Ebullated Bed: Setup and Analysis

CPFD Software

www.cpfd-software.com

Ebullated Bed Reactor

Model of an ebullated bed used to hydrocrack vacuum resid (VR) with hydrogen gas

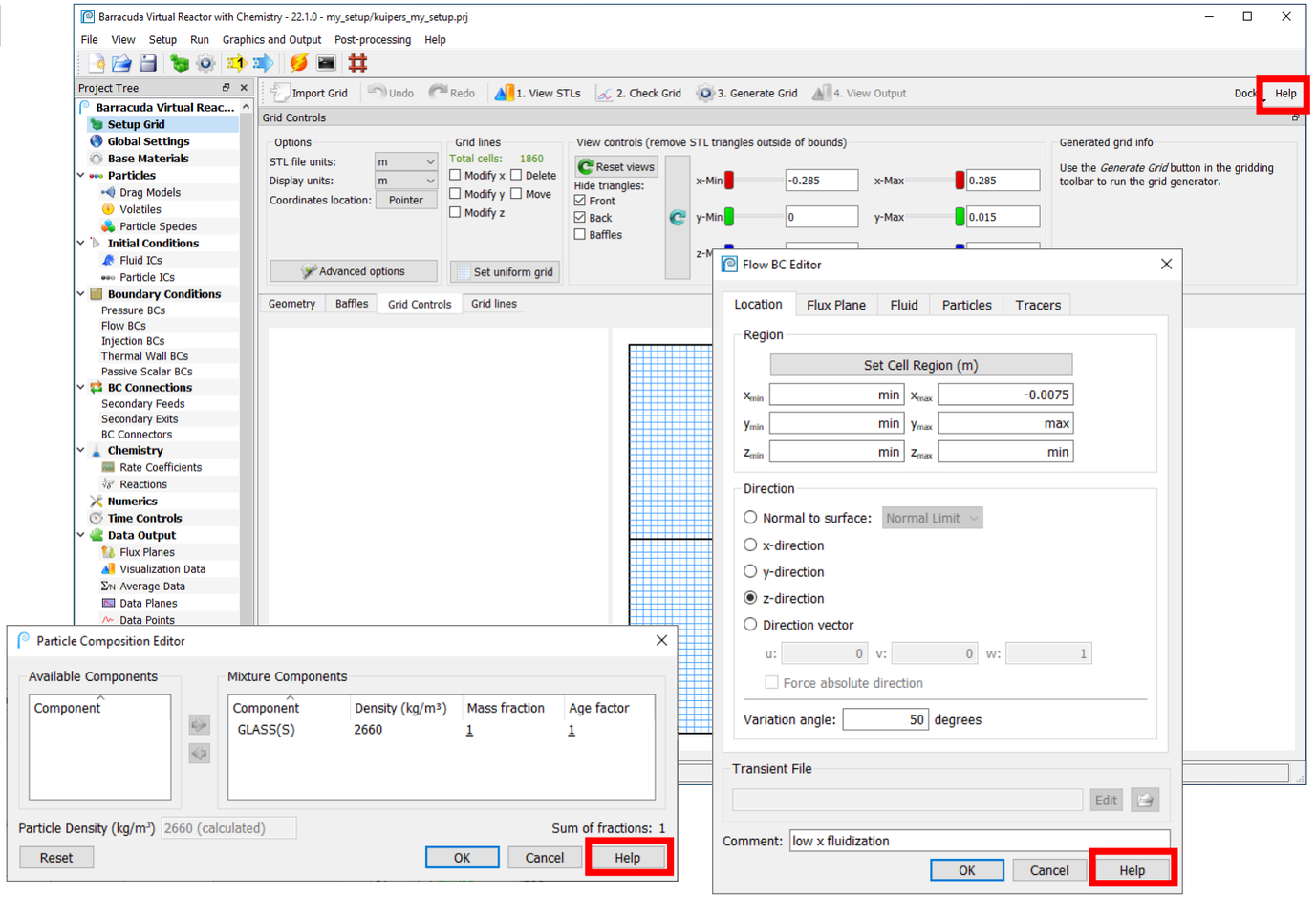
3-phase VLS (vapor, liquid, solid) with liquid domain

Isothermal and reacting system

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.



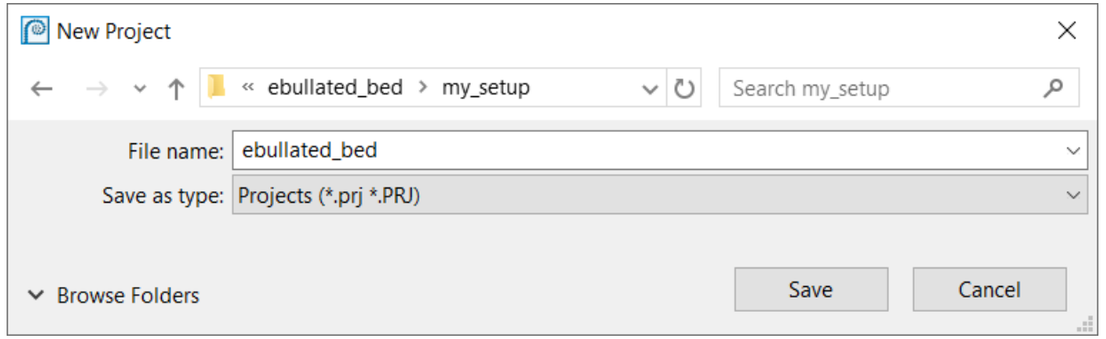
Project File

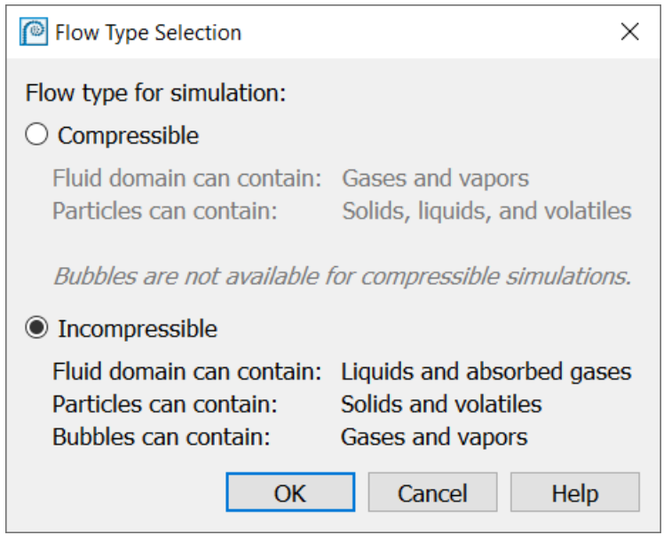
Make a new incompressible project file in the supplemental training directory:

\ebullated_bed\my_setup

With the project name:

ebullated_bed.prj





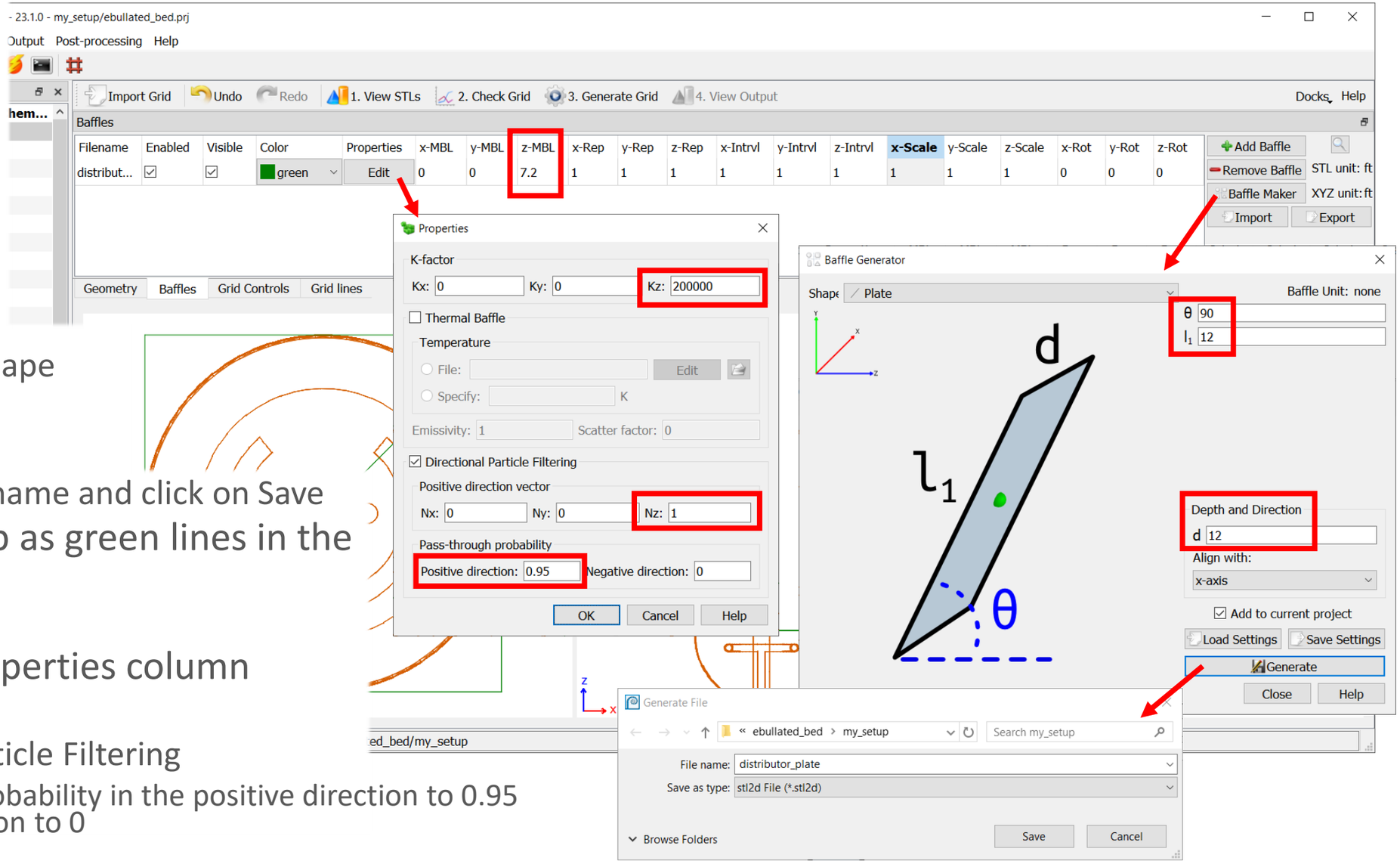
Setup Grid

Geometry tab:

- Add ebullated_bed.stl

Baffles tab:

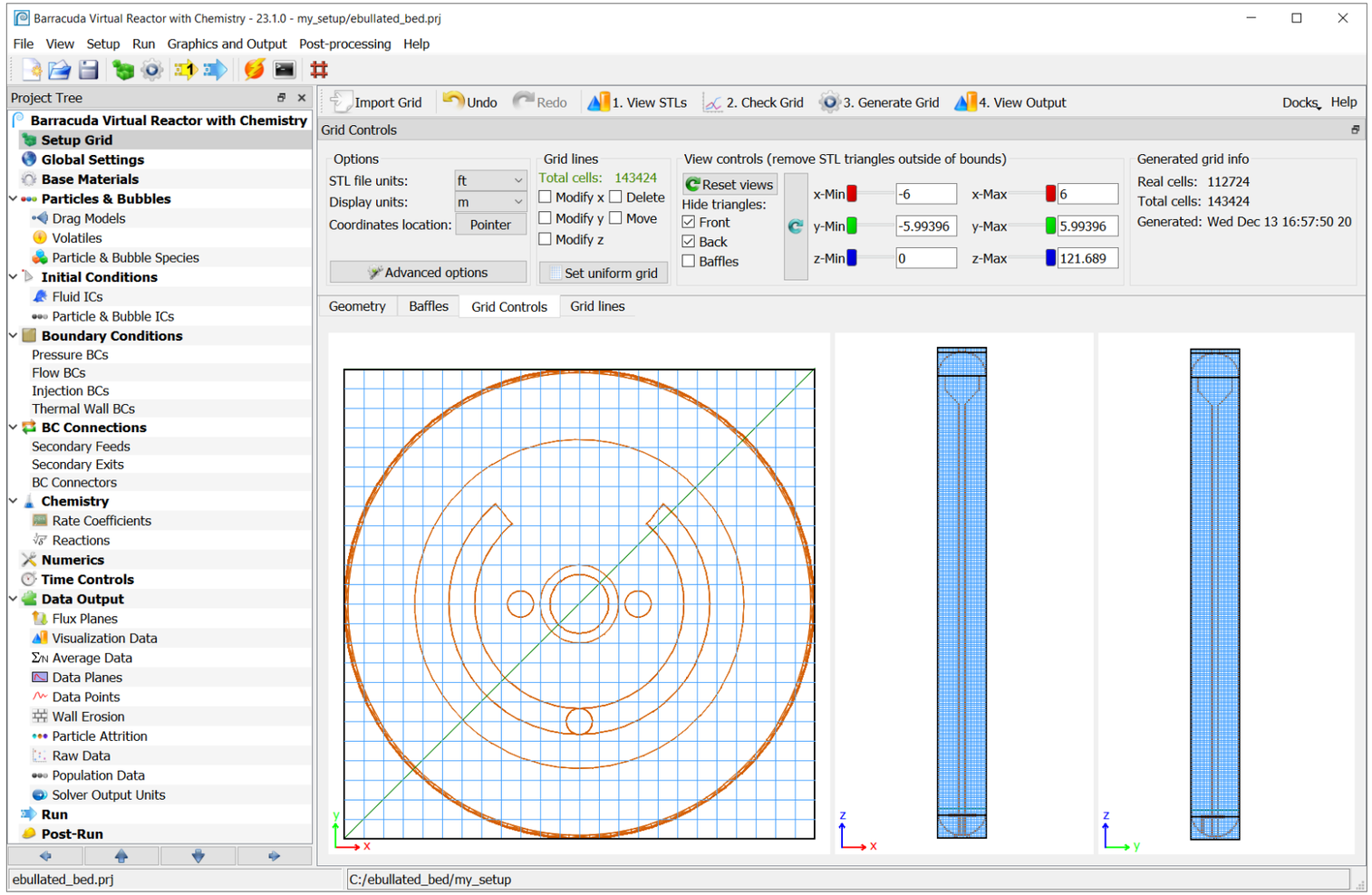
- Click on Baffle Maker
  - Select Plate for the Shape
  - Set l_1 and d to 12
  - Click Generate
  - Give the baffle a File name and click on Save
- The baffle will show up as green lines in the three grid panes
- Set the z-MBL to 7.2
- Click on Edit in the Properties column
  - Kz = 200000
  - Select Directional Particle Filtering
    - Set Pass-through probability in the positive direction to 0.95 and negative direction to 0
  - Click OK



