete and gridless
- Bi-directional coupling between the Eulerian and Lagrangian phases

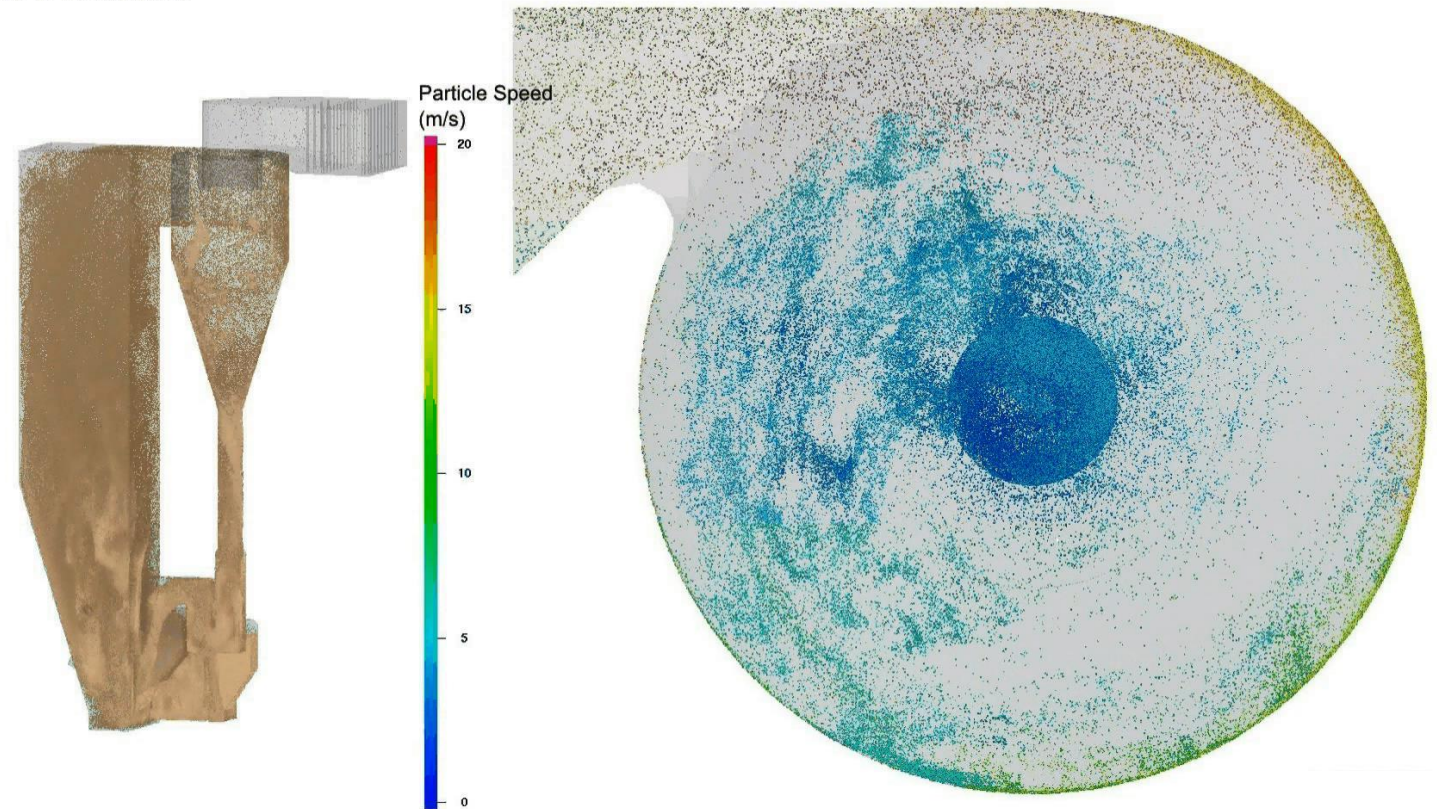


Benefits of the CPFD Approach

Virtual Reactor can model:

- Industrial scale systems with hundreds of millions of particles
- Discrete particle and bubble properties – size, temperature, composition, position
- Full size distributions for particle and bubble species
- Wide range of particulate loadings, from fully dilute to fully dense
- Heat transfer and multiphase chemical reactions

CFB Simulation



Numerical Method Publications

This introductory presentation is meant to provide a general overview of the CPFD implementation of the MP-PIC method.

For detailed discussions of the mathematics behind CPFD, please refer to our published journal and conference papers: cpfd-software.com/publications-about-barracuda-virtual-reactor/



System Requirements for Deploying Virtual Reactor

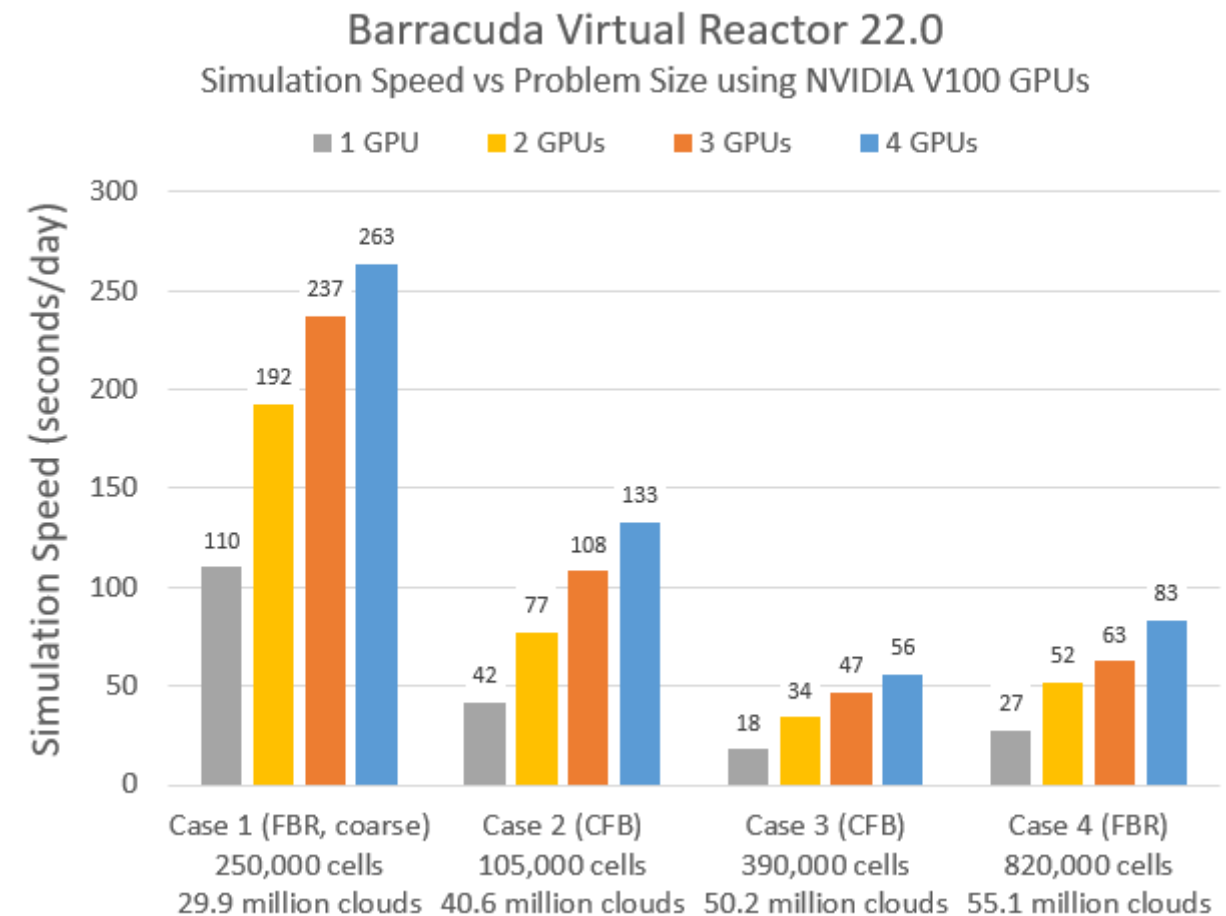
Windows and Linux OS support

GPU acceleration on NVIDIA GPUs

- Single-GPU acceleration up to 100X
- Multi-GPU acceleration up to 500X
- CPF D is a preferred ISV partner with NVIDIA

On-premise, in the cloud, or both

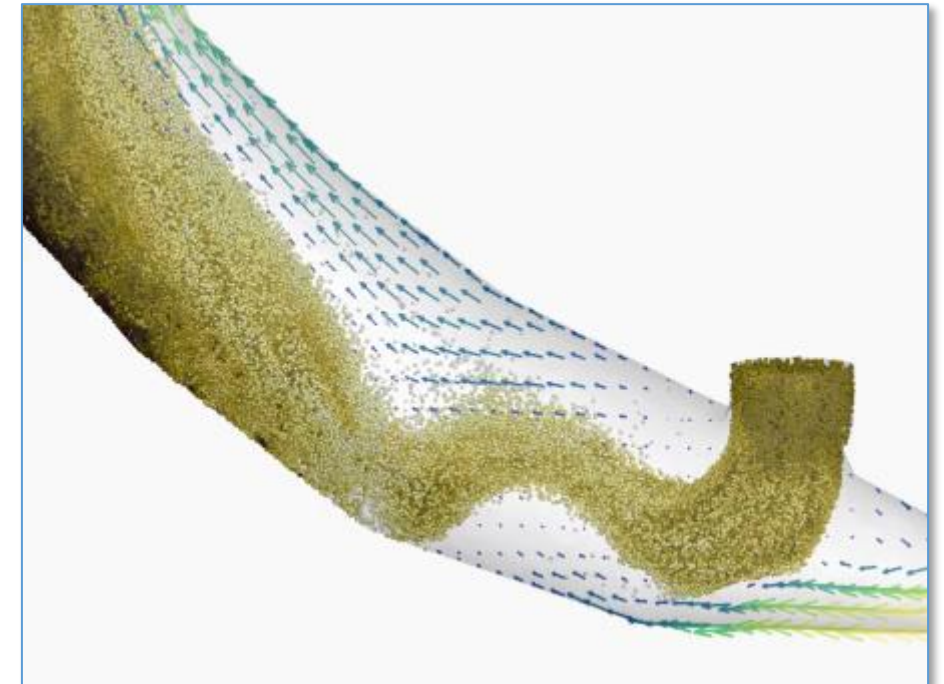
- CPF D partners with Mark III Systems, AWS, Azure, and Rescale



Summary of Introduction

Barracuda Virtual Reactor:

- Is a complete physics-based engineering software package
- Is used to model large-scale fluid-particle systems across a wide variety of industries
- Uses the CPFD Method to model fluid-particle flow
 - Eulerian-Lagrangian
 - Distinct advantages over traditional CFD
- Runs on Linux or Windows, and uses NVIDIA GPUs for parallelization



Kuipers Training Example Goals and Objectives

This training example is designed to provide a quick introduction to the overall problem set-up process and explanations are minimal. The purpose is to give the user an overall feel for the process and tools involved.

- Setup
- Run Solver
- Post-Processing
- Analyze Results

The training problem is based on a “2D” fluidized bed experiment reported by Kuipers, et. al (1992). We will simulate the experiment and observe the results.

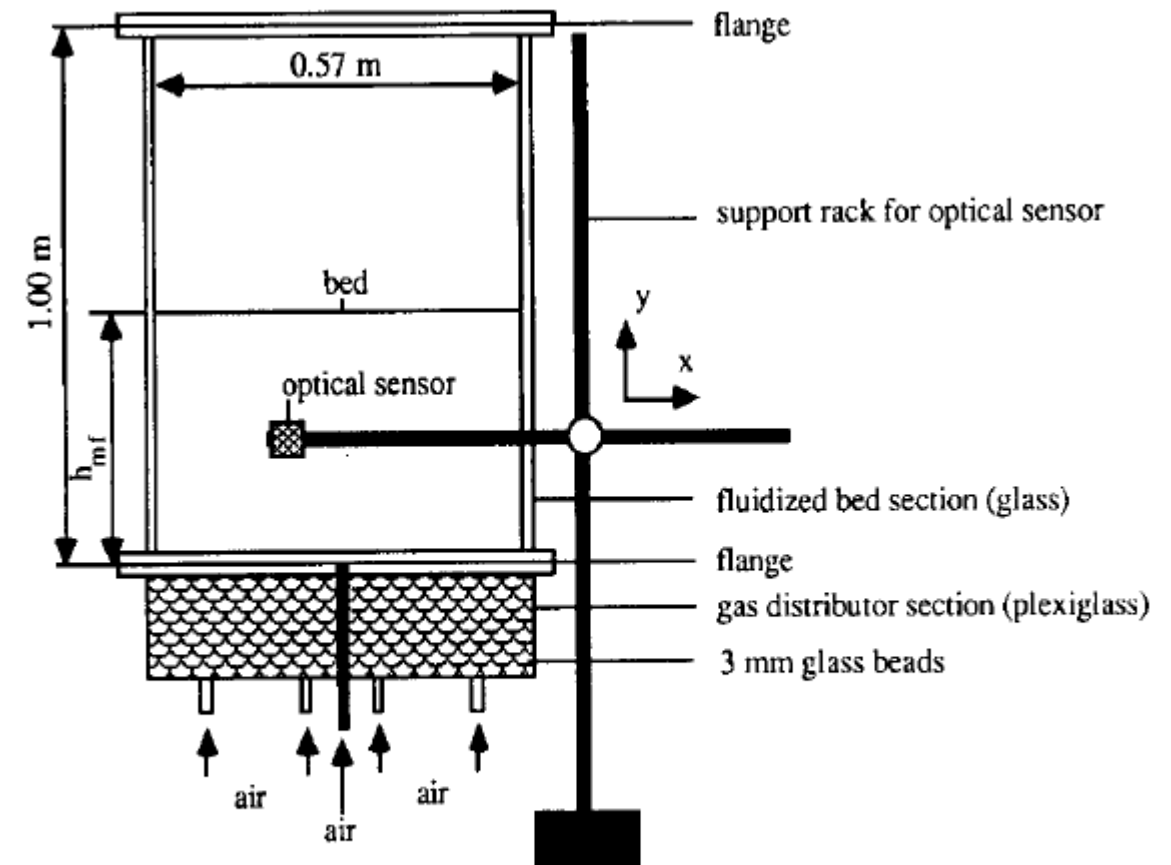
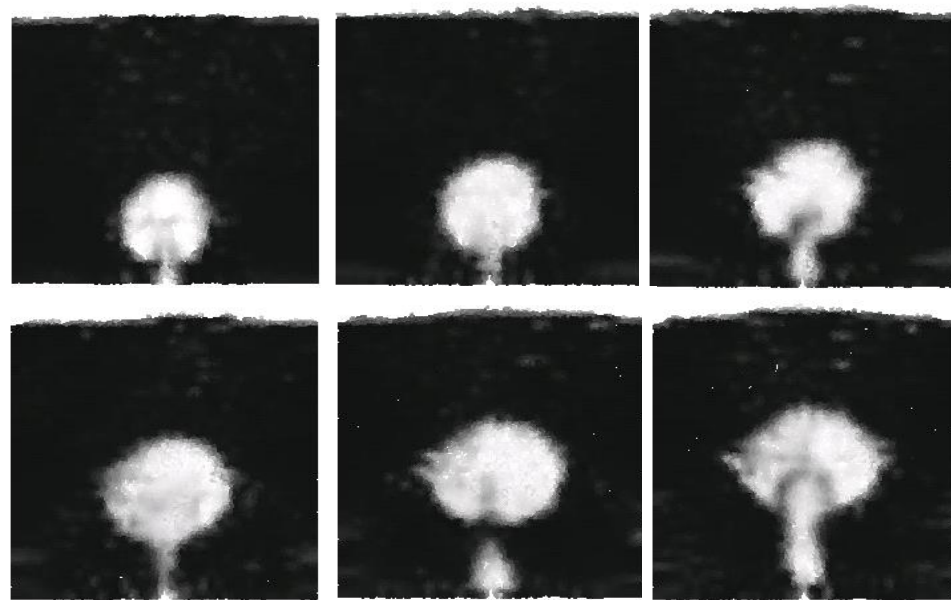


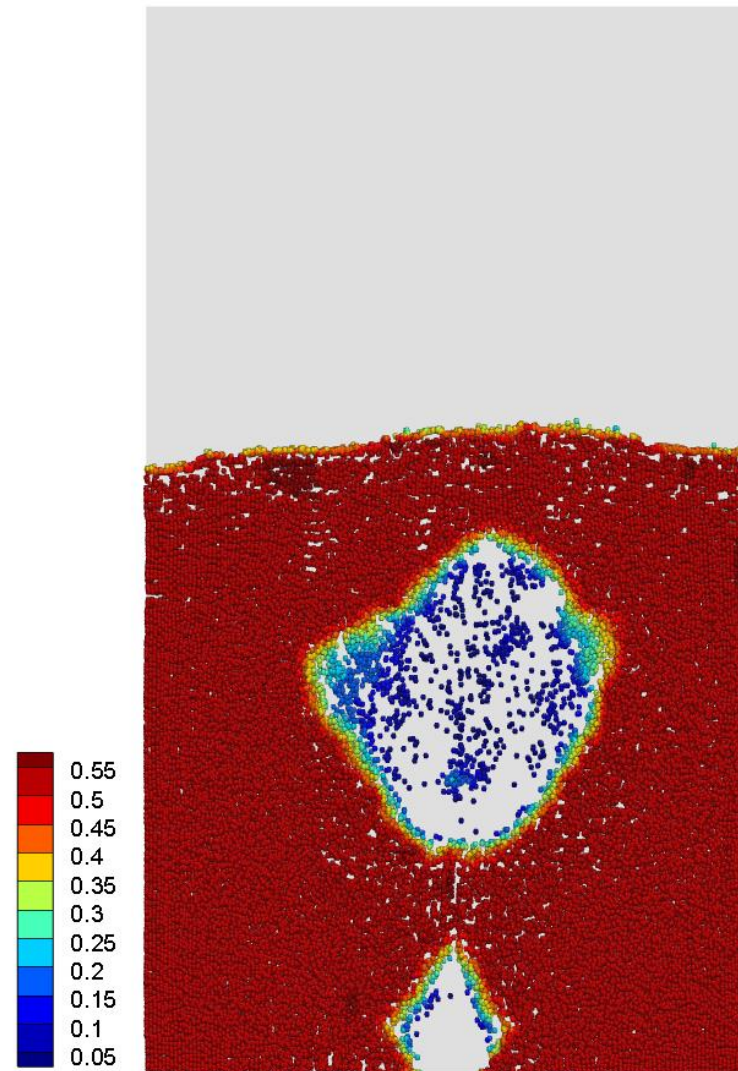
Fig. 1. Schematic representation of the experimental set-up used for the porosity measurements.

Kuipers, J, Tammes, Prins, and Swaaij (1992). Powder Technology 71: 87-99

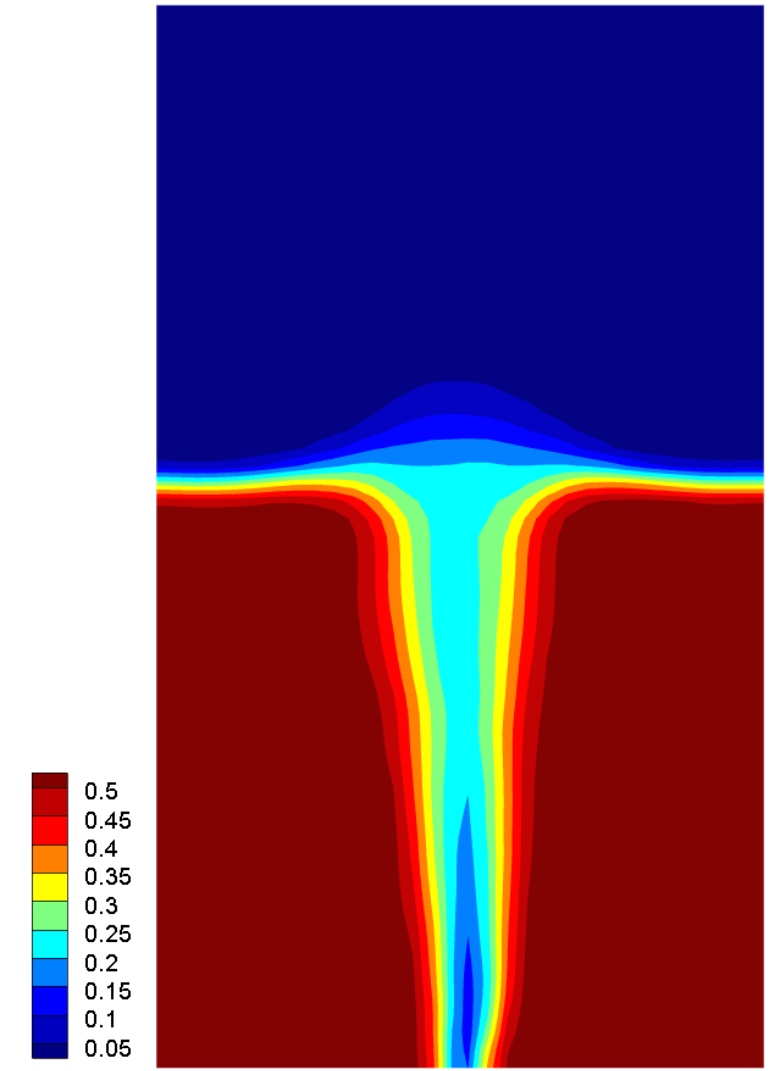
Results: Experimental vs. Simulation



Kuipers, J, Tammes, Prins, and Swaaij (1992). Powder Technology 71: 87-99



Instantaneous Particle Volume Fraction



Time Averaged Particle Volume Fraction

Process Sheet

Geometry

- 0.57m x 1.0m x 1.5cm
- 50 cm initial bed height
- 1.5cm x 1.5cm jet centered at bottom

Particles

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

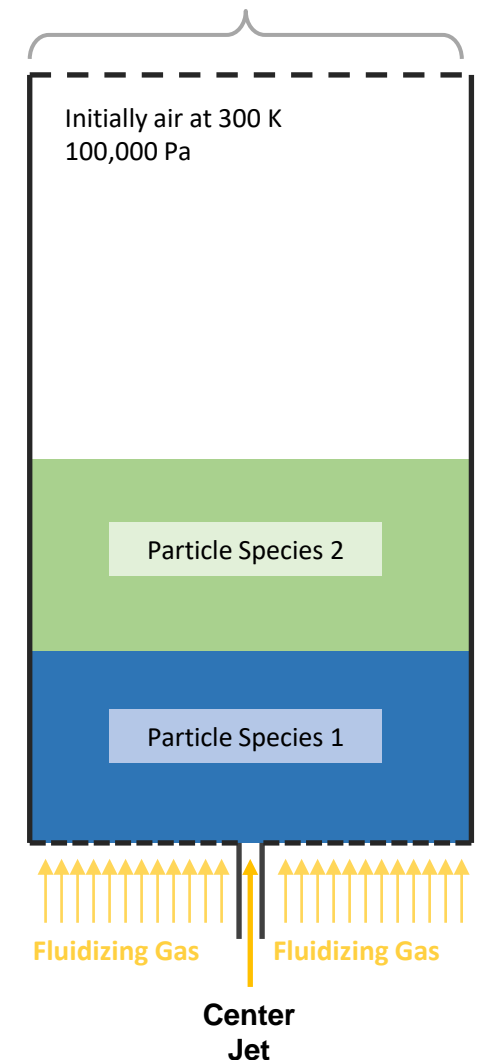
Initial conditions

- Fluid phase: air at atmospheric pressure
- Solid phase: particles in bottom ½ of bed at close-pack ($\theta_{cp} = 0.55$)

Boundary conditions

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

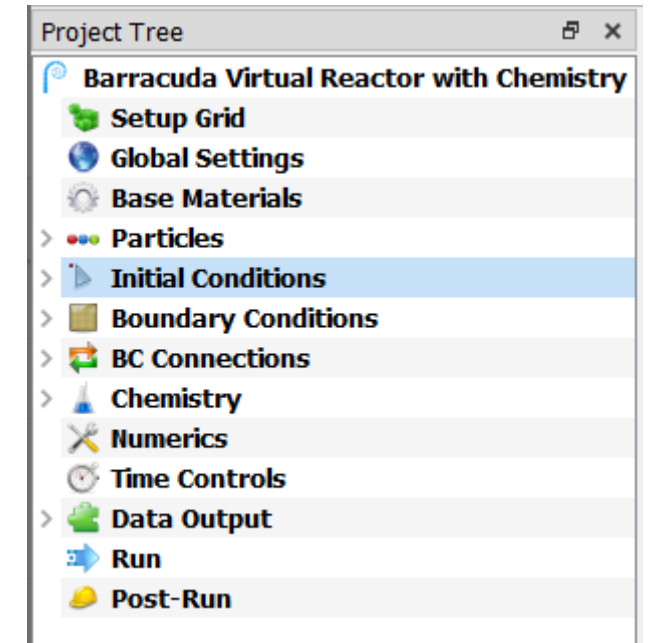
Pressure at outlet: 100,000 Pa



Setting up the Kuipers Bed Simulation

The Barracuda GUI Project Tree allows for convenient setup of the Kuipers bed simulation:

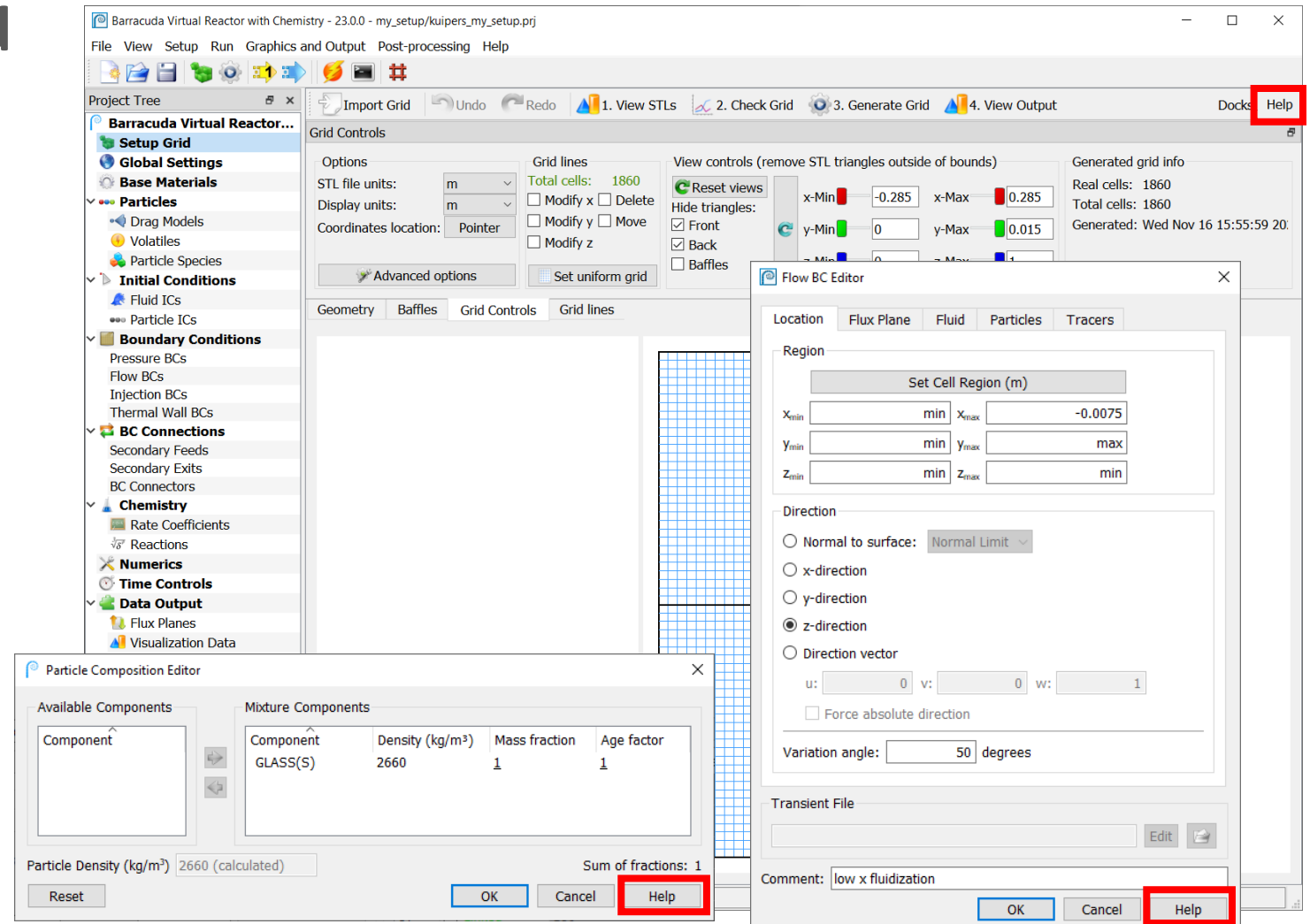
- Setup Grid – Create the computational grid from a CAD file of the physical geometry
- Global Settings – Set gravity and select isothermal calculations
- Base Materials - Add materials to simulation and edit physical properties
- Particles - Specify materials and particle size distributions for the particles in the model
- Initial Conditions - Specify initial fluid and particle conditions. Specify initial particle locations
- Boundary condition - Specify fluid velocities and pressures at model boundaries
- Time Controls - Specify simulation time, time step and restart interval
- Data Output - Select data to be written during simulation for later analysis
- Run - Check the model setup and run the simulation



How to Get More Information

All training materials have a limited amount of information about Barracuda and the GUI.

If you want to learn more, click on the Help button in the relevant dialog. This brings up the corresponding section of the User Manual.

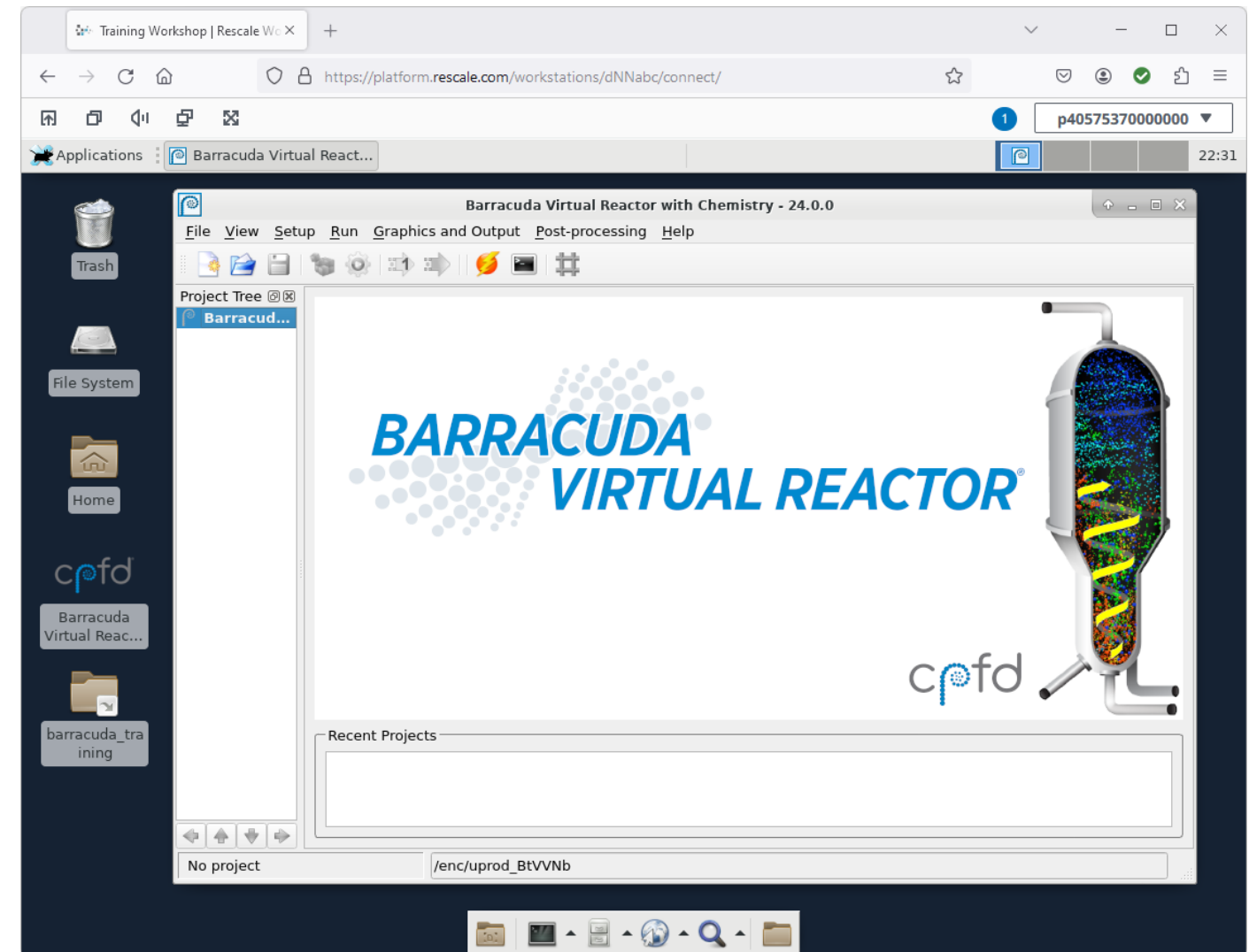


Cloud-based Linux VMs Provided by rescale

CPFD thanks Rescale for sponsoring cloud-based Linux VMs for training attendees to use

Log in based on instructions provided during the training workshop

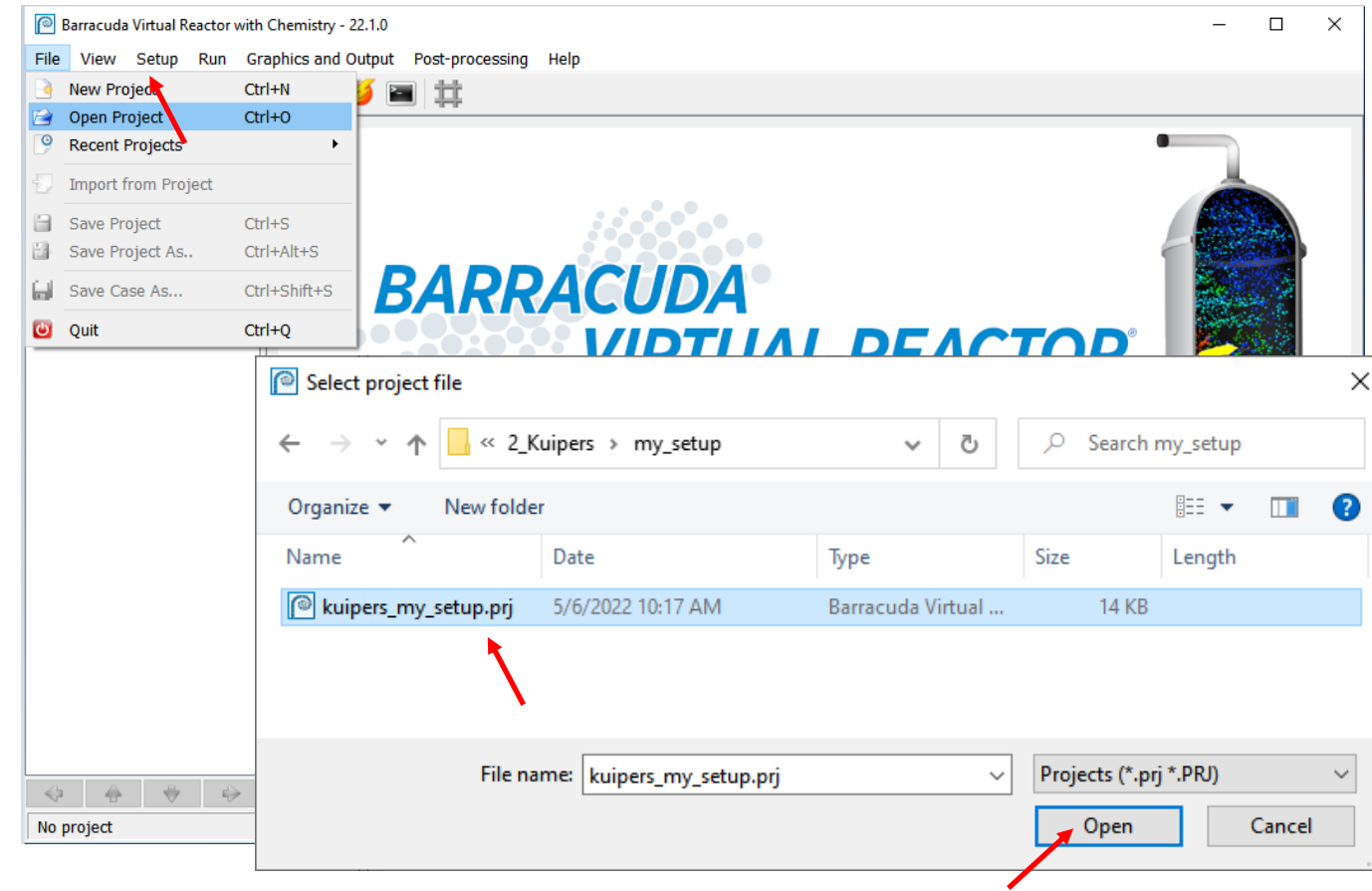
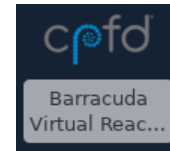
NVIDIA GPU cards are available on the VMs, make sure to take advantage of them when running the training example!



