FCC Riser: Setup and Analysis

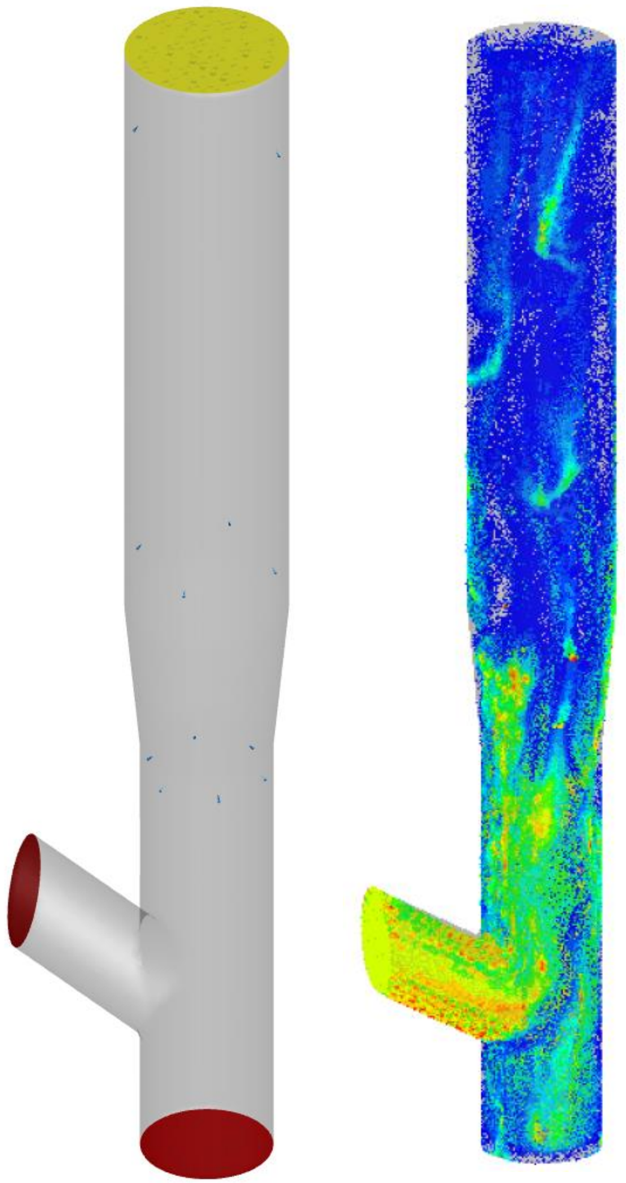
CPFD Software

www.cpfd-software.com

Fluid Catalytic Cracking (FCC) Riser

Model of an FCC Riser used to crack large hydrocarbon molecules into smaller molecules suitable for use in fuels. These reactions take place on the surface of catalyst particles that flow through the riser.

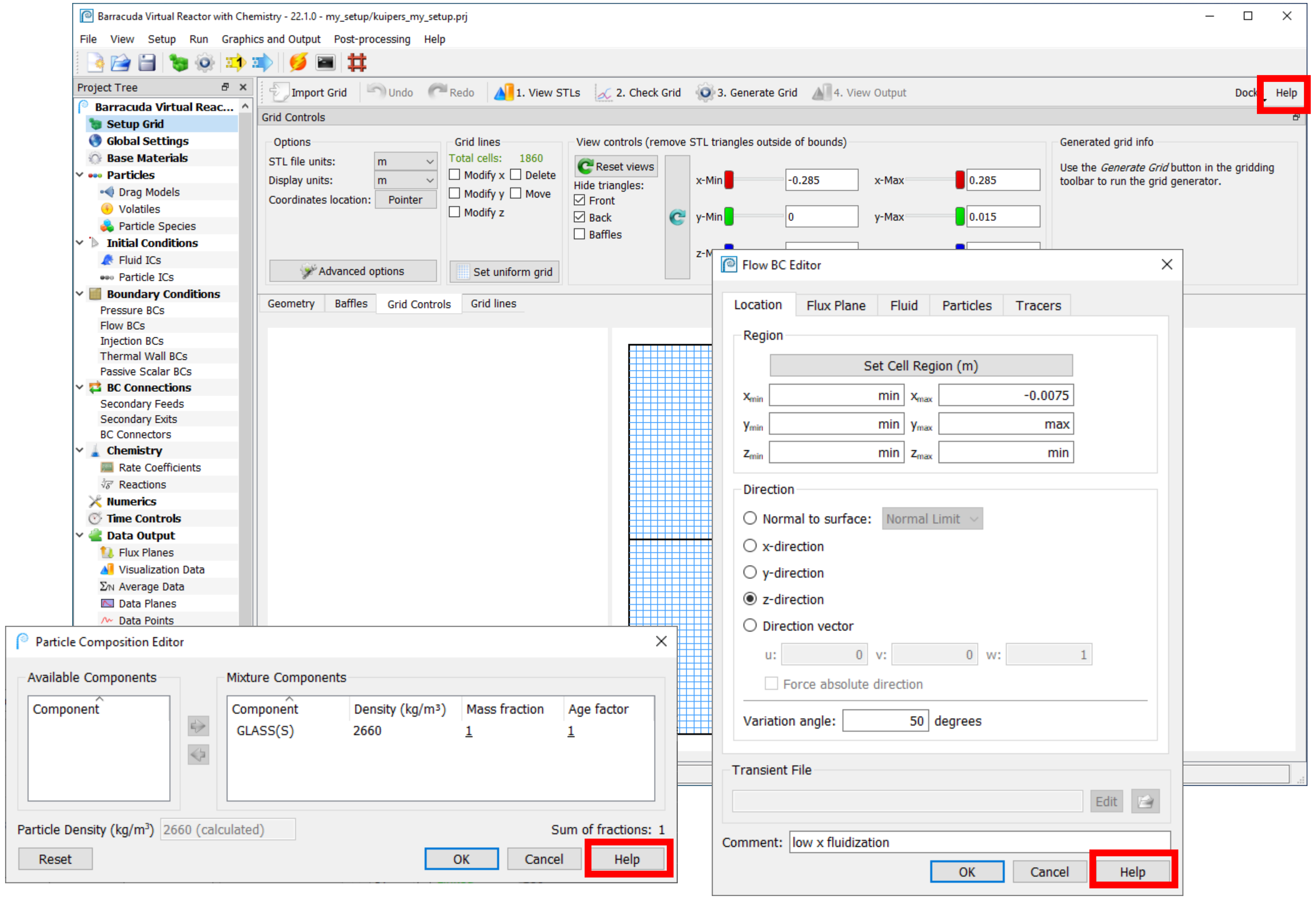
This is a thermal and reacting system with a four-lump model in which the hydrocarbons present are divided into four groups: heavy gas compounds, product gas compounds, light gas compounds, and solid carbon.