Setup Grid

Grid Controls tab:

- Set STL file units to ft
- Select Merge and remove small cells in Advanced options
- Set uniform grid of 150,000 cells
- Modify z grid lines to capture the outlet pipe, recycle pan, and bubble ring
- Click on Generate Grid



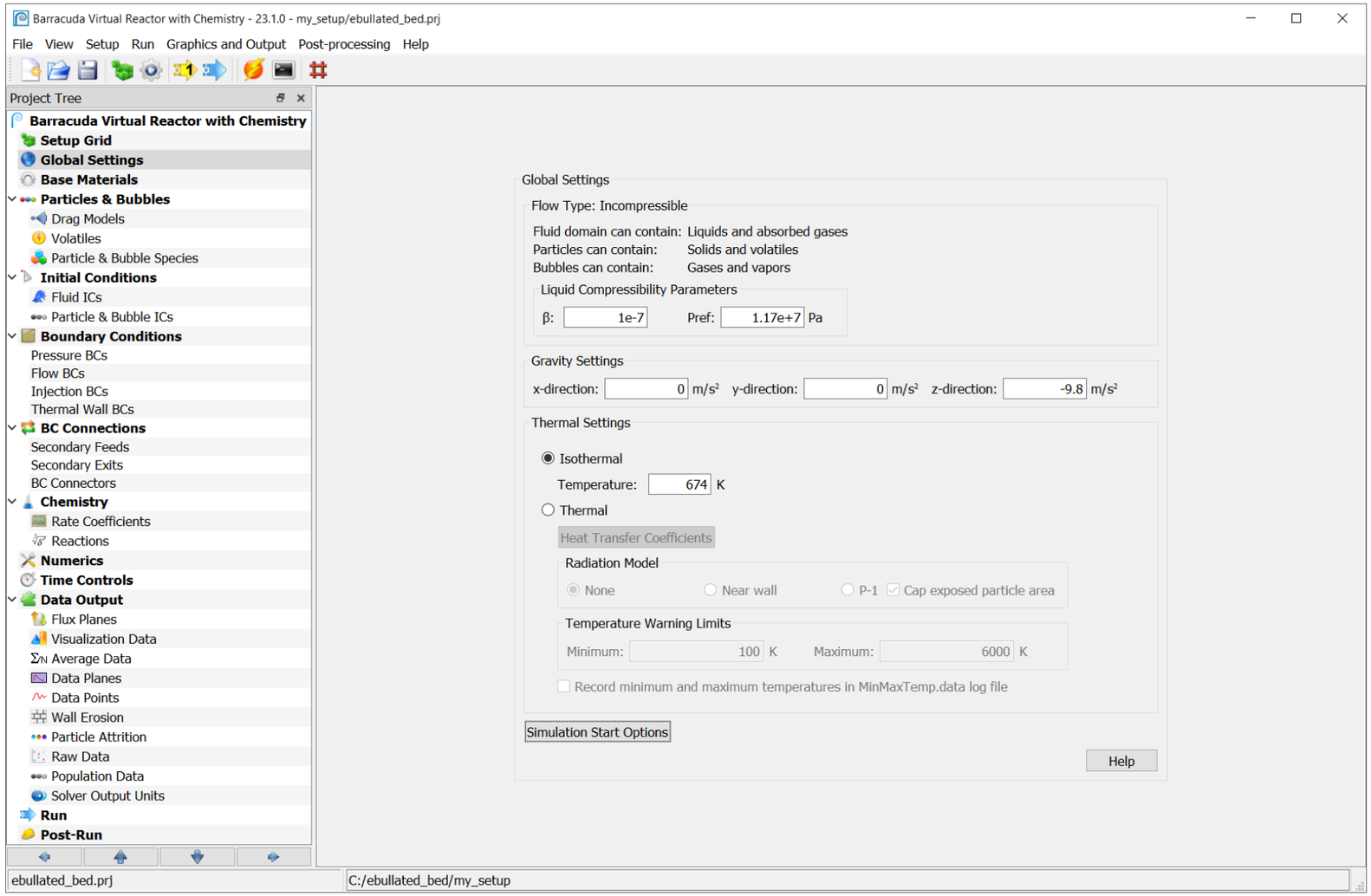
Global Settings

Liquid Compressibility Parameters:

- ß = 1e-7
- Pref = 1.17e+7

Set Gravity in negative z-direction

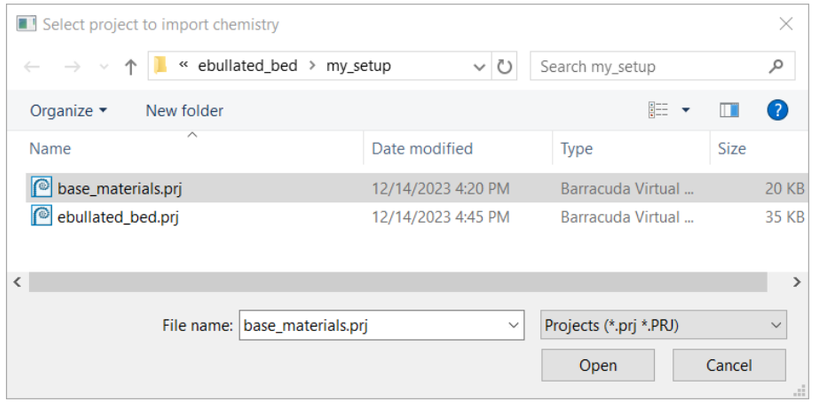
Select Isothermal and set the temperature to 674 K

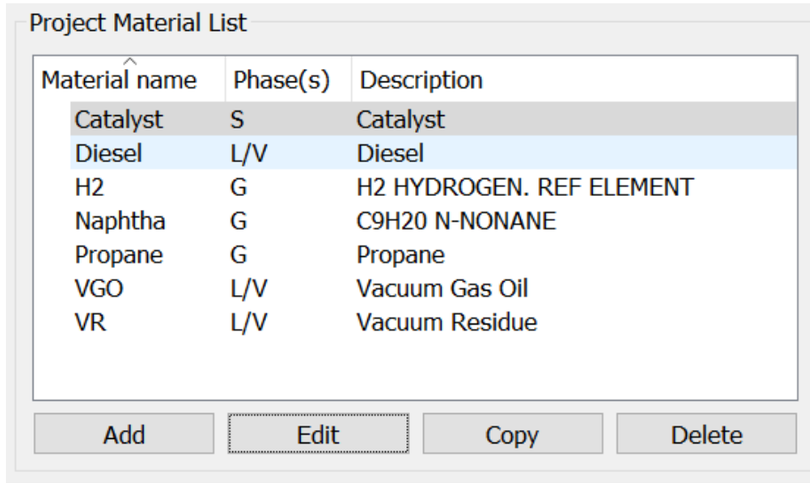


Base Materials

The materials in this project have adjusted values for many physical properties. Import the base materials for this project:

- Click on File →Import from project
- Browse to select base_materials.prj and click Open
- Select Import Base Materials with Append option
- Click OK
- Verify that the materials match the list on the right





Particles & Bubbles

Close pack volume fraction: 0.6

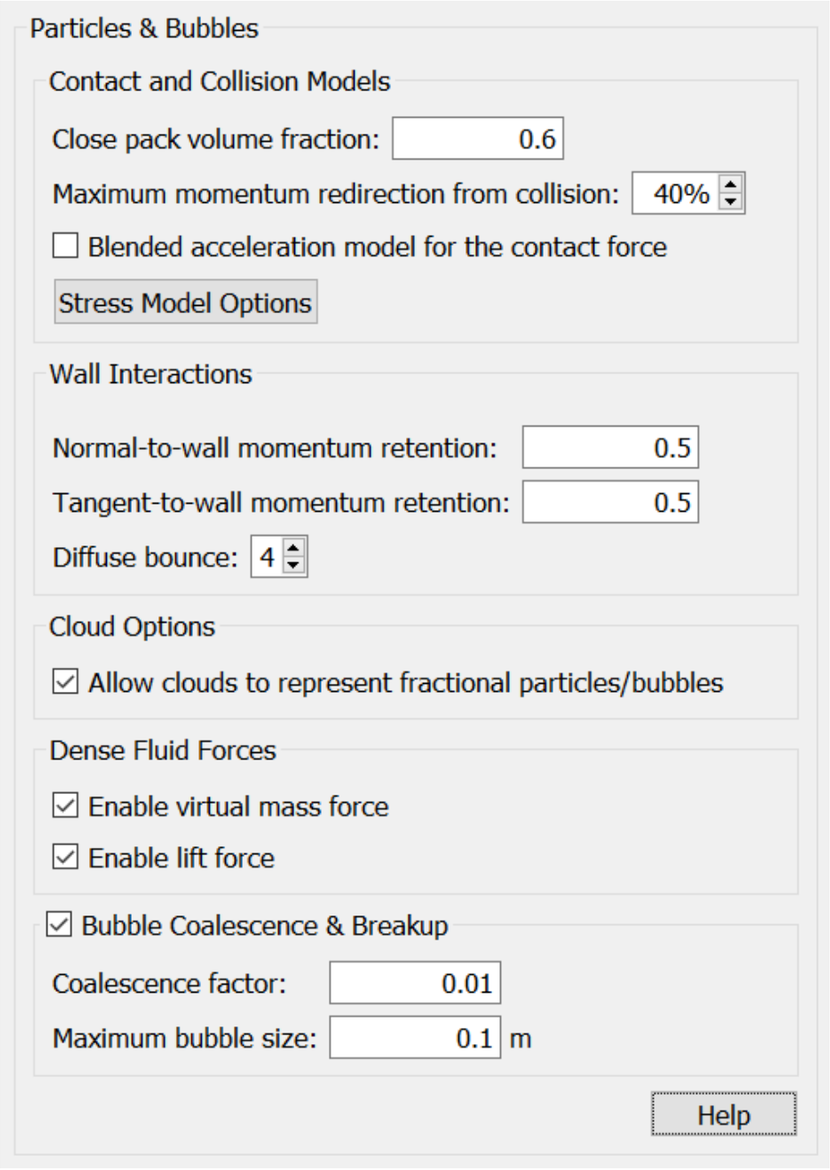
Normal-to-wall momentum retention: 0.5

Tangent-to-wall momentum retention: 0.5

Diffuse bounce: 4

Select Bubble Coalescence & Breakup

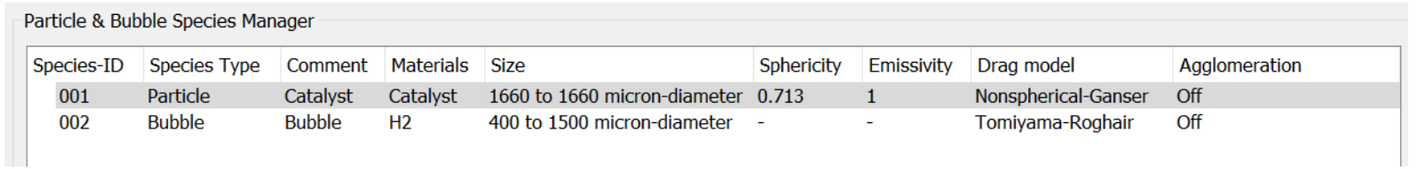
- Coalescence factor: 0.01
- Maximum bubble size: 0.1