Opening a Project File

Launch Barracuda:

- Double-click on the Barracuda desktop icon
- Click on File → Open Project
- Navigate to the training directory, and go into the folder: `2_Kuipers/my_setup/`
- Choose the project file: `kuipers_my_setup.prj`
- Click Open



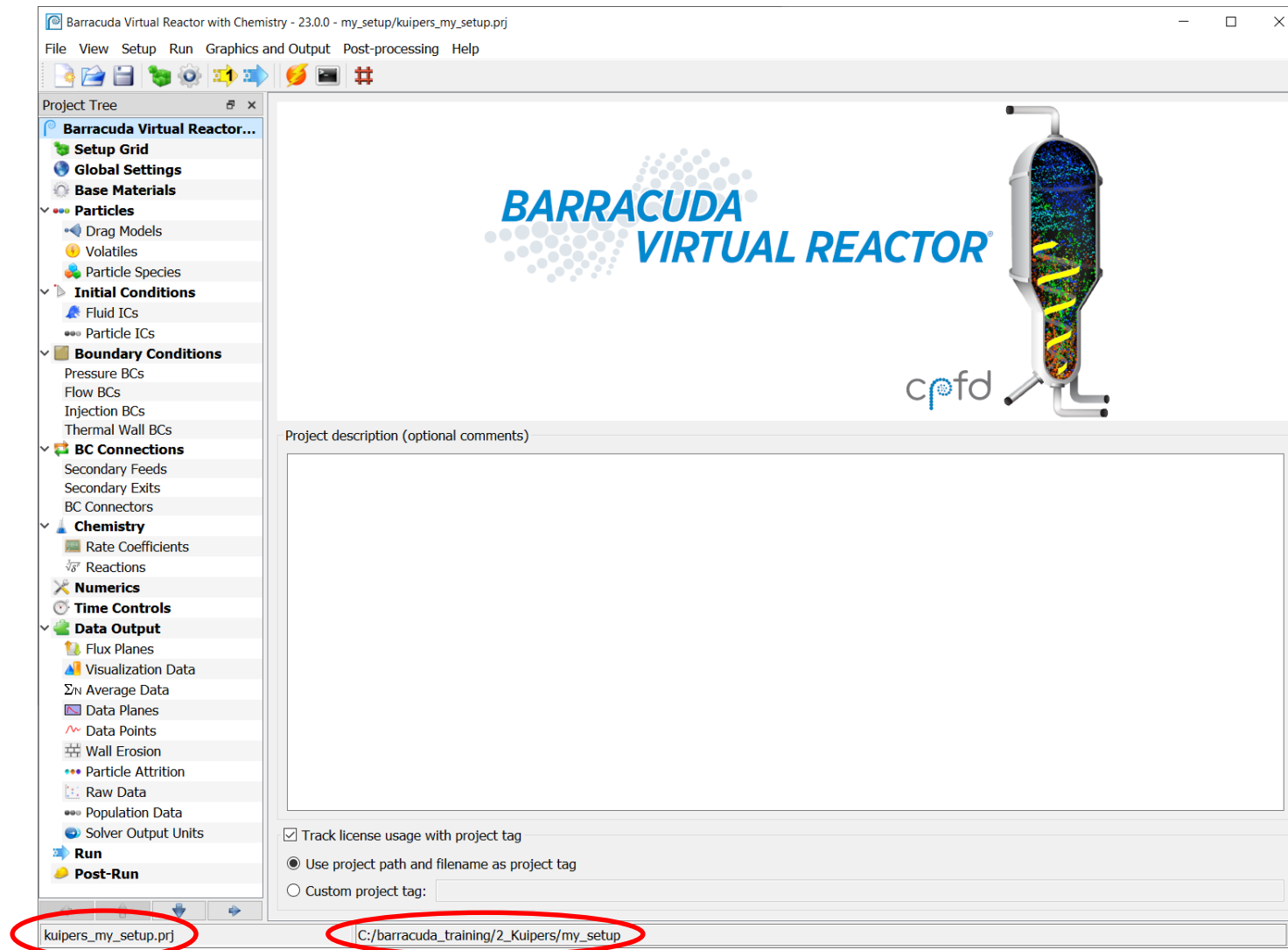
If you are using Rescale in a CPFD-led training class, links to the `barracuda_training` directory are on the Desktop.

Suggested location for the Barracuda training directory if you are working on your own local computer:

- Linux: `~/barracuda_training/`
- Windows: `C:\barracuda_training\`

Navigating the Barracuda GUI

Notice the project file and working directory are listed at the bottom of the main Barracuda GUI window



Setup Grid

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

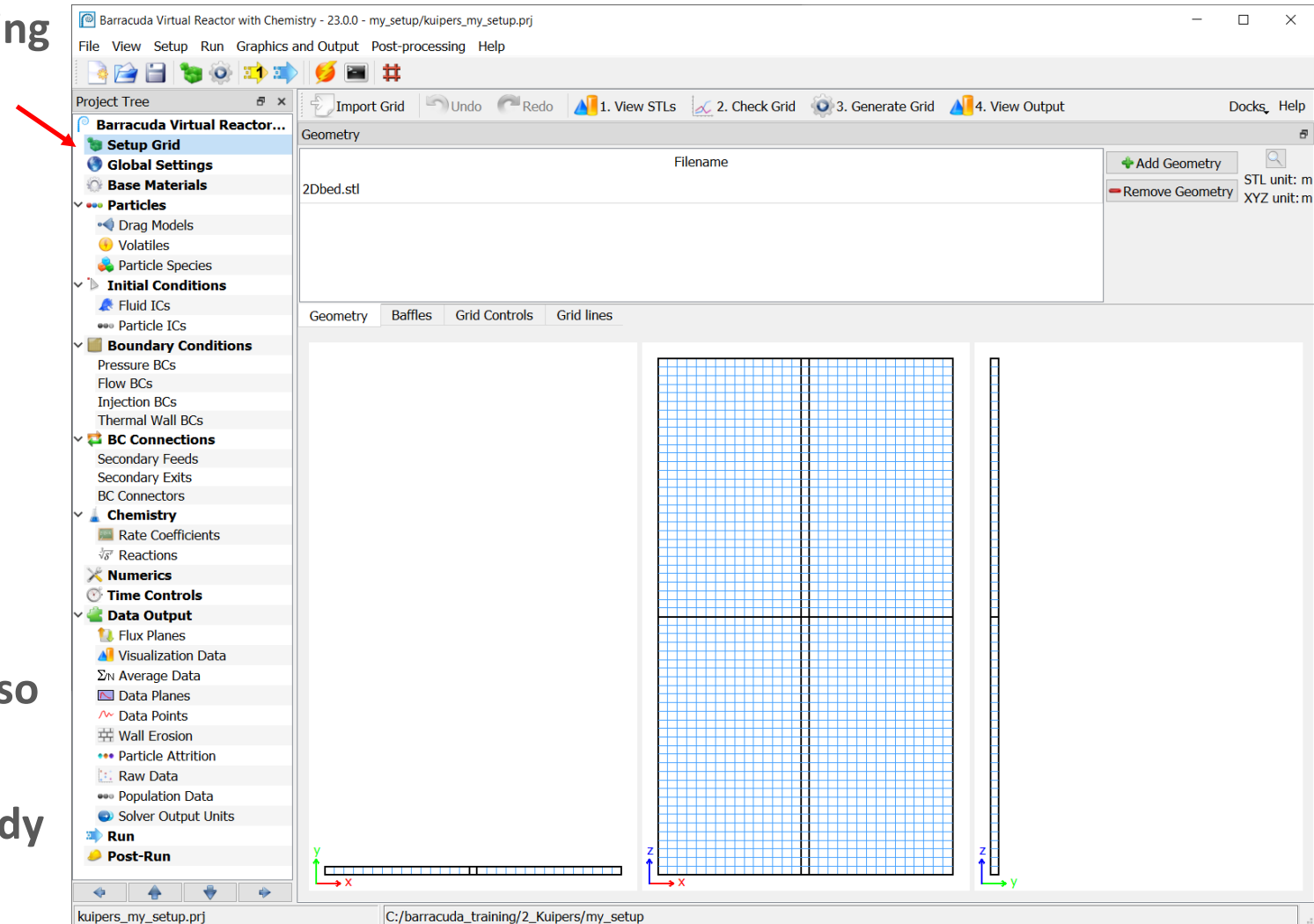
Each cell within the grid provides a location for the solver to calculate Eulerian values:

- 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, but also increase the computational time required.

For the Kuipers problem, gridline locations are already provided in the `kuipers_my_setup.prj` file.

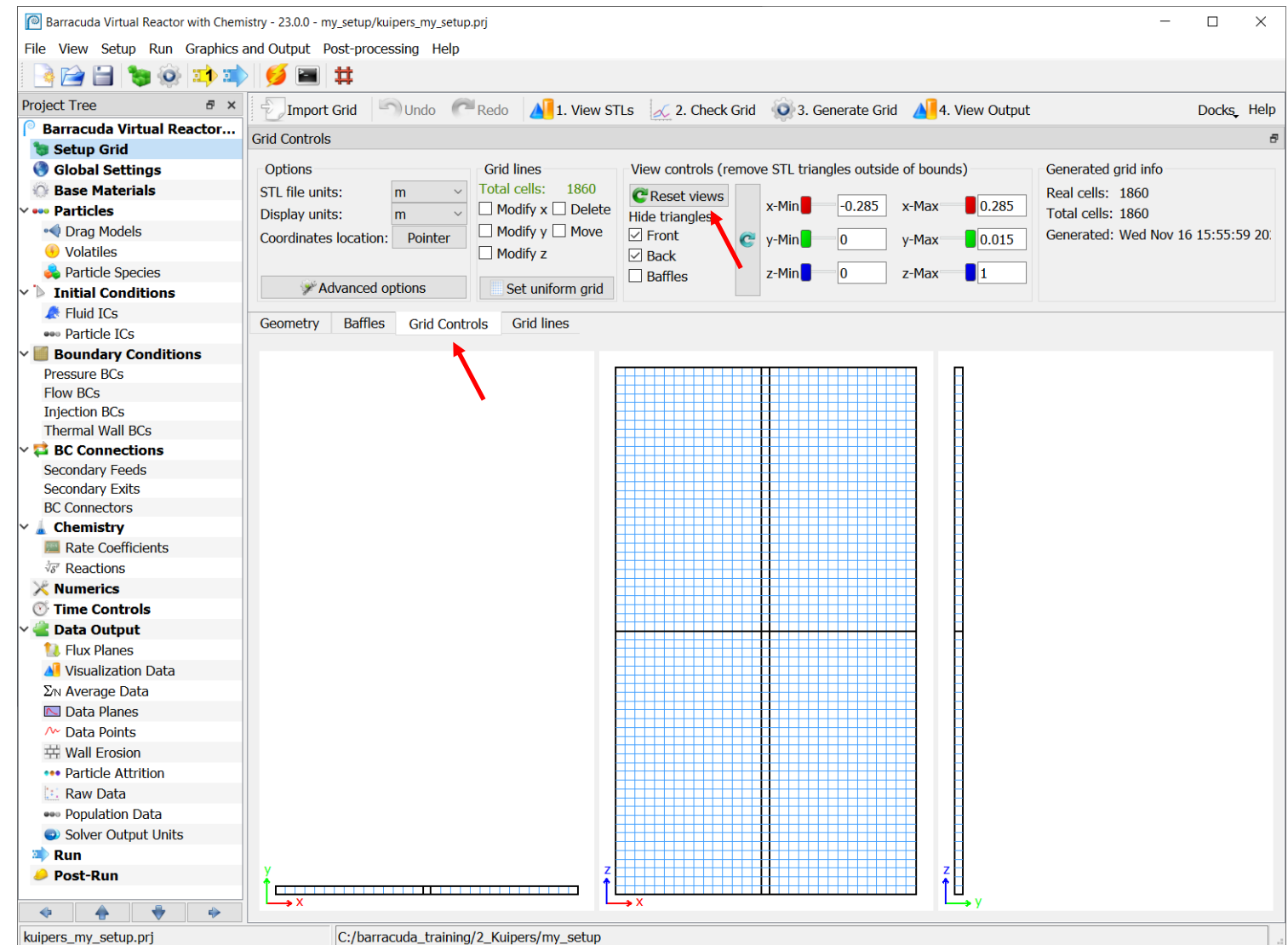


Grid Controls

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

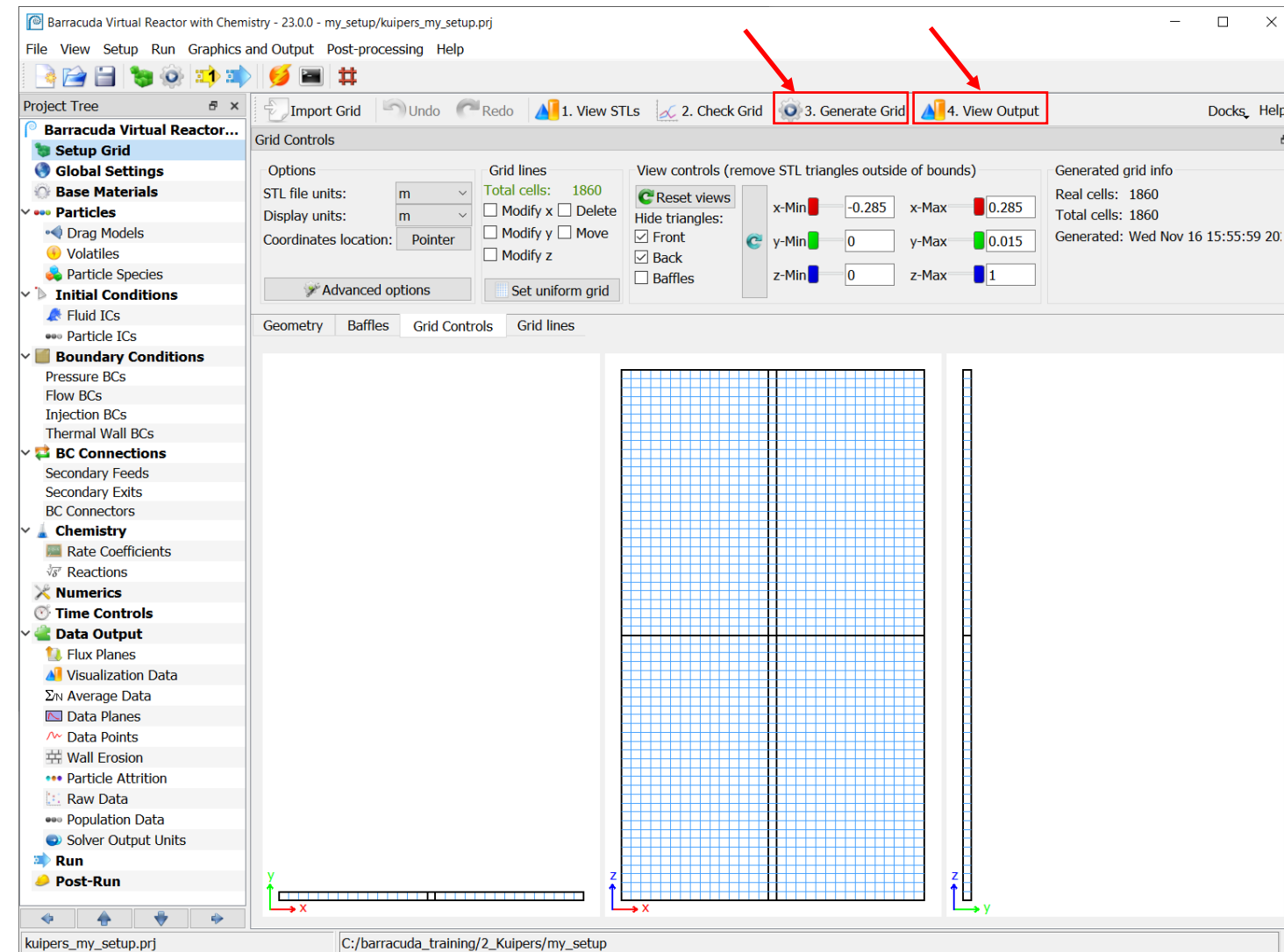
Reset views button in Grid Controls tab will return pane views to default position



Generating and Viewing the Grid

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

- Click Generate Grid
 - This automatically saves the project file
- Once the grid generator runs, click View Output. This opens the Grid: Transparent Model view in Tecplot for Barracuda.



Viewing the Grid

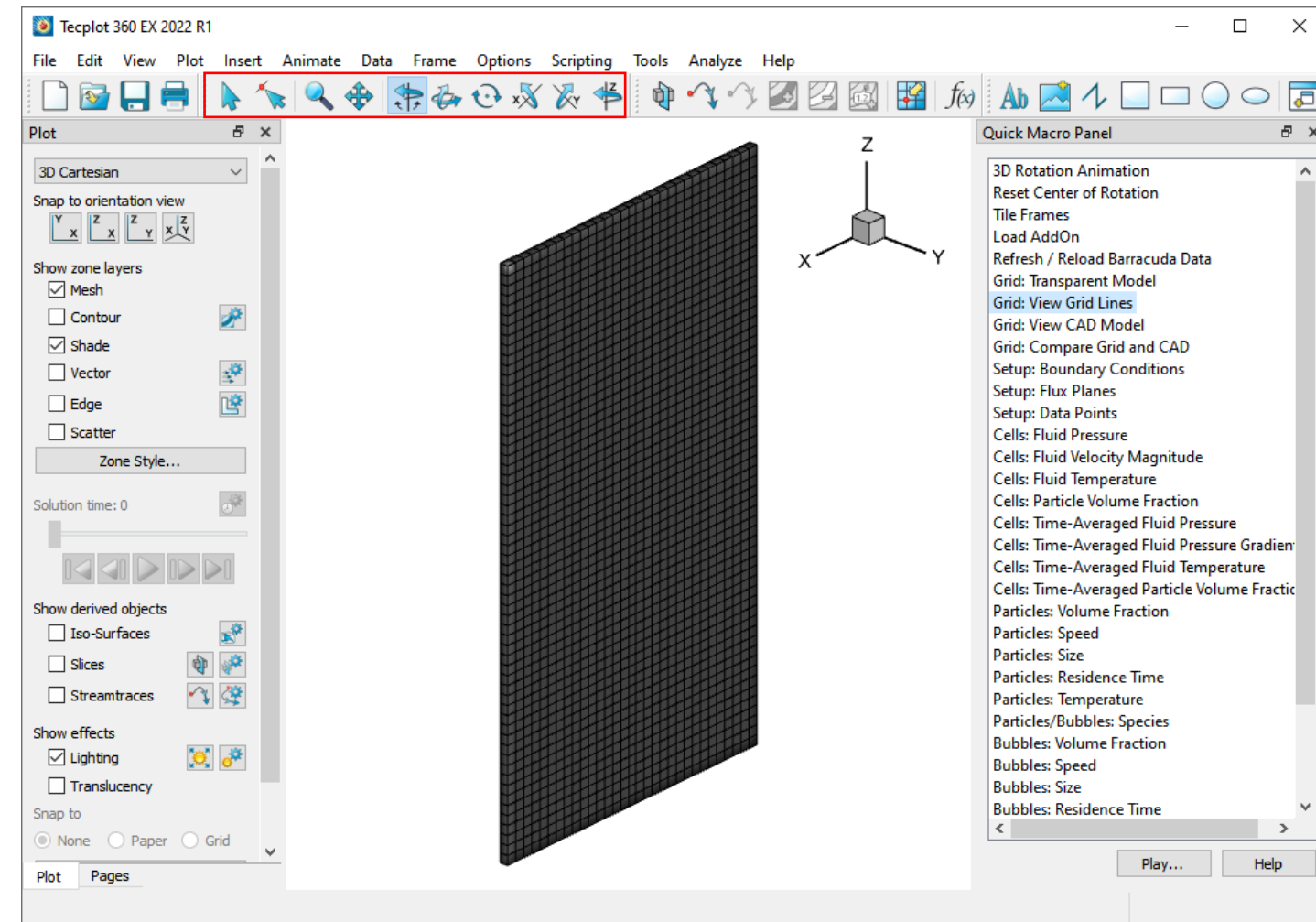
Double-click on Grid: View Grid Lines in the Quick Macro Panel

To rotate, translate, or adjust the zoom on the grid, use the buttons in the top tool bar.

Note:

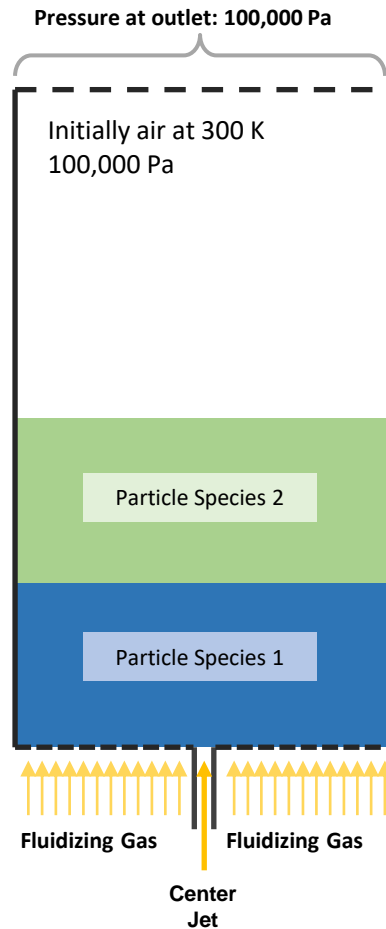
- This is the coarsest grid possible for this problem (resolving the center jet with a single cell).
- This is not necessarily the recommended grid resolution, but rather intended to illustrate how the CPFD method obtains resolution from both the computational cells (grid) and computational particles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

Close the Tecplot window and select Discard when prompted.

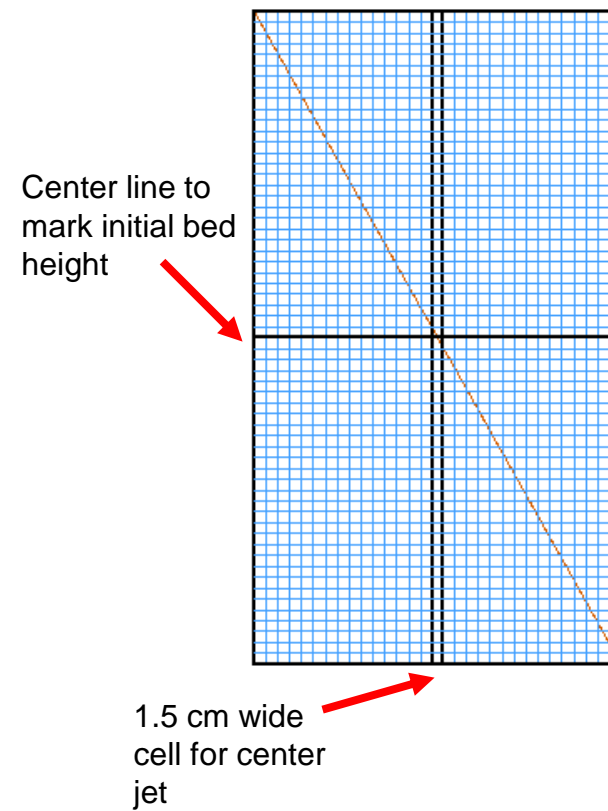


Overview of the Kuipers Bed Grid

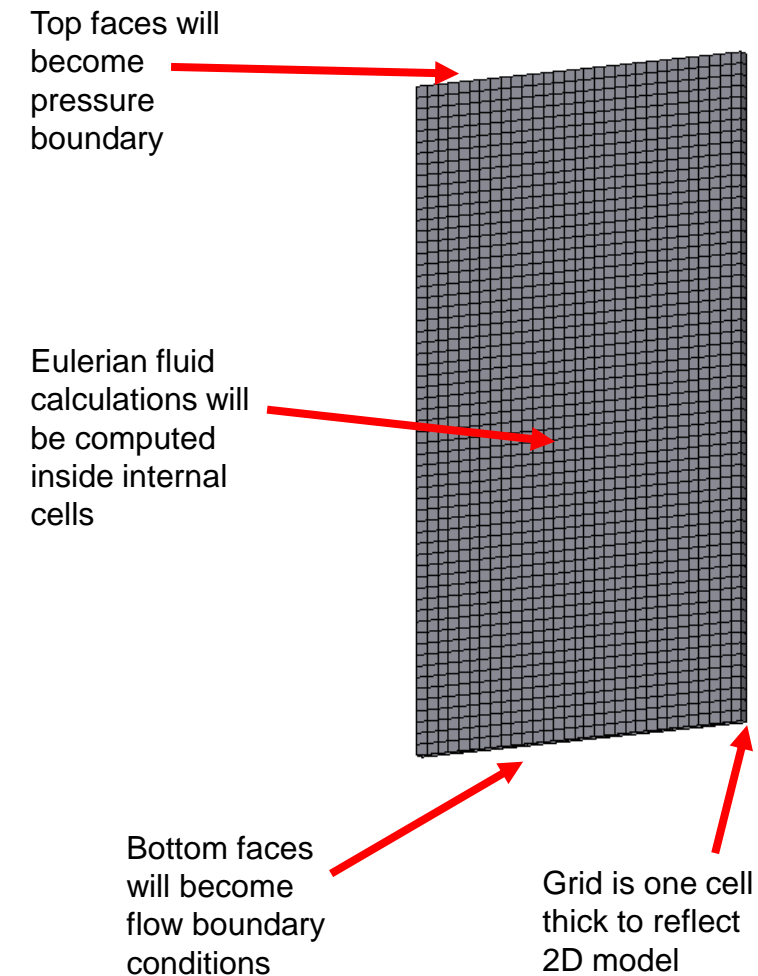
Physical Setup



Grid Setup



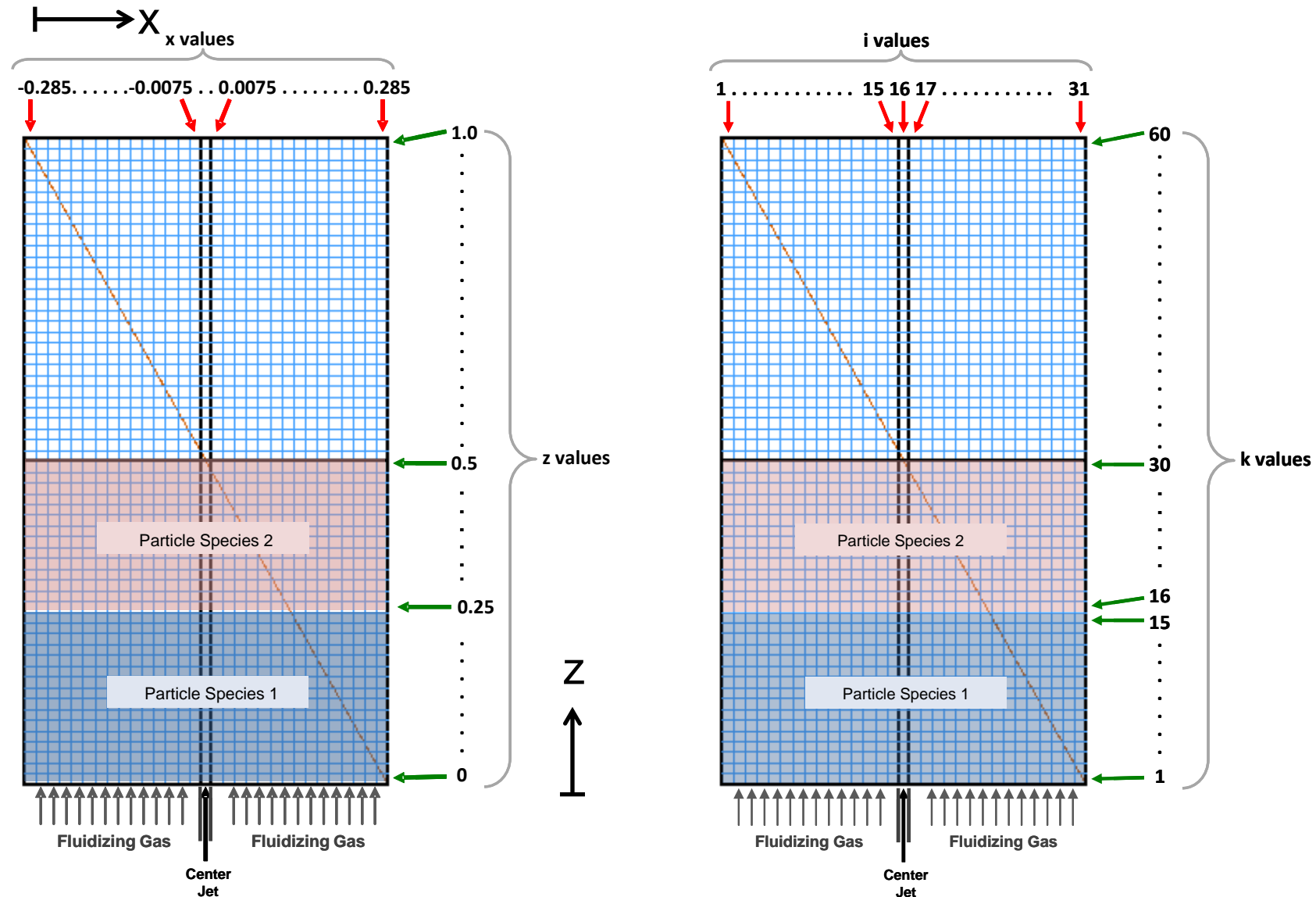
Generated Grid



Grid Coordinates

Grid cells are located by x,y,z values

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, which reference the cell in the x-, y-, and z- directions, respectively.



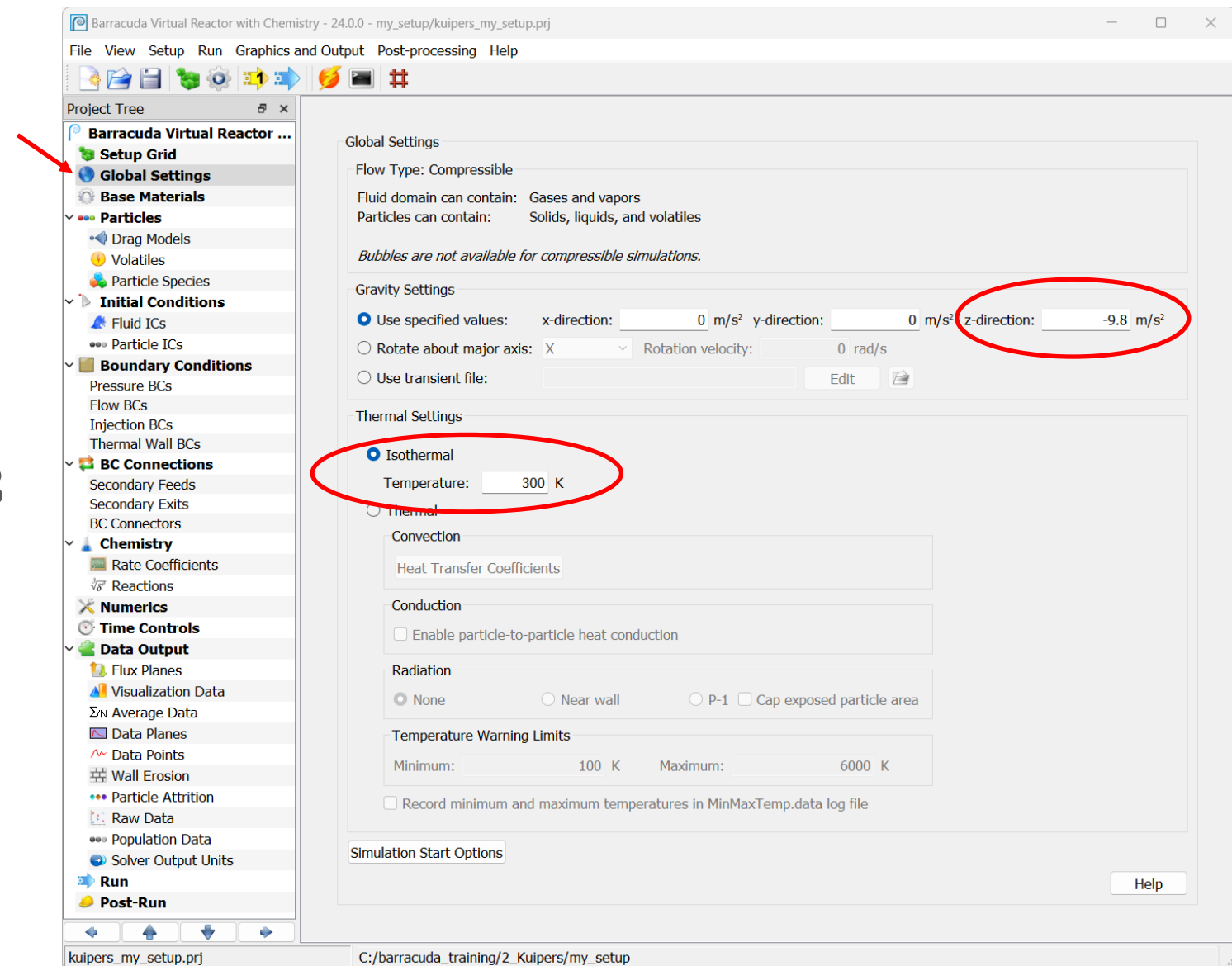
Global Settings

Click on Global Settings

Set Gravity vector

- In this example, gravity is in the negative z direction
- Notice the vector magnitude is 9.8 m/s^2

Isothermal flow should be selected.