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.



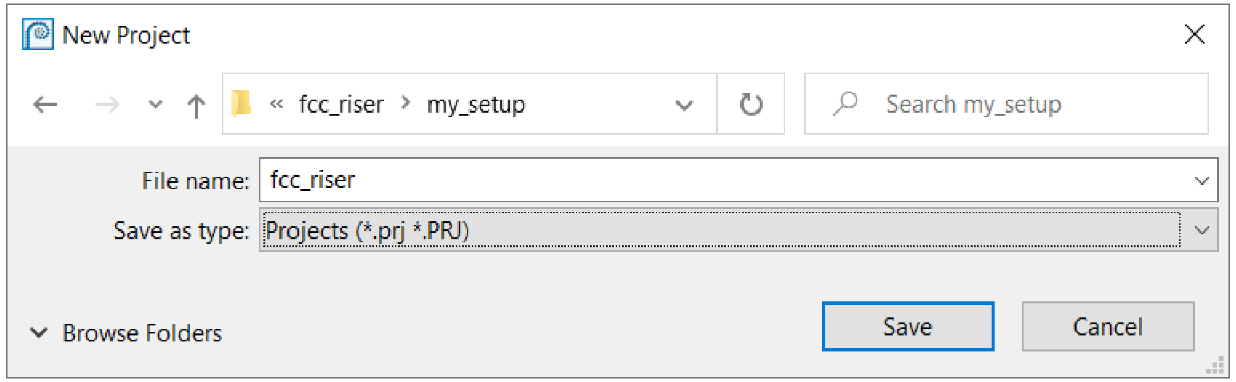
Project File

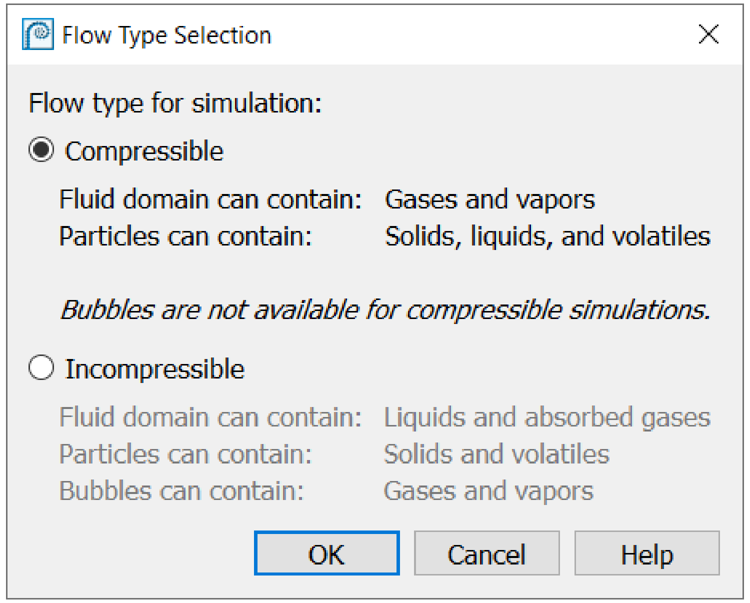
Make a new compressible project file in the supplemental training directory:

\fcc_riser\my_setup

With the project name:

fcc_riser.prj





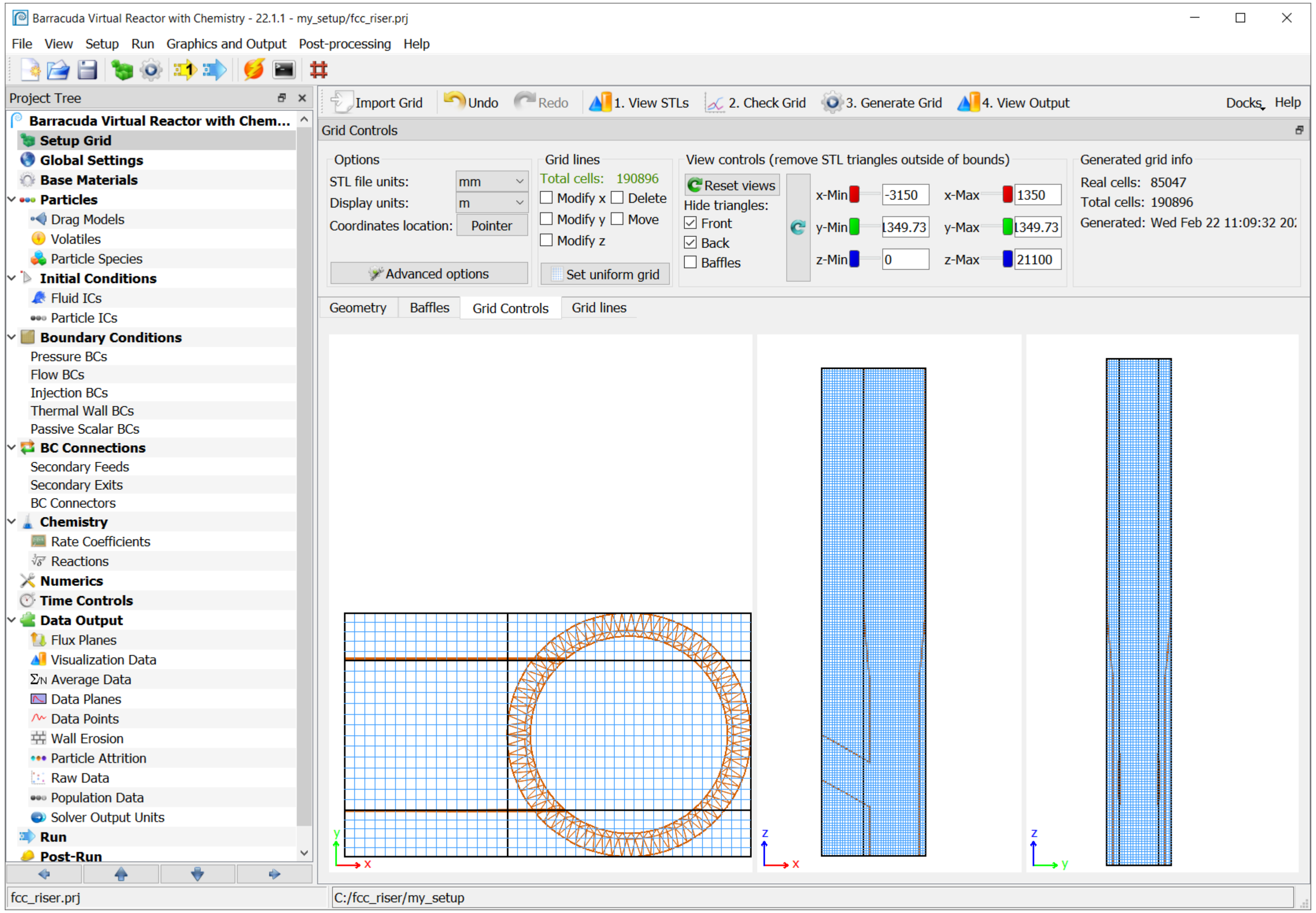
Setup Grid

Geometry tab:

- Add fcc_riser.stl

Grid Controls tab:

- Set STL file units to mm
- Select Merge and remove small cells in Advanced options
- Set uniform grid of 200,000 cells
- Modify x and y grid lines to capture the catalyst inlet pipe