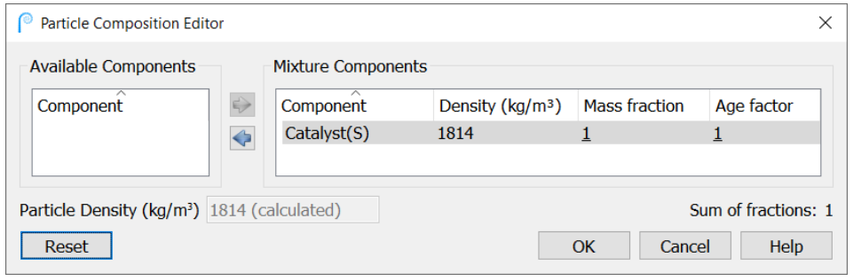


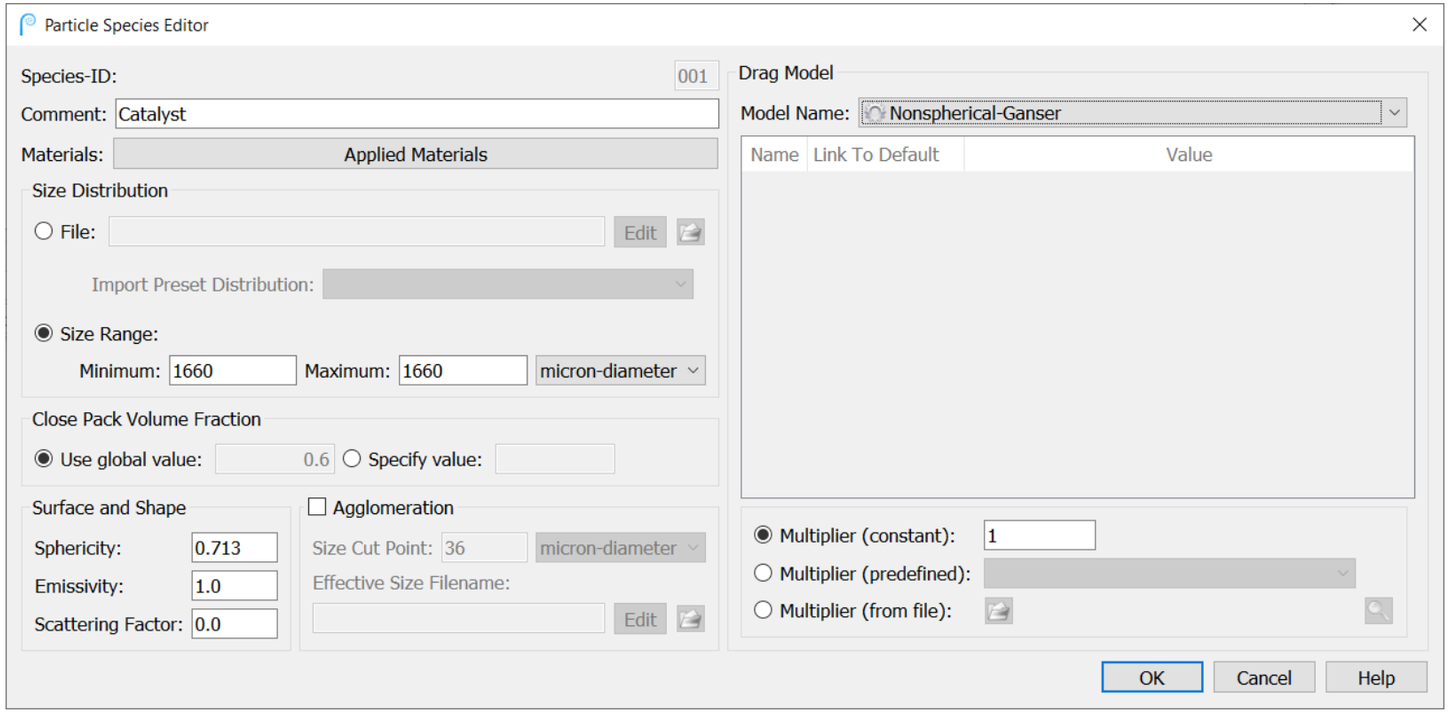
Particle Species

Create the Catalyst particle species:

- Click on Add Particle
- 100% Catalyst(S)
- 1660 micron diameter
- Use global value for close pack volume fraction
- Set sphericity to 0.713
- Use Nonspherical- Ganser drag model



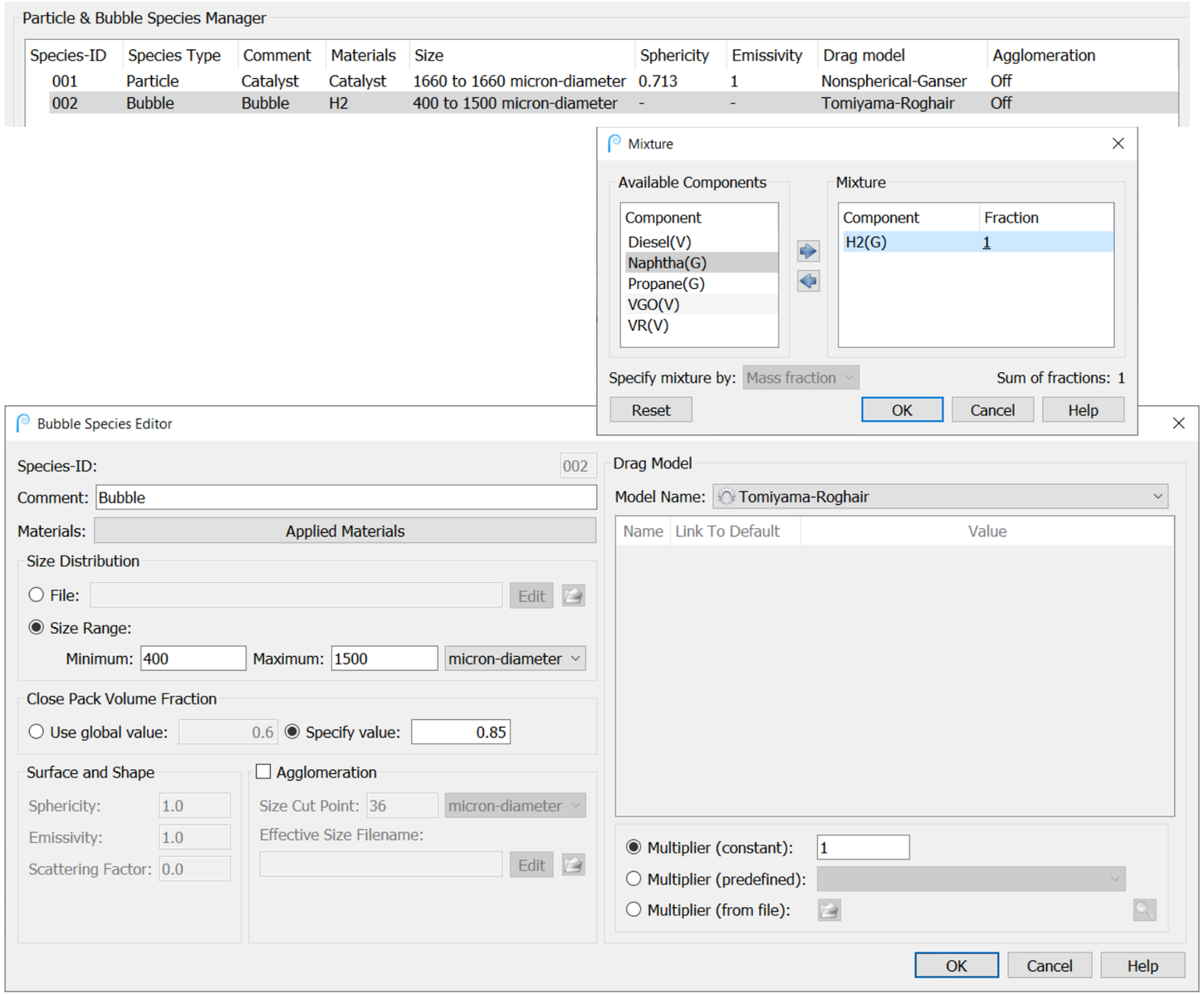




Bubble Species

Create the bubble species:

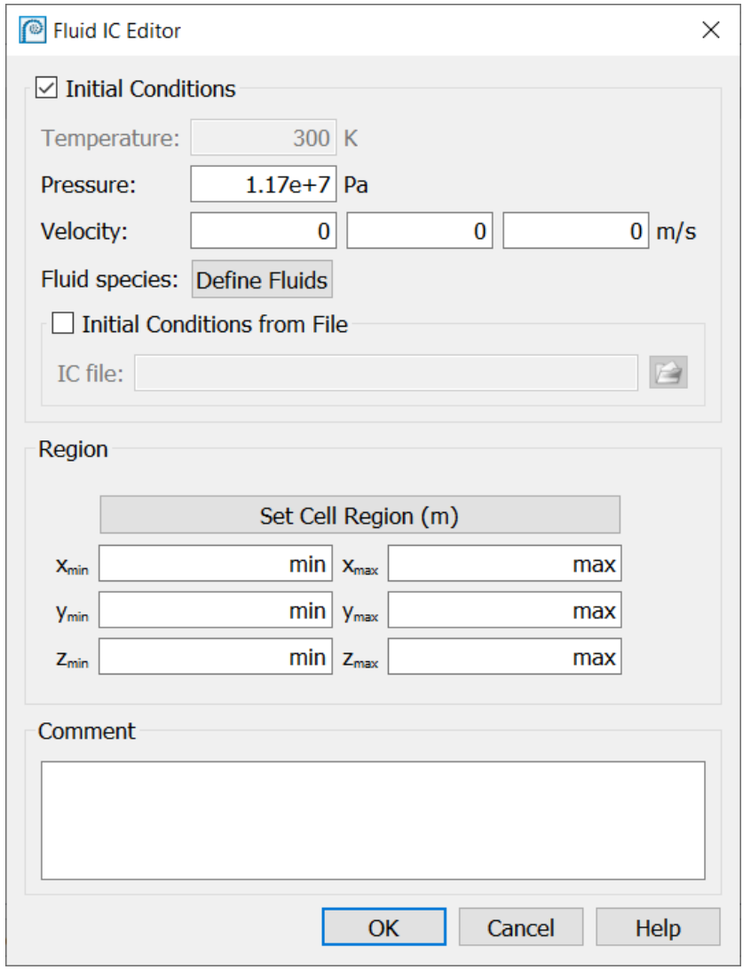
- Click on Add Bubble
- 100% H2(G)
- 400-1500 micron diameter
- Specify a close pack volume fraction of 0.85
- Use Tomiyama-Roghair drag model

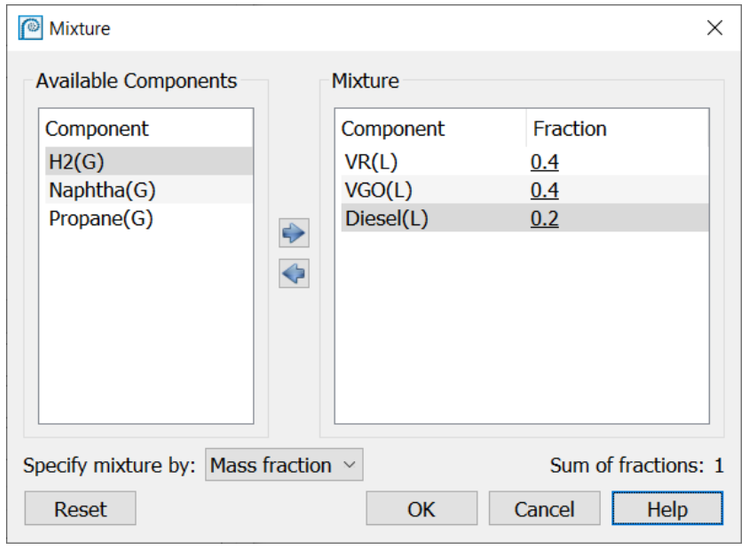


Fluid ICs

Fluid IC

- Pressure = 1.17e+7 Pa
- Fluid species mass fractions
  - 0.4 VR(L)
  - 0.4 VGO(L)
  - 0.2 Diesel(L)