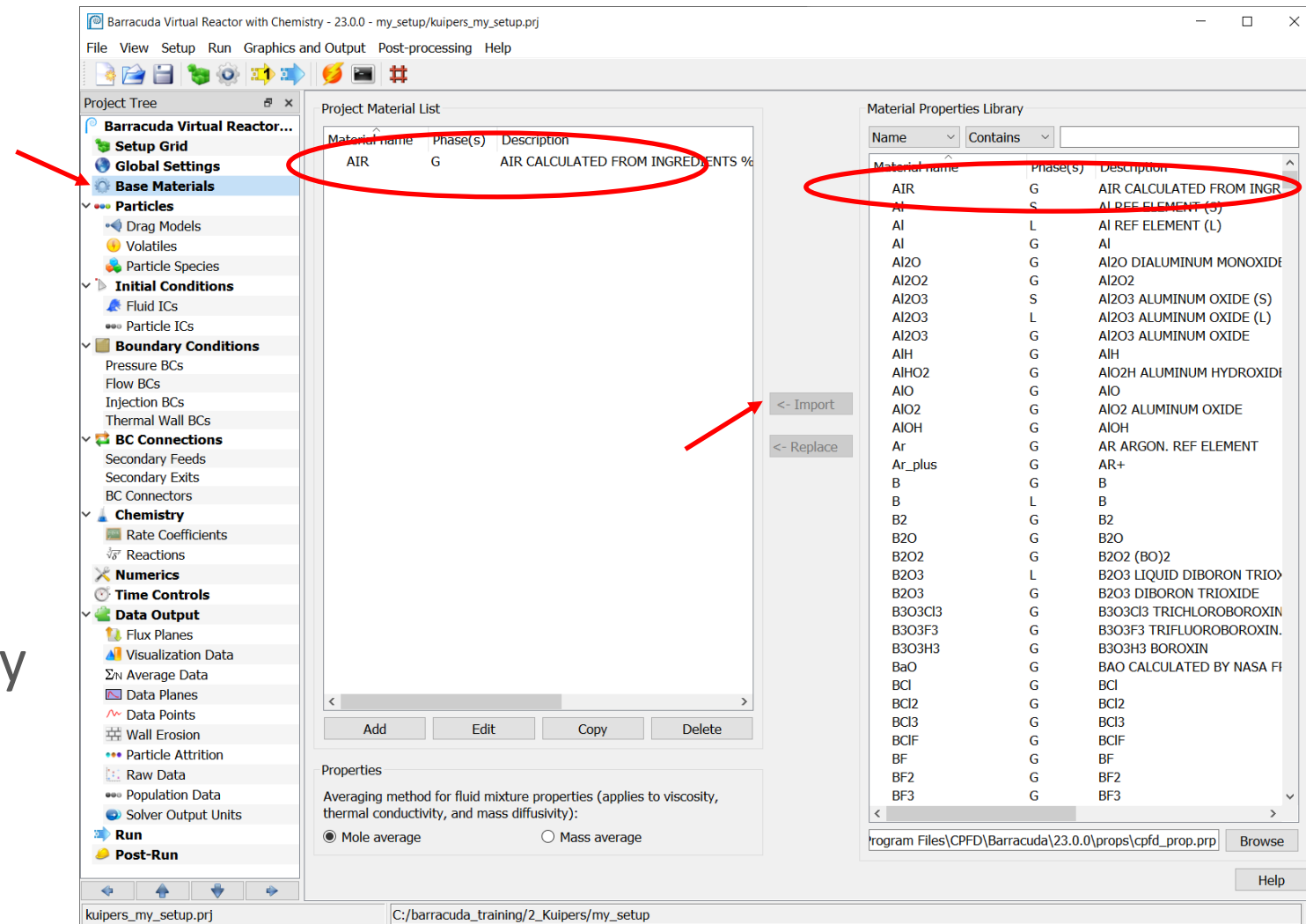
Base Materials

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

To add the fluid:

- Select AIR from the Material Library
- Click Import
- AIR now appears in the Project Material List at the left



Base Materials

All material properties can be defined and edited in the Base Materials window. To define the solid material:

- Click Add
- In the Material Properties window, enter the Chemical name as GLASS.
- Set the Phase to Solid
- Enter an appropriate description
- Set the Molecular weight to 60 g/mol in the Material Tab
- Click on Edit expression to set the Density to 2660 kg/m³ in the Solid Phase Tab
- Click OK

GLASS now appears in the Project Material List at the left

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.
- Other material property data such as thermal conductivity, heat capacity, and heat of formation would have to be specified if this were a thermal or reacting problem. Viscosity is required if the new material is a fluid.

The screenshot displays the Barracuda Virtual Reactor software interface. The main window shows the Project Tree on the left and the Project Material List in the center. The Project Material List contains the following entries:

Material name	Phase(s)	Description
AIR	G	AIR
GLASS	S	GLASS

The Base Materials Editor - GLASS (S) window is open, showing the following fields:

- Name: GLASS
- Phase(s): Solid
- Description: Glass - Soda-lime silica, common for glass beads
- Material: Solid Phase
- Molecular weight: 60 g/mol
- Density: Edit expression
- Heat of formation: 0 J/kg

The Material Property Editor window is also open, showing the following fields:

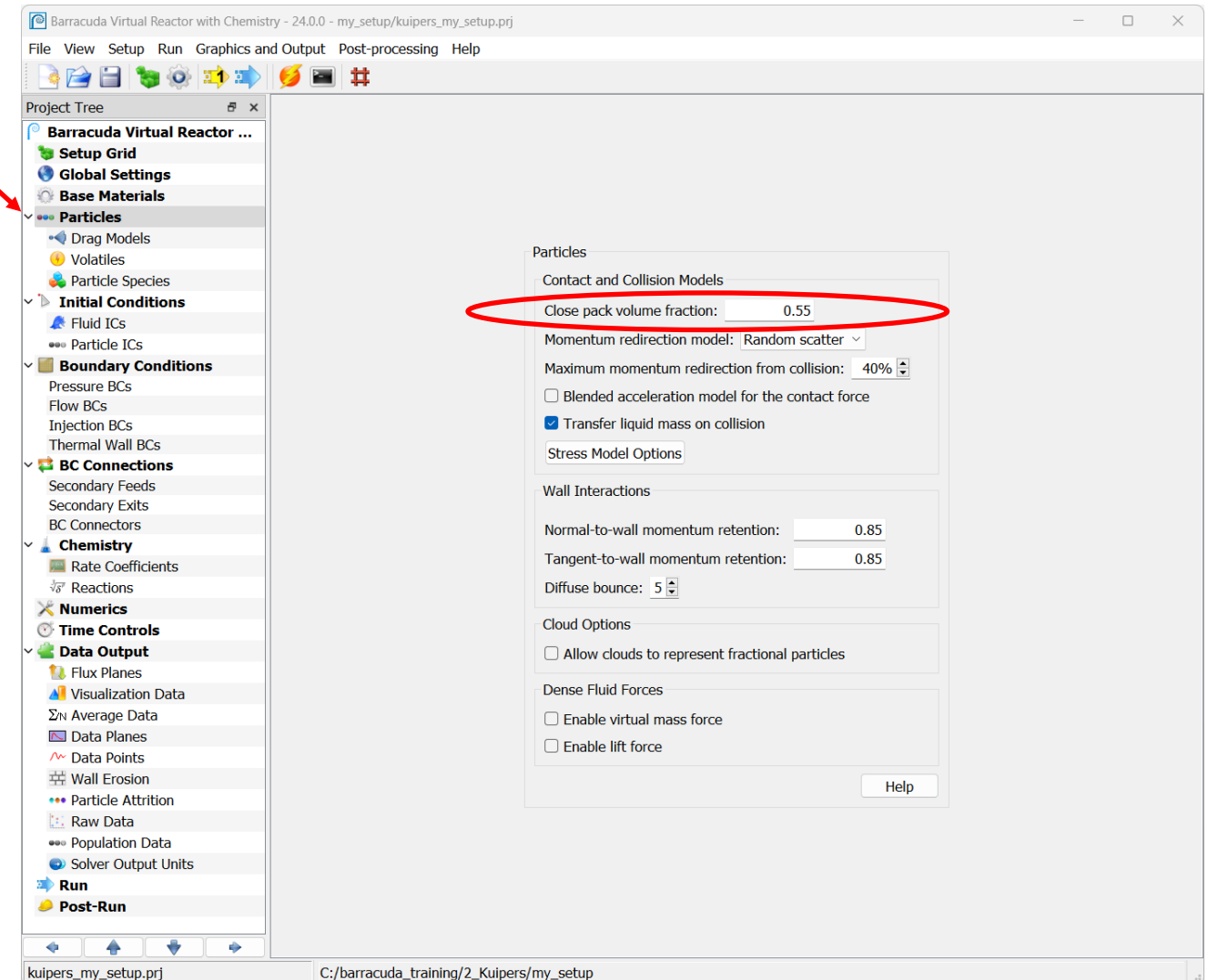
- Material: GLASS (S)
- Property: Density
- Property units: kg/m³
- Temperature units: K
- Expression: Polynomial (4th order)
- Expression: $2660 + 0.0 \cdot T + 0.0 \cdot T^2 + 0.0 \cdot T^3 + 0.0 \cdot T^4$
- Temperature Limits: Min. 0, Max. 6000
- Value Limits: Min. 0, Max. 1
- Verification: Display units as: Specified, SI
- Verification: T = 300 K, Expression = 2660 kg/m³
- Verification: T_{min} = 0 K, T_{max} = 2000 K, ΔT = 1 K
- Messages: Expression is valid
- Buttons: Copy expression, Paste expression, OK, Cancel, Help

Particles

Click on Particles

Enter a Close pack volume fraction of 0.55

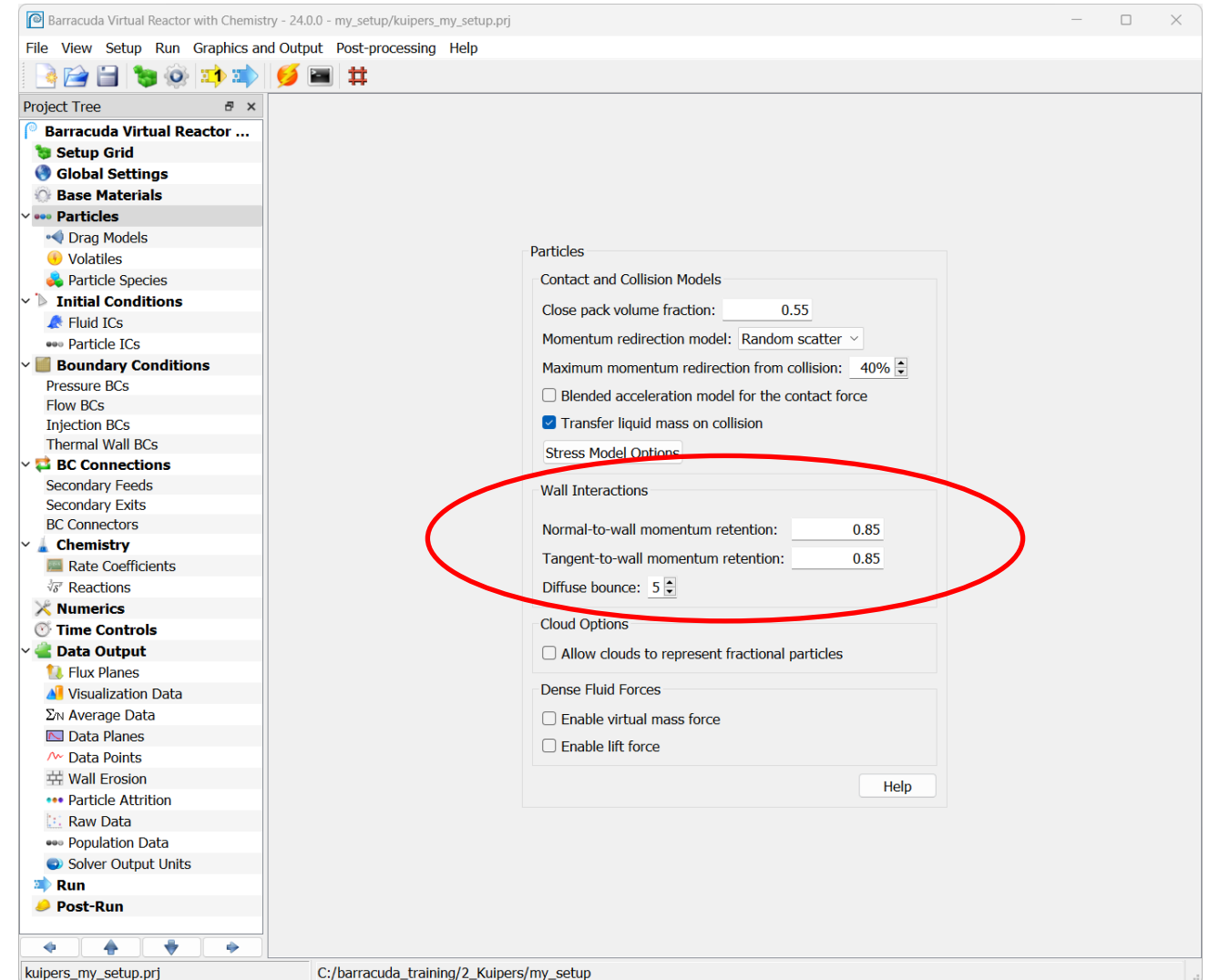
- This is the maximum amount of solids packing permitted in a cell
- This means that up to 55% of a reasonably-sized control volume can be occupied by particles. Conversely, at least 45% of the same volume must be occupied by the fluid.



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

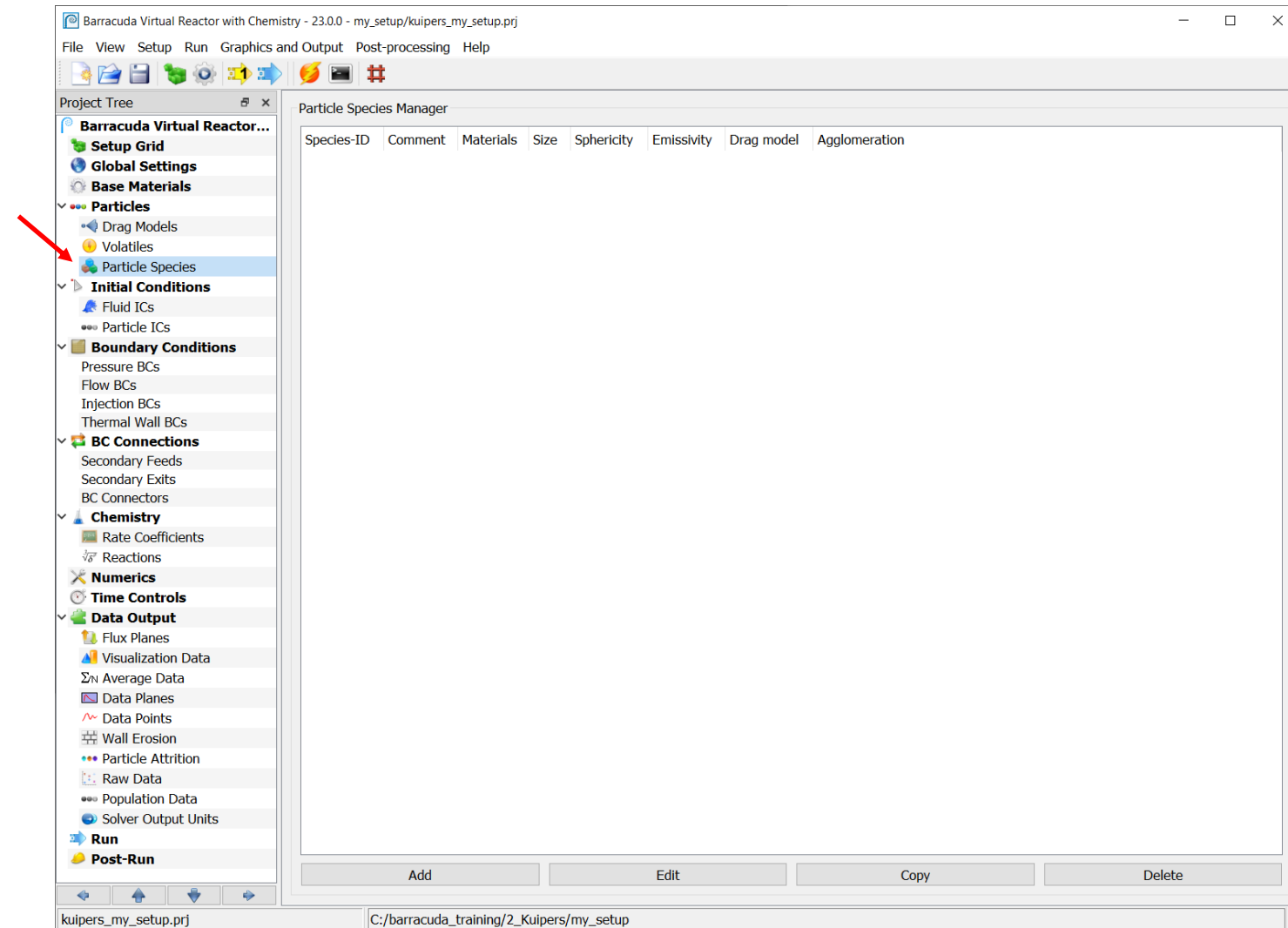


Particle Species

Click on Particle Species

We have only one type of solid particle (GLASS)

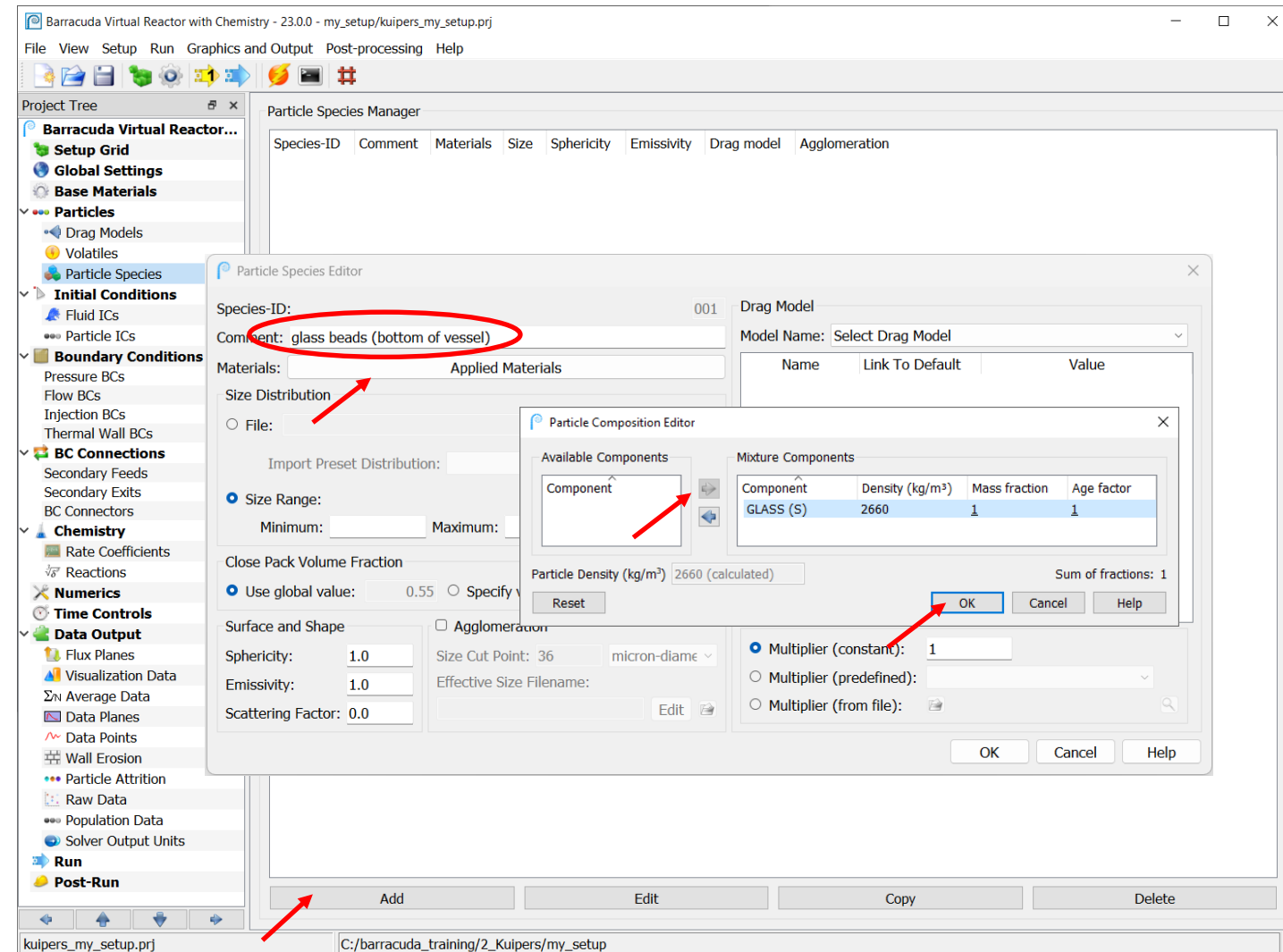
- However, we want to use two colors (one in bottom half of bed, another in top half) to view mixing
- To accomplish this, we must define two separate species of the same material (GLASS)



Particle Species – Applied Materials

To add the first particle species:

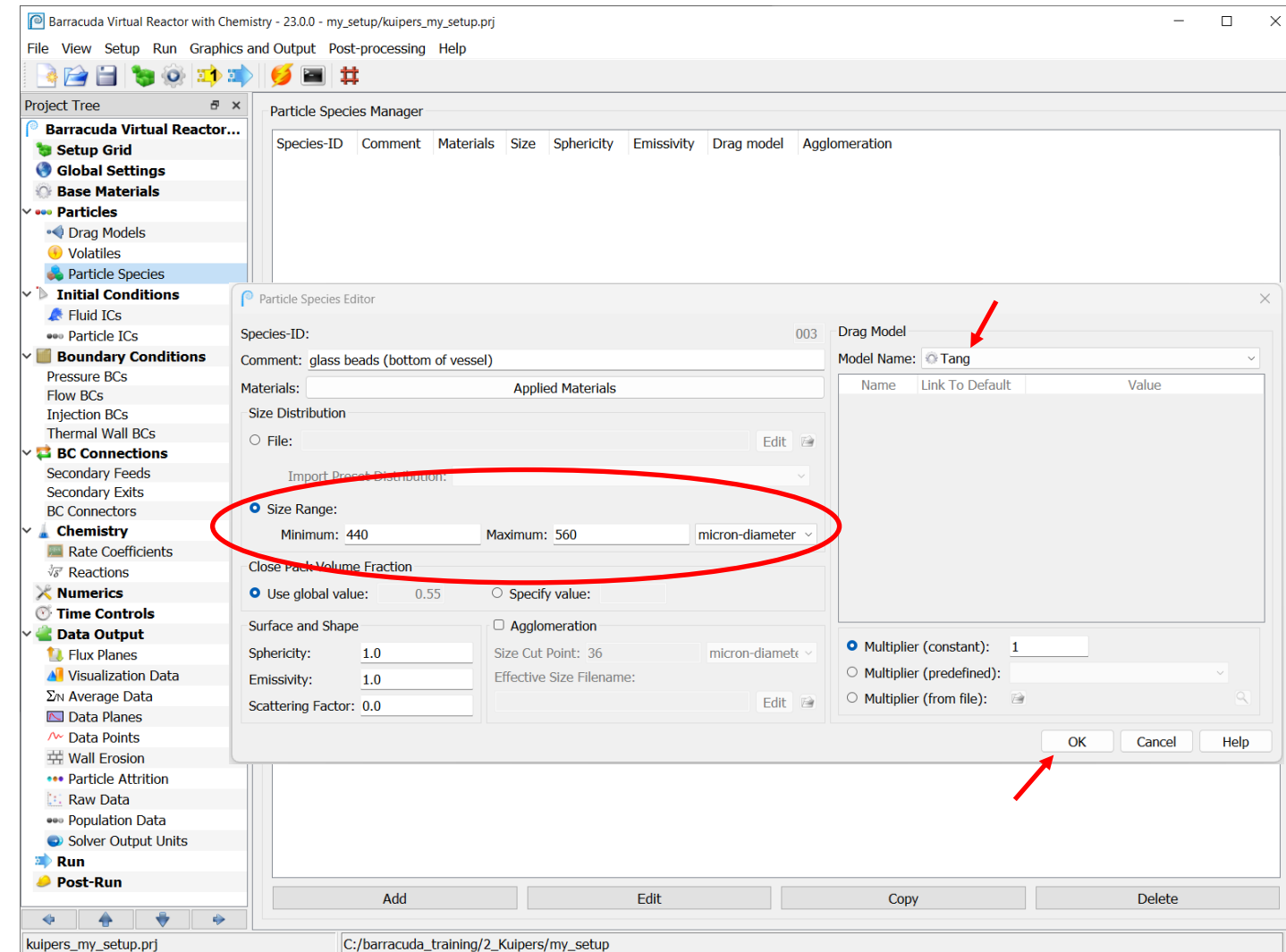
- Click on Add
- Add a description in the Comment section of Particle Species Editor
- Click on Applied Materials
- In the Particle Composition Editor import GLASS from the Available Components to the Mixture Components using the Right Arrow Button
- Click OK



Particle Species – Particle size and Drag Model

For the Kuipers setup:

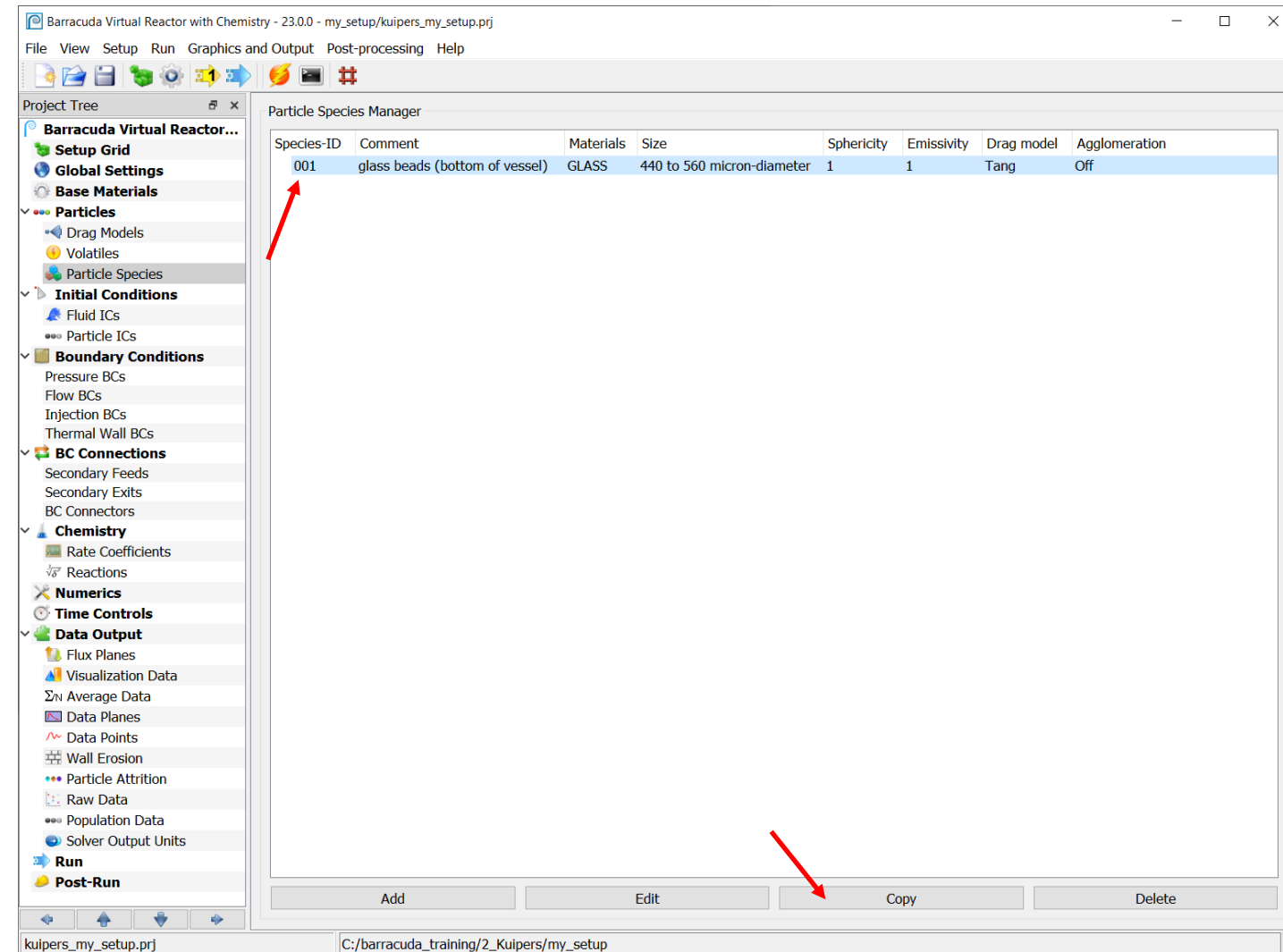
- Set the Size Range to 440 – 560 micron diameter
- Select Tang as Drag model in the drop down menu
- Click OK



Particle Species – Copy Species 001

To define a second, identical particle species:

- Select species 001
- Click Copy



Particle Species – Edit Species 002

To change the comment describing the second particle species:

- Select species 002
- Click Edit (or double-click on species 002)
- Change the Comment
- Click OK

The screenshot shows the Barracuda Virtual Reactor interface. The 'Particle Species Manager' window displays a table with the following data:

Species-ID	Comment	Materials	Size	Sphericity	Emissivity	Drag model	Agglomeration
001	glass beads (bottom of vessel)	GLASS	440 to 560 micron-diameter	1	1	Tang	Off
002	glass beads (top of vessel)	GLASS	440 to 560 micron-diameter	1	1	Tang	Off

The 'Particle Species Editor' window is open for species 002, showing the following fields:

- Species-ID: 2
- Comment: glass beads (top of vessel)
- Materials: Applied Materials
- Size Distribution: Size Range (Minimum: 440, Maximum: 560, micron-diameter)
- Close Pack Volume Fraction: Use global value: 0.55
- Surface and Shape: Sphericity: 1, Emissivity: 1, Scattering Factor: 0
- Agglomeration: Agglomeration: Off, Size Cut Point: 1.8e-05, m-radius
- Multiplier (constant): 1

Red arrows in the image indicate the following actions:

- Clicking on species 002 in the 'Particle Species Manager' table.
- Clicking the 'Edit' button at the bottom of the 'Particle Species Manager' window.
- Clicking the 'Comment' field in the 'Particle Species Editor' window.
- Clicking the 'OK' button in the 'Particle Species Editor' window.

Fluid Initial Conditions – Define Fluid, Pressure, Location

Click on Fluid ICs. Every Barracuda project has a default Fluid IC that needs to be edited.

For this example problem, air is initially at rest at atmospheric pressure:

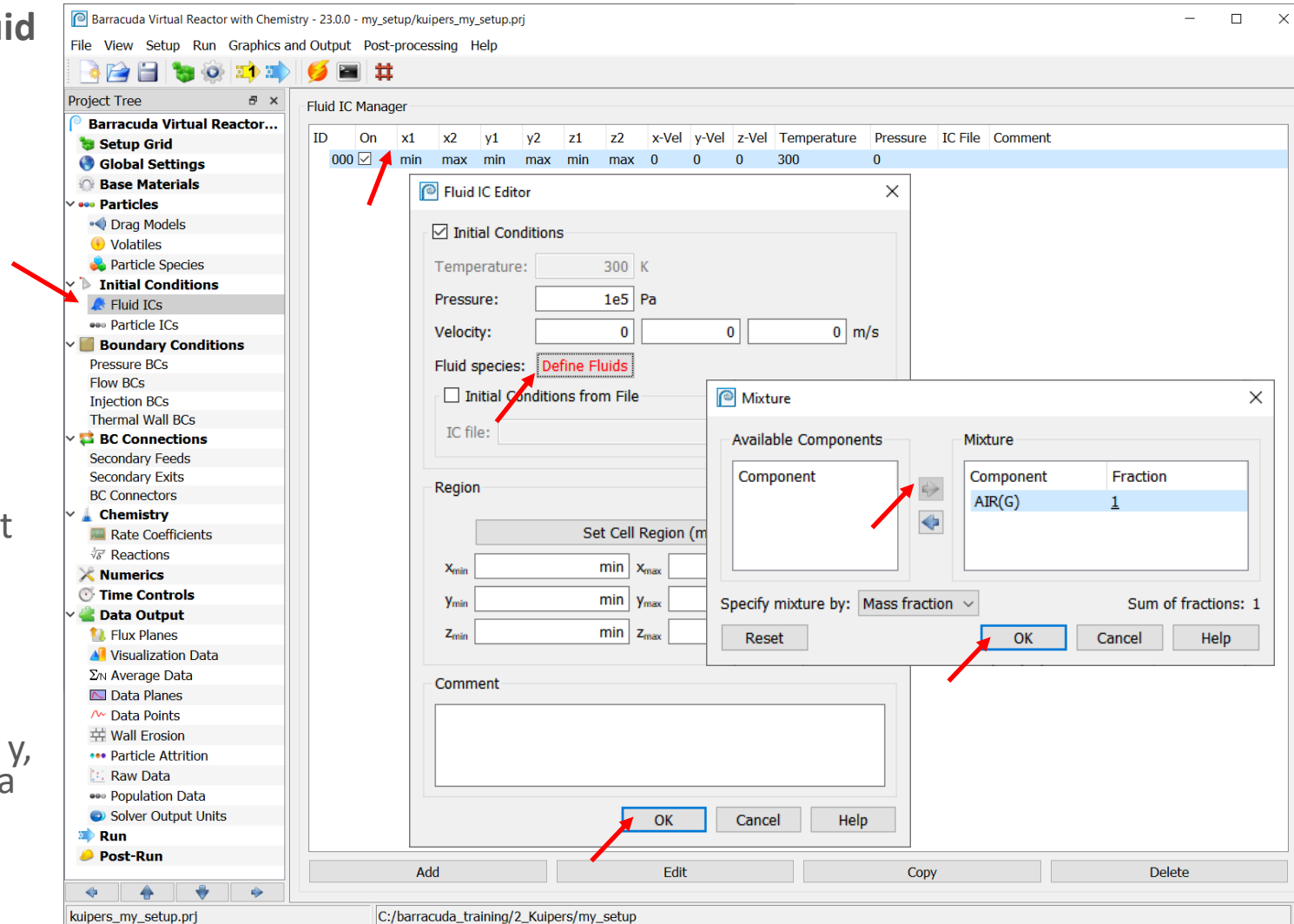
- Double-click on the default fluid IC
- Specify the pressure as 1e5 Pa
- Leave the x, y, and z fluid velocities at zero
- Click on Define Fluids

In the Mixture window:

- Select AIR (G) and use the Right arrow button to import from Available Components to Mixture
- Click OK

In the Fluid IC Editor:

- Leave the Region set from minimum to maximum for x, y, and z, since the air initially occupies the entire bed (area above and in between glass particles)
- Click OK