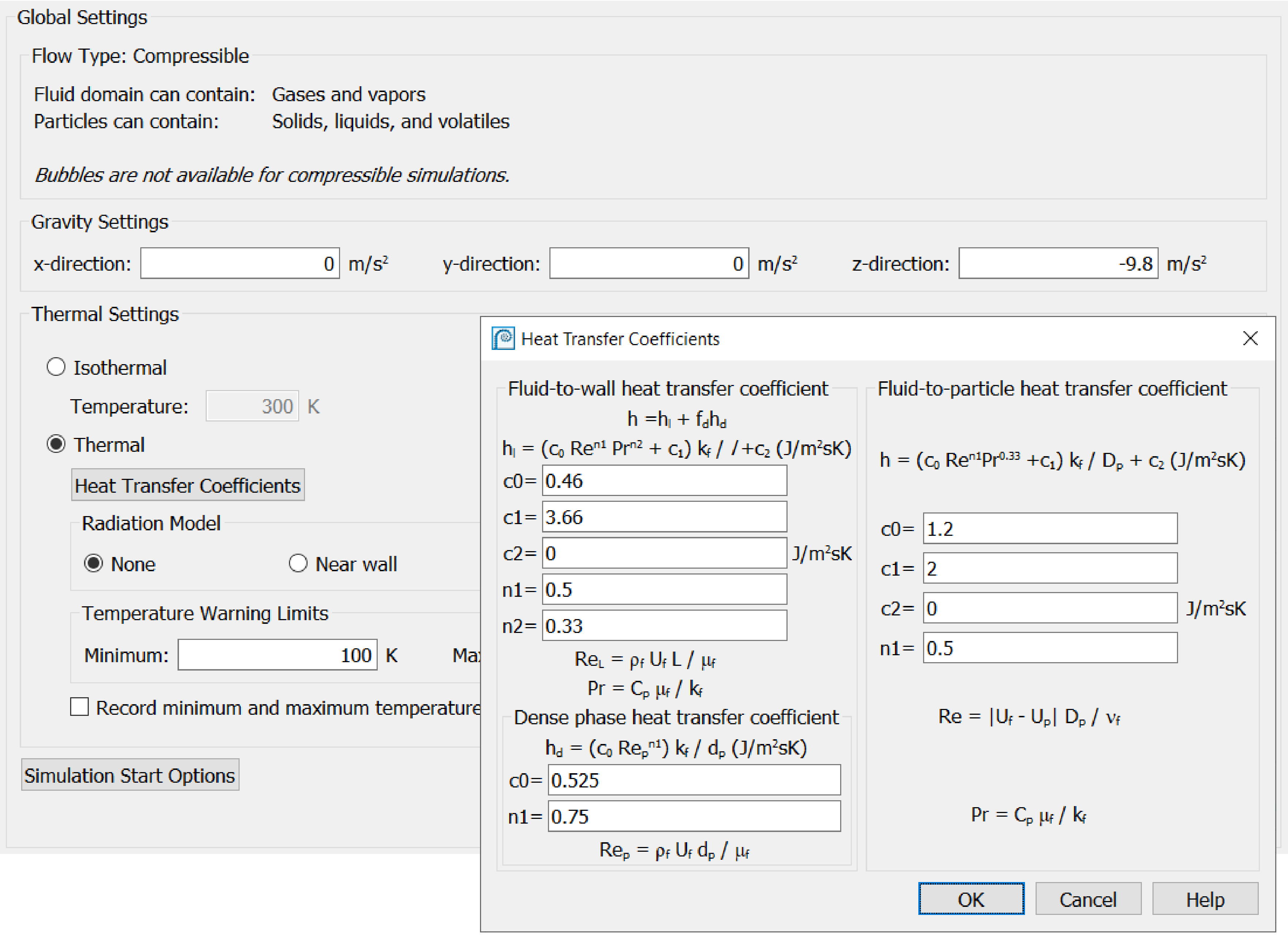


Global Settings

Set Gravity in the z-direction

Select Thermal

Set Heat Transfer Coefficients as shown for Fluid-to-particle



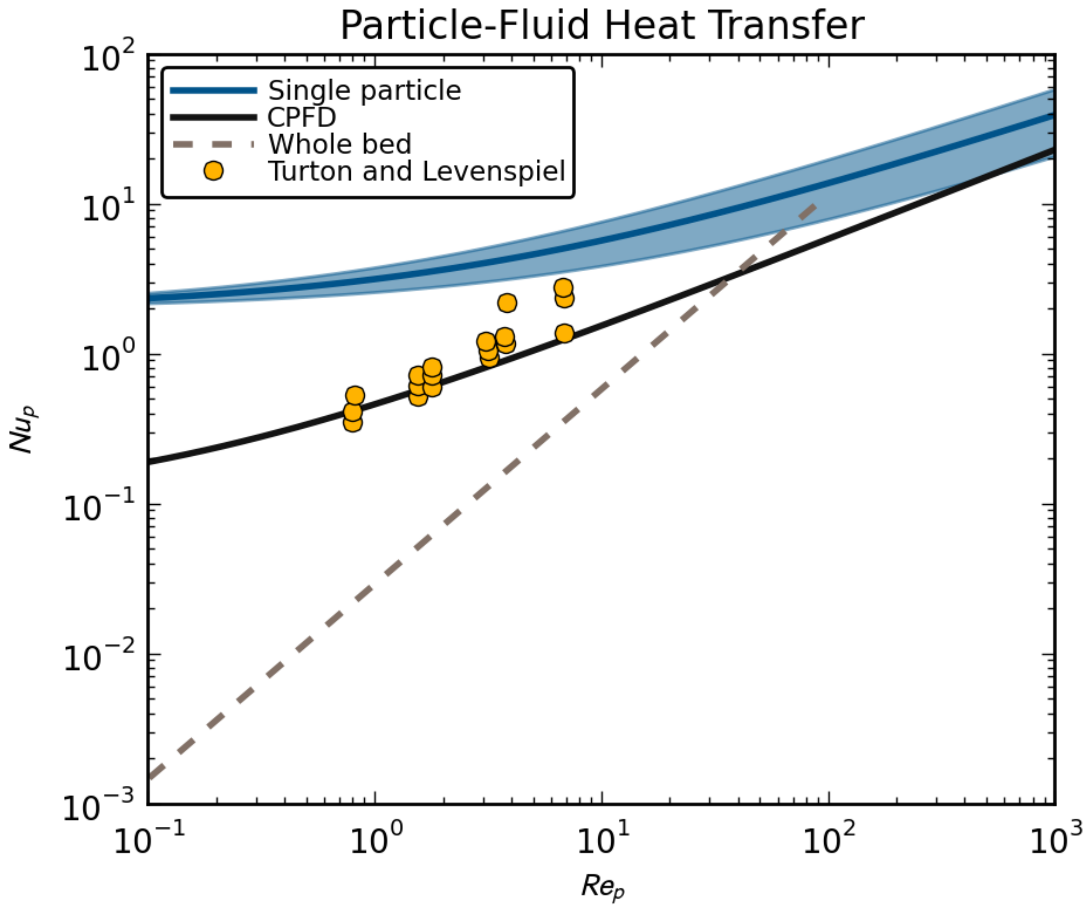
Heat Transfer Coefficients

In this thermal and reacting problem, particle – fluid heat transfer is an important consideration and a different heat transfer correlation is occasionally used for FCC catalyst.

$$Nu_p = \frac{h\, d_p}{k_f} = 2 + 1.2Re^{0.5}Pr^{0.33}$$

Use the single particle Nusselt number correlation for Fluid-particle heat transfer recommended by Kunii and Levenspiel in [Fluidization Engineering](#).