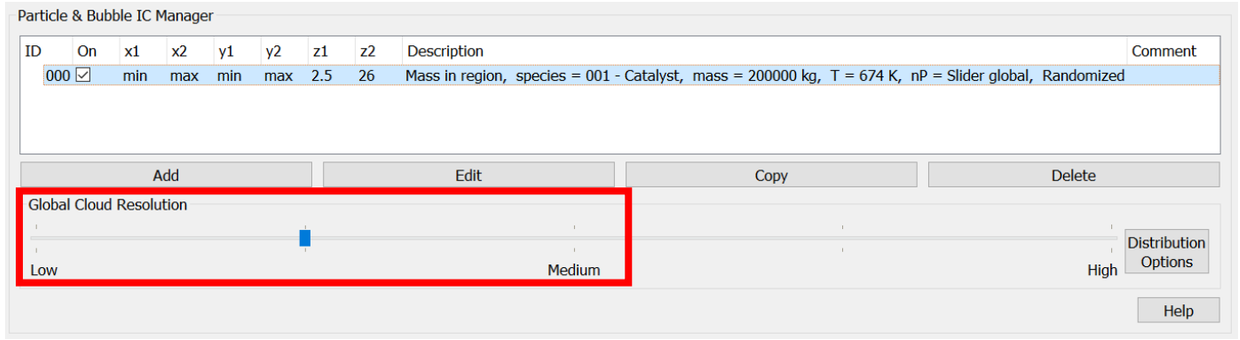


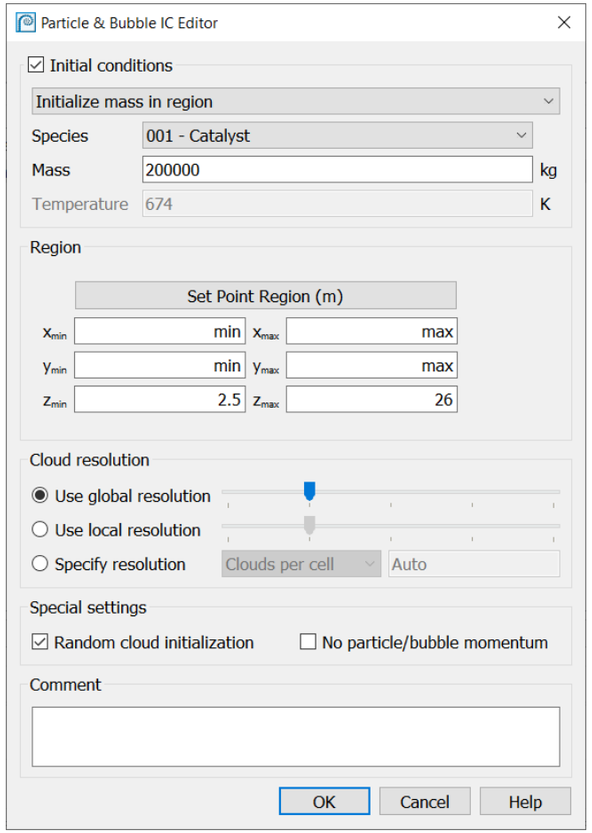
Particle & Bubble ICs

Set the Global Cloud Resolution between Low and Medium

Catalyst Particle IC

- Click on Add
- Initialize mass in region
- Species = 001 - Catalyst
- Mass = 200,000 kg
- Region
  - min, max for x-direction
  - min, max for y-direction
  - 2.5, 26 for z-direction
- Use global resolution





Pressure BCs

Add a pressure BC with information shown here for the outlet

Use 100% VR(L) for Applied Fluids

Pressure BC Editor

Location | Flux Plane | Fluid | Particles/Bubbles | Tracers

Region

Select region (m)

x_{min} min x_{max} max

y_{min} min y_{max} max

z_{min} max z_{max} max

Direction

- x-direction
- y-direction
- z-direction

Pressure BC Editor

Location | Flux Plane | Fluid | Particles/Bubbles | Tracers

Name: FLUXBC_pressure_outlet

Fluid species behavior:

Mass flow rate

Bin by particle/bubble size 100 bins

Output raw particle/bubble data

Output tracer data

Pressure BC Editor

Location | Flux Plane | Fluid | Particles/Bubbles | Tracers

Behavior at Boundary

- No outflow
- Outflow with size filtering:
  - Minimum: 0
  - Maximum: UNLIMITED
  - Units: micron-diameter
- Feed specified as volume fraction
- Feed specified as mass flux
- Feed specified as mass flow rate

Feed Settings

Edit Feed | Feed Control

Comment:

OK | Cancel | Help

Pressure BC Editor

Location | Flux Plane | Fluid | Particles/Bubbles | Tracers

- Off
- Use BC Connector data
- Tracer feed
  - Species: 2000
  - Resolution: 100

Comment:

OK | Cancel | Help

Pressure BC Editor

Location | Flux Plane | Fluid | Particles/Bubbles | Tracers

Flow Conditions

- Transient file: outlet_pressure.sff Edit
- Specify values:

Pressure Boundary Conditions Editor

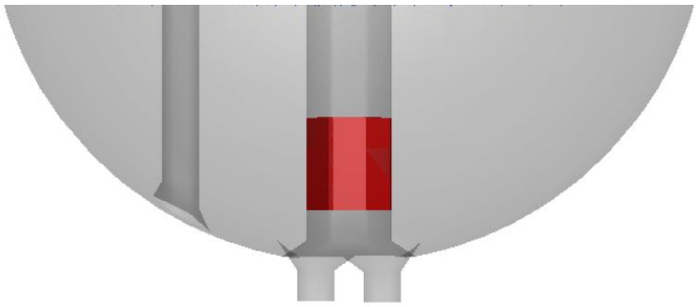
	Time (s)	Pressure (Pa)	Temperature (K)	Area Fraction	Particle Feed	K-Factor
1	0	1.17e7	674	1	On	0
2					On	

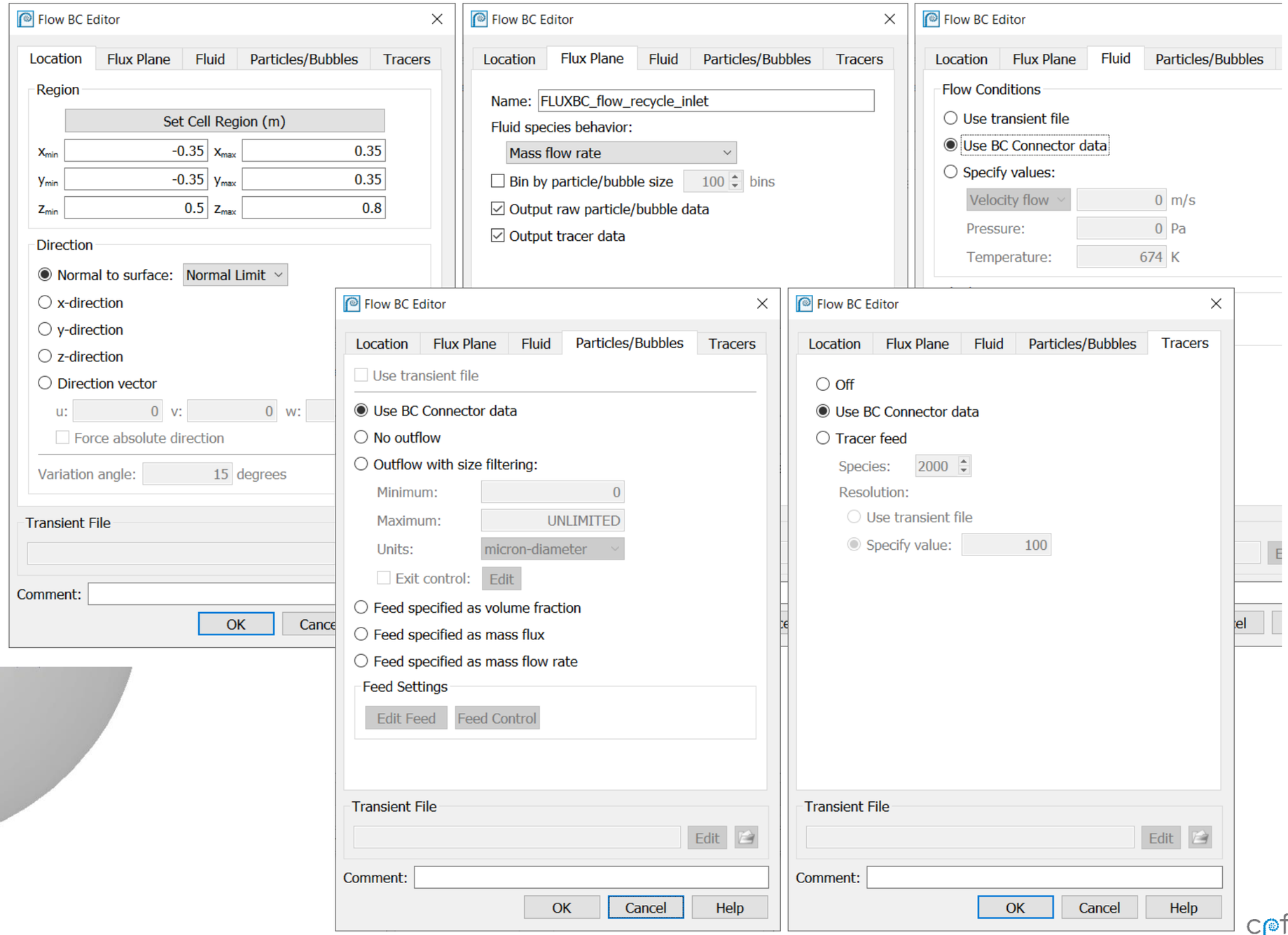
Add Row | Delete Row | Check Data | Graph | Update Simulation

File: outlet_pressure.sff | Save | Save As | Close | Help

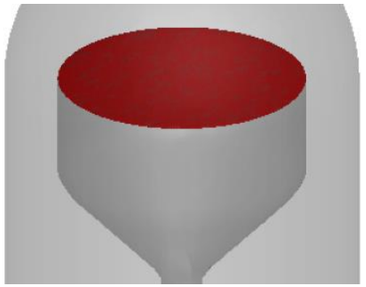
Flow BCs

Add flow BC with information shown here for liquid recycle inlet under the baffle distributor