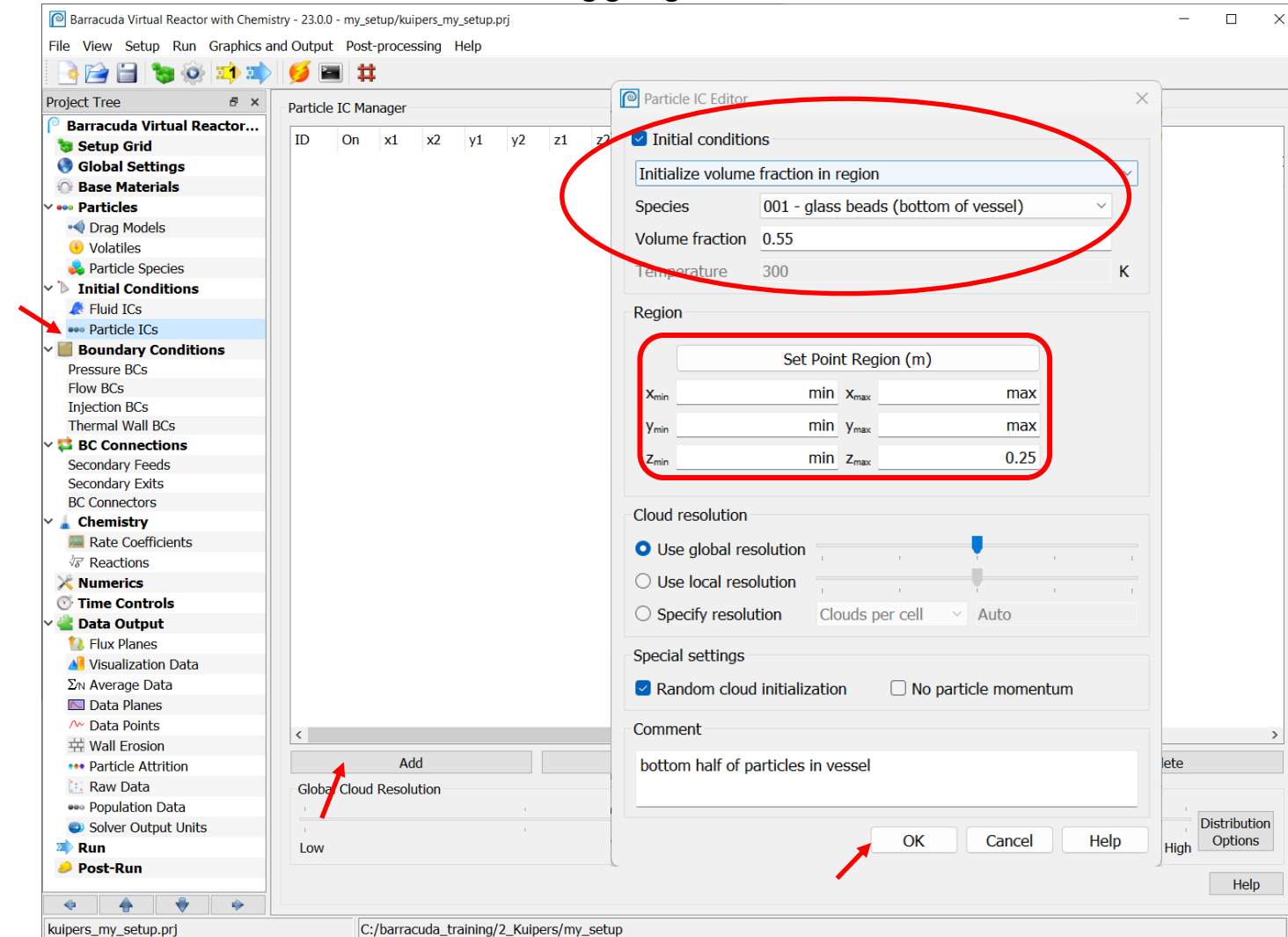
Particle Initial Conditions

X _{min}	X _{max}	Y _{min}	Y _{max}	Z _{min}	Z _{max}
[]	[]	[0.25

*Note: The [and] keys are shortcuts for the min and max values defined during grid generation

To show mixing add two distinct layers of particles:

- Click on Particle ICs
- Click Add, which pops up a Particle IC dialog
- Select Initialize volume fraction in region
- Select 001 – glass beads in Species
- Set Volume fraction to 0.55
- Set Point Region as shown in the table
 - [and] (for min and max)
- Add descriptive comment
- Click OK



Particle Initial Conditions

X _{min}	X _{max}	Y _{min}	Y _{max}	Z _{min}	Z _{max}
[]	[]	0.25	0.5

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

- Click Add
- Select Initialize volume fraction in region
- Select 002 – glass beads in Species
- Set the Volume fraction to 0.55
- Set Point Region as shown in the table
- Add descriptive comment
- Click OK

Pressure Boundary Condition

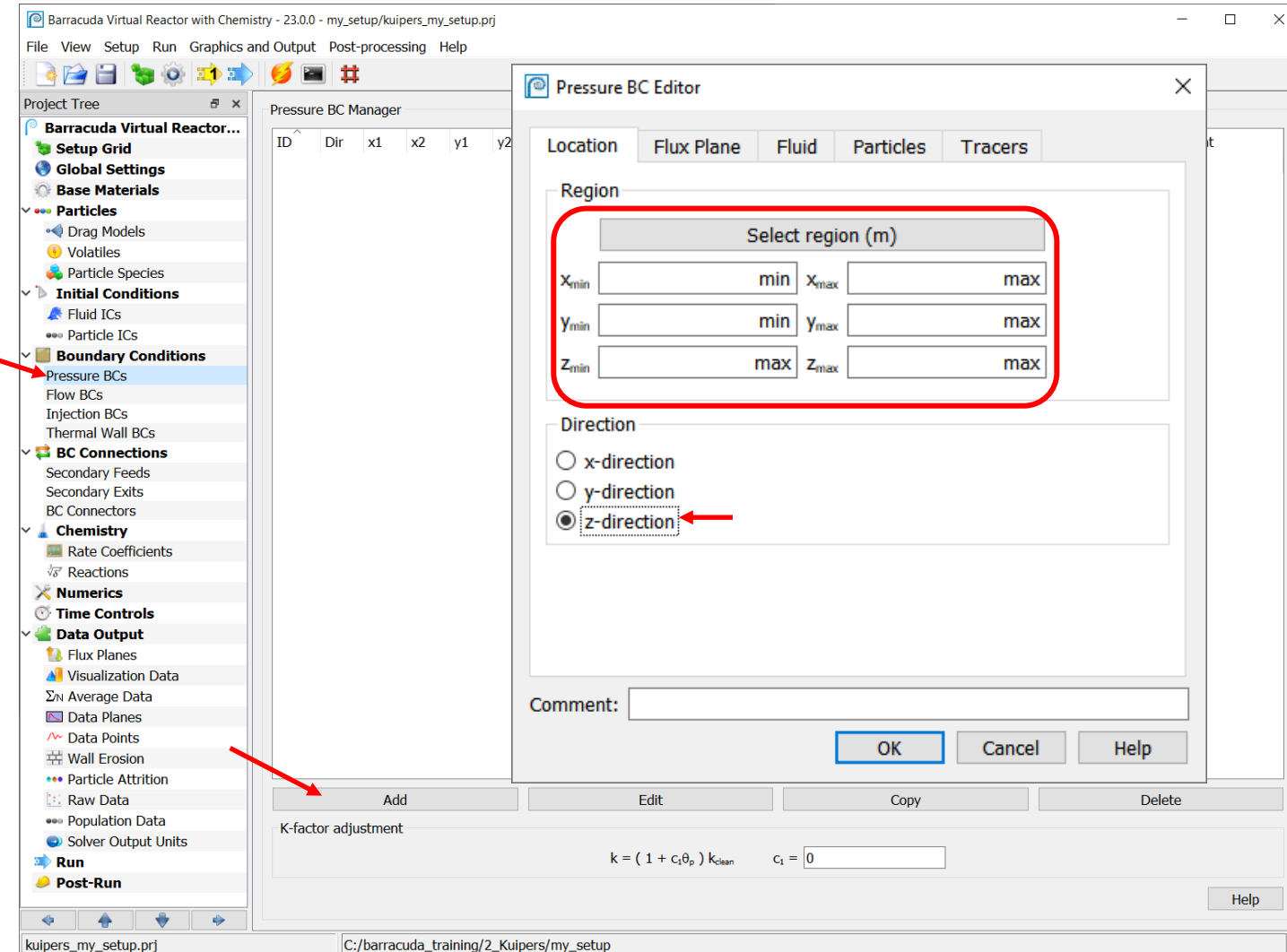
x_{min}	x_{max}	y_{min}	y_{max}	z_{min}	z_{max}
[]	[]]]

To specify that the top of the system is open to the atmosphere, define a Pressure BC:

- Click on Pressure BCs
- Click Add

In the Pressure BC Editor Location tab:

- Set Direction to z
- Set x and y region using [and] (for min and max)
- Set z region using] (for max) for both z_{min} and z_{max} so that the BC is placed on the top surface of the geometry
- Enter a comment (optional)



Pressure Boundary Condition

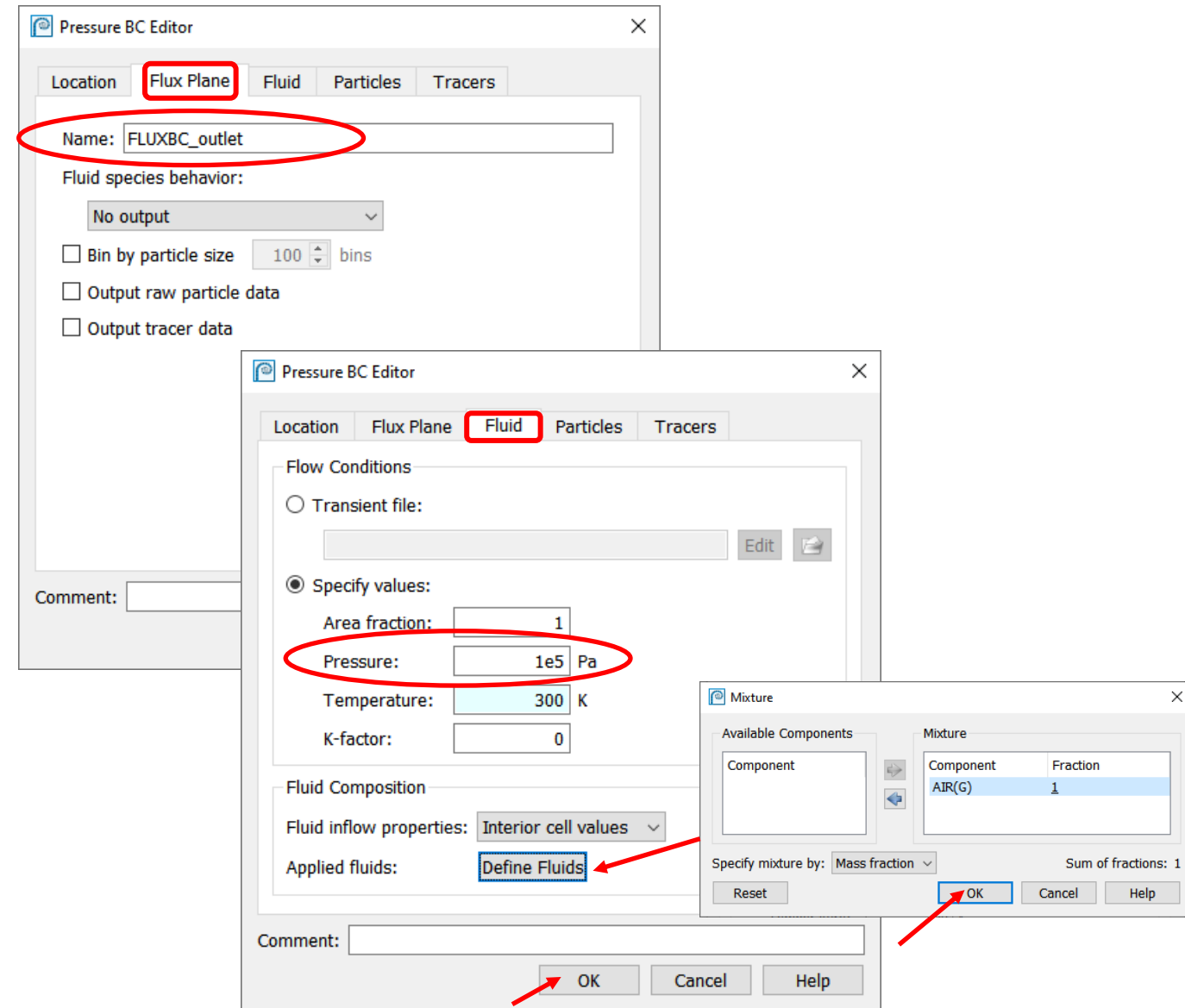
Flux Plane tab:

- Provide a name for the Flux plane
 - Best practice is to start a boundary condition flux plane file name with **FLUXBC_** for ease of post-processing

Fluid tab:

- Specify the pressure as 1e5 Pa
- Click on Define fluid species
 - Import AIR(G) from Available Component to Mixture using the Right Arrow Button
- Click OK in the Mixture editor

Click OK in the Pressure BC Editor



Flow Boundary Conditions

X _{min}	X _{max}	Y _{min}	Y _{max}	Z _{min}	Z _{max}
[-0.0075	[]	[[

To specify the inlet flow boundaries (2 fluidizing gas and one center jet) define a separate Flow BC for each one:

- Click on Flow BCs
- Click on Add

In the Flow BC Editor Location tab:

- Set x and y region using the values in the table
 - Set z region using [(for min) for both z_{min} and z_{max} so that the BC is placed on the bottom surface of the geometry
- Set Direction to z
- Enter a comment (optional)

The screenshot shows the Barracuda Virtual Reactor software interface. The main window displays a project tree on the left with 'Flow BCs' selected under 'Boundary Conditions'. The 'Flow BC Manager' window is open, showing a table with columns for ID, Dir, x1, x2, y1, and y2. Below the table are 'Add', 'Edit', 'Copy', and 'Delete' buttons. A red arrow points to the 'Add' button. The 'Flow BC Editor' dialog box is open, showing the 'Location' tab. The 'Set Cell Region (m)' section is highlighted with a red box, showing input fields for X_{min} (min), X_{max} (-0.0075), Y_{min} (min), Y_{max} (max), Z_{min} (min), and Z_{max} (min). The 'Direction' section has the 'z-direction' radio button selected. The 'Variation angle' is set to 15 degrees. The 'Comment' field contains 'low x fluidization'. The 'OK', 'Cancel', and 'Help' buttons are at the bottom of the dialog.

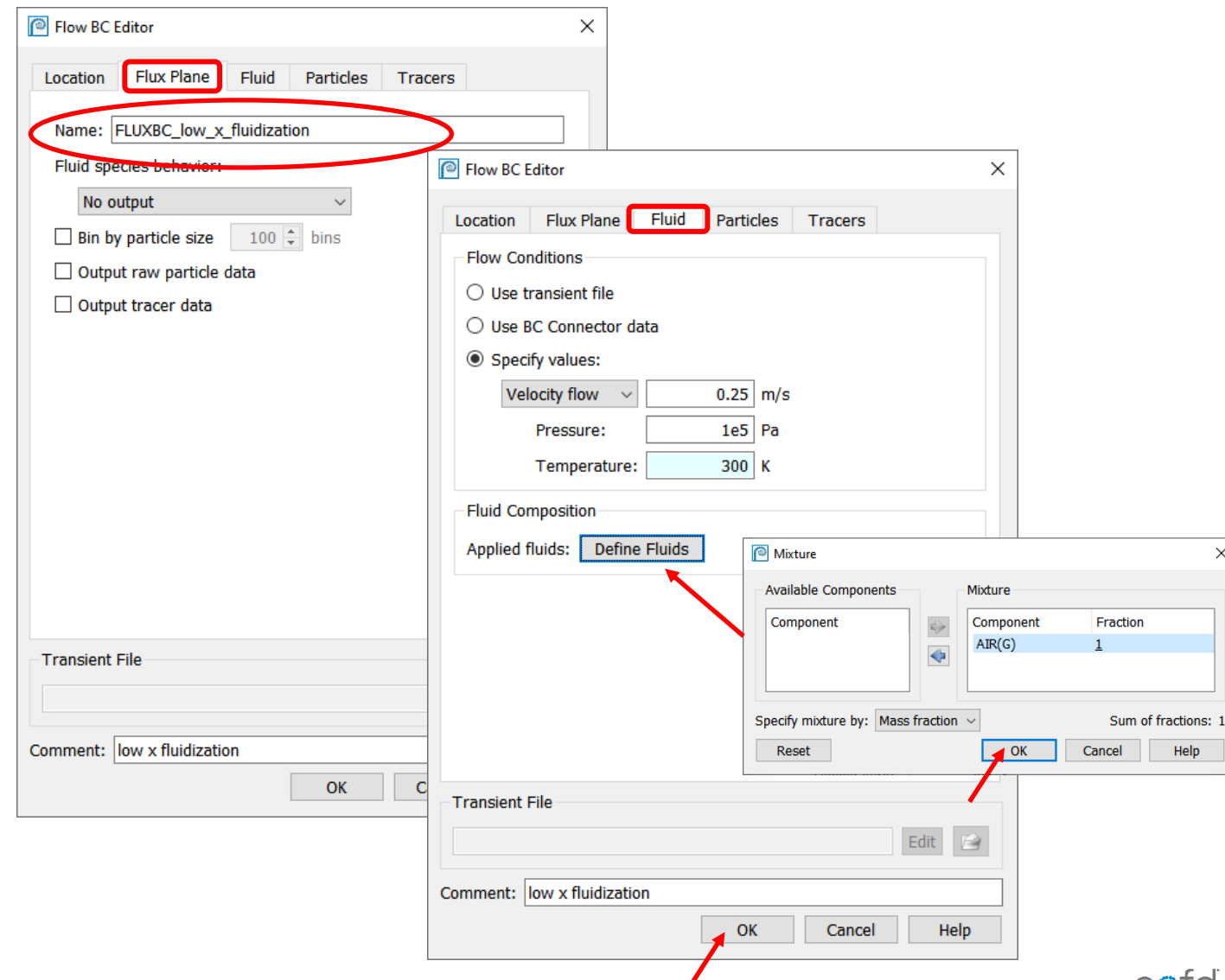
Flow Boundary Conditions – Low x Fluidizing Gas

Flux Plane tab:

- Provide a name for the Flux plane

Fluid tab:

- Set Velocity flow to 0.25 m/s
 - 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 Pressure to 1e5 Pa
- Click on Define Fluids
 - Select AIR (G)
 - Use the Right arrow button to import from Available Components to Mixture
 - Click OK in the Mixture editor
- Click OK in the Flow BC Editor



Flow Boundary Conditions - High x Fluidizing Gas

Create the boundary for fluidizing air entering at high indices in x-direction:

- Copy the first Flow BC
- Select the copy and click on Edit
- Location tab
 - Enter region values shown in table
 - Enter a Comment (optional)
- Flux Plane tab
 - Edit the Flux plane name to correspond with the boundary
- Click OK

X _{min}	X _{max}	Y _{min}	Y _{max}	Z _{min}	Z _{max}
0.0075]	[]	[[

The screenshot shows the Barracuda Virtual Reactor software interface. The 'Flow BC Manager' window is open, displaying a table of boundary conditions. The first entry is selected, and the 'Flow BC Editor' dialog is open. The 'Location' tab is active, showing the 'Set Cell Region (m)' dialog with the following values: X_{min} = 0.0075, X_{max} = max, Y_{min} = min, Y_{max} = max, Z_{min} = min, Z_{max} = min. The 'Flux Plane' tab is also visible, showing the name 'FLUXBC_high_x_fluidization'. The 'Comment' field contains 'high x fluidization'. Red arrows point to the 'Copy' button at the bottom and the 'OK' button in the dialog.

Flow Boundary Conditions – Center Jet

X _{min}	X _{max}	Y _{min}	Y _{max}	Z _{min}	Z _{max}
-0.0075	0.0075	[]	[]

Create the boundary for center jet:

- Copy the first Flow BC
- Select the copy and click on Edit
- Location tab
 - Enter region values shown in table
 - Enter a Comment (optional)
- Flux Plane tab
 - Edit the Flux plane name to correspond with the boundary
- Fluid tab
 - Set Velocity flow to 10 m/s
- Click OK

The screenshot displays the Barracuda Virtual Reactor interface. At the top, the 'Flow BC Manager' window shows a table of boundary conditions:

ID	Dir	x1	x2	y1	y2	z1	z2	Area	Flow rate	Temperature	Pressure	Particles	Flux plane name	Comment
000	z	min	-0.0075	min	max	min	min	1	0.25	300	100000	No exit	FLUXBC_low_x_fluidization	low x fluidization
001	z	0.0075	max	min	max	min	min	1	0.25	300	100000	No exit	FLUXBC_high_x_fluidization	high x fluidization
002	z	min	-0.0075	min	max	min	min	1	10	300	100000	No exit	FLUXBC_center_jet	center jet inlet

Below the table, three 'Flow BC Editor' dialog boxes are shown, illustrating the configuration steps:

- Flow BC Editor (Location tab):** The 'Set Cell Region (m)' section is highlighted with a red box, showing X_{min} = -0.0075, X_{max} = 0.0075, Y_{min} = min, Y_{max} = max, Z_{min} = min, and Z_{max} = min. The 'Direction' section has 'z-direction' selected. The 'Comment' field contains 'center jet inlet'.
- Flow BC Editor (Flux Plane tab):** The 'Name' field is highlighted with a red circle and contains 'FLUXBC_center_jet'.
- Flow BC Editor (Fluid tab):** The 'Fluid' tab is highlighted with a red box. Under 'Flow Conditions', 'Specify values' is selected, and 'Velocity flow' is set to 10 m/s. 'Pressure' is 100000 Pa and 'Temperature' is 300 K.

Time Controls

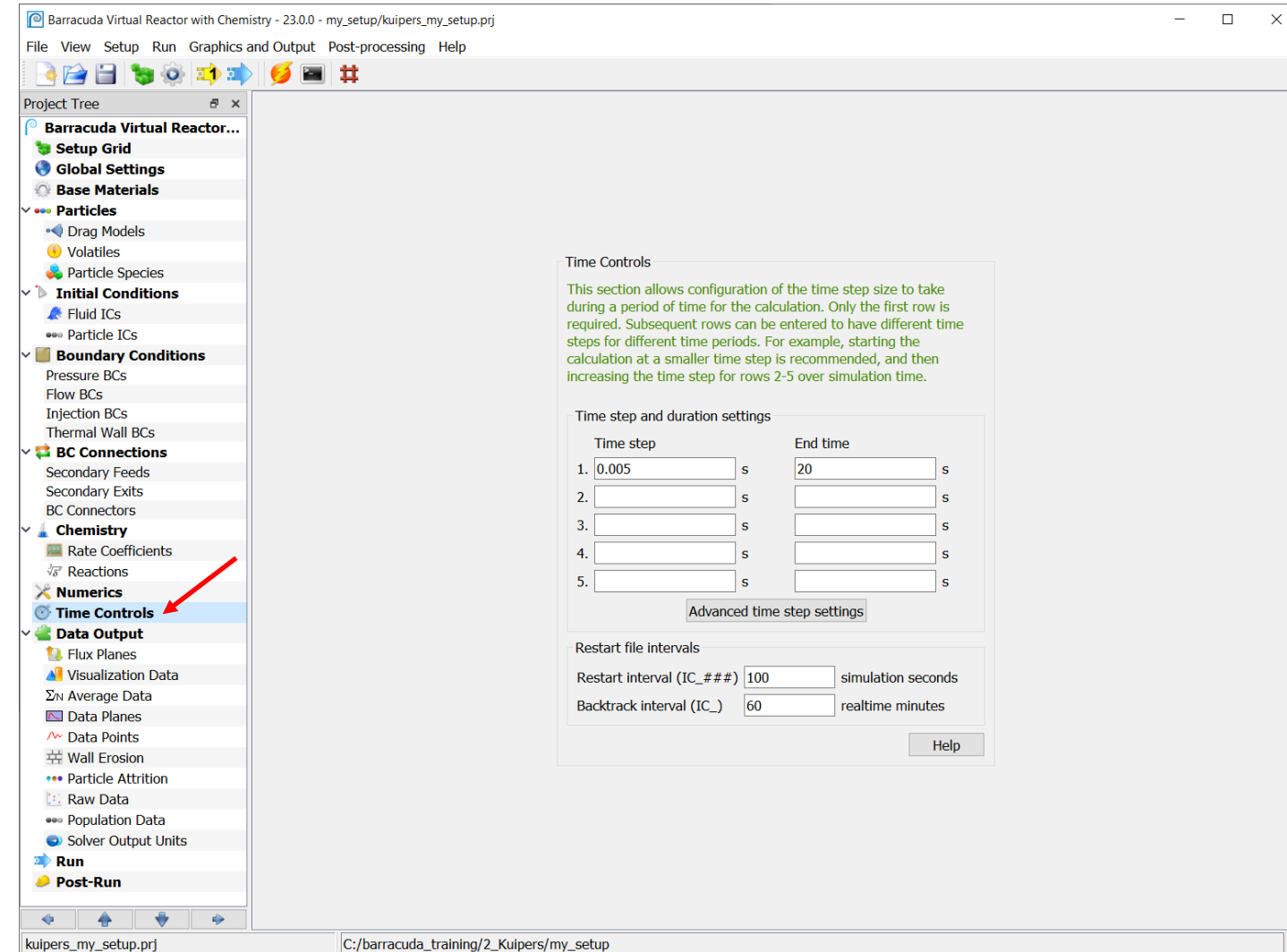
Click on Time Controls:

- Set the Time step to 0.005 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

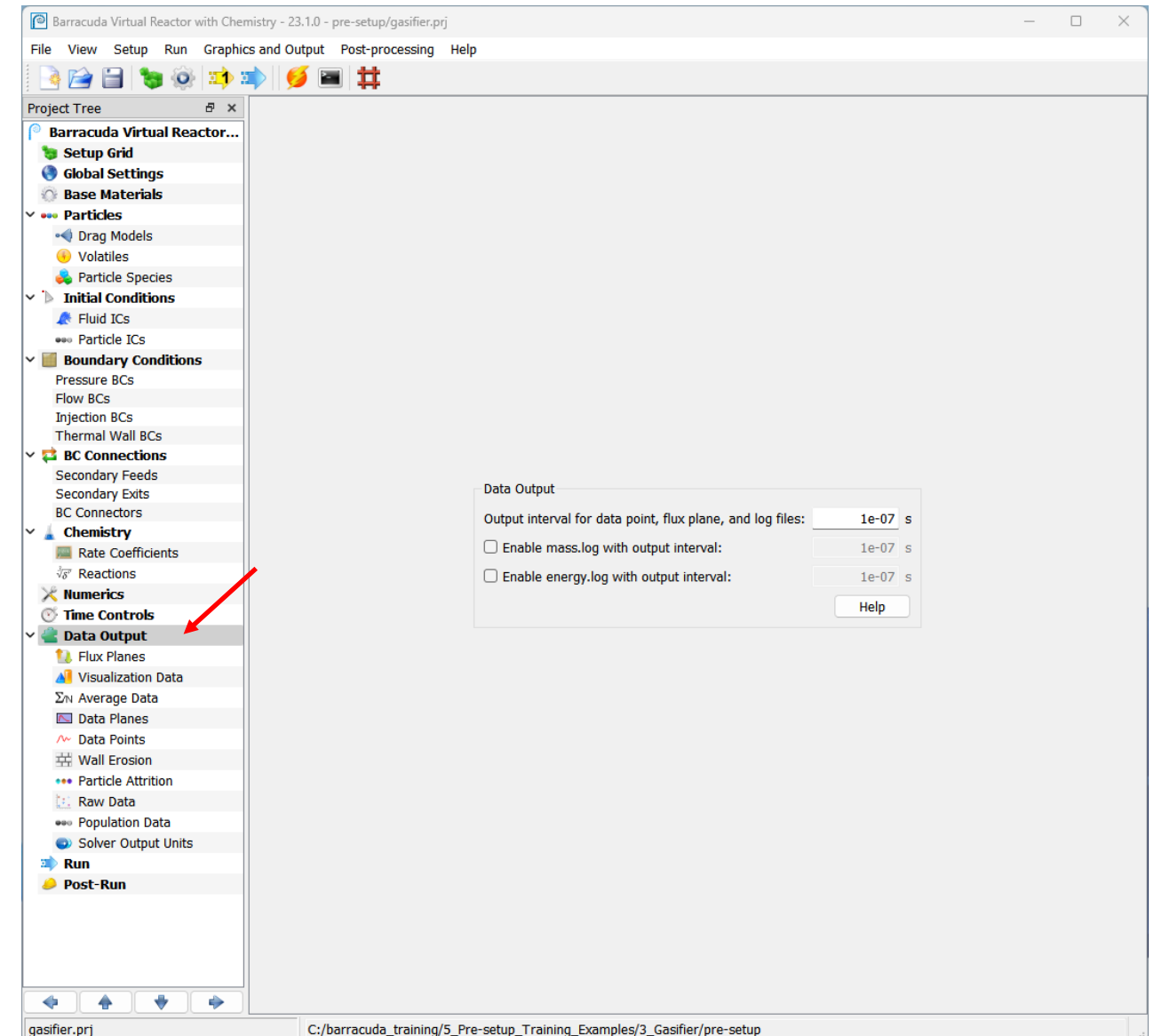


Data Output Options

Click on Data Output

For the Kuipers problem, the following types of data will be output:

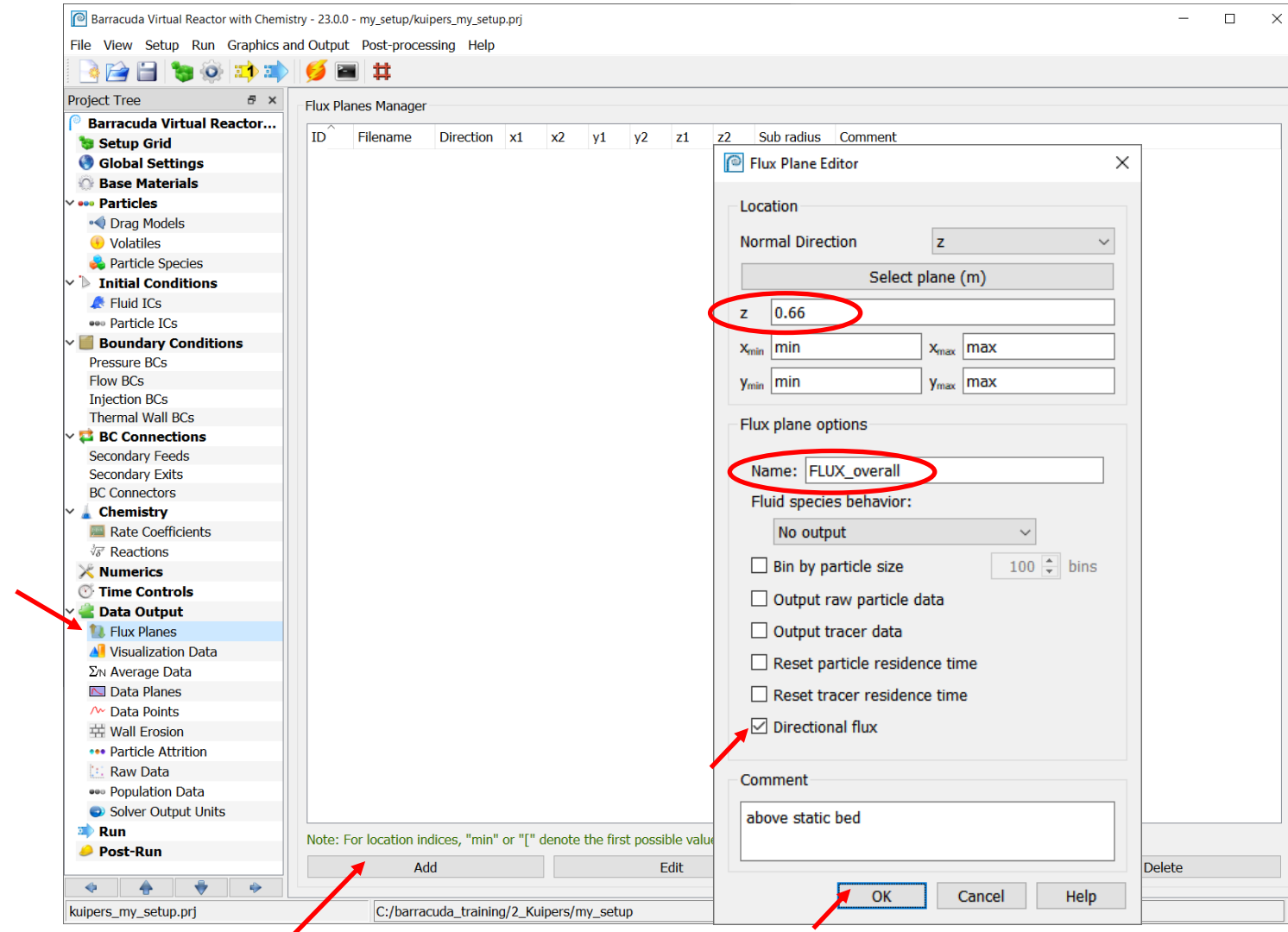
- Flux planes – Track the transport of fluid and solids through a defined plane in the model
- Visualization Data – Select variables for visualization of fluid and solid states in Tecplot
- Average Data – Select some Tecplot output data to be averaged as the simulation runs
- Data Points – High frequency tracking of data at a specified location in a model



Data Output: Flux Planes

Click on Flux Planes to create interior flux planes:

- Click Add
- Select z for the Normal Direction
- Enter the z location as 0.66 m
- Provide a descriptive Name for the flux plane
- Select Directional flux
- Enter a Comment (optional)
- Click OK

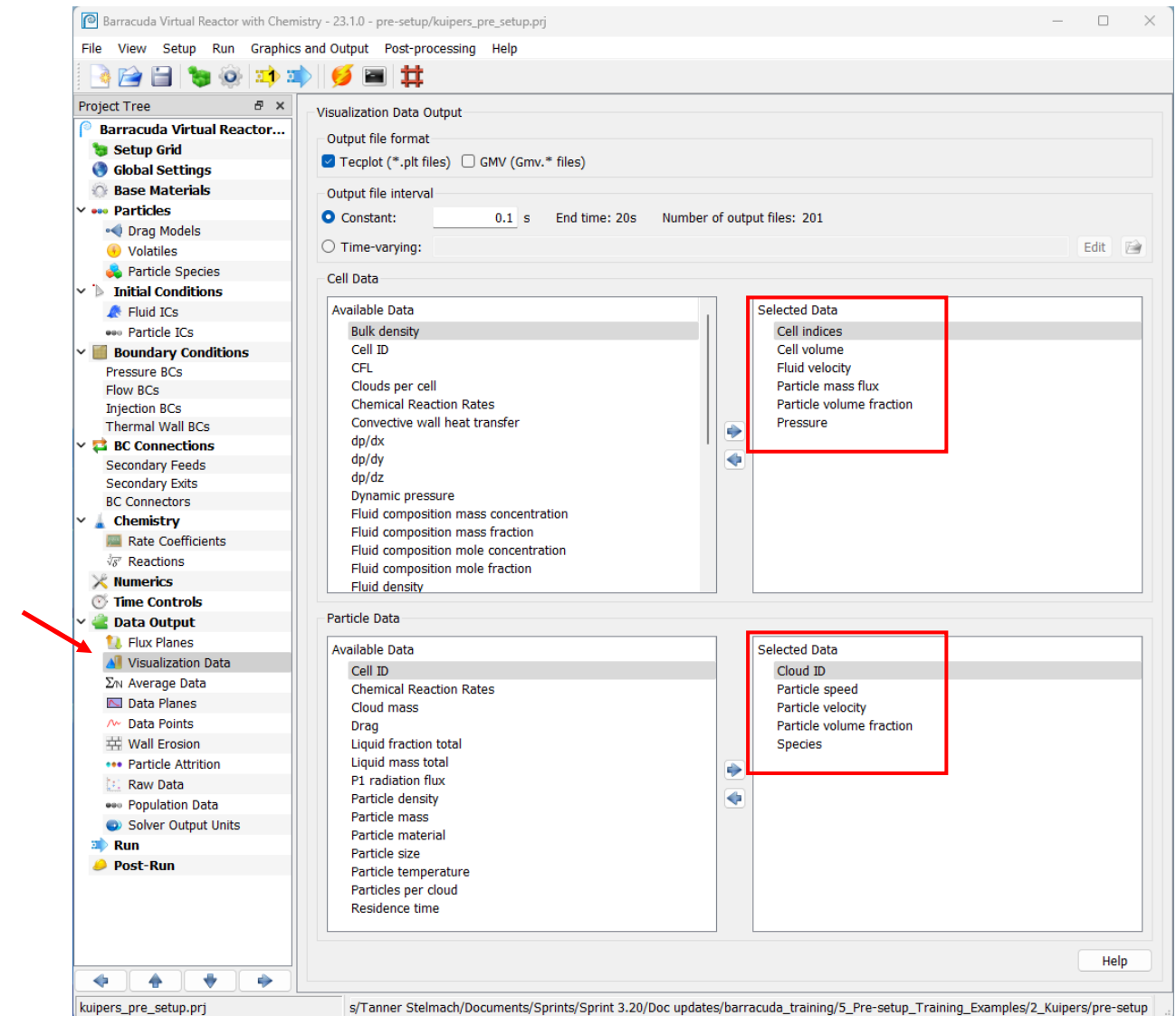


Data Output: Visualization Data

Click on Visualization Data. The information selected here will be written to your Tecplot output files