Find more info in our support site post:
[Fluid to Particle Heat Transfer in Barracuda](#)

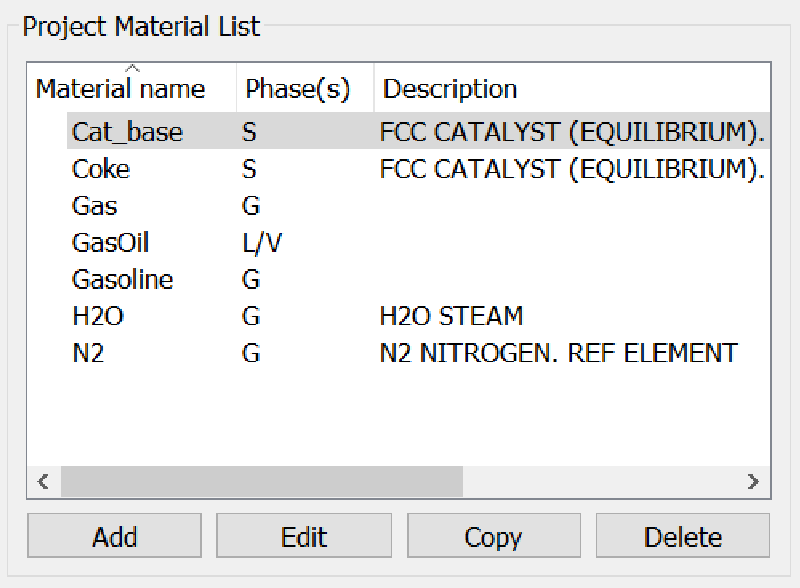


Base Materials

Import H2O and N2 gas from the material properties library

Import SiO2&Al2O3_2 twice and change the following properties:

Name	MW (g/mol)	Density (kg/m^3)
Cat_base	-	1620
Coke	12.5	1200



Add the following materials:

Name	Phase	MW (g/mol)	Density (kg/m^3)	Viscosity (Pa•s)	ΔH_f (J/kg)	Heat Capacity (J/kg/K)	Therm. Cond. (W/m/K)
GasOil*	Liquid/	400	900	5.00E-02	-692000	2798	0.15
	Vapor	400		5.00E-05	-905000	3406	0.025
Gas	Gas	50		1.66E-05	-75000	1040	0.025
Gasoline	Gas	100		1.66E-05	-550000	1040	0.025

* Further material setup is on next slide

Base Materials – Evaporation

To fully define the GasOil as an evaporating droplet within your system, you will need to do the following in the Base Material Editor:

- Enable evaporation model
- Vapor pressure, input the Antoine Equation*:

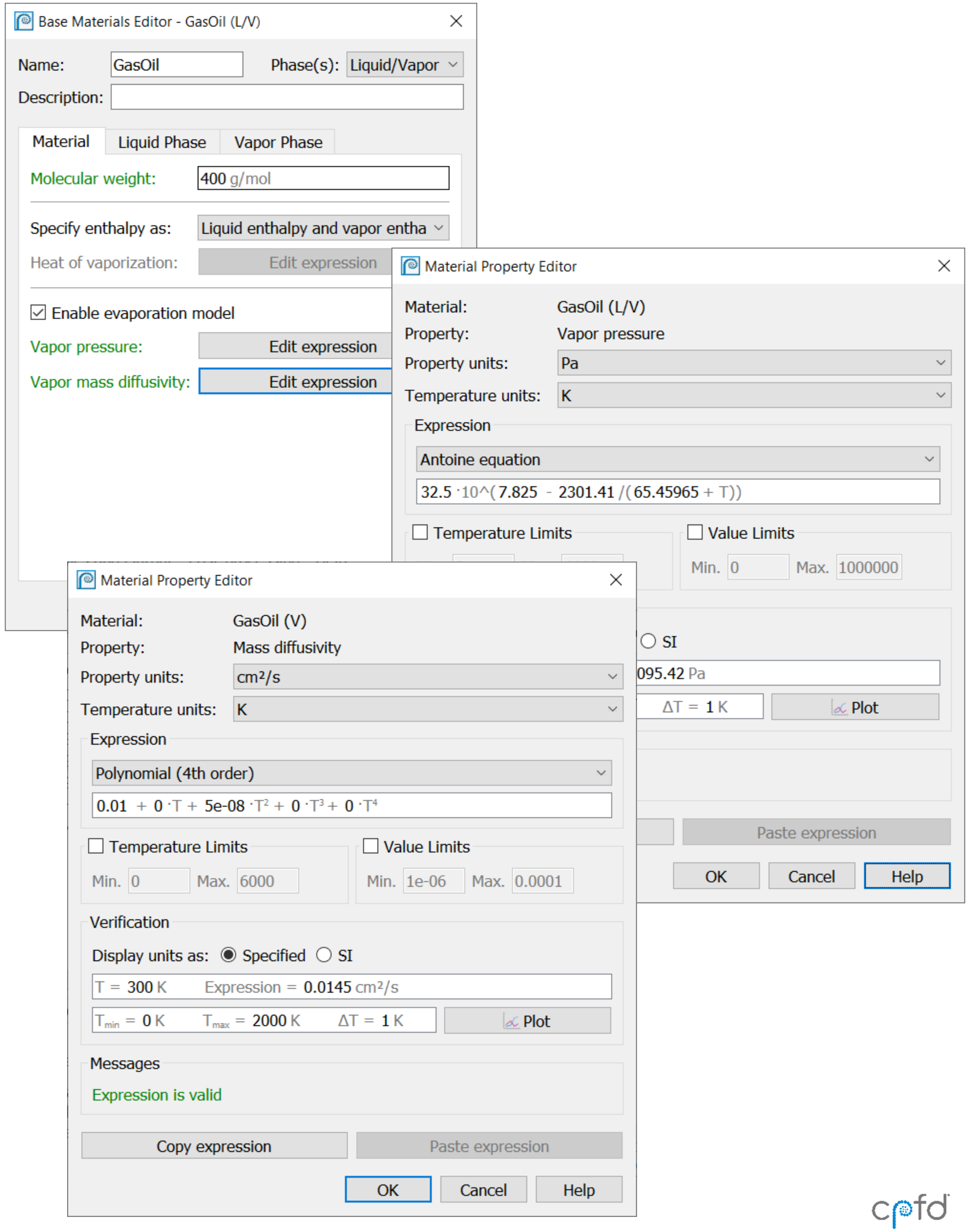
$$P_{vap} = 32.5 \cdot 10^{A-\frac{B}{C+T}}$$