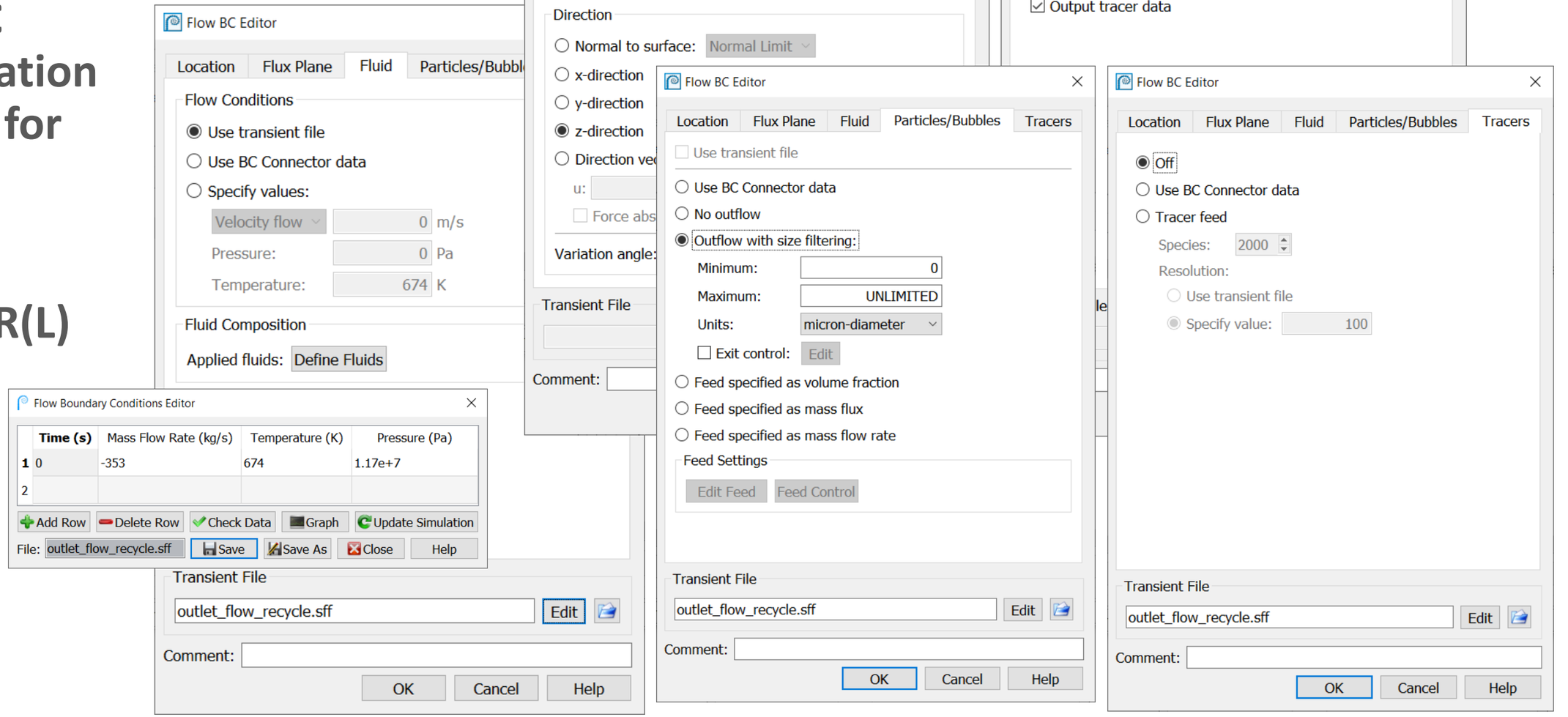


Flow BCs

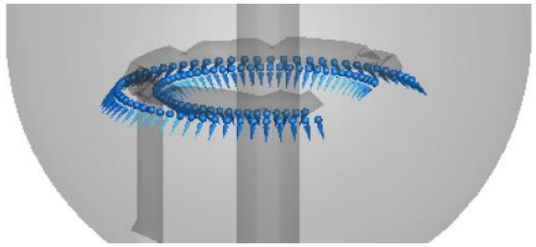


Add flow BC with information shown here for recycle pan outlet

Use 100% VR(L) for Applied Fluids



Injection BCs



Add H2 bubble injection BC

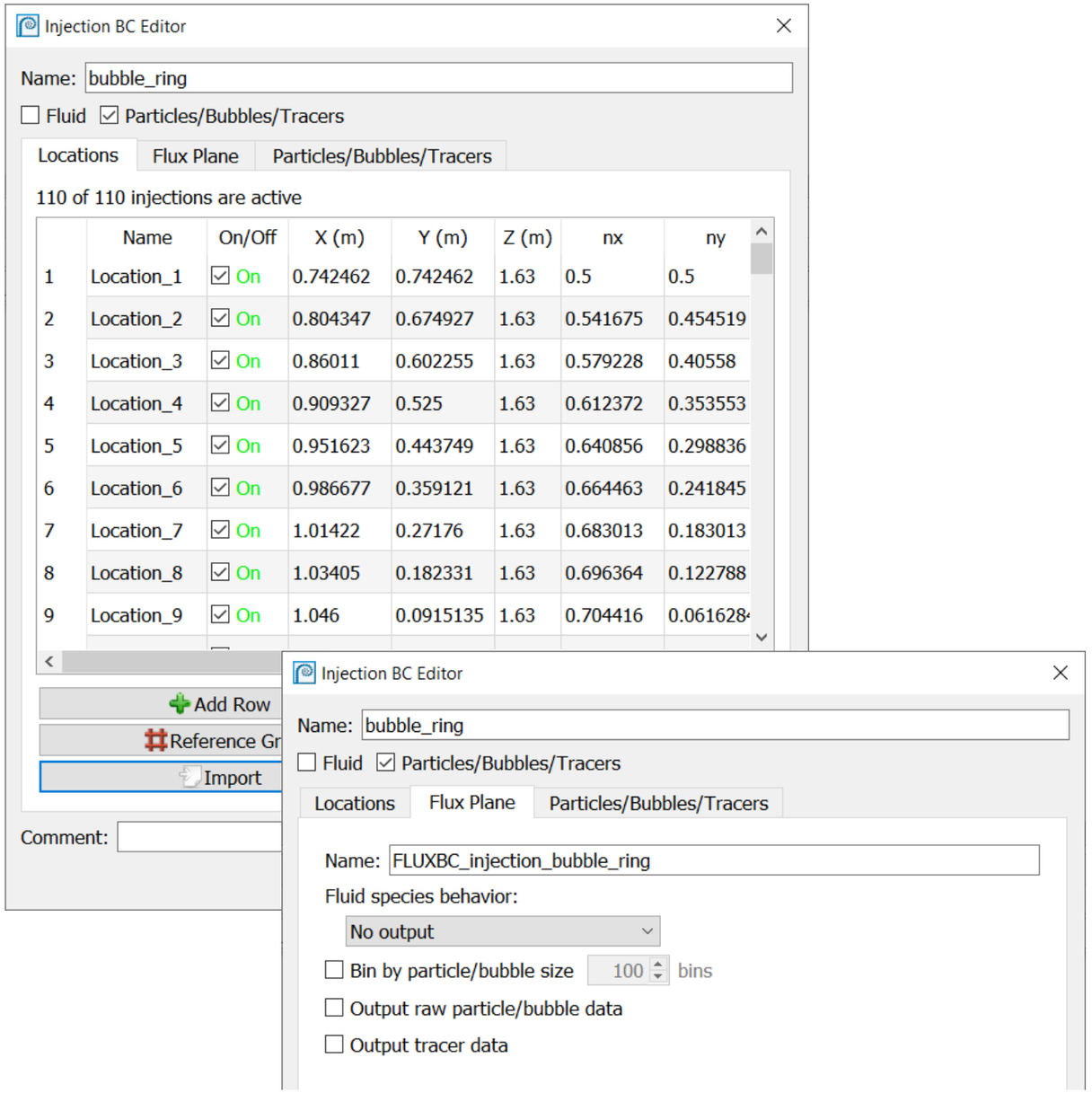
- Name = bubble_ring
- Select Particles/Bubbles/Tracers

Locations tab

- Import bubble_ring_locations.csv

Flux Plane tab

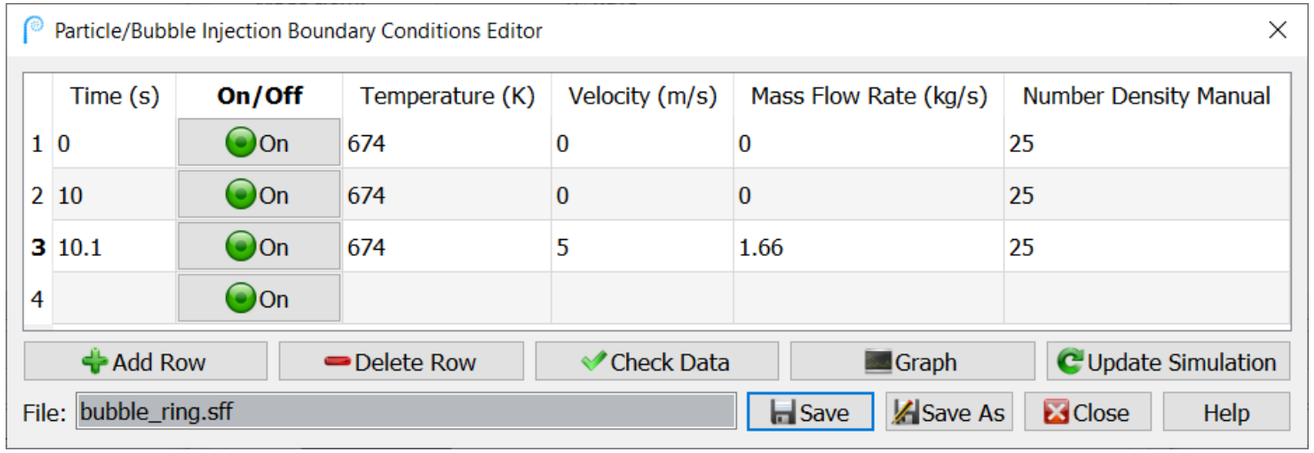
- Add a flux plane name

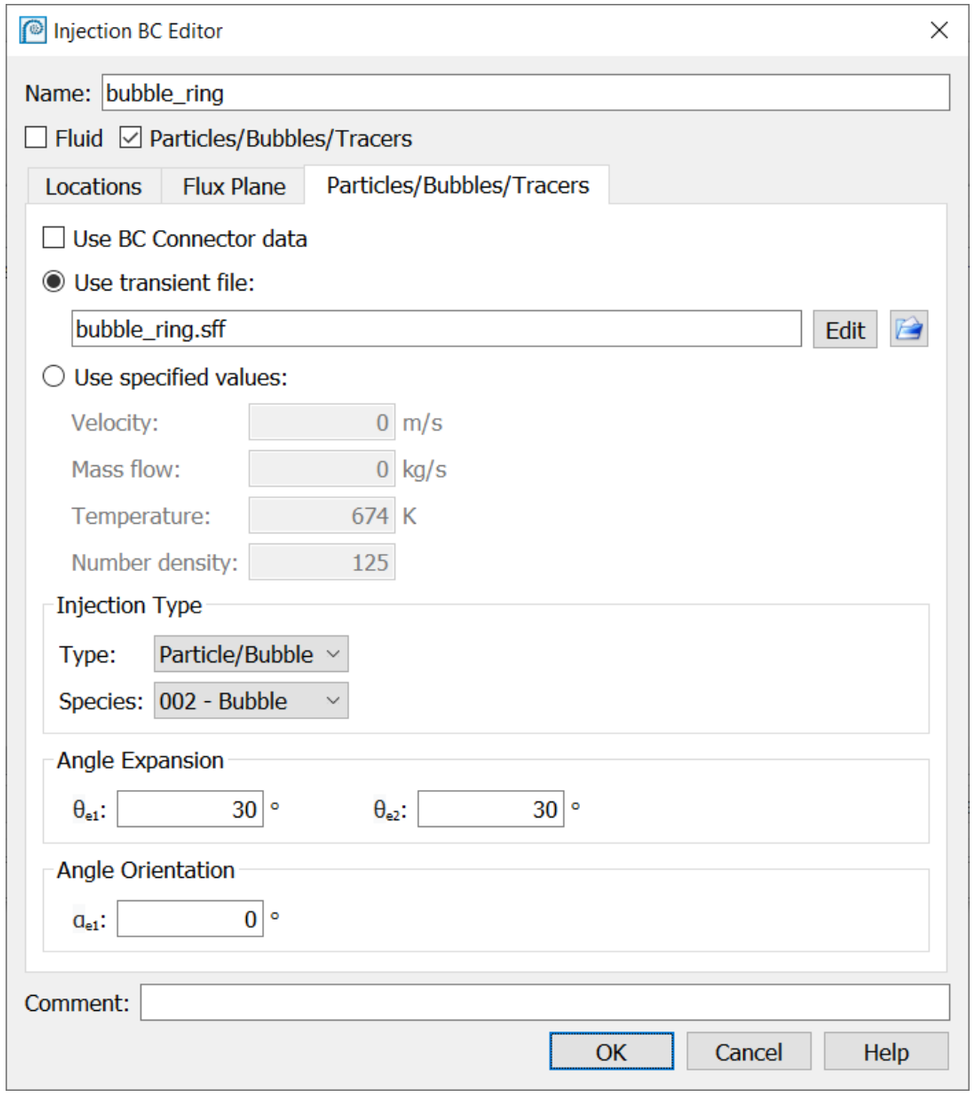


Injection BCs

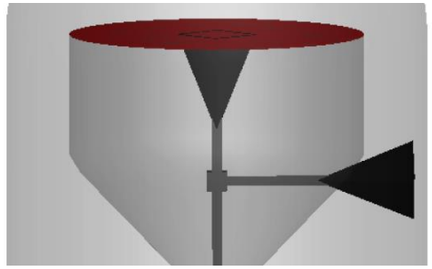
Particles/Bubble/Tracers tab

- Set up transient file as shown, turning on bubble flow after 10 seconds
- Select 002 - Bubble
- Set the Angle Expansion to 30˚





Secondary Feeds



Add secondary feed to use with BC Connector

- Select Fluid and Tracers

Flux Plane tab

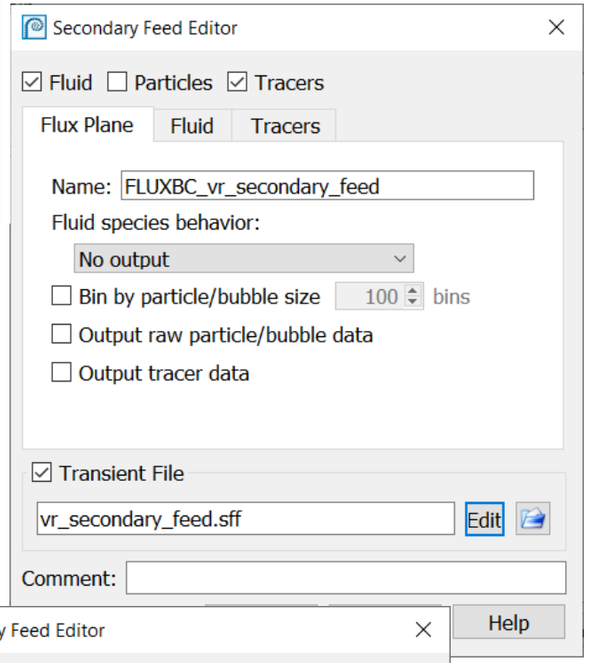
- Add flux plane name
- Set up transient file as shown