- Cell Data is mapped to the grid
 - Cell indices
 - Cell volume
 - Fluid velocity
 - Particle mass flux
 - Particle volume fraction
 - Pressure
- Particle Data is mapped to particle locations
 - Cloud ID
 - Particle speed
 - Particle velocity
 - Particle volume fraction
 - Species

Make sure all the options highlighted here are in the Selected Data columns of your project



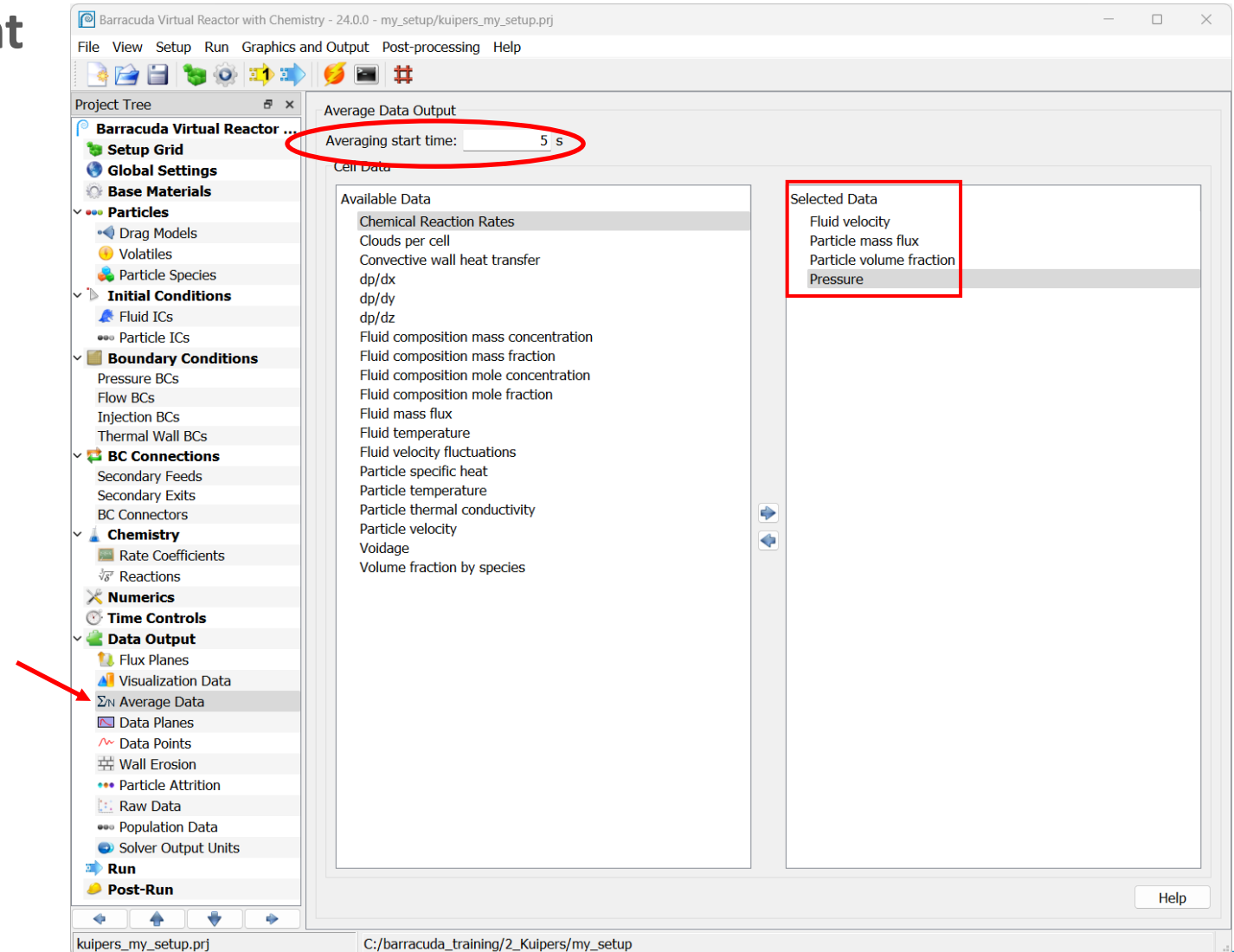
Data Output: Average Data

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

Click on Average Data

- Set Averaging start time to 5 s
- Select the following options for time-averaging:
 - Fluid velocity
 - Particle mass flux
 - Particle Volume Fraction
 - Pressure



Data Output: Data Points

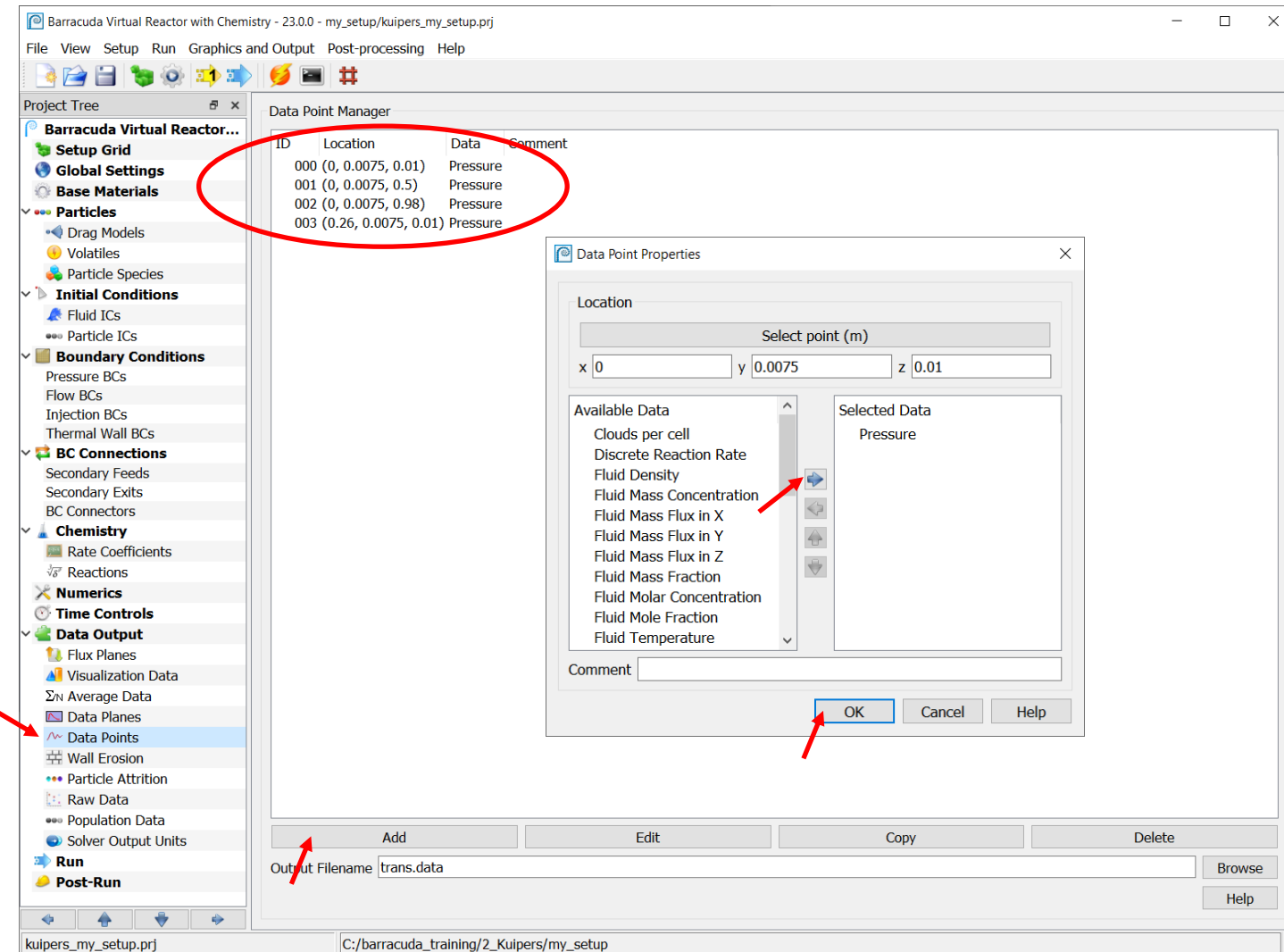
Barracuda can output high-frequency data at point locations in the computational domain

Data will be written to the file: `trans . data00`

To create the four data points used in post-processing:

- Click on Data Points
- Click on Add
- Enter the coordinates shown in the Location column for Point 1 in table below
- Import Pressure from Available Data to Selected Data
- Click OK
- Repeat for additional three data points using the corresponding location for each point

Point #	x	y	z
1	0	0.0075	0.01
2	0	0.0075	0.5
3	0	0.0075	0.98
4	0.26	0.0075	0.01

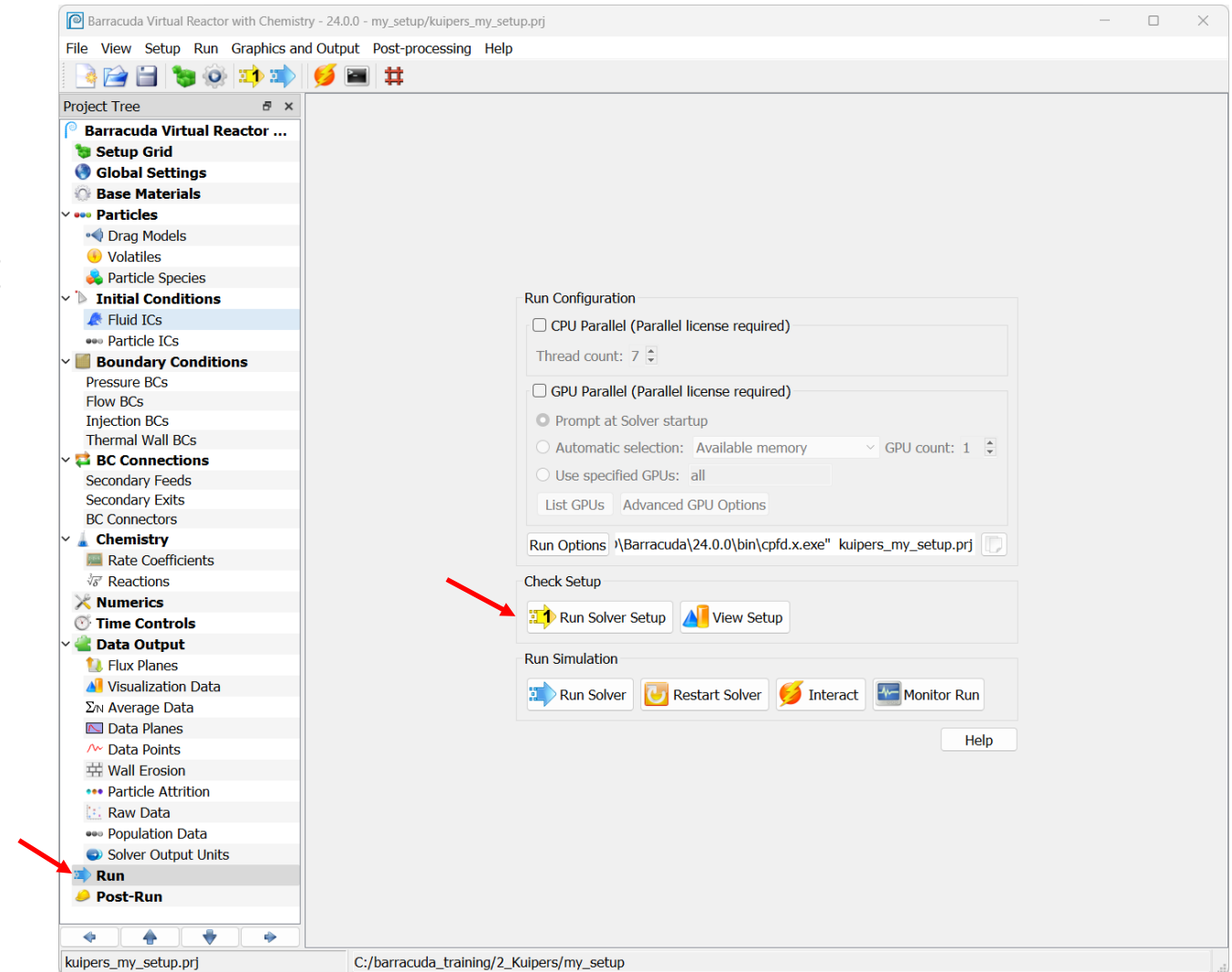


Run Solver Setup

Click on Run

Click on Run Solver Setup

- This automatically saves the project file
- This will run the simulation for one time step and write a single Tecplot file
- All boundary and initial conditions are stored in the Tecplot file
- This first Tecplot file is needed to check the problem setup



Run Solver Setup

Solver information will be output to the run window

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. Once this happens, then you can close the run window.

```

Barracuda Virtual Reactor - 22.1.0 - my_setup/kuipers_my_setup.prj
Barracuda release 22.1.0
Solver version 22.1.0.x088
Build date 2022-10-20 01:02:47 UTC
Restart IC version 2210

Particle randomization ... 100%

Particle randomization ... 100%

Particle initialization adjustment ... 100%

Attempting to checkout required licenses: barracuda-15-setup (1)
Connecting to license server "myRLMserver" at 27015@arcee
Server contains the following product licenses: arena-7, arena-7-setup, arena-openmp, tecplot360-arena, barracuda-15, barracuda-15-setup, barracuda-15-chem, barracuda-15-setup-chem, barracuda-gpu, tecplot360-bvr
Checking out barracuda-15-setup (1)... license checked out from arcee
License(s) checked out from specified server: myRLMserver (27015@arcee)

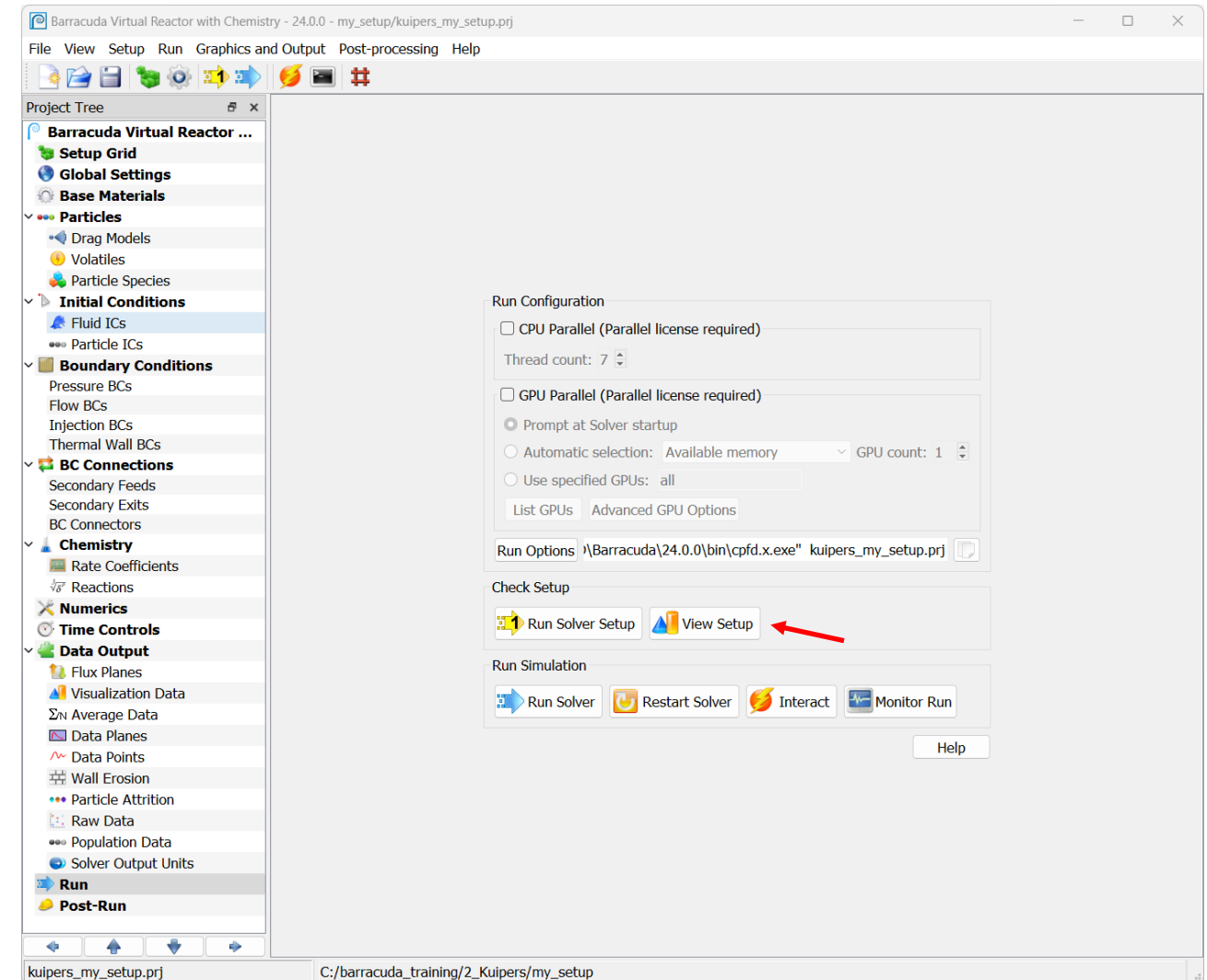
# Reprise Project tag: path:C:\barracuda_training\2_Kuipers\my_setup/kuipers_my_setup.prj
-----
      t      dt  Vol  Vol  u    u    v    v    w    w    p    p    CFL  Low Med  Hi  R
      s      s  itr  err  itr  err  itr  err  itr  err  itr  err
-----
0.00000e+00 5.000e-03 000 0.00e+00 000 0.00e+00 000 0.00e+00 000 0.00e+00 0 0.00e+00 0.00 344 0 0 0
Writing bvr.setup.plt
Writing bvr.grid.plt
Writing bvr.cells.00000.plt
Writing bvr.particles.00000.plt
# Decrease dt from CFL. Old = 5.000e-03 New = 2.541e-03 (16 1 1)
5.00000e-03 2.541e-03 010 9.61e-08 001 0.00e+00 000 0.00e+00 002 3.55e-10 300 4.47e-07 2.95 332 0 0 0
Thu Nov 17 13:23:07 2022
C:\barracuda_training\2_Kuipers\my_setup>
    
```

Checking your Setup

Before letting your calculation run, check the following:

- Are your boundary conditions in the right place?
- Are your particles defined correctly and located where you want them?
- Are your data points and flux plane located where you want them?

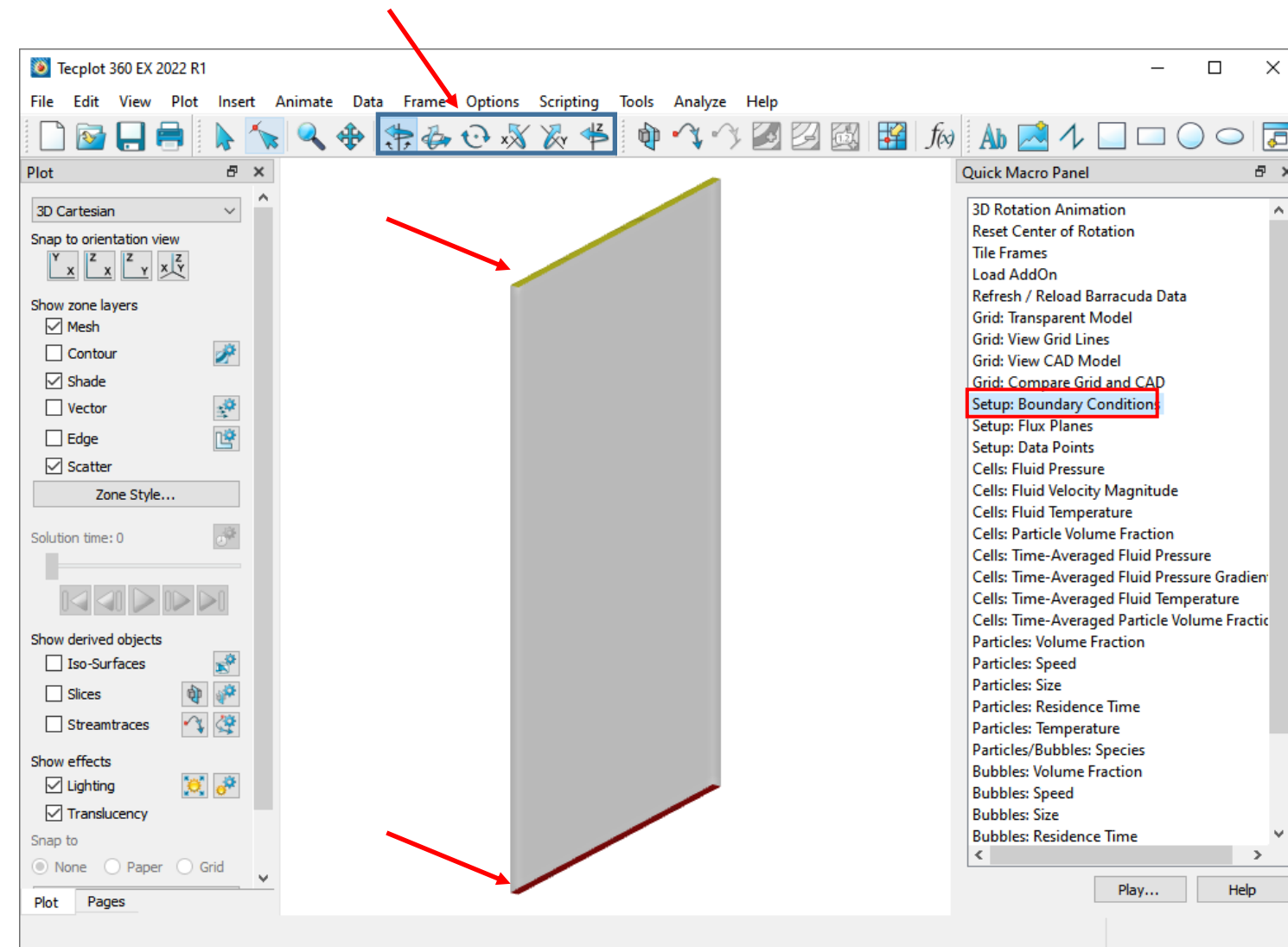
To check, click on **View Setup** which brings up Setup: Boundary Conditions view in Tecplot for Barracuda



Checking your Setup – Boundary Conditions

Verify that the boundary conditions are in the right place.

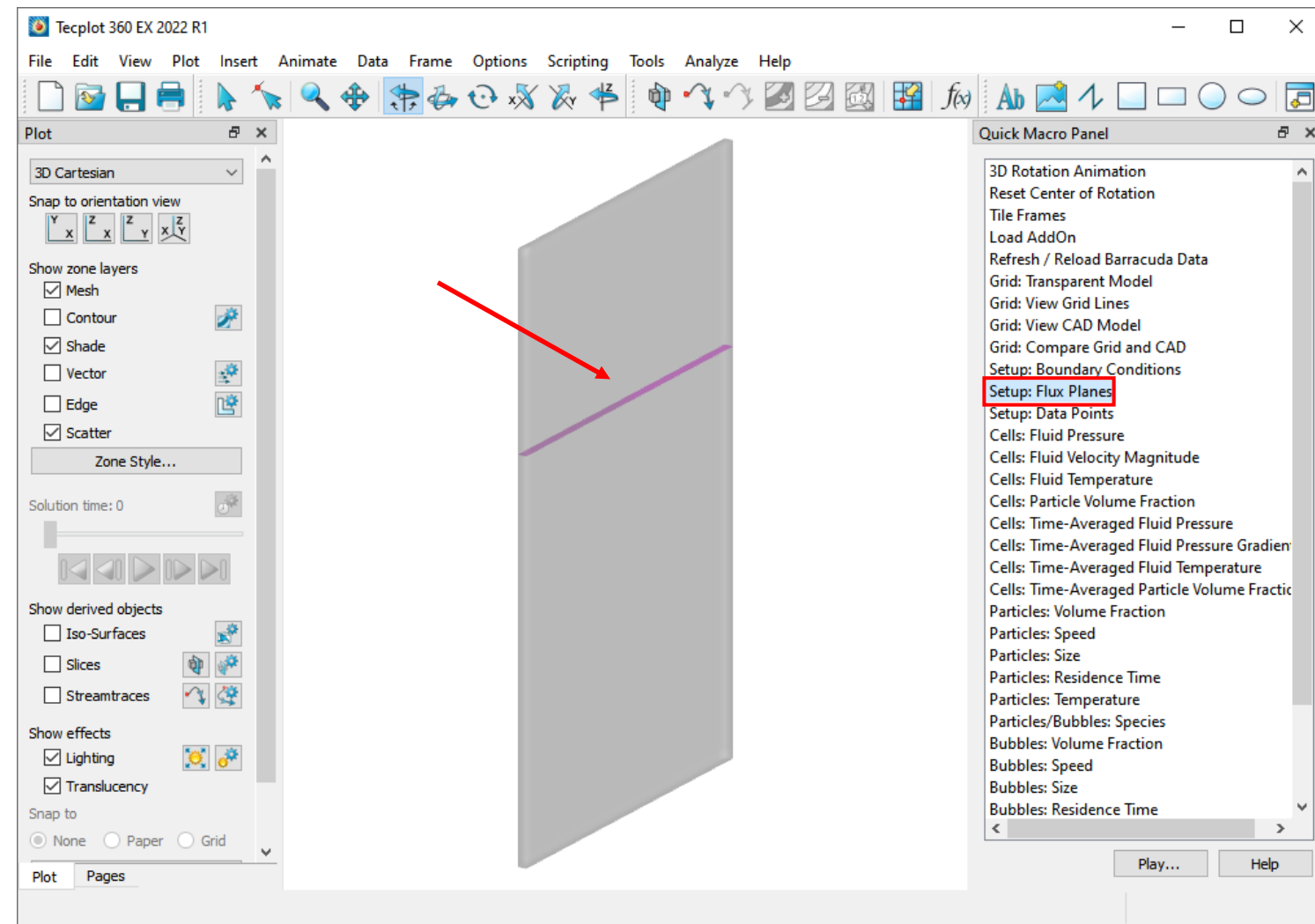
To change the view, use the rotation tools in the toolbar



Checking your Setup – Flux Plane Location

Double-click on Setup: Flux Planes in the Quick Macro Panel.

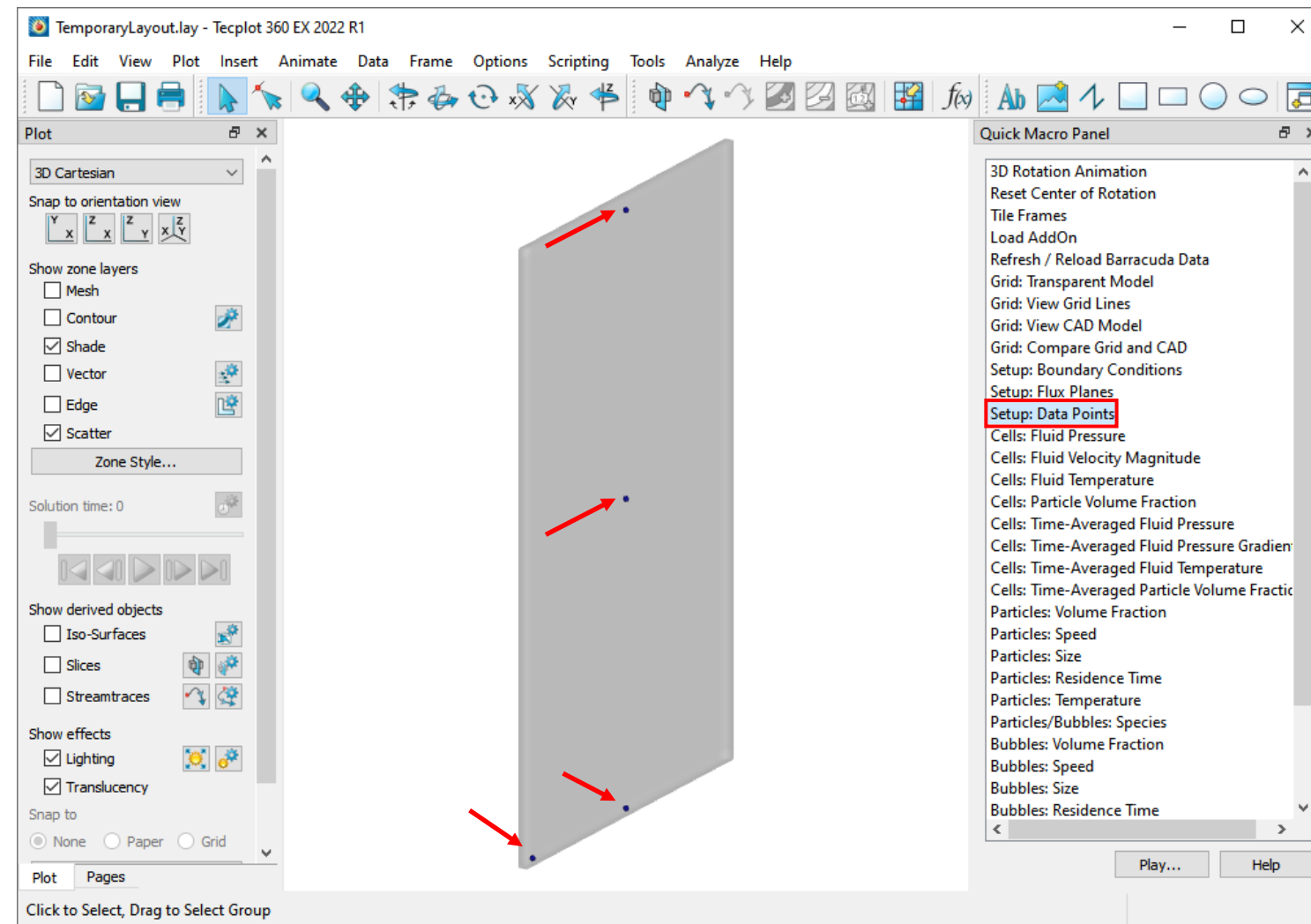
Verify that the flux plane is in the right place.



Checking your Setup – Data Points Location

Double-click on Setup: Data Points in the Quick Macro Panel.

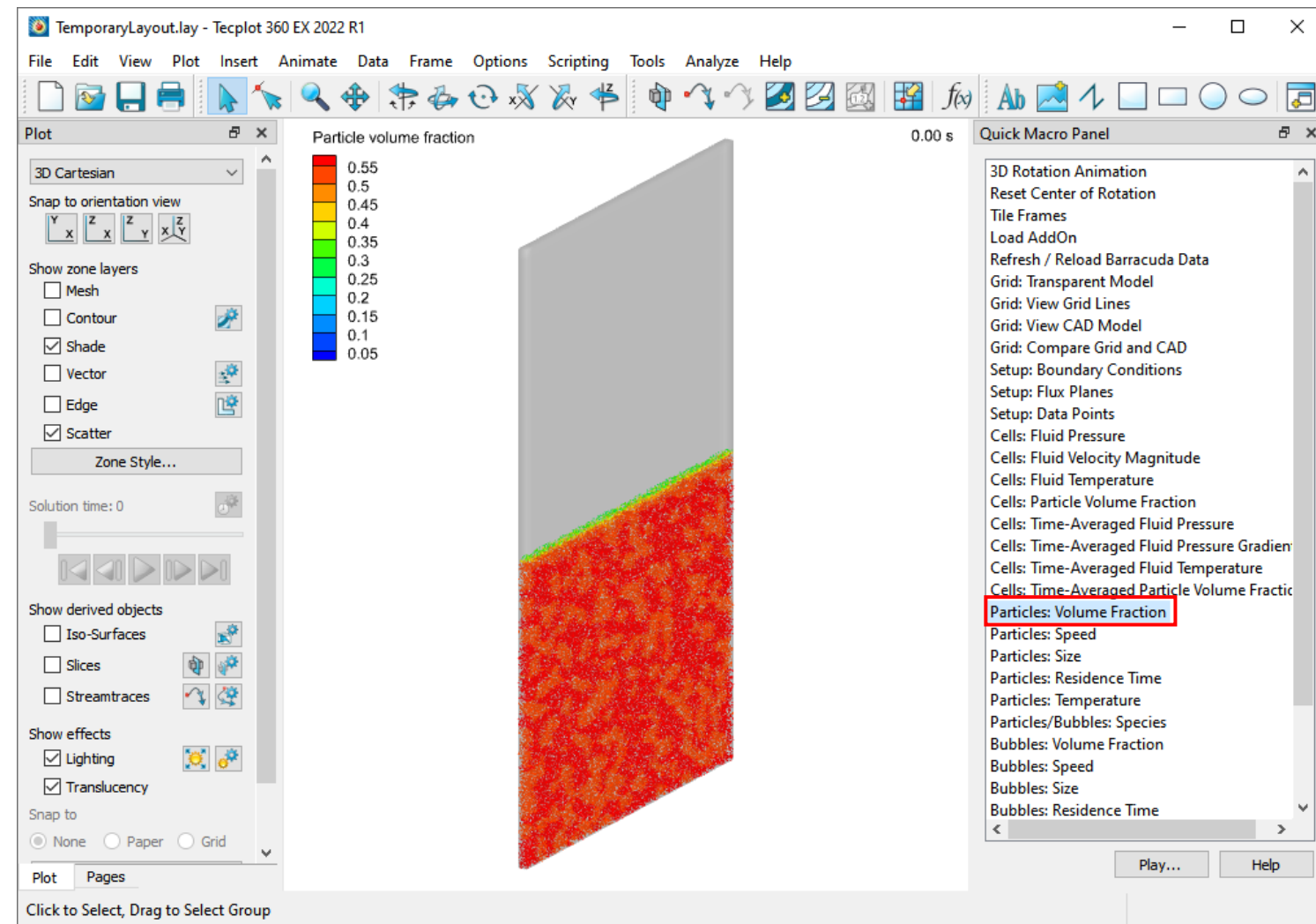
Verify that the data points are in the right place.



Checking your Setup - Particles

Double-click on Particles: Volume Fraction.

Verify the initial location of the particles in the bed.