where A = 7.825, B = 2301.41, C = 65.45965

- Vapor mass diffusivity, input the polynomial equation* and change property units:

$$D = 0.01 + \left(5 \times 10^{-8}\right)T^2$$

* Values used are approximate and for illustrative purposes only. For more accurate values, independent research will be required.



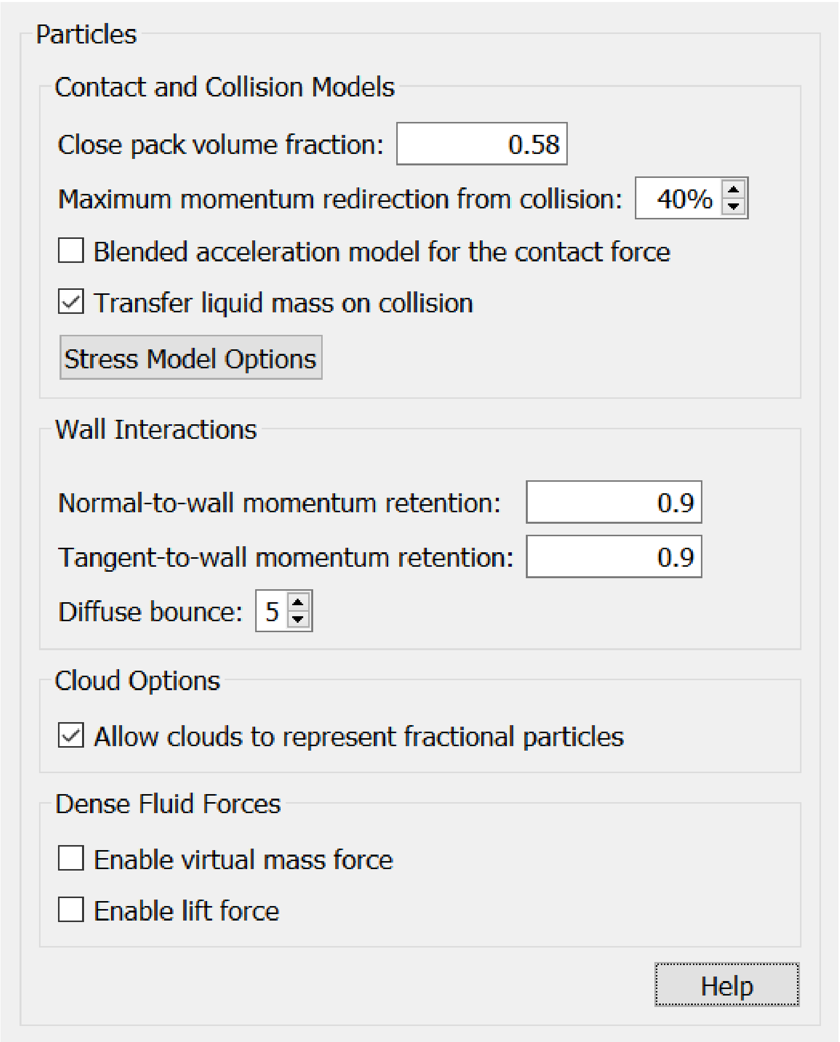
Particles

Close pack volume fraction: 0.58

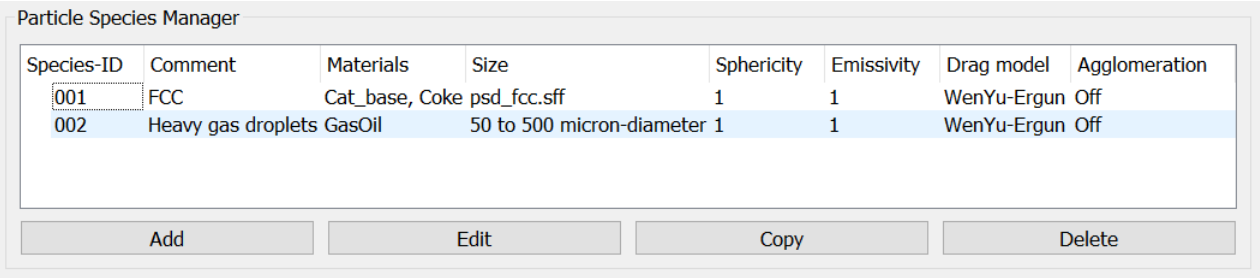