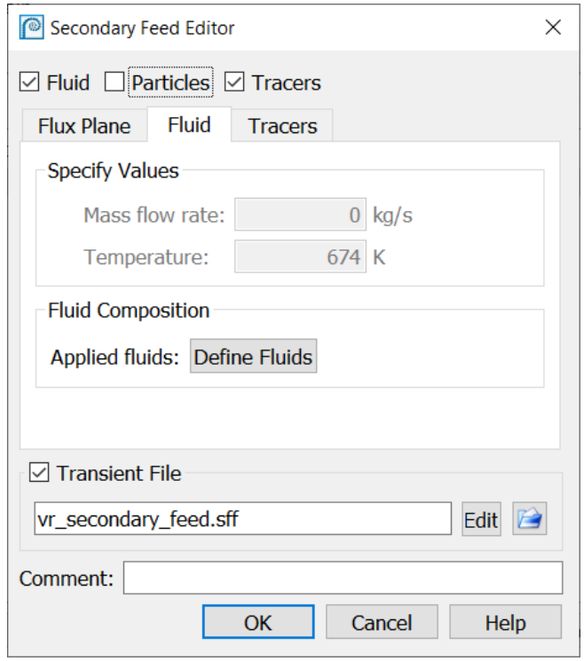
Fluid tab

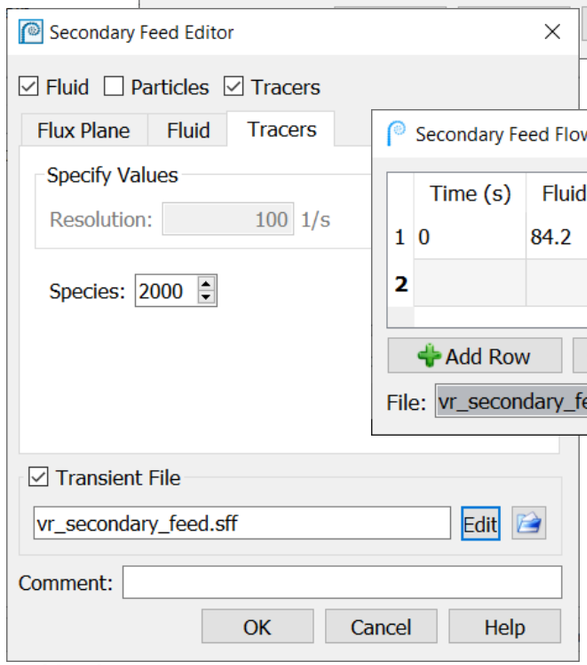
- 100% VR(L) for Applied Fluids

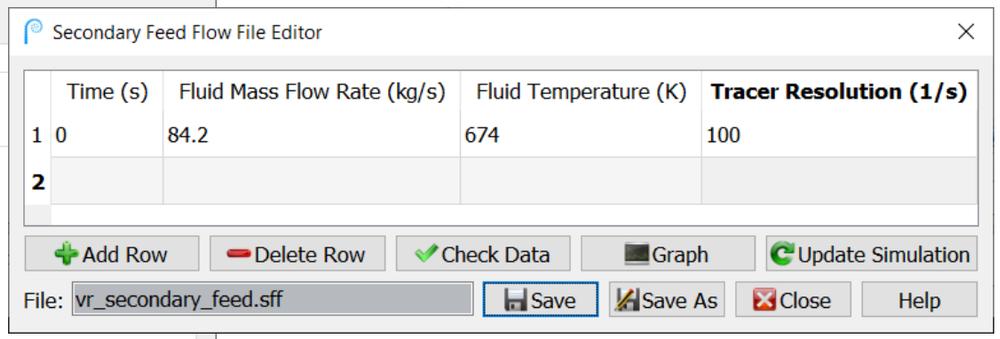
Tracers tab

- Verify species is set to 2000









BC Connectors

Add BC Connector

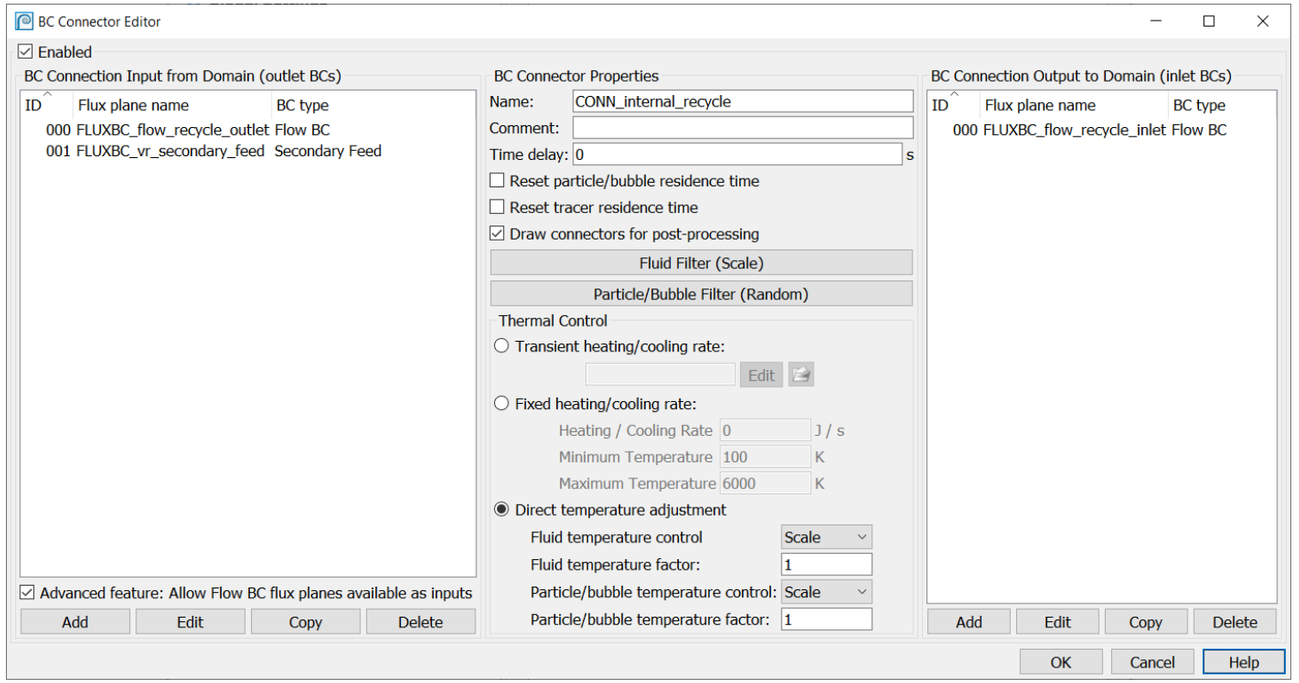
- Name = CONN_internal_recycle
- Select Draw connectors for post-processing

Input

- Select Advanced feature: Allow Flow BC flux planes available as inputs
- Add Flow BC
- Add Secondary Feed

Output

- Add Flow BC



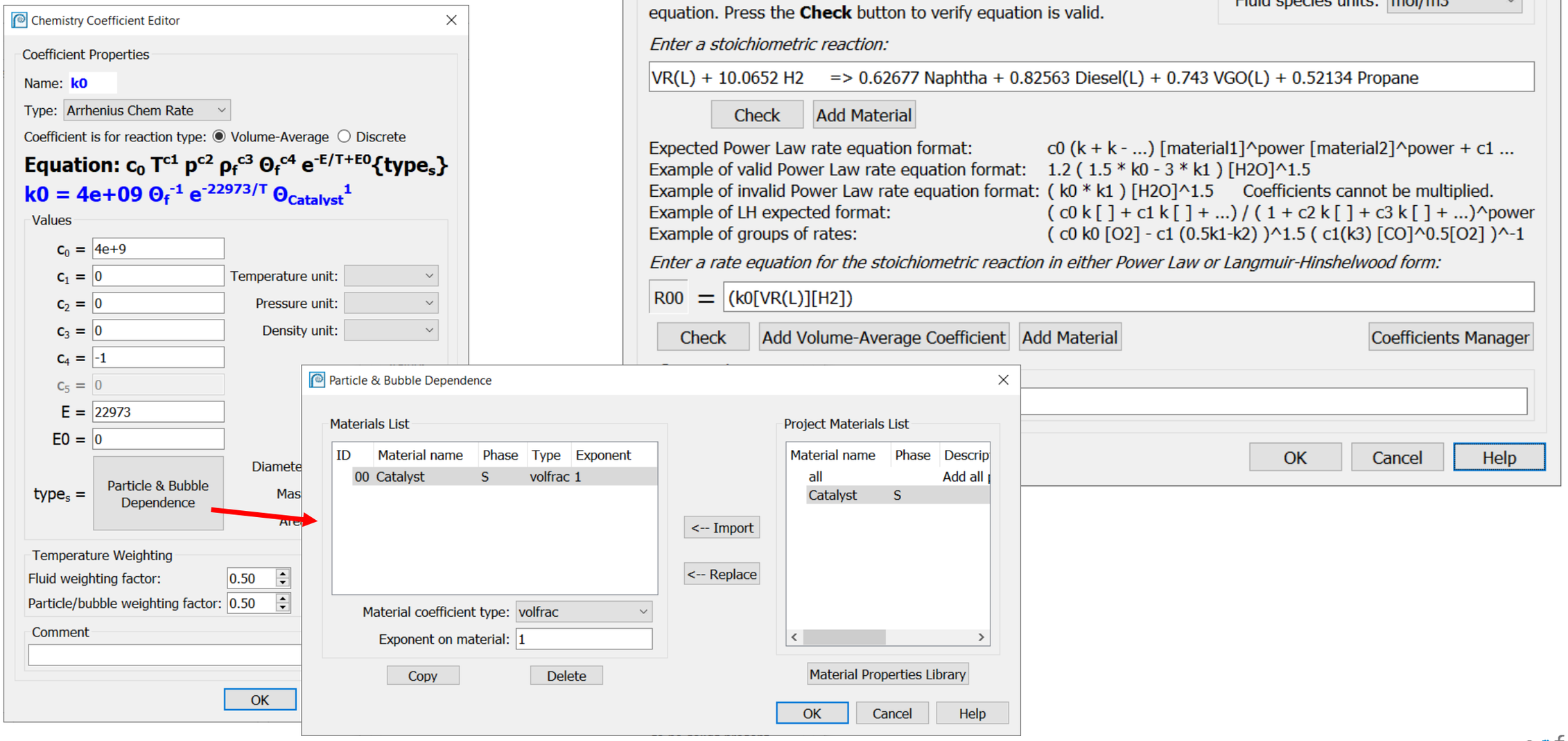
Reaction Chemistry

The kinetics have been adapted from Stratiev et al (2019). This model assumes that the vacuum residue reacts with the hydrogen gas bubbles to form Naphtha, Diesel, Vacuum Gas Oil (VGO), and Propane.

Take note of the following when defining your chemistry:

- Volume average will be used with these units
  - Reaction rate: $mol/m^3/s$
  - Fluid species: mol/m^3
- One rate coefficient and one reaction will be defined as shown on the next slide