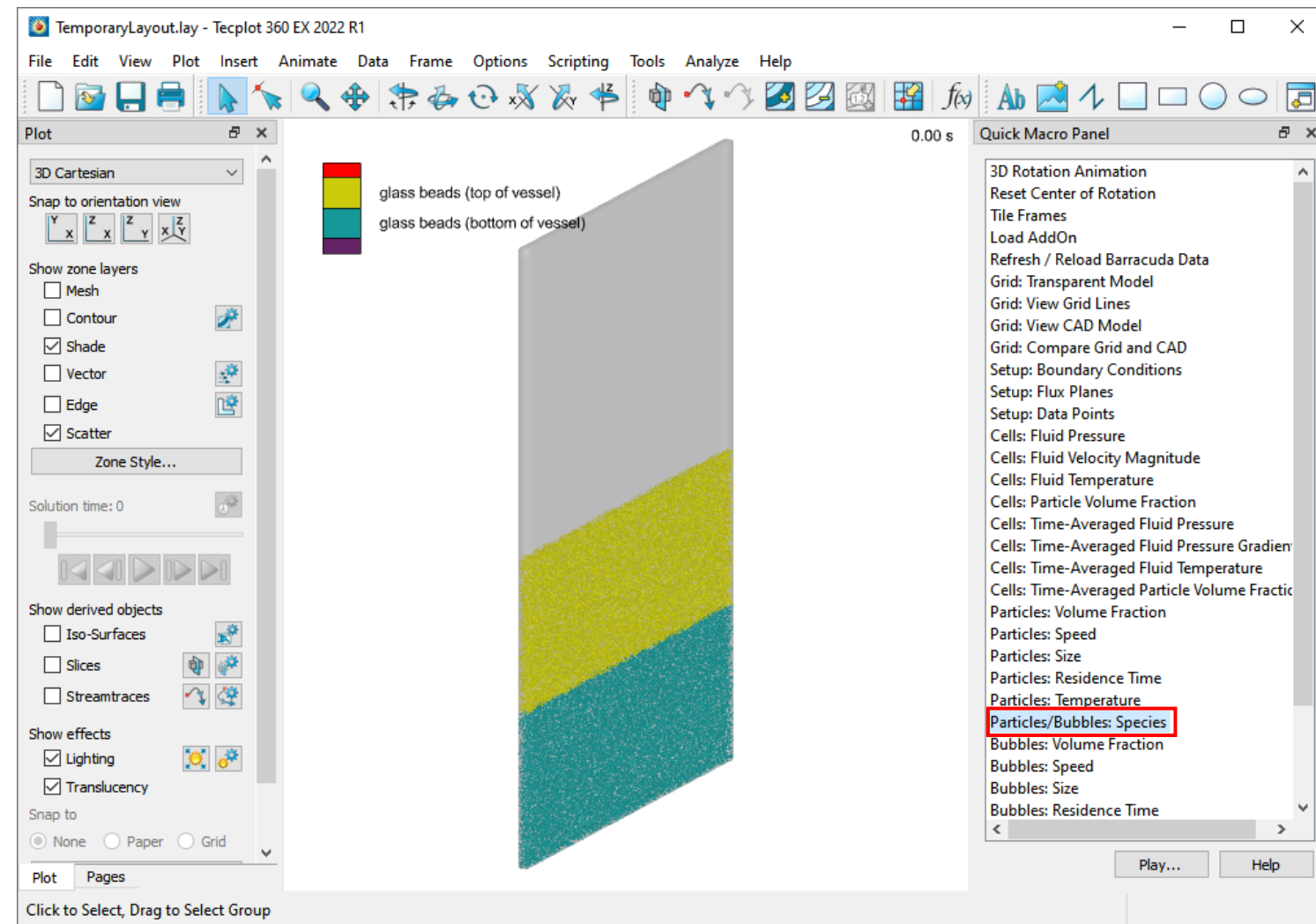


Checking your Setup – Particle Species

Double-click on Particles/Bubbles:
Species in the Quick Macro Panel.

Verify the initial location of the two
particle species in the bed.

Close the Tecplot window and select
Discard when prompted.



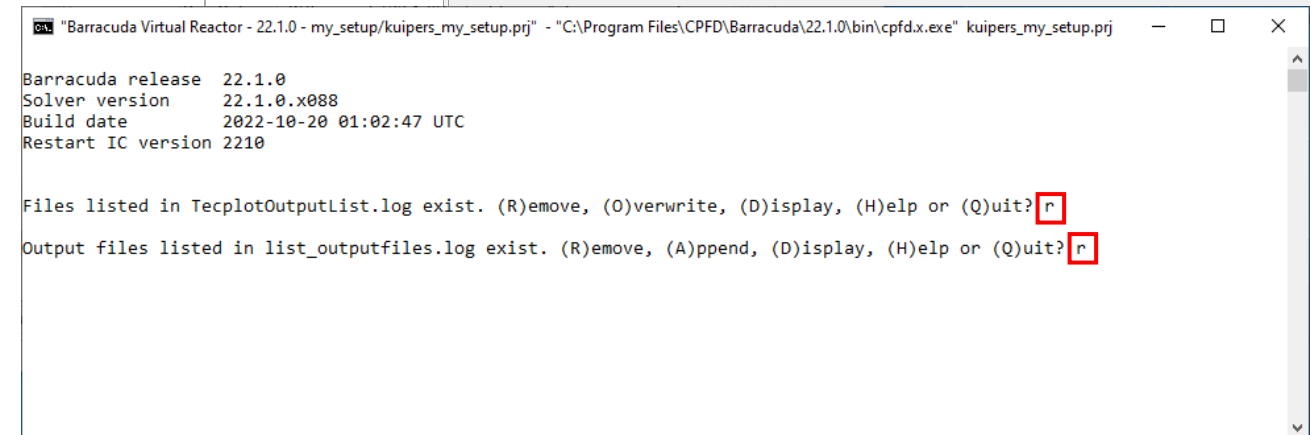
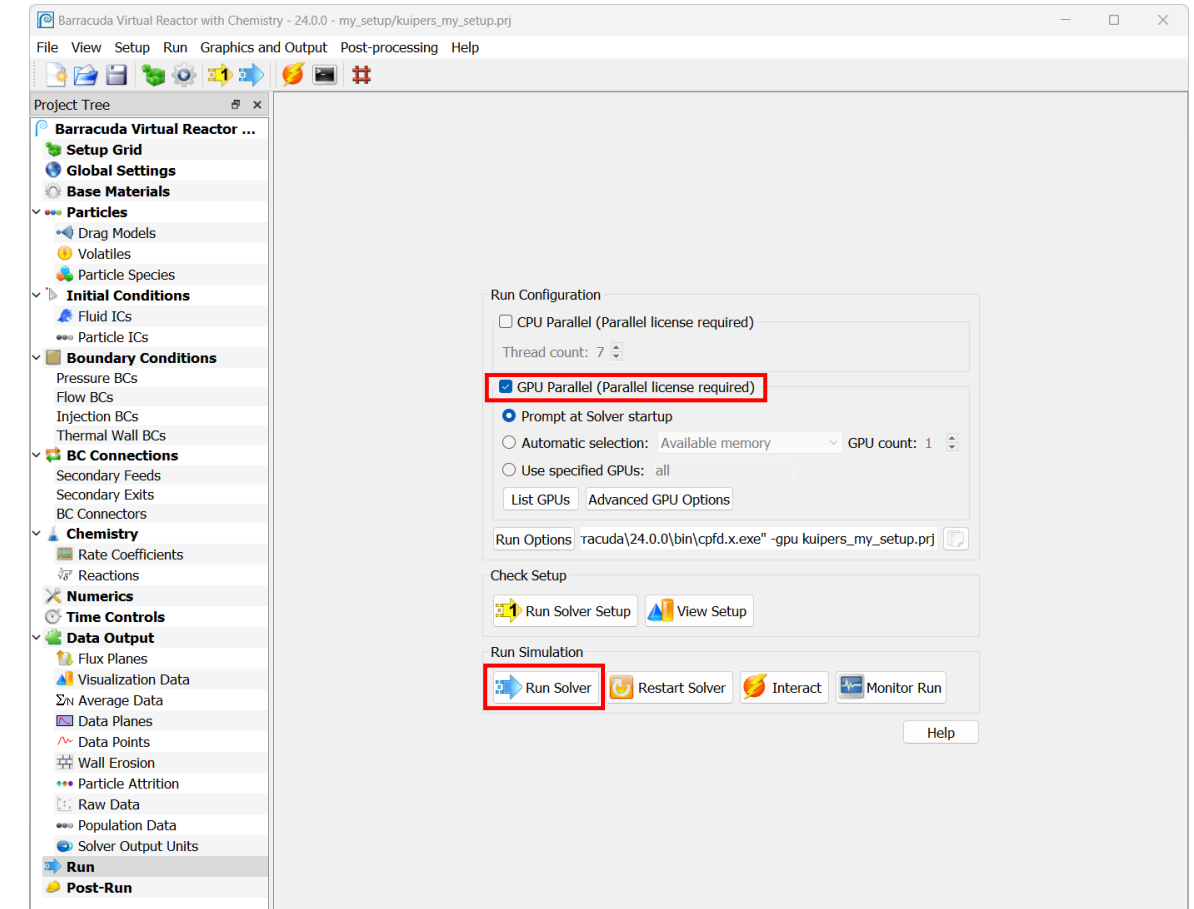
Executing the Simulation

After checking the setup, return to the Run window

- If your computer has an NVIDIA GPU card, select the “GPU Parallel” check box. The simulation will run much faster in GPU Parallel mode!
- To start the simulation click Run Solver

The run window will prompt to Remove, Overwrite, Display, Help or Quit. The files can be removed since they were all created during the Run Solver Setup.

- Type r when prompted



Solver Output Window

While running, the Solver Output Window will continuously scroll as the simulation proceeds.

Once the Solver has reached a simulation time of 20 seconds, the output will stop.

Run times can be lengthy and will vary based on computer hardware, so please move on to Part 4 while the simulation runs.

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

```

Select "Barracuda Virtual Reactor - 22.1.0 - my_setup/kuipers_my_setup.prj" - "C:\Program Files\CPFD\Barracuda\22.1.0\bin\cpfd.exe" kuipers_my_setup.prj
Barracuda release 22.1.0
Solver version 22.1.0.x888
Build date 2022-10-10 01:02:47 UTC
Restart ID version 2210

Files listed in TecplotOutputList.log exist. (R)emove, (O)verwrite, (D)isplay, (H)elp or (Q)uit? r
Output files listed in list_outputfiles.log exist. (R)emove, (A)ppend, (D)isplay, (H)elp or (Q)uit? r
Particle randomization ... 100%
Particle randomization ... 100%
Particle initialization adjustment ... 100%

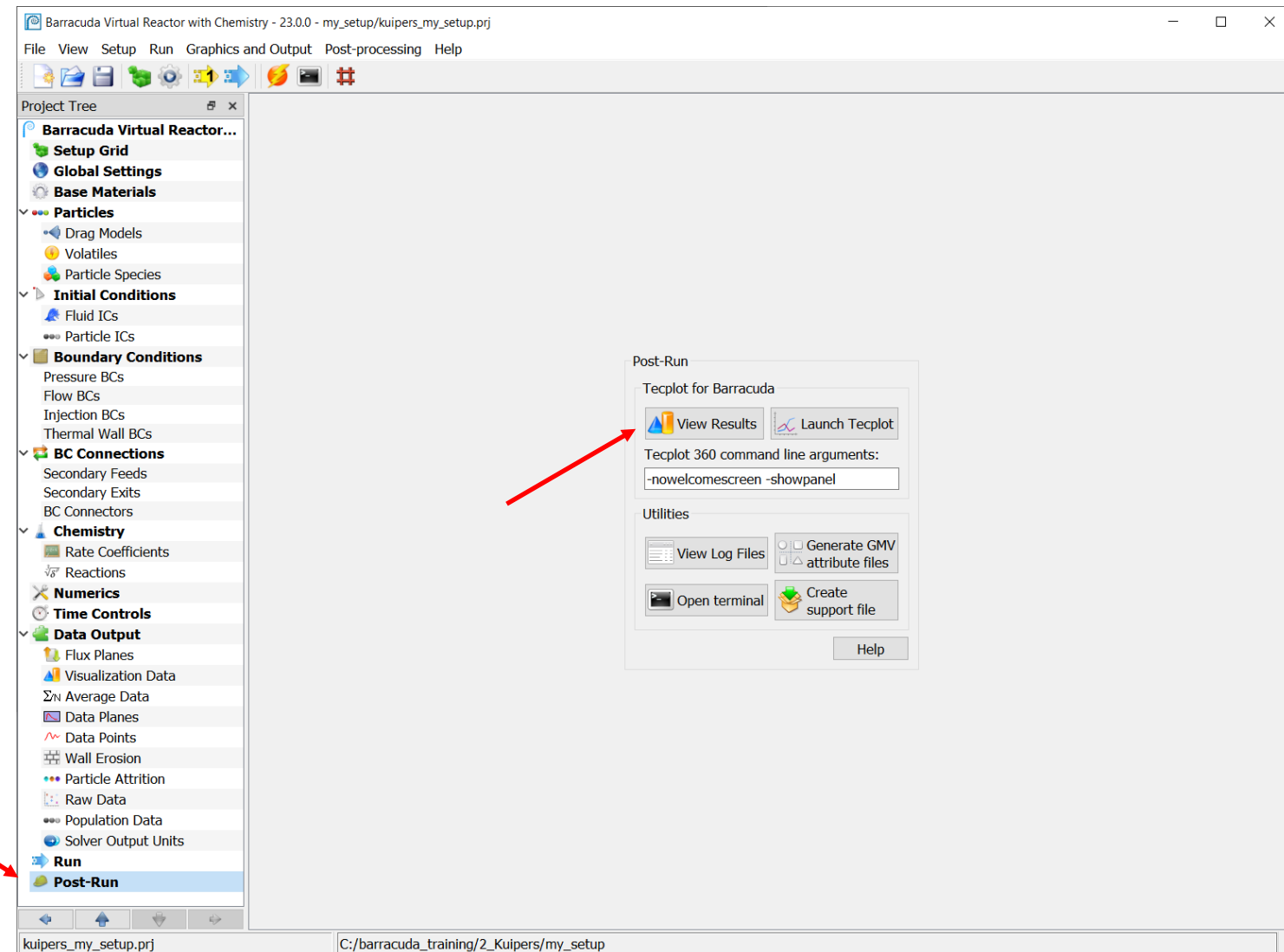
Attempting to checkout required licenses: barracuda-15 (1)
Connecting to license server "myRLMserver" at 27015@arcee
Server contains the following product licenses: arena-7, arena-7-setup, arena-openmp, tecplot360-arena, barracuda-15, barracuda-15-setup, barracuda-15-chem, barracuda-15-setup-chem, barracuda-gpu, tecplot360-bvr
Checking out barracuda-15 (1)... license checked out from arcee
License(s) checked out from specified server: myRLMserver (27015@arcee)

# Reprise Project tag: path:C:\barracuda_training\2_Kuipers\my_setup\kuipers_my_setup.prj
-----
t      dt  Vol  Vol  u    u    v    v    w    w    p    p    CFL  Low  Med  Hi  R
s      s  itr  err  itr  err  itr  err  itr  err  itr  err
-----
0.00000e+00 5.000e-03 000 0.00e+00 000 0.00e+00 000 0.00e+00 000 0.00e+00 0 0.00e+00 0.00 344 0 0 0
Writing bvr.setup.plt
Writing bvr.grid.plt
Writing bvr.cells.00000.plt
Writing bvr.particles.00000.plt
# Decrease dt from CFL. Old = 5.000e-03 New = 2.541e-03 (16 1 1)
5.00000e-03 2.541e-03 010 9.61e-08 001 0.00e+00 000 0.00e+00 002 3.55e-10 300 4.47e-07 2.95 332 0 0 0
7.54096e-03 2.541e-03 011 1.68e-08 003 6.11e-08 000 0.00e+00 004 1.68e-09 240 8.37e-08 0.94 319 0 0 0
1.00819e-02 2.541e-03 002 1.64e-08 003 1.77e-08 000 0.00e+00 003 2.46e-08 242 8.56e-08 0.94 285 0 0 0
1.26229e-02 2.541e-03 002 1.80e-08 003 8.93e-09 000 0.00e+00 003 6.35e-09 243 9.60e-08 0.94 266 0 0 0
1.51639e-02 2.541e-03 002 1.39e-08 003 3.89e-09 000 0.00e+00 003 2.17e-09 241 8.75e-08 0.93 239 0 0 0
    
```

Post-Run

During and after a Barracuda simulation, examine your results by clicking on the Post Run tab. You can view Tecplot files while the solver is operating.

Click on View Results in the Post-Run window to open the Particles: Volume Fraction view.

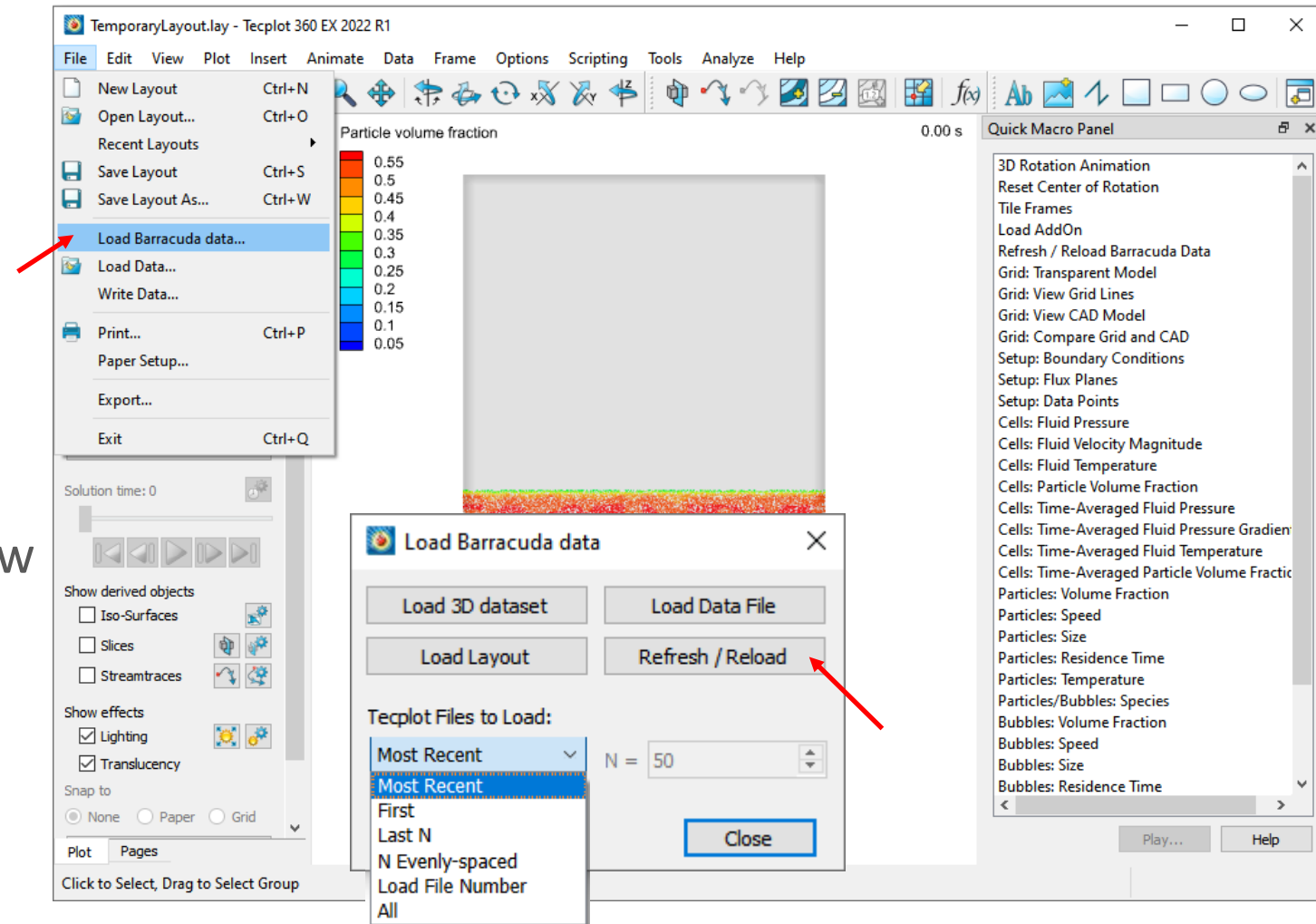


Using the Load Barracuda Data Dialog

When launched from the Barracuda GUI, Tecplot will load only the most recent solution time in order open the view as quickly as possible.

To load more solution times:

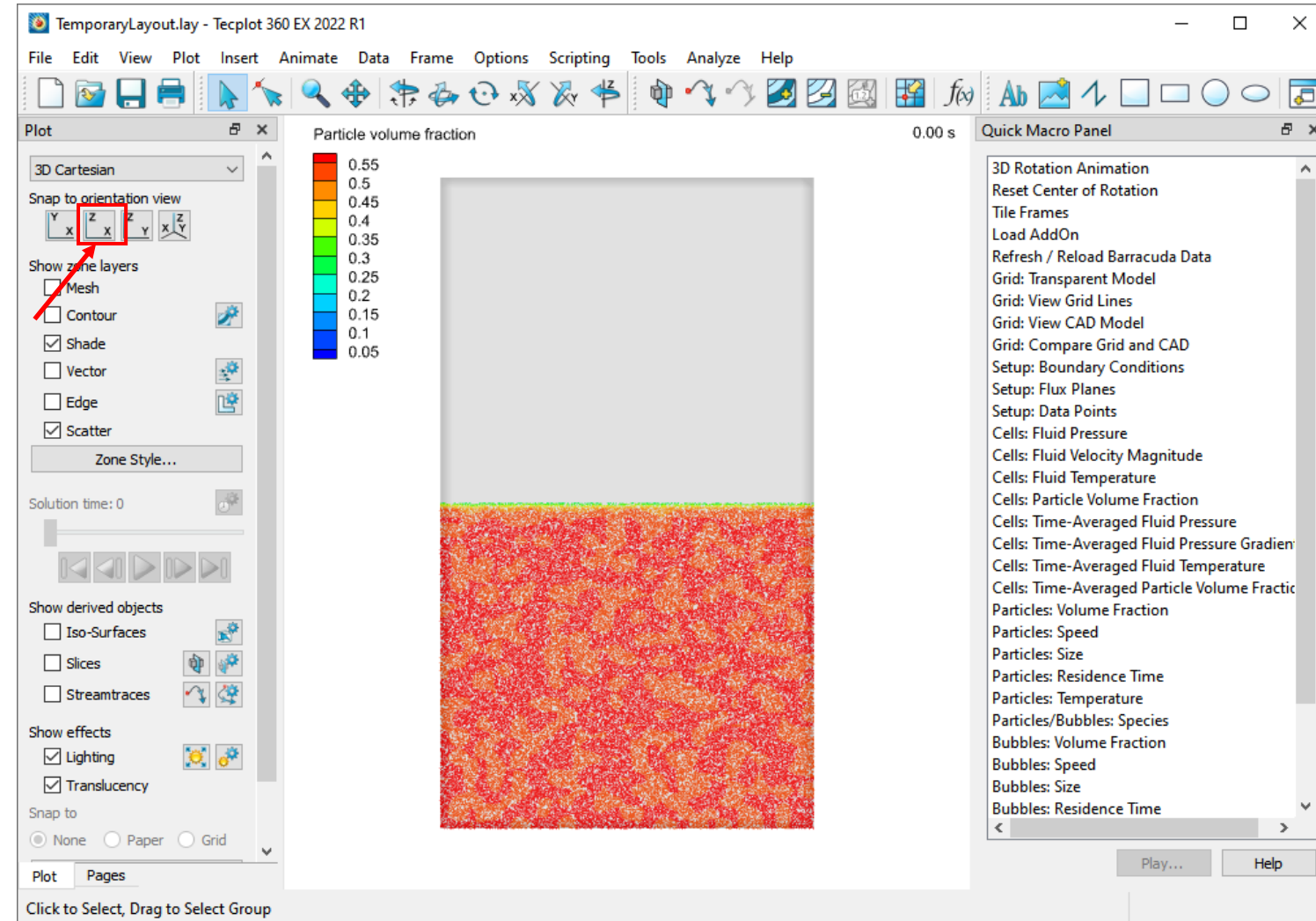
- Click on File → Load Barracuda Data
- Under Tecplot Files to Load there are a few options
 - All is most commonly used for animations
- Click on Refresh / Reload in order to load the .plt files



Particle Volume Fraction View

Rotate the image into view

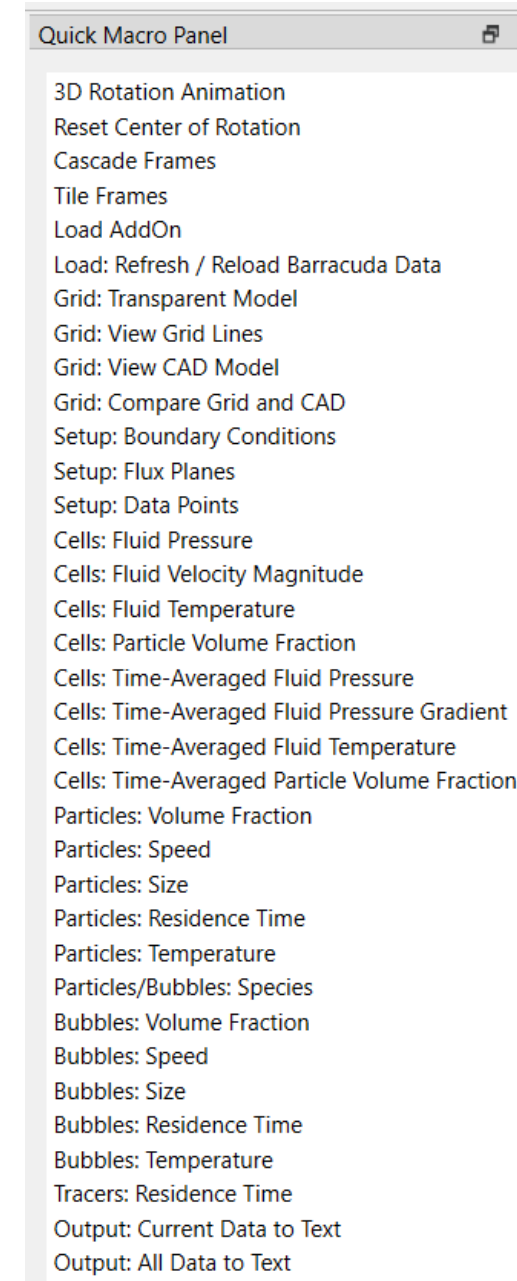
- This can be accomplished quickly by selecting the “ZX plane” view



Tecplot Quick Macro Panel

Once in Tecplot, use the Quick Macro Panel to easily view commonly used results.

- Not all options are available for all simulations. If the data is not available, Tecplot will warn you (e.g. clicking on average data buttons, when averaging has not been set)
- Do the results reflect the behavior you expected?
- How does the average volume fraction compare to the instantaneous volume fraction?
- How does the cell volume fraction compare to the particle volume fraction?



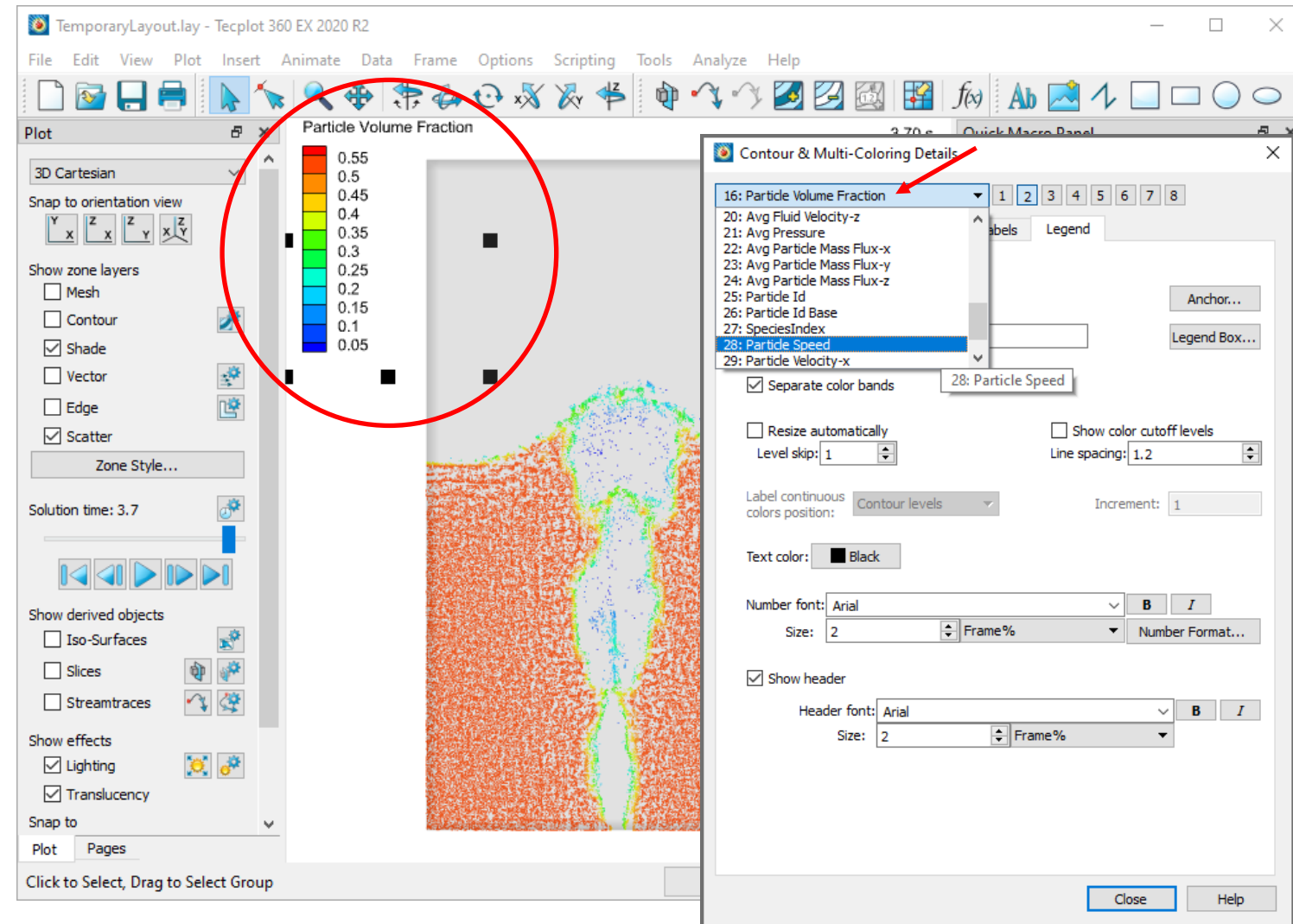
Coloring by a Different Variable

To change which data is being presented, double-click on the legend

In the drop down menu at the top left, select the data you would like to see displayed (for the next few slides, we will be using Particle Volume Fraction)

For a scatter zone, you should select particle-dependent data. Likewise, for a Contour or Vector zone, you should select cell-dependent data.

Note: Only data selected for visualization data output during the setup will be available



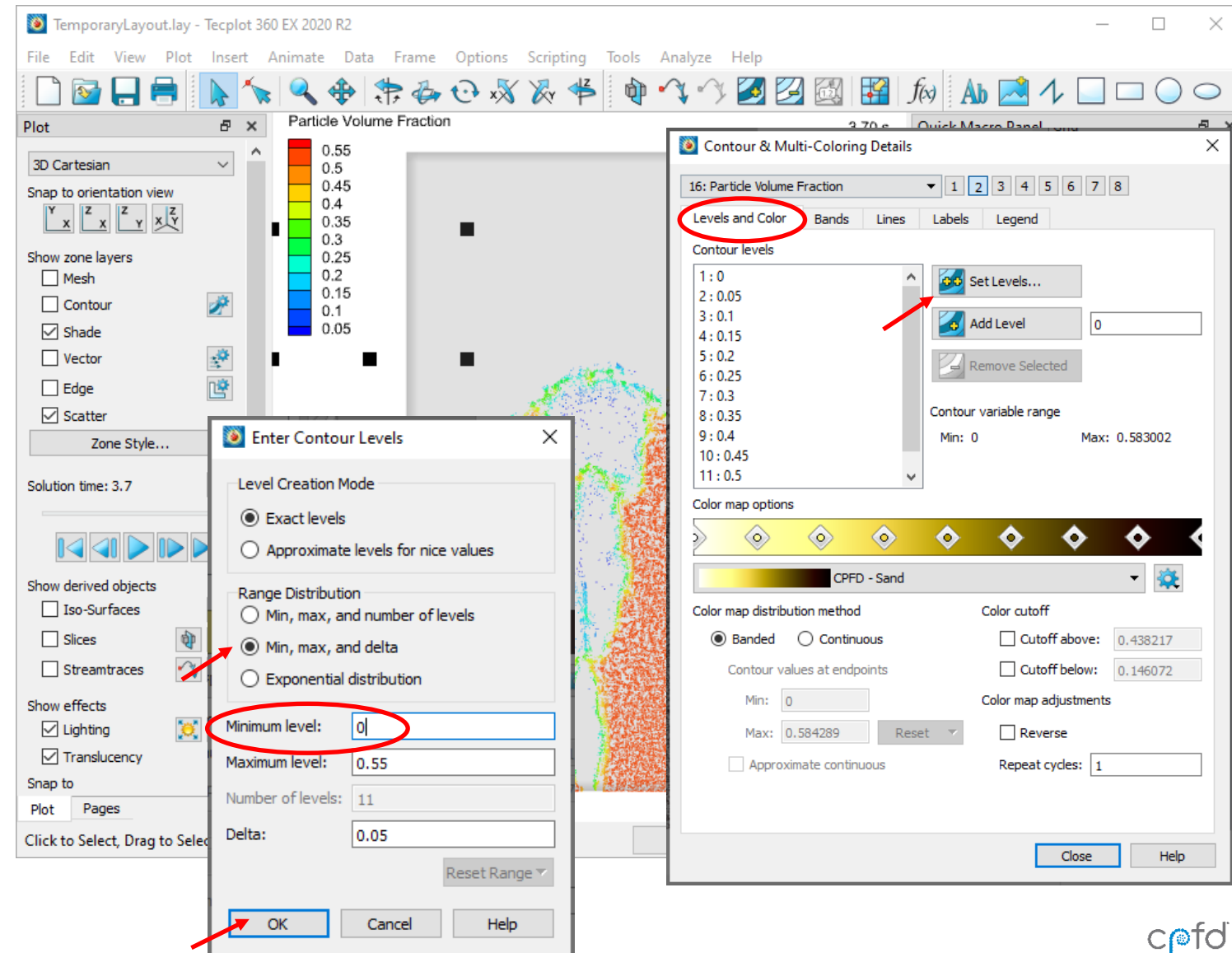
Setting Data Limits

We can control the minimum and maximum values to display

- Note: Any values above or below these respectively will be colored as if they are at this value

To change the data limits:

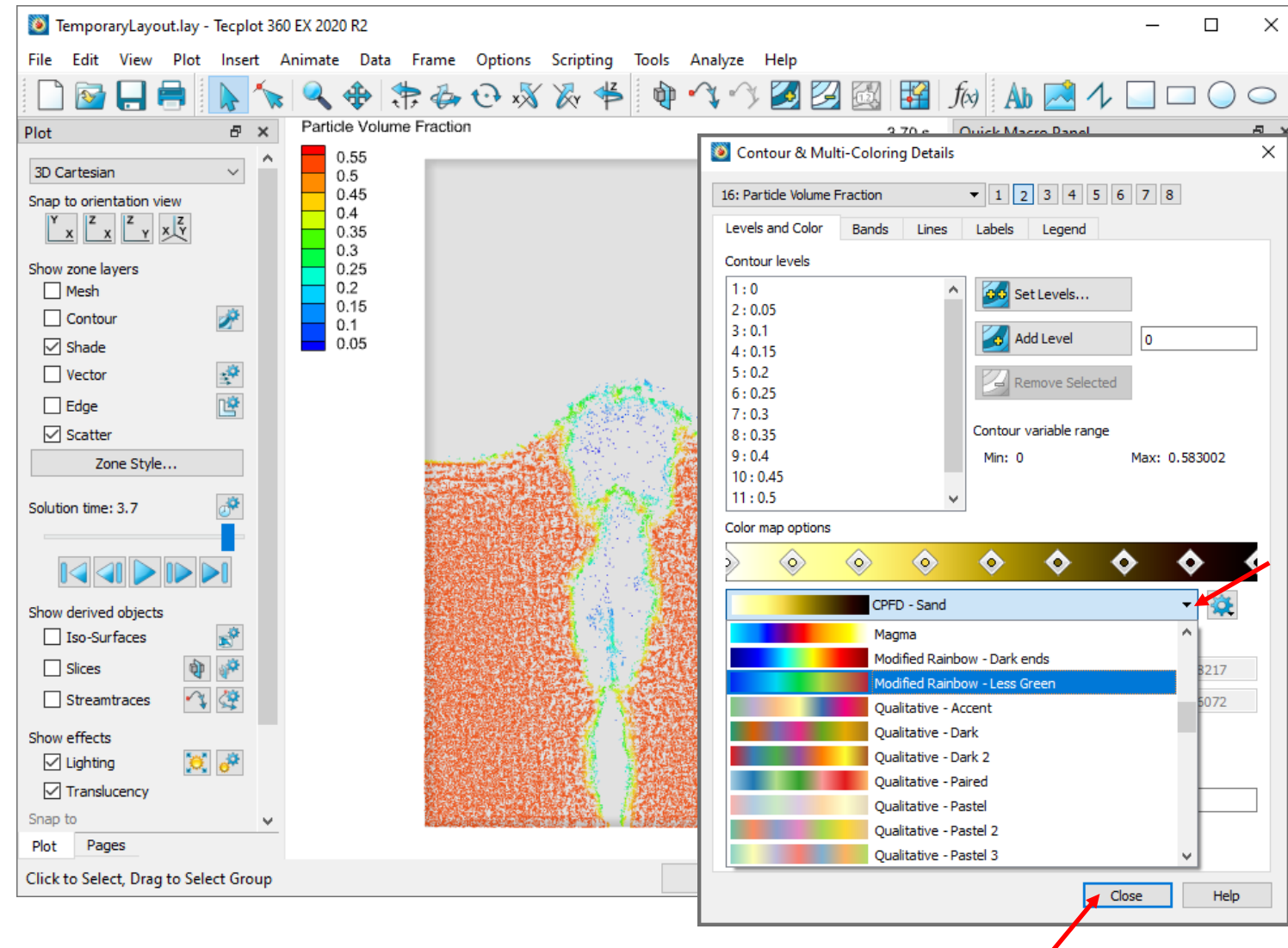
- Navigate to the Levels and Color tab
- Click on the Set Levels... button, which will bring up the Enter Contour Levels dialog
- Select Min, max, and delta for Range Distribution
- Change the Minimum level to 0
- Click OK
- Observe the minimum in the legend has changed to 0