Normal-to-wall momentum retention: 0.9

Tangent-to-wall momentum retention: 0.9

Diffuse bounce: 5

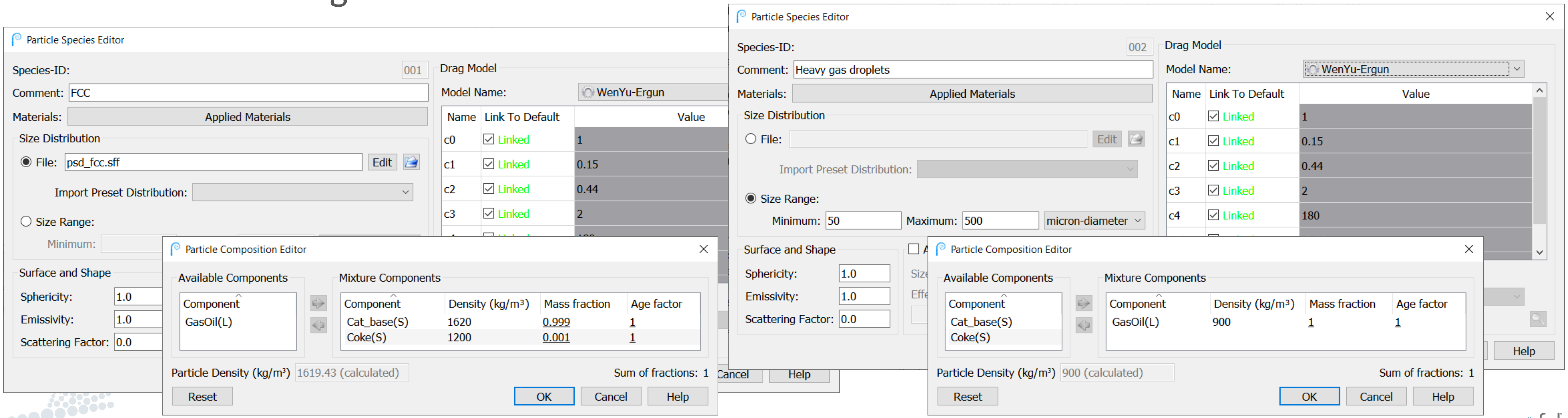


Particle Species



Create the following particles species:

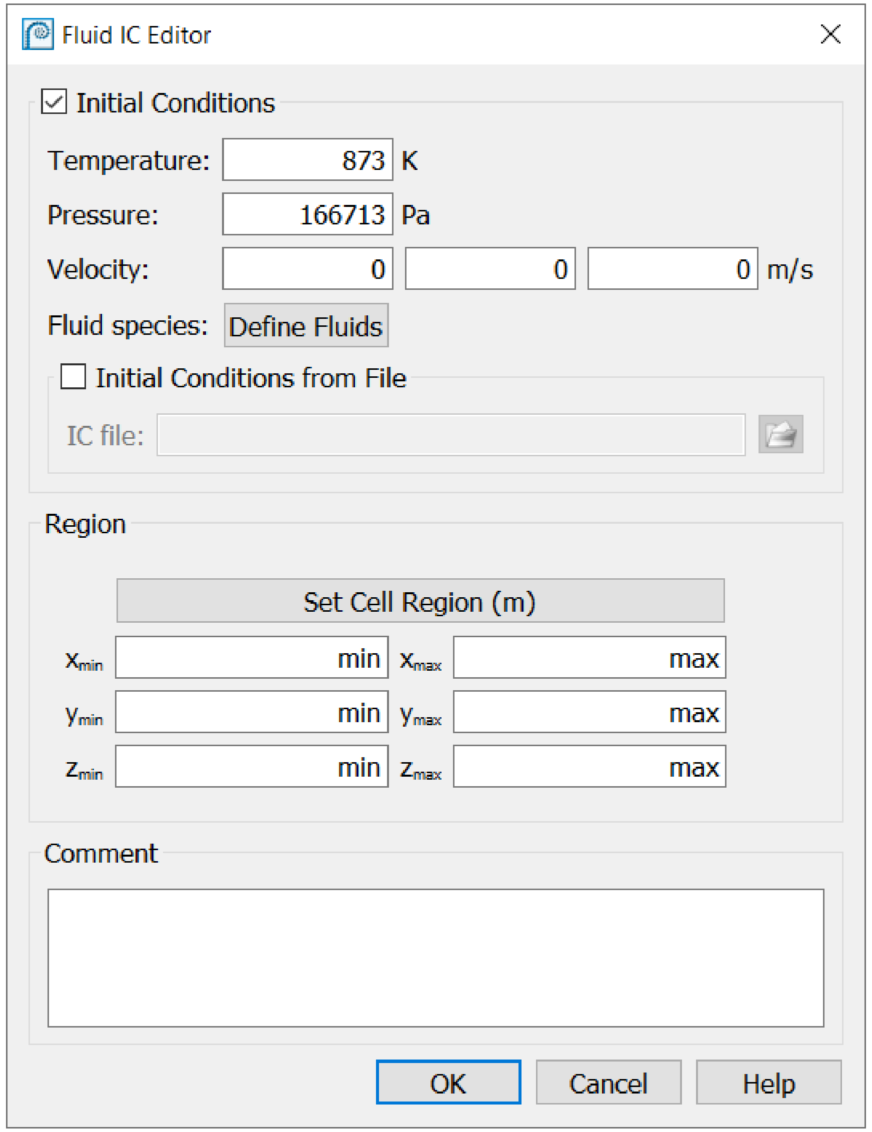
- FCC, 0.999 Cat_base(S), 0.001 Coke(S), psd_fcc.sff, WenYu-Ergun
- Heavy gas droplets, 100% GasOil (L), Size range: 50-500 micron diameter, WenYu-Ergun