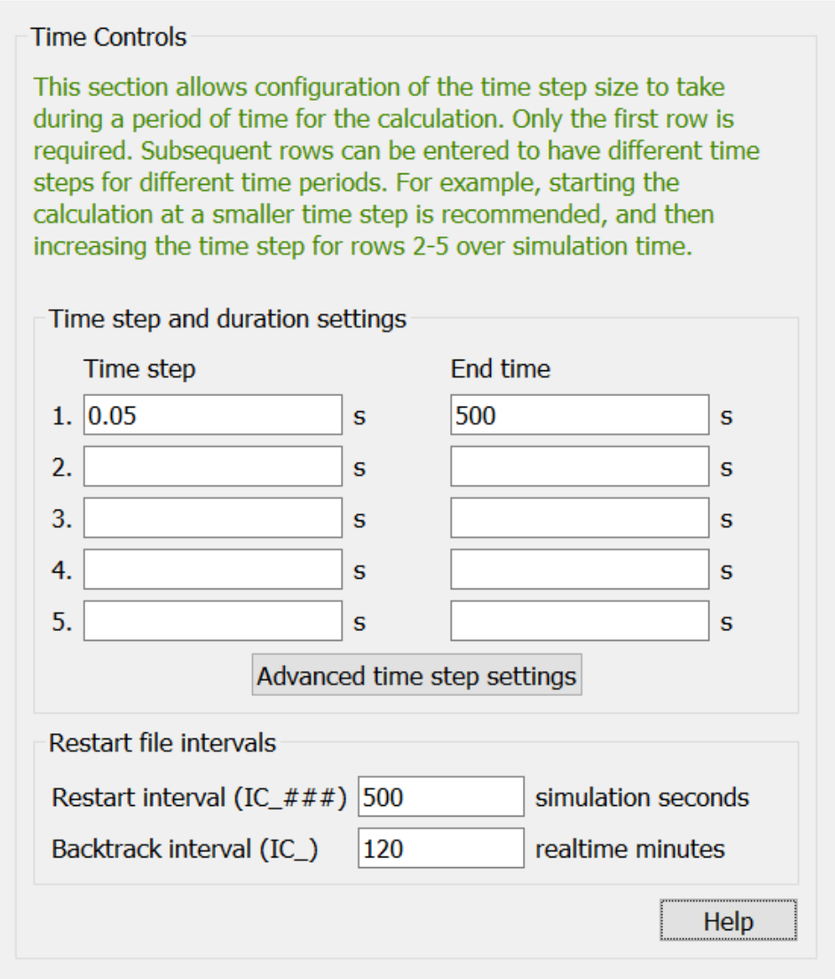
Reaction Chemistry



Time Controls

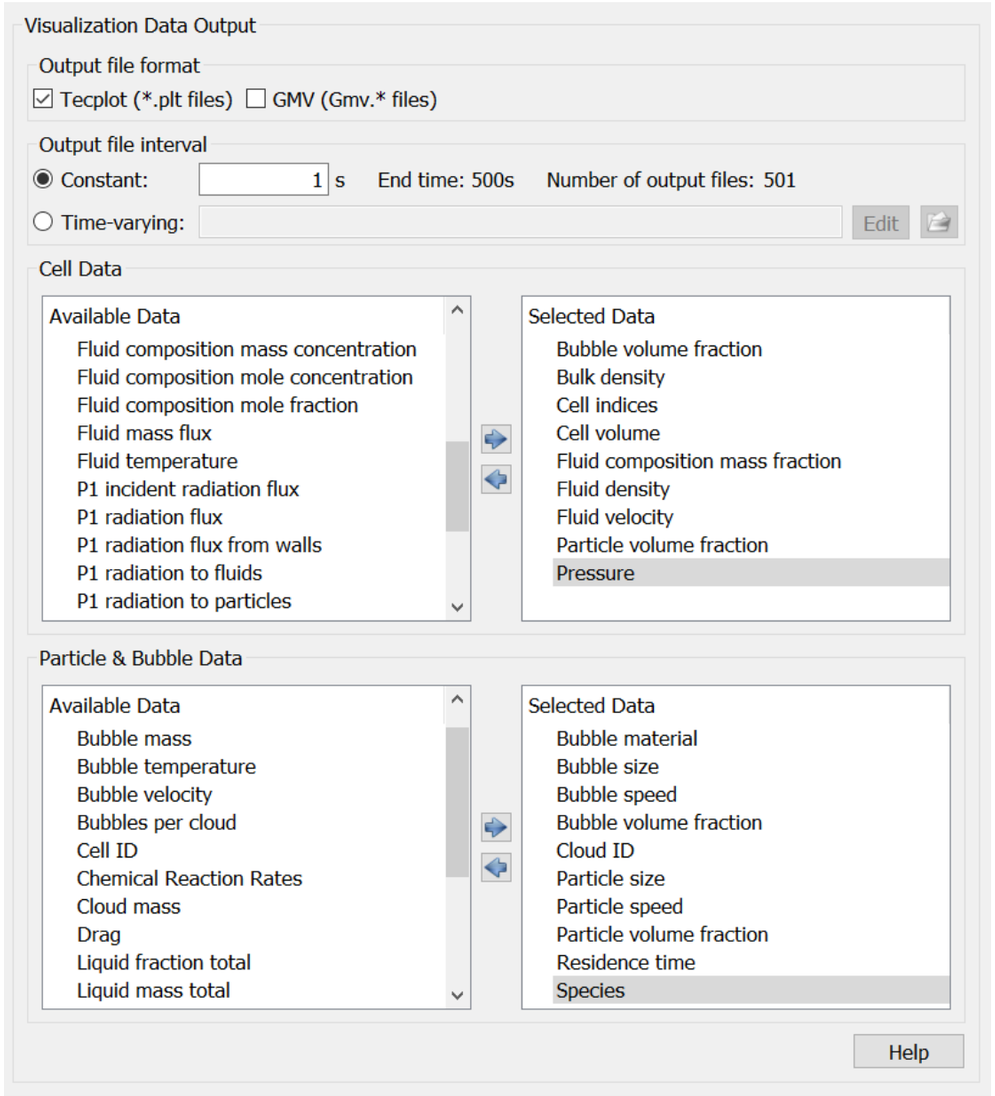
Set Time step and End time

Set Restart intervals



Visualization Data Output

Set Output file interval and select options shown for Visualization Data Output



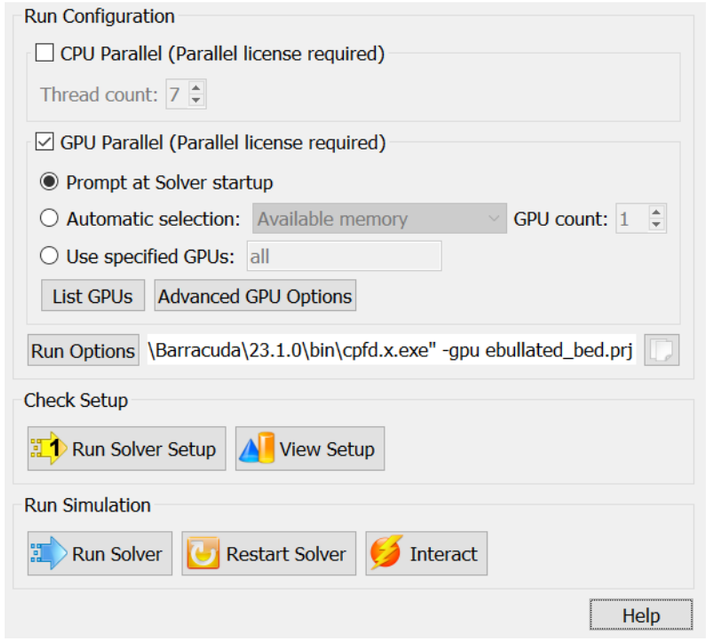
Run

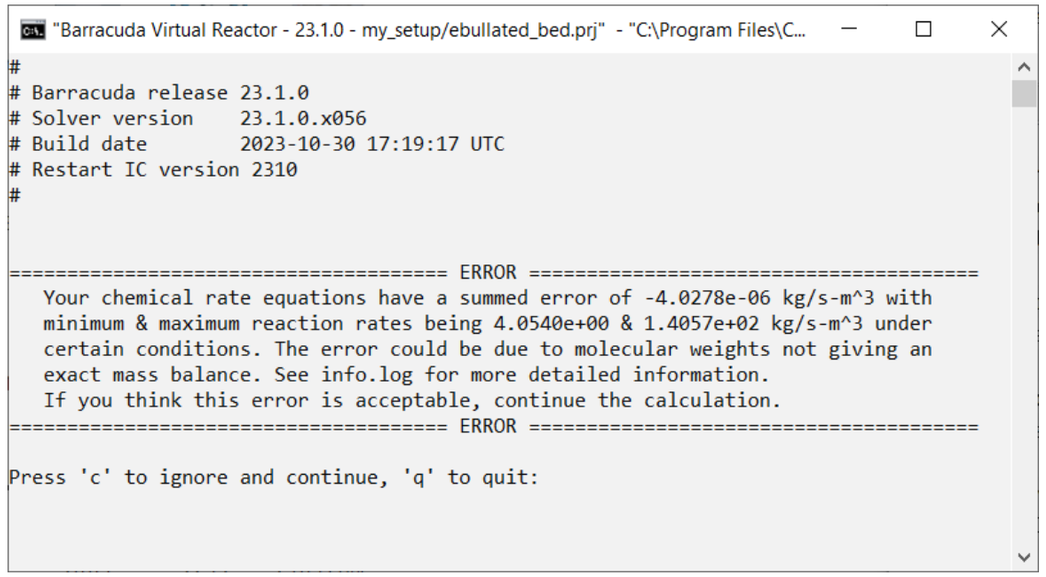
If NVIDIA GPU card is available, select GPU Parallel

Run Solver Setup and View Setup

Once you have checked the setup, Run Solver to start the simulation

Due to the complexity of the chemistry, the following error may pop up when the solver starts up. It is safe to press ‘c’ to ignore this error.





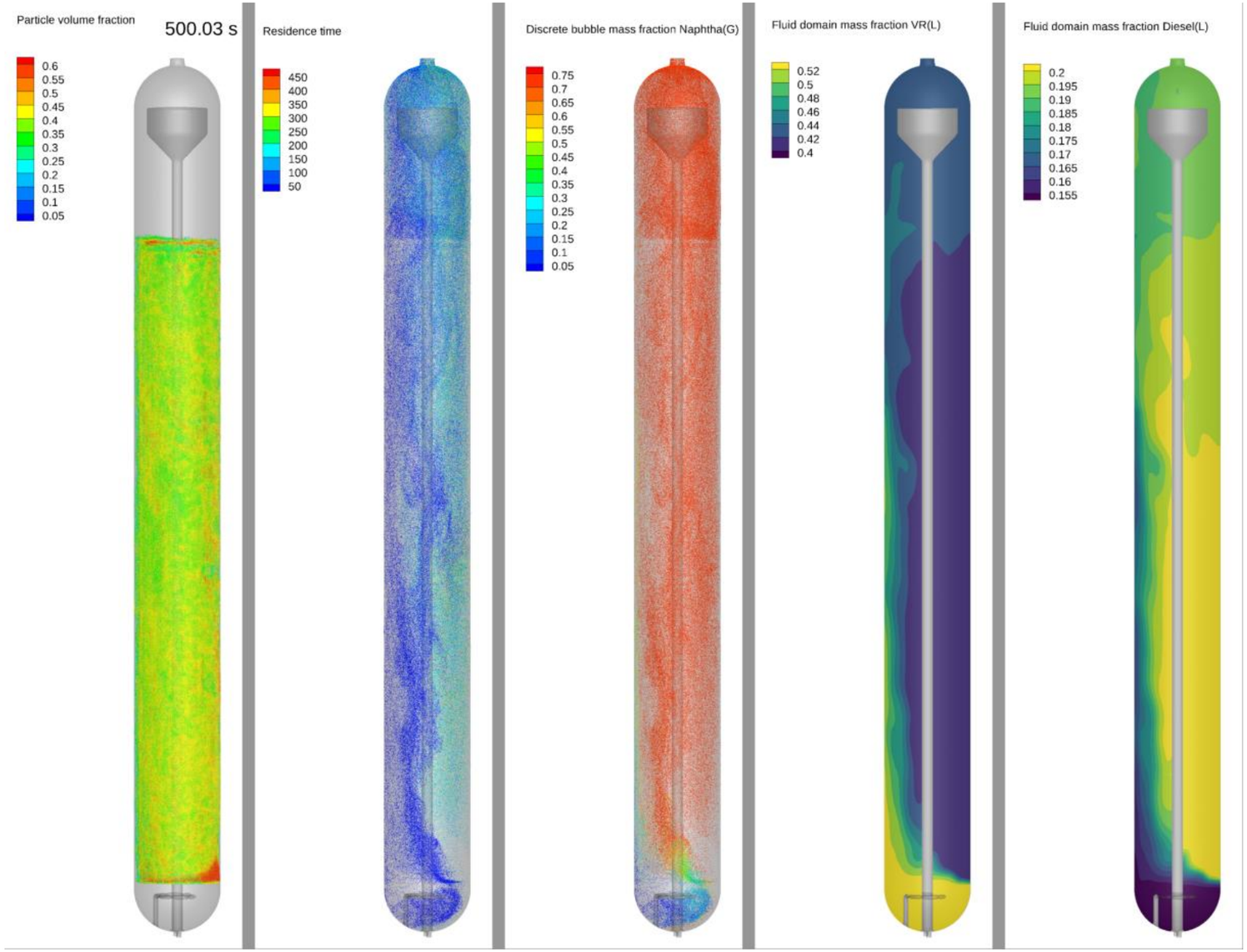
Post-Processing

Create a 5 frame view of the ebullated bed behavior as shown to the right

Specific hints for obtaining the desired views are on the following slides

Also see the following videos:

- Frames
- Slices
- Contour legend

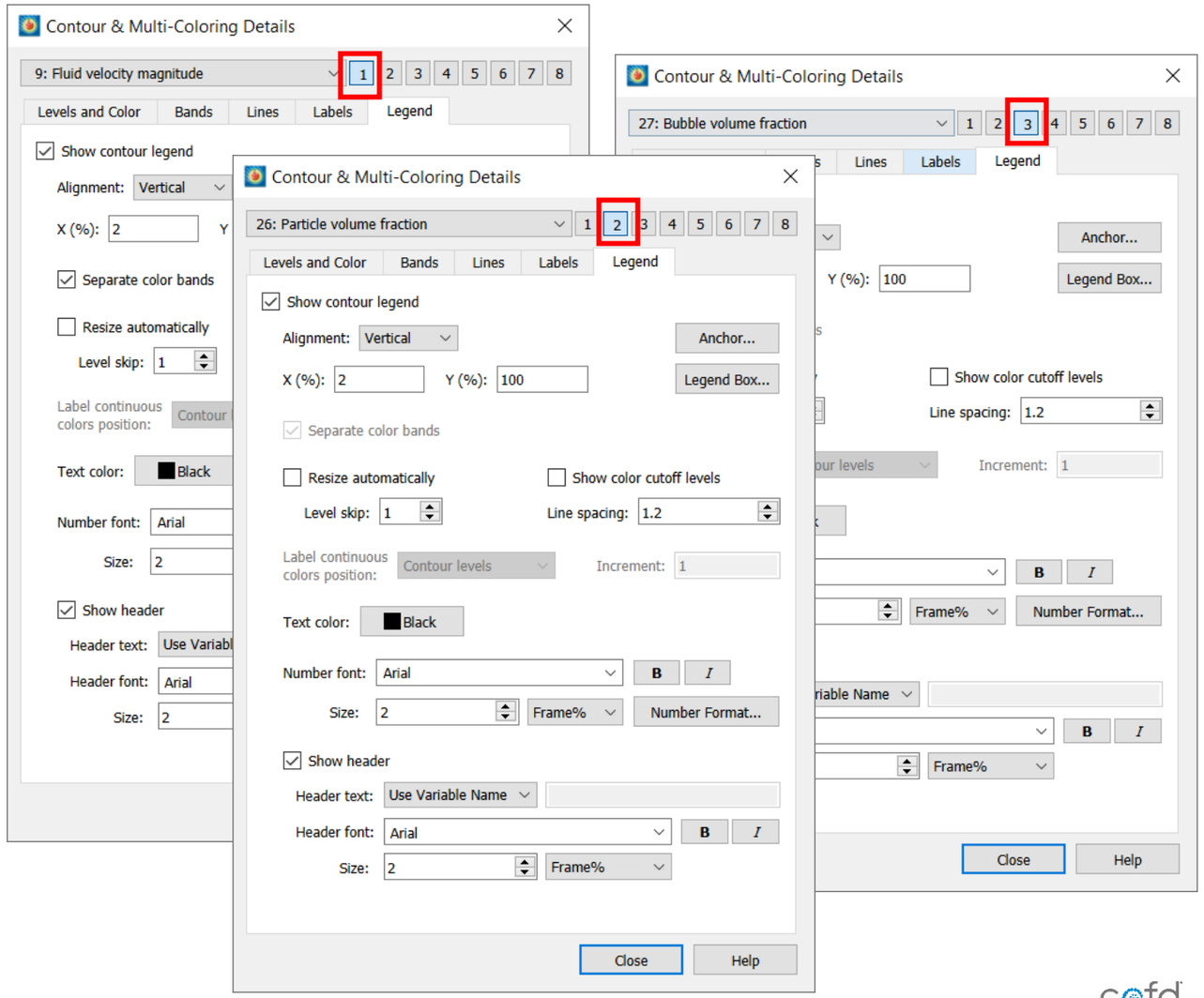


Using Contour Groups

When using fluid, particles, and bubbles in Barracuda, the contour groups in Tecplot become more important.

- Fluid is contour group 1
- Particles are group 2
- Bubbles are group 3

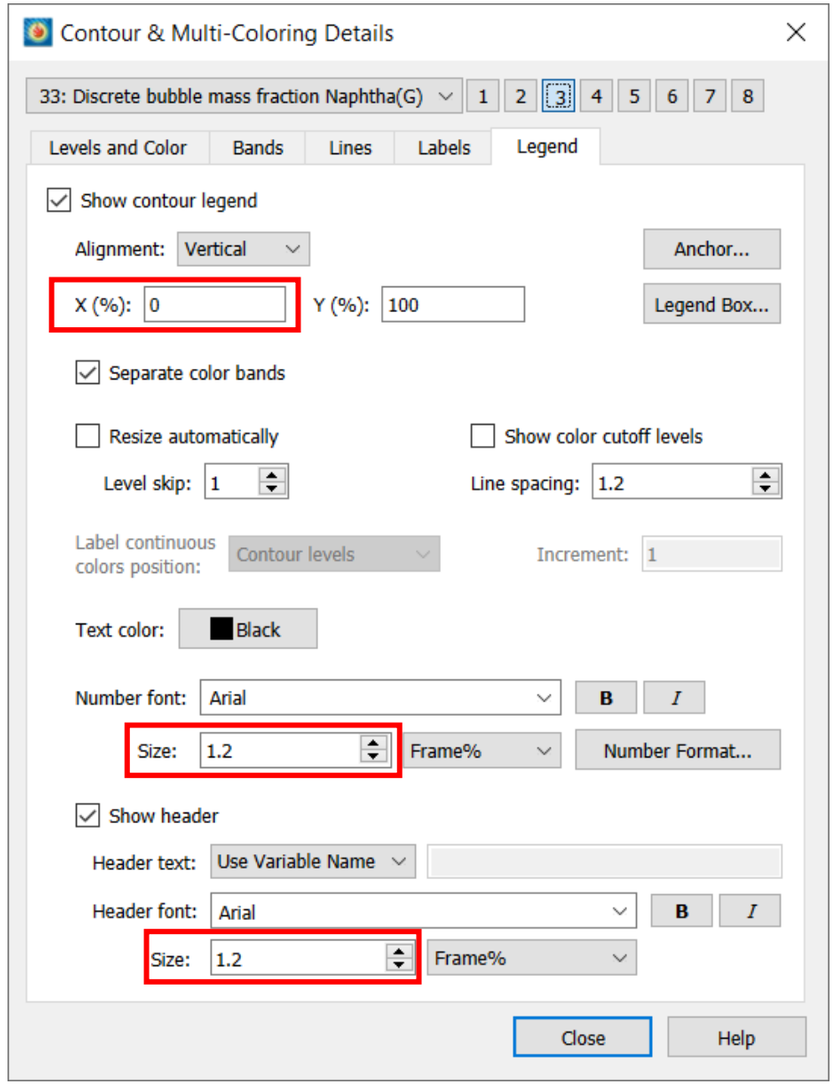
For views with multiple frames, ensure that the group is correct when adjusting the frame contour legend

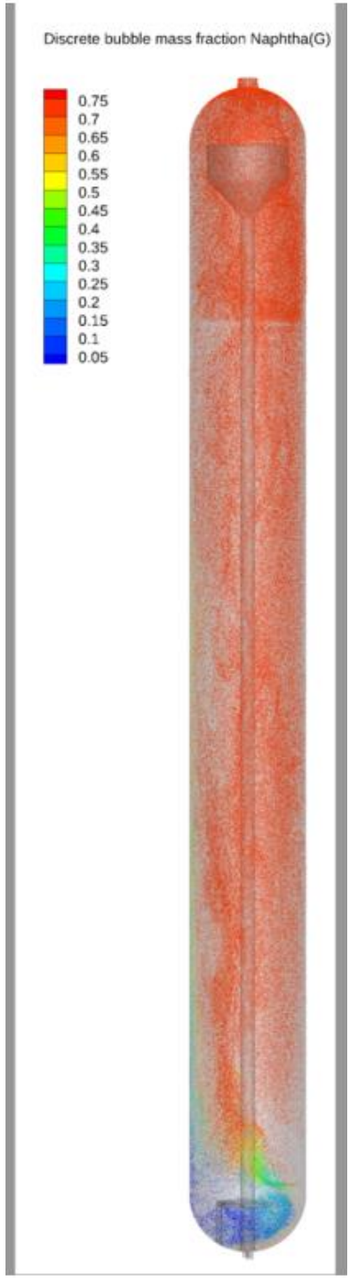


Adjusting Legend Text Sizes

When using multiple frames in a view, the text size may need to be adjusted. To do this:

- Legend tab of Contour editor
- Set X(%) to 0
- Adjust size of “Number font” and “Header font” until the legend label fits the size of your frame





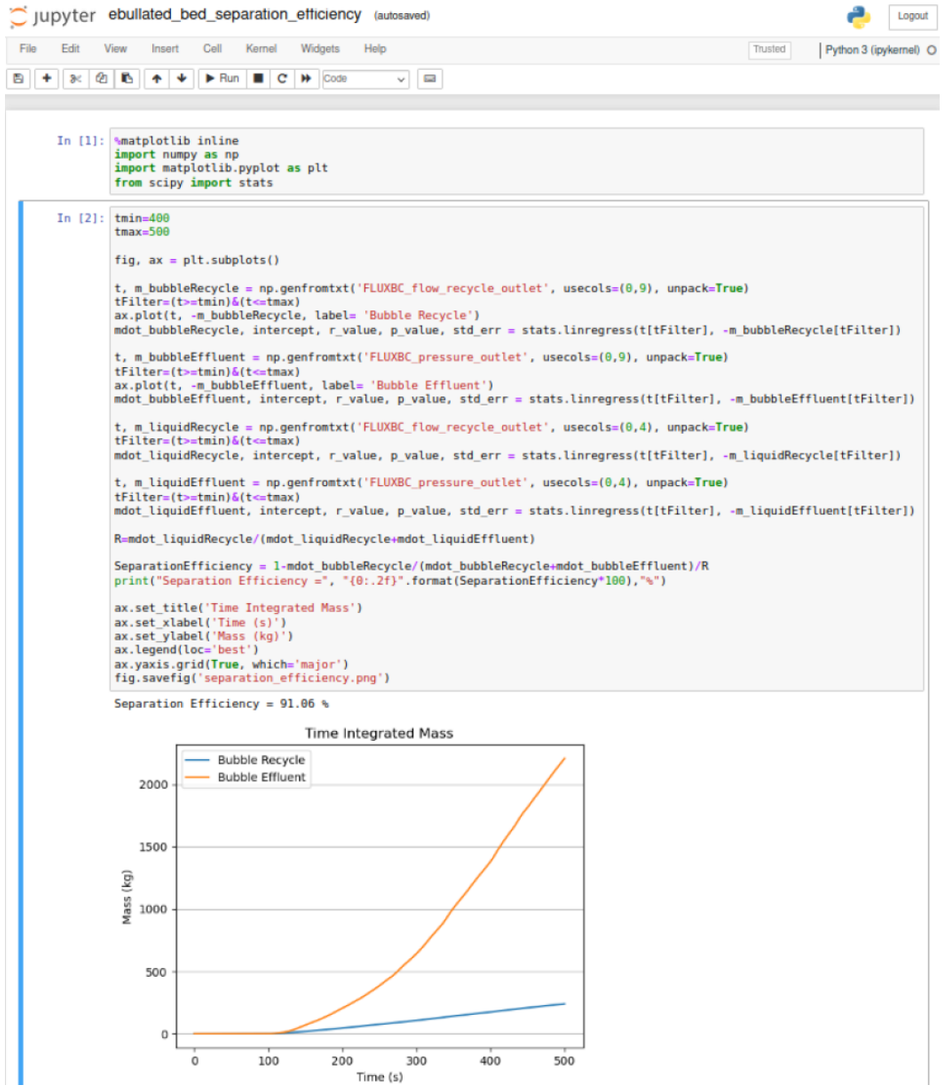
Post-Processing: Separation Efficiency

The separation efficiency of the reactor can be calculated using the included Jupyter notebook:

`ebullated_bed_separation_efficiency.ipynb`

Helpful support site posts:

- Using Jupyter Notebook
- Installing Anaconda Python



Post-Processing: Calculating Fluid Residence Time

Tracers were introduced in the secondary feed of VR(L). This support post shows how to create a histogram of fluid residence time using tracers.

https://cpfd-software.com/using-tracers-in-a-barracuda-virtual-reactor-model/

jupyter 2022-12-01_tracer_residence_time (autosaved)

Logout

File Edit View Insert Cell Kernel Widgets Help

Not Trusted | Python 3 (ipykernel)

Run Code

In [3]:
```
%matplotlib inline
import matplotlib.pyplot as plt
import numpy as np
```

In [4]:
```
# Example 1: Analysis of tracer residence time at one flux plane

# Gather data from raw tracer flux plane file
fluxPlaneName = 'FLUXBC_pressure_outlet_raw_tracer'
resTimeCol = 4  # Specify column number for residence time here
resTime = np.genfromtxt(fluxPlaneName, usecols=resTimeCol-1)

# Create Histogram of residence time
numBins = 50  # Change this number if you want more or fewer bins
# For more info on histograms, see https://matplotlib.org/stable/gallery/statistics/hist.html
n, bins, patches = plt.hist(resTime, numBins)
plt.xlabel('Residence Time (s)')
plt.ylabel('Tracer Count')
plt.title('Tracer Residence Time Distribution')
plt.show()
```