Changing the Color Bar

To change how the view is colored:

- Click on the drop-down menu in the Color map options section to view the many options to choose from
- For this example we will be using Modified Rainbow – Less Green
- Click on Close

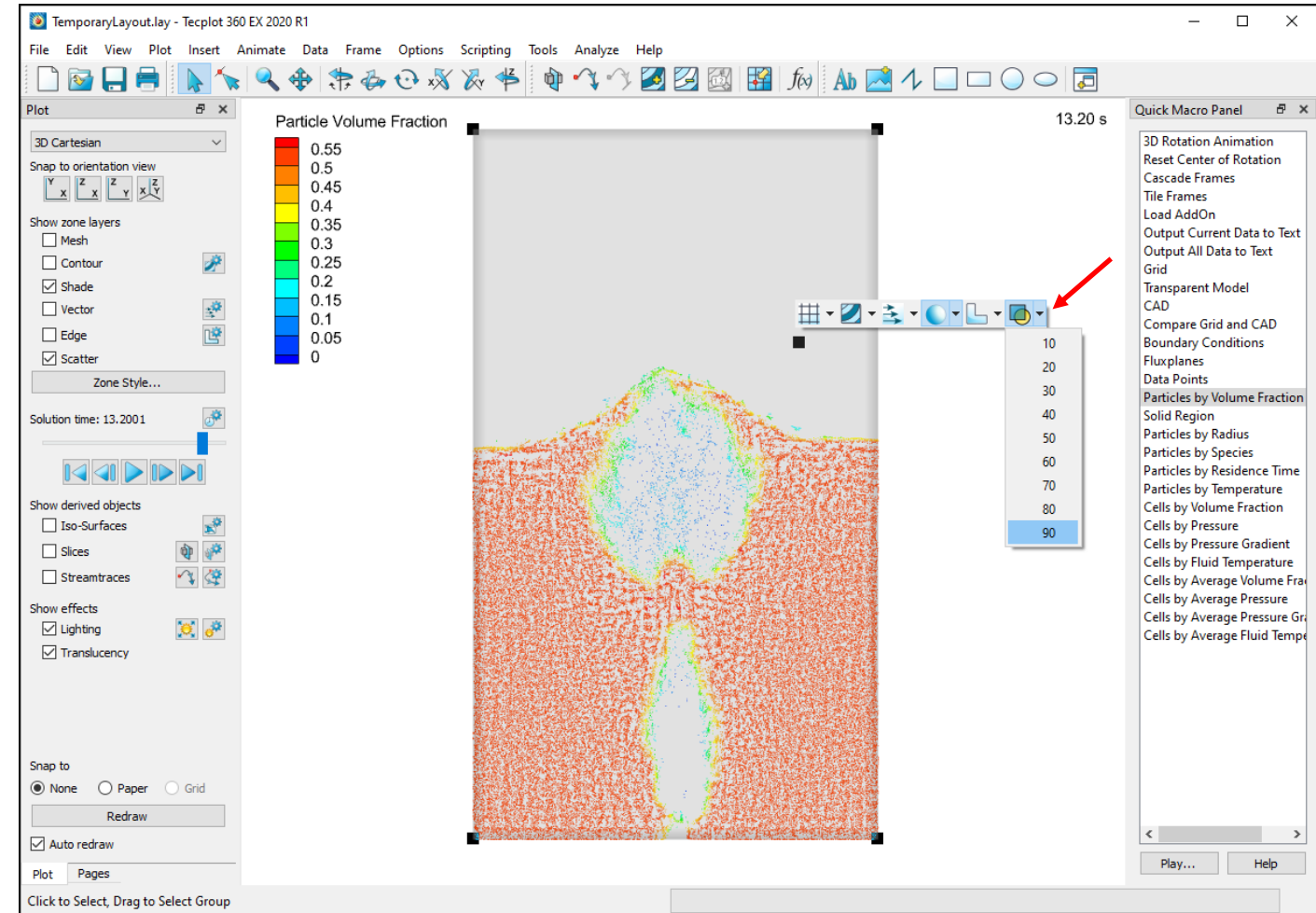


Translucent Geometry

The default view of model geometry is at 80% translucency

While this often looks good for many views, in some situations you will want to modify this value:

- Right-click the geometry
- Click the rightmost figure to toggle the translucency
- Click the dropdown menu next to it to select a translucency value
- Try out different values for the model geometry translucency and see which looks best for this project (90% is shown in the next slides)

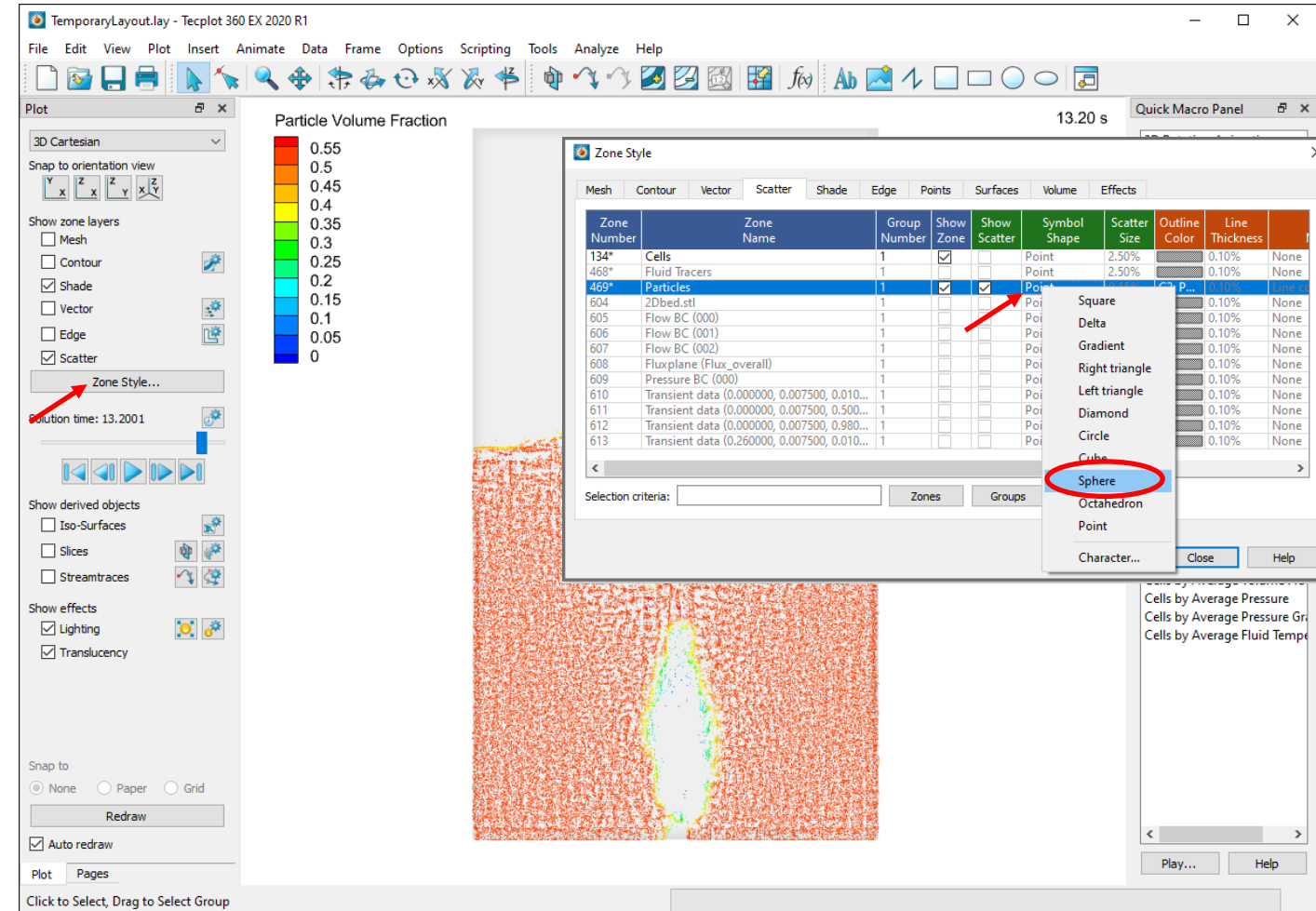


Changing Scatter Symbol Shape and Size

The default scatter symbol shape is one-pixel points, which is great for rendering a very large number of particles in a reasonable amount of time.

If you have fewer particles and want to show them a little larger:

- Click on Zone Style...
- On the Scatter tab, right-click on Point in the Symbol Shape column of the Particles row
 - Select Sphere
- Right-click on Scatter Size column of Particles row
 - Click on Enter...
 - Enter 0.3
 - Click OK

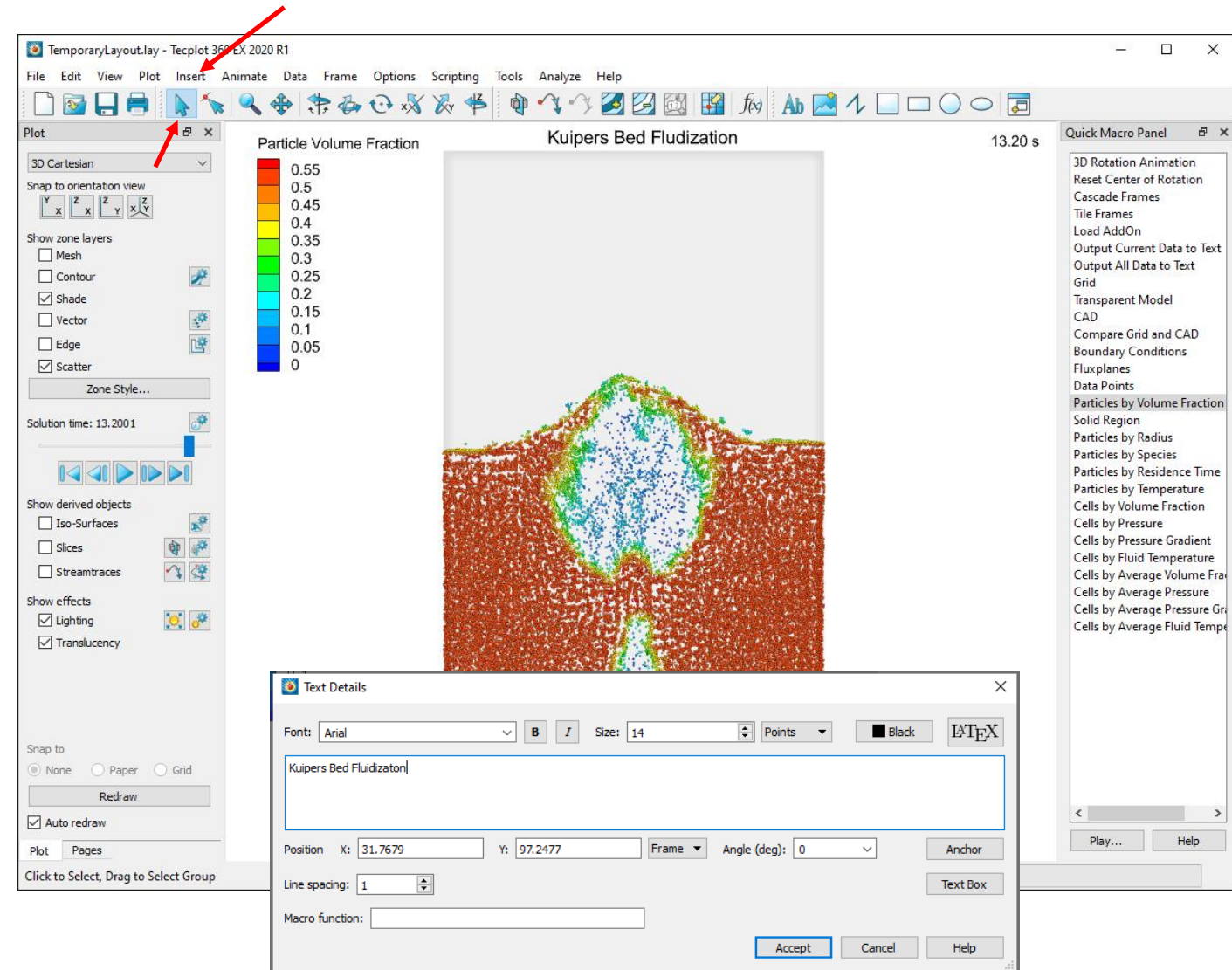


Adding a Title

Select Insert → Text and select a location in the view to raise the Text Details window

- Here you can adjust the font, size, color, location, etc of the text
- Click Accept when your text is ready

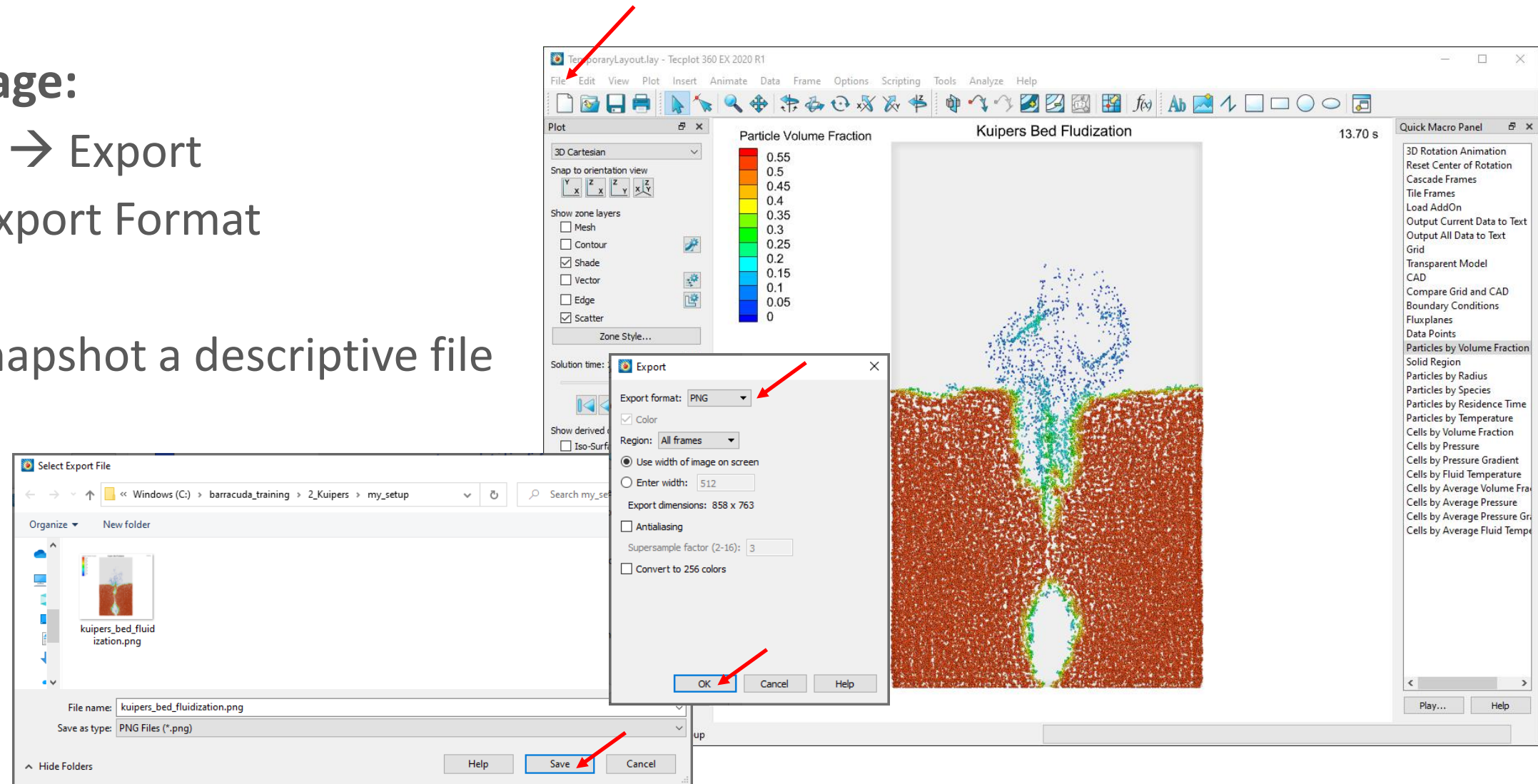
Once entered, any text can be moved around with the selection tool



Exporting an image

To create an image:

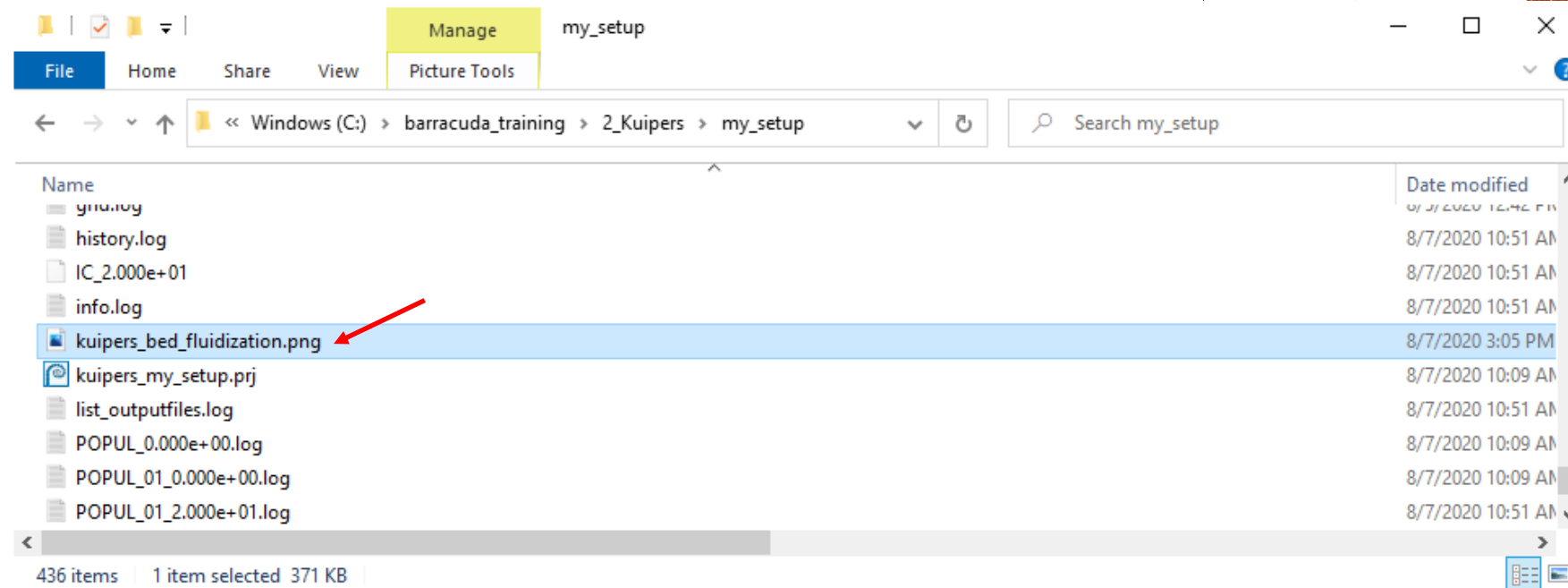
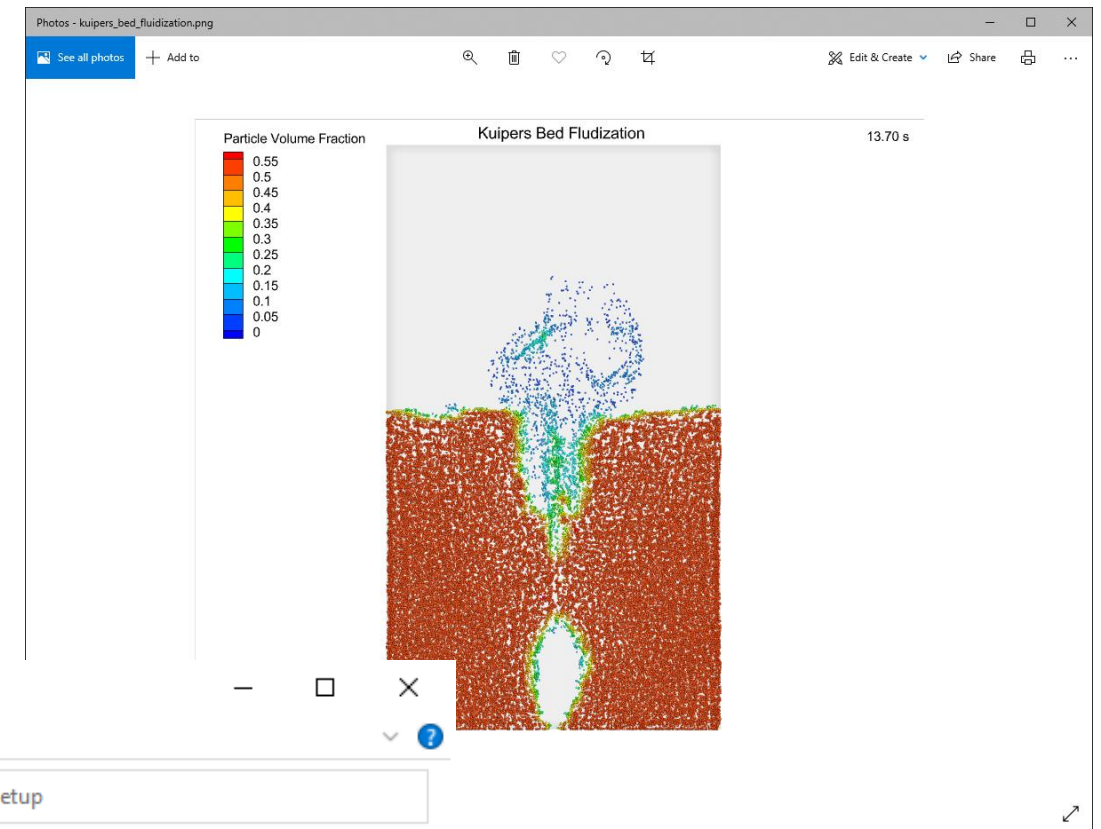
- Click on File → Export
- Select the Export Format
- Click OK
- Give your snapshot a descriptive file name
- Click Save



Viewing an image

To view your snapshot:

- Navigate to your project file directory
- Double-click on snapshot file name



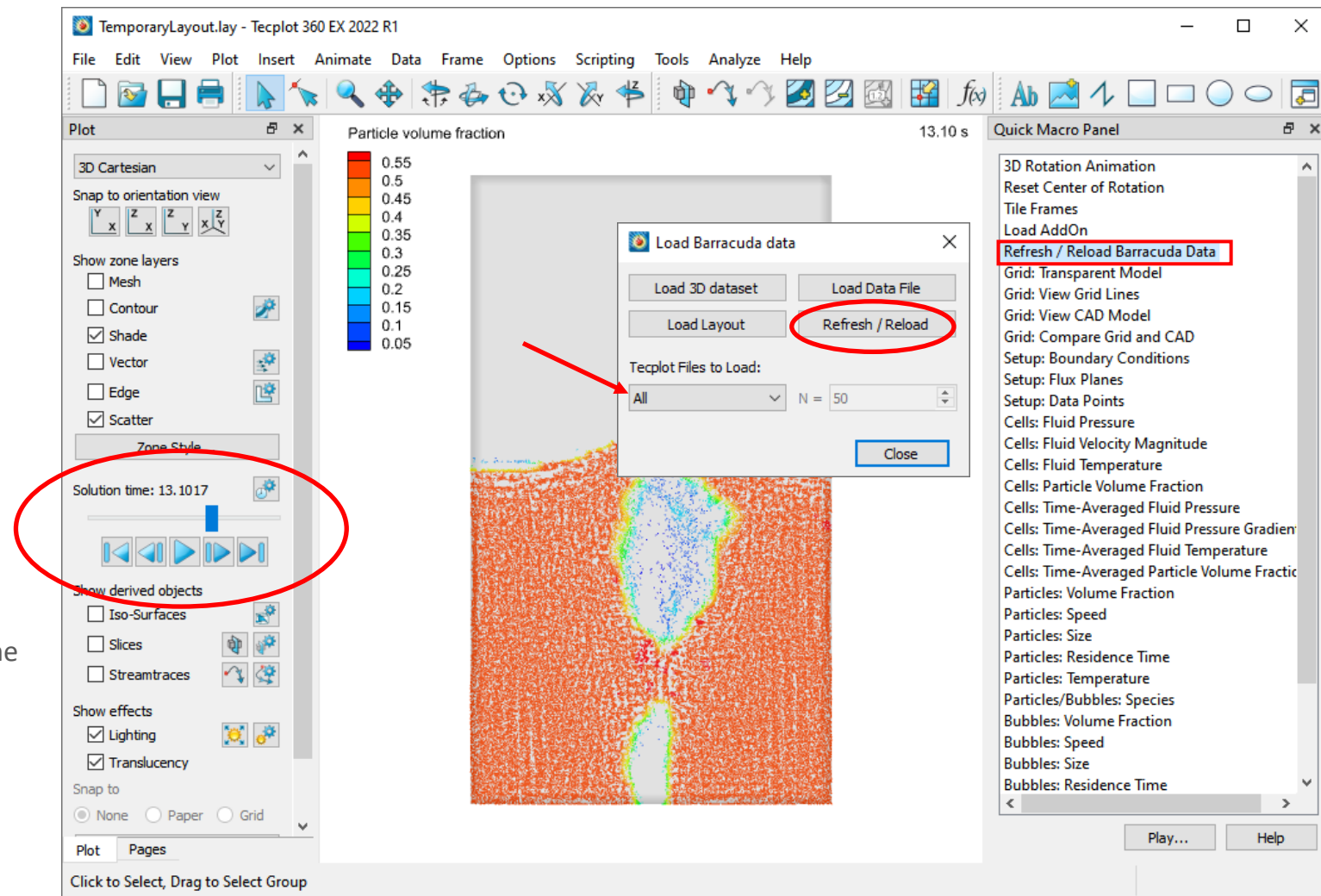
Navigating through Time

If more than one solution time is loaded in Tecplot, use the time controls located in the Plot sidebar to navigate through time:

- Use the Play button in the center to view your simulation through time
- Use the slider to quickly navigate to a certain point in time
- The left- and right-most buttons skip to the beginning and end, and the buttons just inside them navigate to the previous or next file

If more solution time has elapsed and more .plt files have been created, you can scan for more files to view in two ways:

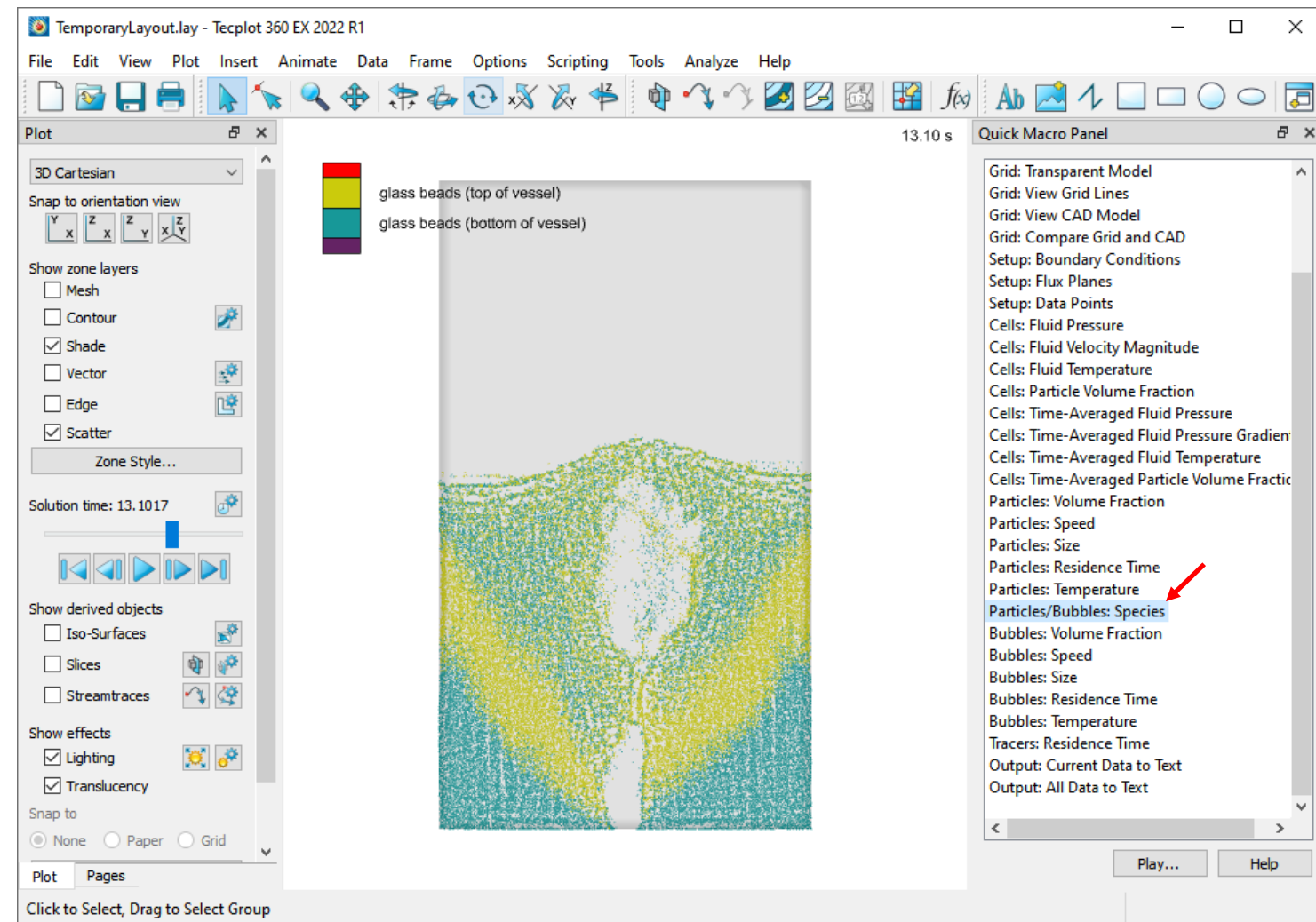
- Make sure that **All** is selected for Tecplot Files to Load
 - Then double-click Load: Refresh / Reload Barracuda Data in the Quick Macro Panel
 - Or click on File → Load Barracuda data → Refresh / Reload



Particle Mixing in Kuipers Bed

Particle mixing can be shown best with an animation of the Kuipers bed through time.

Double-click on Particles/Bubbles: Species in the Quick Macro Panel.



Making an Animation

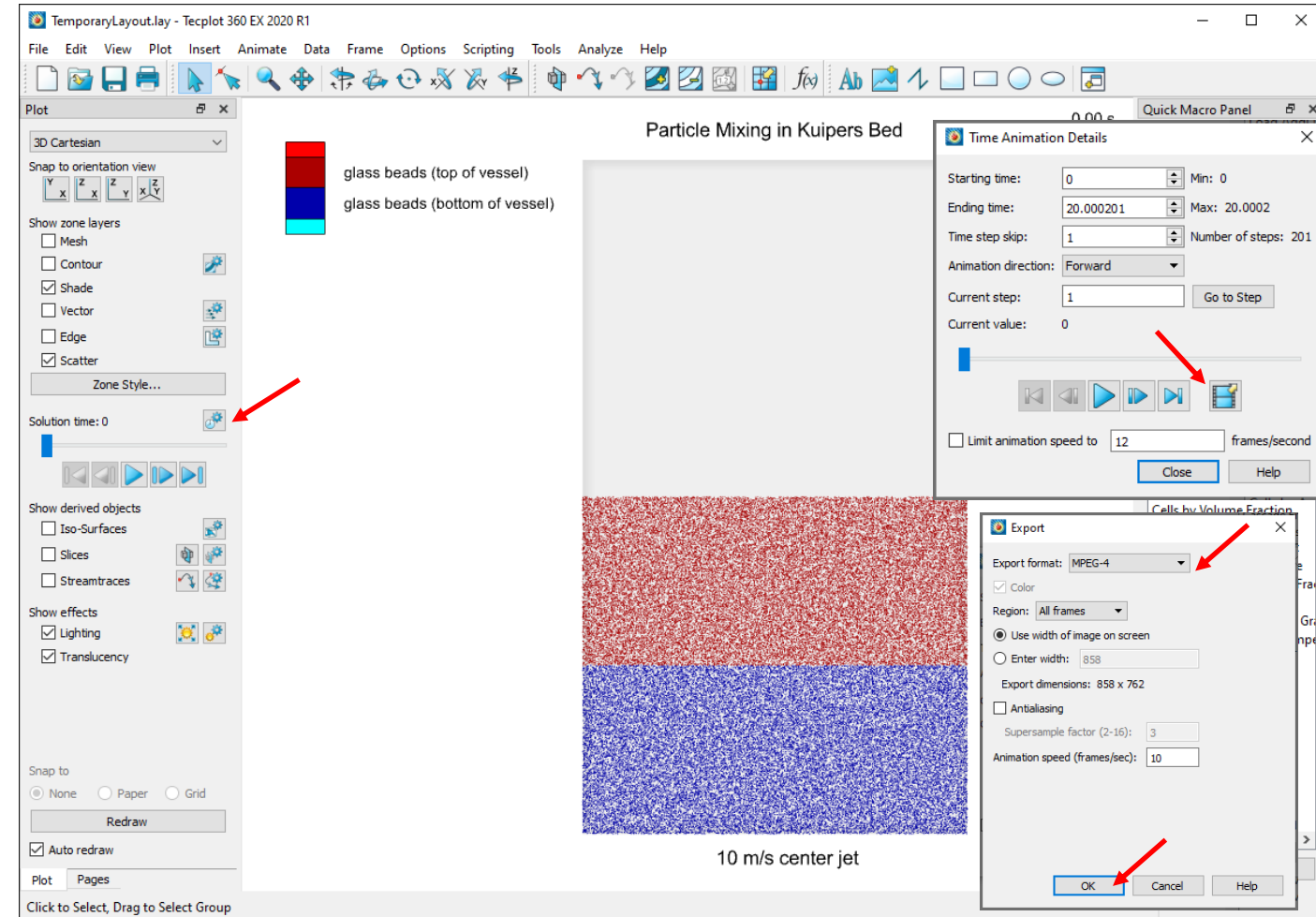
Create this view:

- Color map : Doppler
- Adjust zoom and location of geometry
- Add top and bottom title

Create an animation:

- Ensure all time step .plt files are loaded (File → Load Barracuda data → Tecplot Files to Load: All → Refresh / Reload)
- Click on gear icon next to Solution time
- Verify the settings in the Time Animation Details dialog
- Click on the Film Reel icon
- Select the Export format → OK
- Give descriptive file name → Save

To view the animation, navigate to the simulation directory and double-click on animation file name.



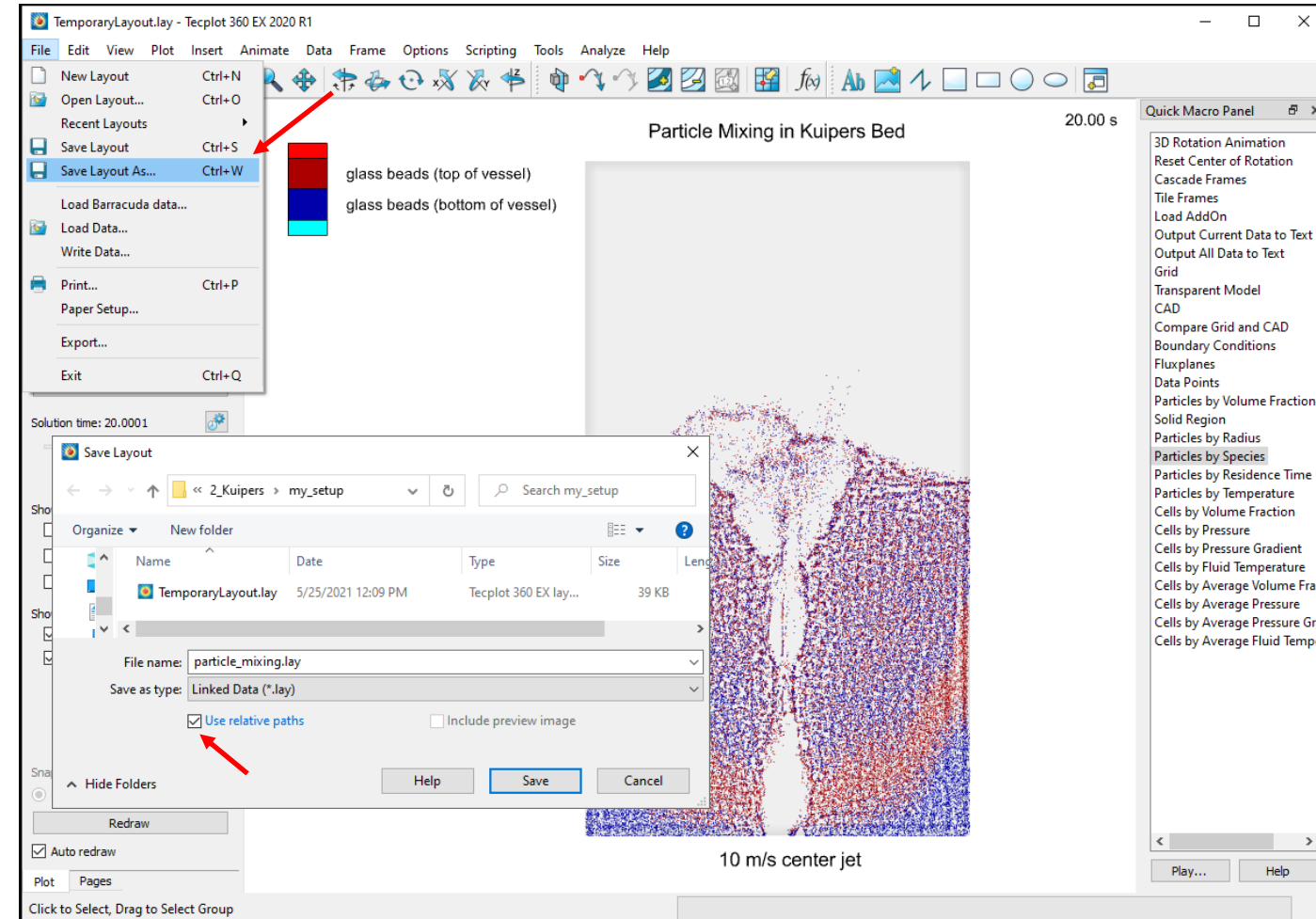
Saving an Layout File

When setting up a non-default data view, it's good practice to save it.

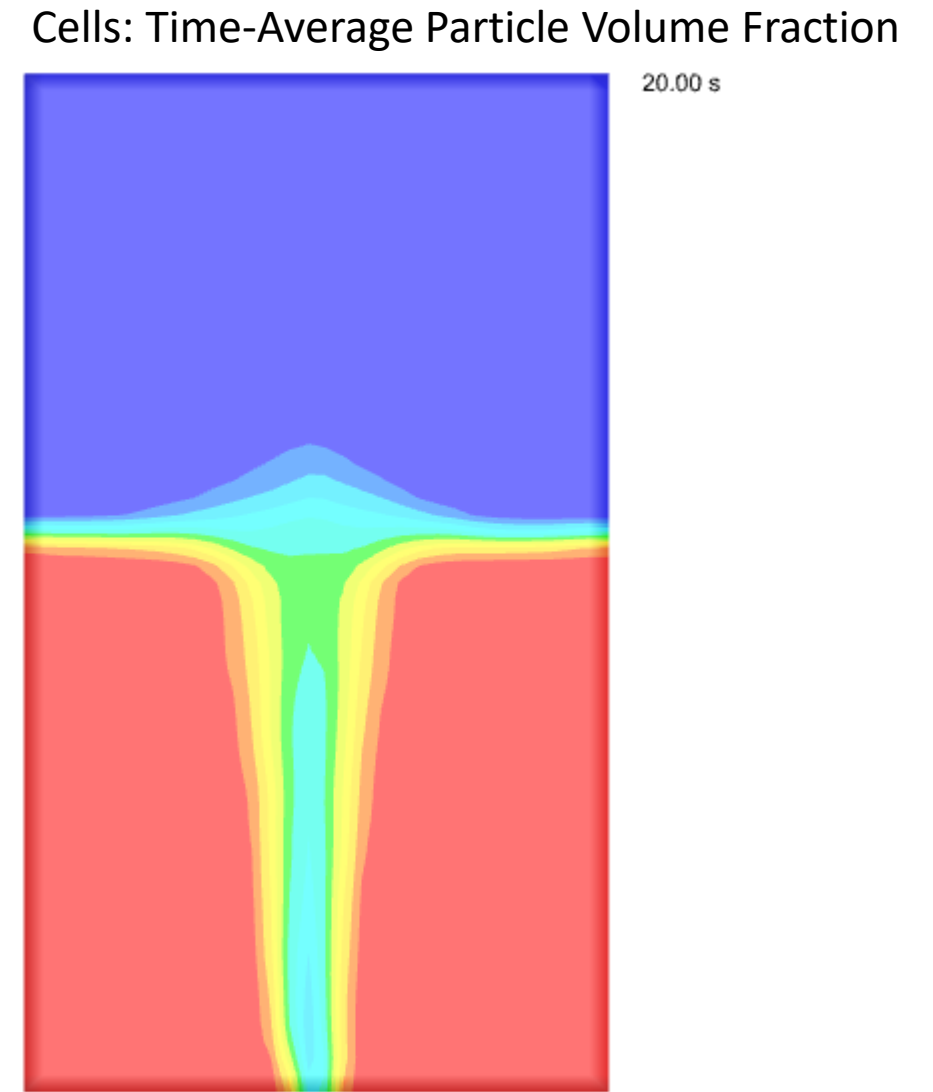
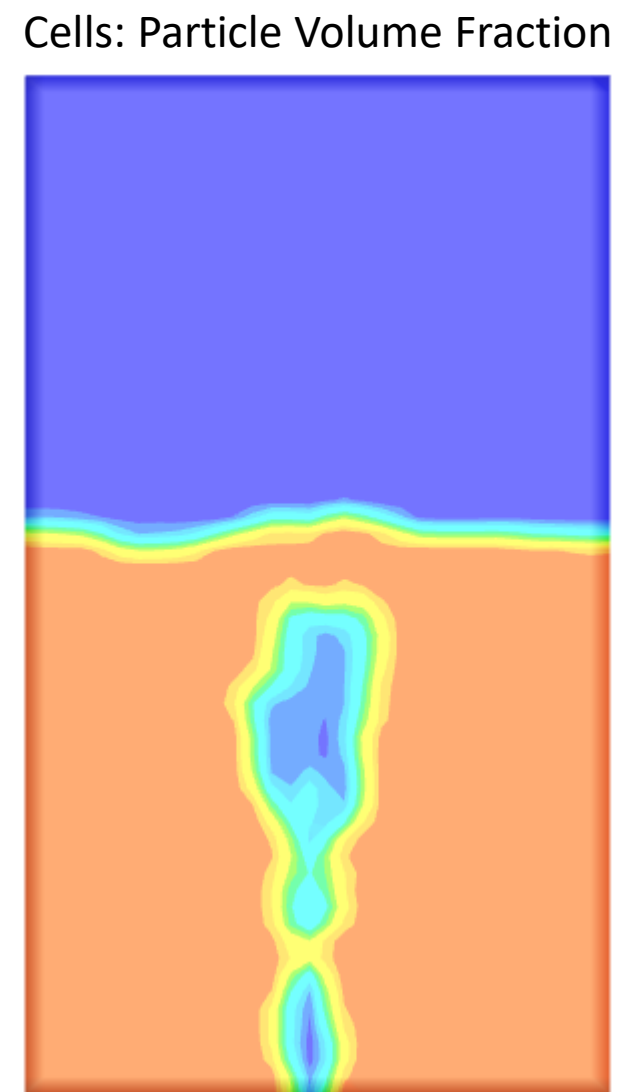
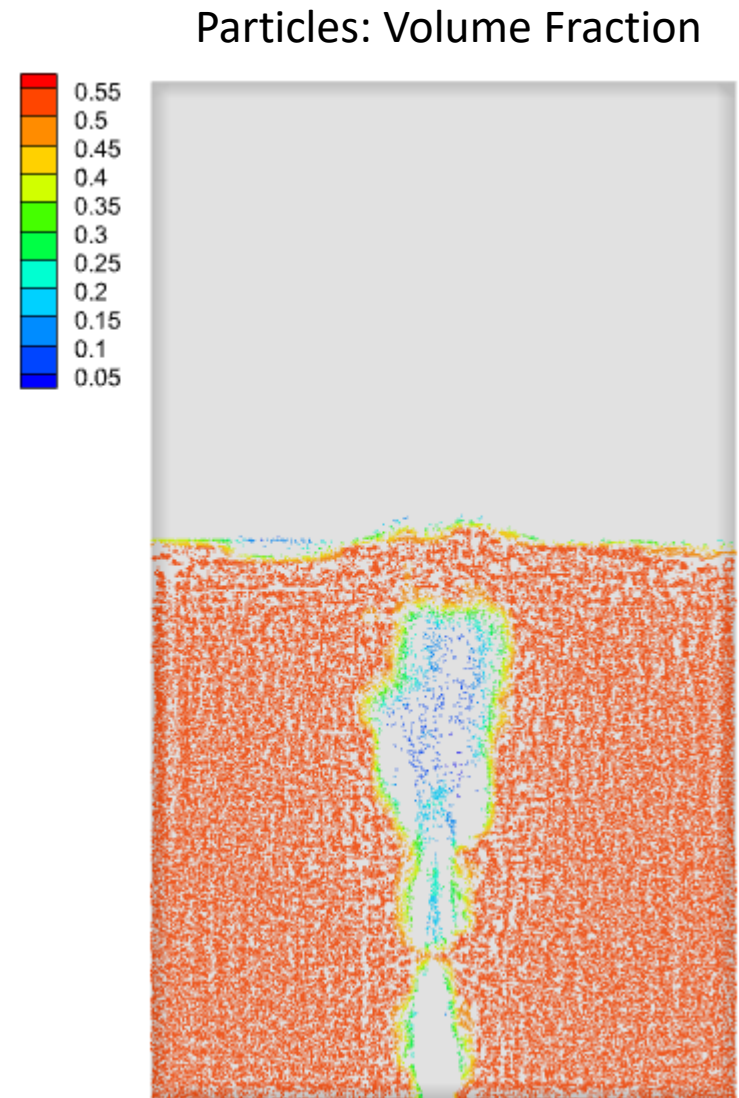
Select File → Save Layout As... to name and save a custom layout.

A layout file will save all the requisite information to recreate the view.

Note: Layout files can be applied to other projects with different data and different geometry. This can be helpful for quickly creating animations and snapshots in multiple directories. When you want to use a layout file in other projects, always check the “Use relative paths” option in the Save Layout window.

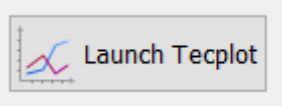


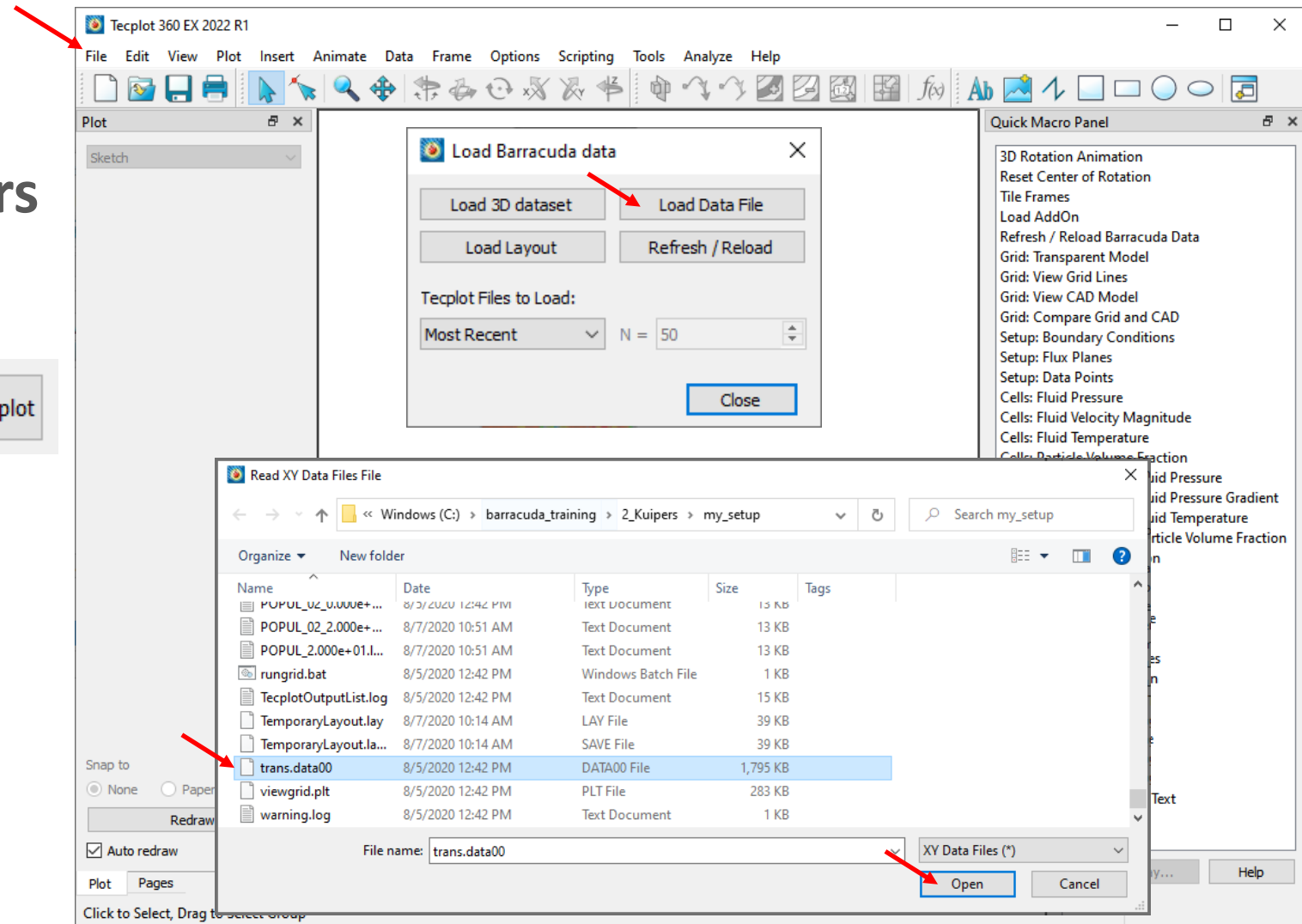
Comparing Results



Loading Barracuda Data for xy plots

When setting up the simulation, we defined Data Points to measure pressure at specific cells in the Kuipers bed. Let's plot the data from those points.

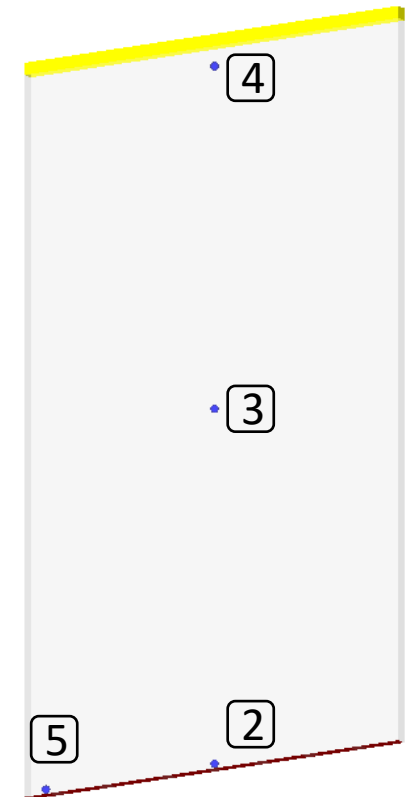
- Click File → New Layout or  button in the Post-Run window
- Click File → Load Barracuda Data...
- Click Load Data File
- Select trans.data00
- Click Open



Data Points File Contents

The file trans.data00 header text lists the data collected in each column of the file:

- Column 1 corresponds to Time
- Column 2 corresponds to Pressure at cell (16, 1, 1)
- Column 3 corresponds to Pressure at cell (16, 1, 31)
- Column 4 corresponds to Pressure at cell (16, 1, 59)
- Column 5 corresponds to Pressure at cell (30, 1, 1)



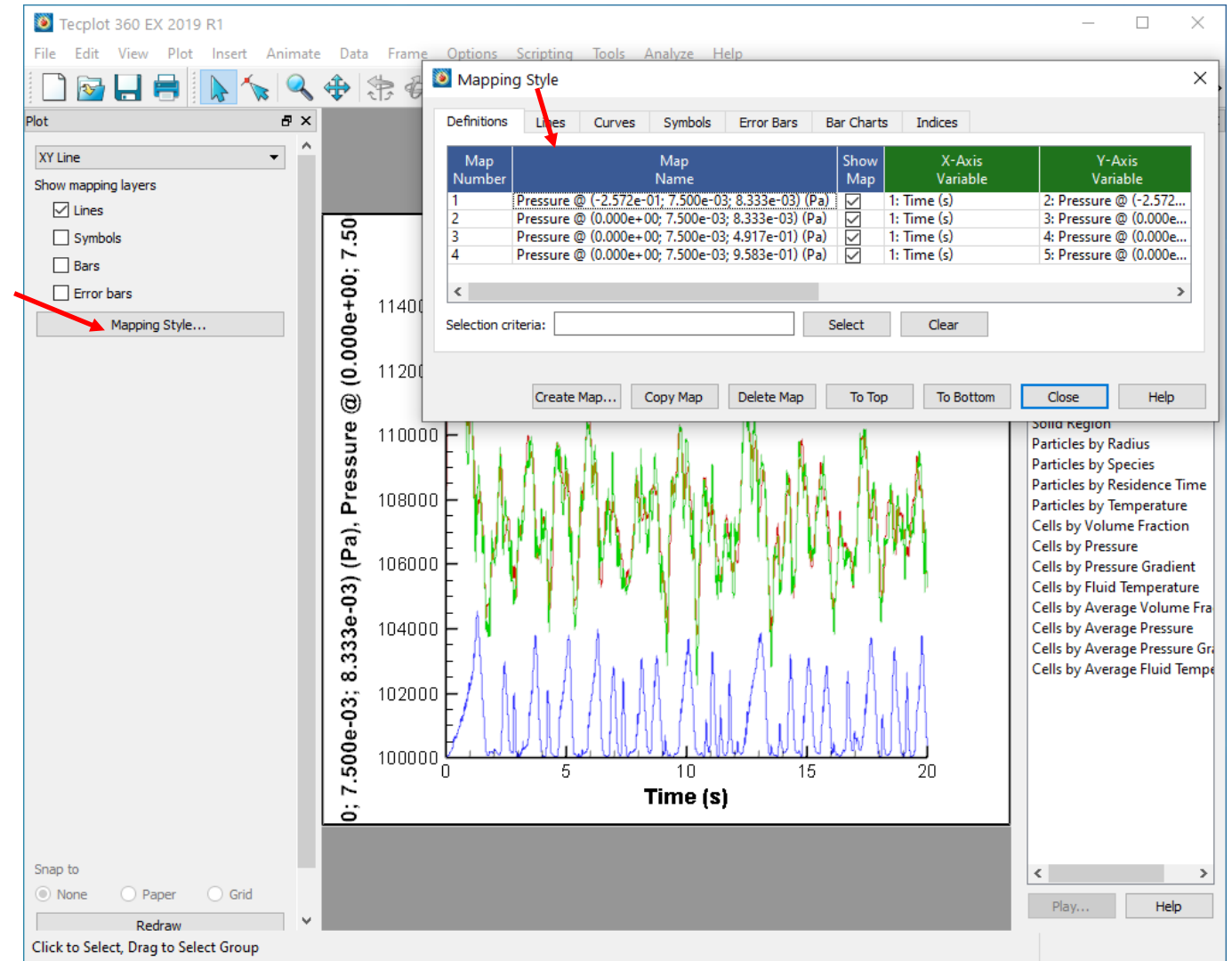
```

C:\barracuda_training\2_Kuipers\my_setup\trans.data00 - Notepad++
File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?
trans.data00
1 # Thu Nov 17 13:46:45 2022
2 #
3 # Barracuda release 22.1.0
4 # Solver version 22.1.0.x088
5 # Build date 2022-10-20 01:02:47 UTC
6 #
7 # Variable name @ location in m Units ijk xyz (m) Comment
8 #
9 # 1 "Time" "s"
10 # 2 "Pressure @ (0.000e+00, 7.500e-03, 8.333e-03)" "Pa" " 16 1 1" " 0.00000e+00 7.50000e-03 8.33333e-03" ""
11 # 3 "Pressure @ (0.000e+00, 7.500e-03, 5.083e-01)" "Pa" " 16 1 31" " 0.00000e+00 7.50000e-03 5.08333e-01" ""
12 # 4 "Pressure @ (0.000e+00, 7.500e-03, 9.750e-01)" "Pa" " 16 1 59" " 0.00000e+00 7.50000e-03 9.75000e-01" ""
13 # 5 "Pressure @ (2.572e-01, 7.500e-03, 8.333e-03)" "Pa" " 30 1 1" " 2.57250e-01 7.50000e-03 8.33333e-03" ""
14 0.000000e+00 1.0000000000e+05 1.0000000000e+05 1.0000000000e+05 1.0000000000e+05
15 5.000000e-03 1.0578421451e+05 1.0001768011e+05 1.0000087552e+05 1.0176502503e+05
16 7.540964e-03 1.1043355369e+05 1.0000600579e+05 1.0000037180e+05 1.0275273004e+05
Normal text file length : 848,539 lines : 9,752 Ln: 1 Col: 1 Sel: 0|0 Windows (CR LF) UTF-8 INS
    
```

Plotting Data Points

Click the Mapping Style... button

- Go to the Definitions tab
- Select the boxes in the Show Map column for all four pressure data points
- If a line of data is not visible in the plot, click on the frame and press Ctrl+F to autoscale the axes



Editing the Plot Legend

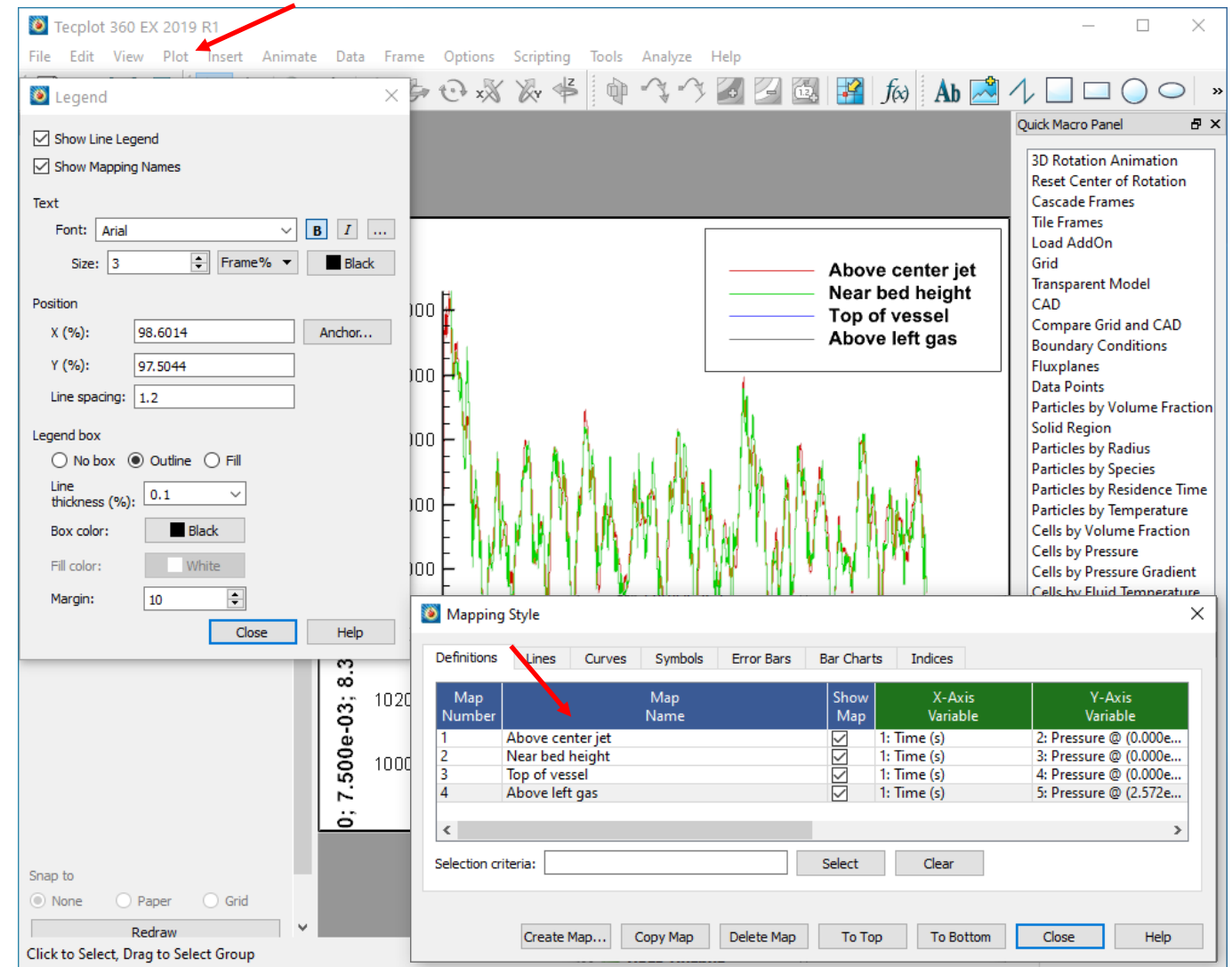
Navigate to Plot → Line Legend...

- Select Show Line Legend to display the legend

In Legend dialog, you can edit other aspects of the legend's appearance

To change the names of the lines in the legend, you must change the names of the variables in the Mapping Style dialog

- Double-click the Map Name for each line to edit the text

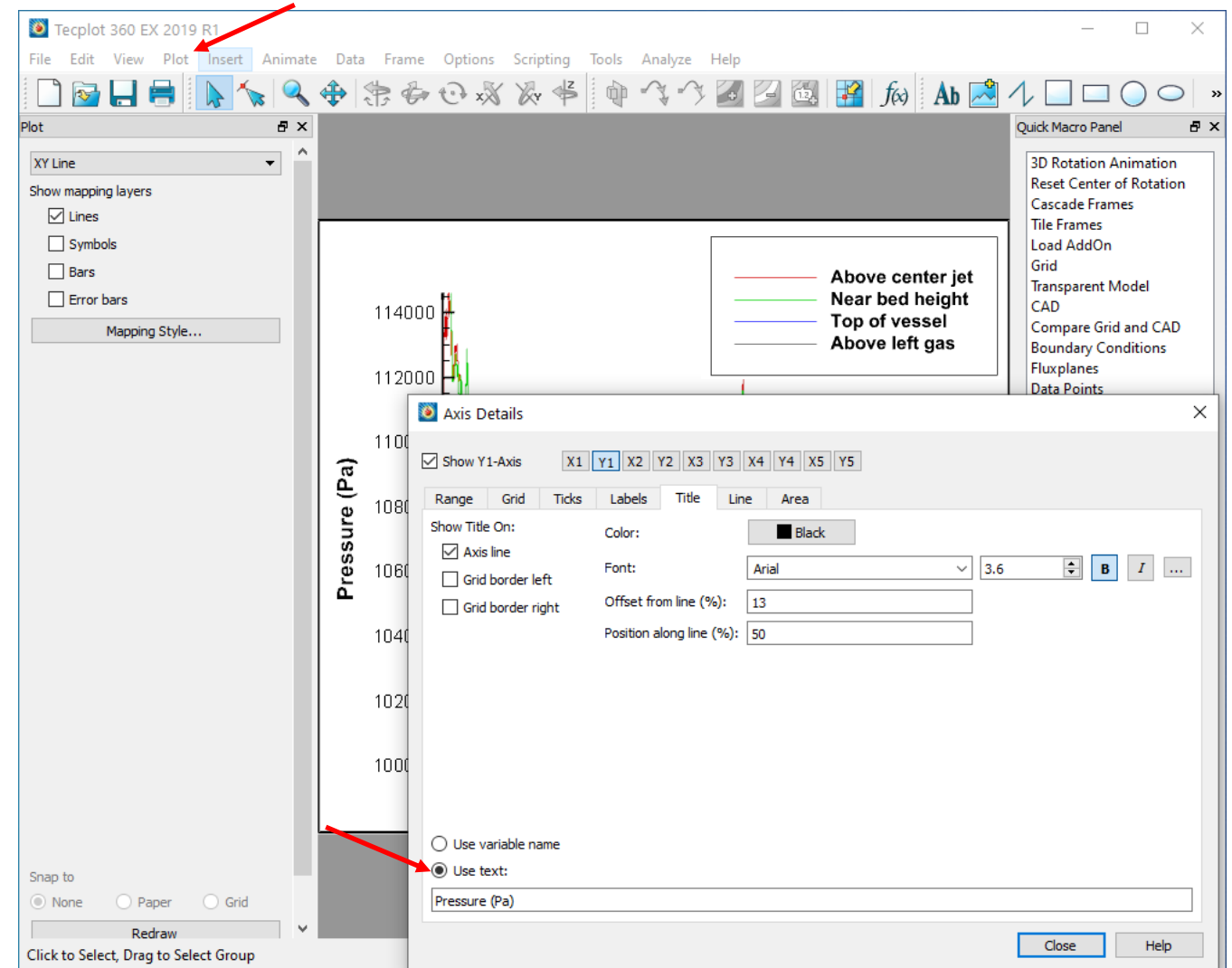


Editing the Axis Labels

Navigate to Plot → Axis...

- Go to the Title tab
- Click on Y1
- Select Use text
- Enter a custom axis title
- Click Close

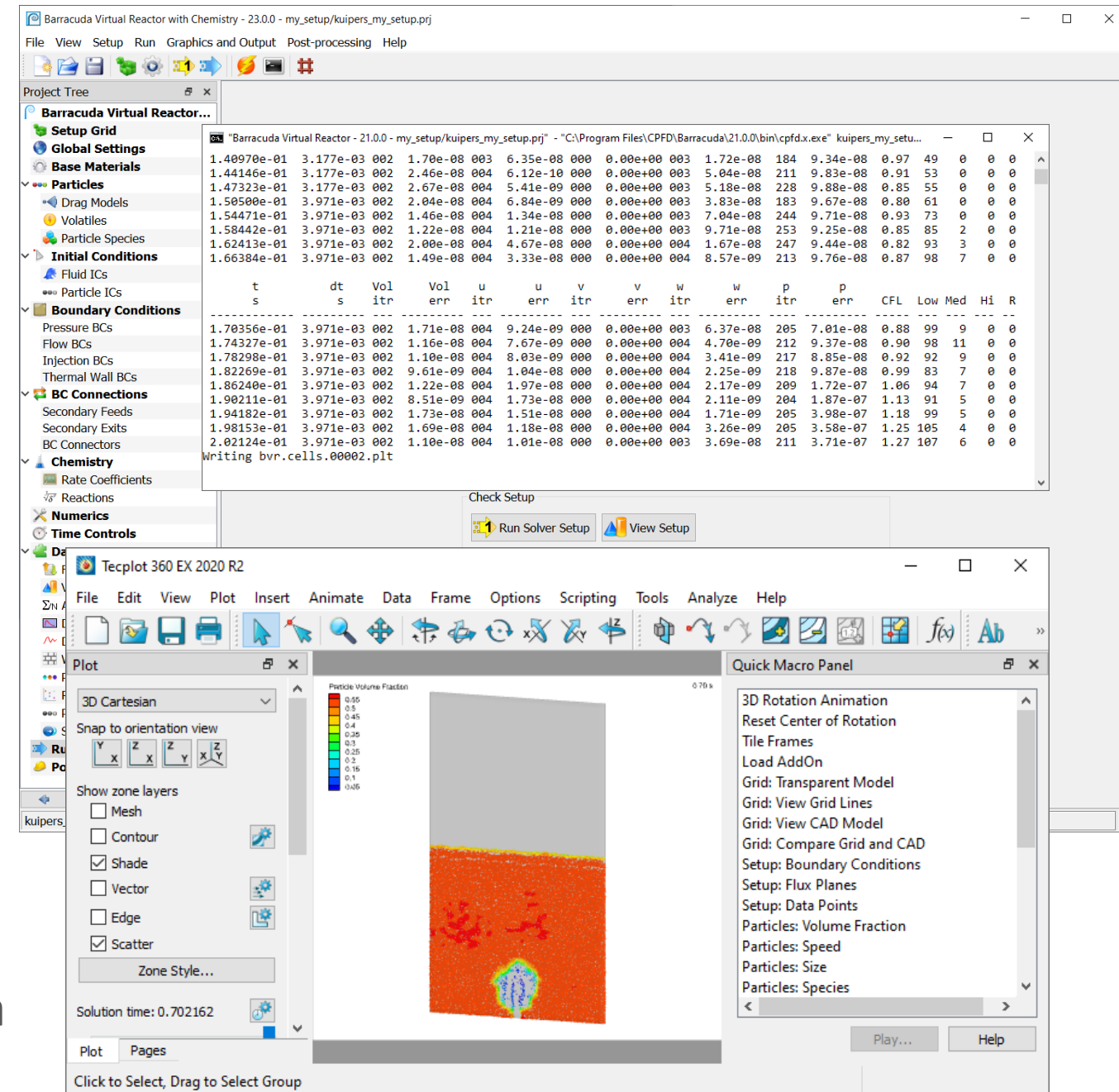
The Axis Details window allows you to edit other aspects of axis appearance



Kuipers Example Conclusion

You've now seen many aspects of the typical workflow for setting up, running, and post-processing a Barracuda Virtual Reactor simulation

- Working with the Barracuda GUI
 - Navigating the project tree
 - Defining base materials and particle species
 - Defining initial and boundary conditions
- Running the Barracuda solver
 - Single time-step run for checking setup
 - Run simulation for full time-period
- Post-processing with Tecplot for Barracuda



Conclusions

If you are interested in joining a full Barracuda Virtual Reactor New User Training Class, please email us at:

training@cpfd-software.com

Future training class dates can be found at:

<https://cpfd-software.com/events-calendar/>