Fluid ICs

Fluid IC

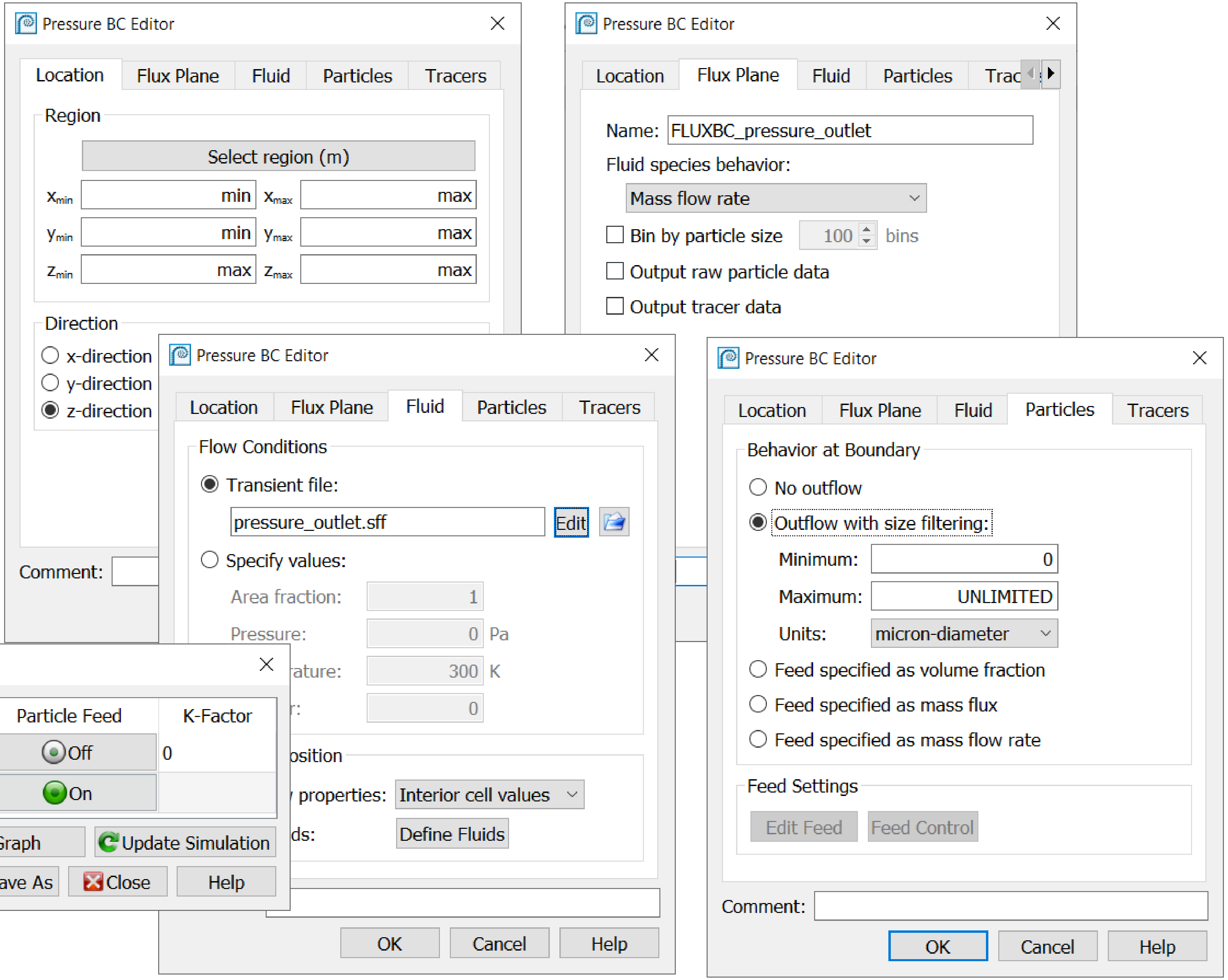
- Temperature = 873 K
- Pressure = 166713 Pa
- Fluid species = 100% N2

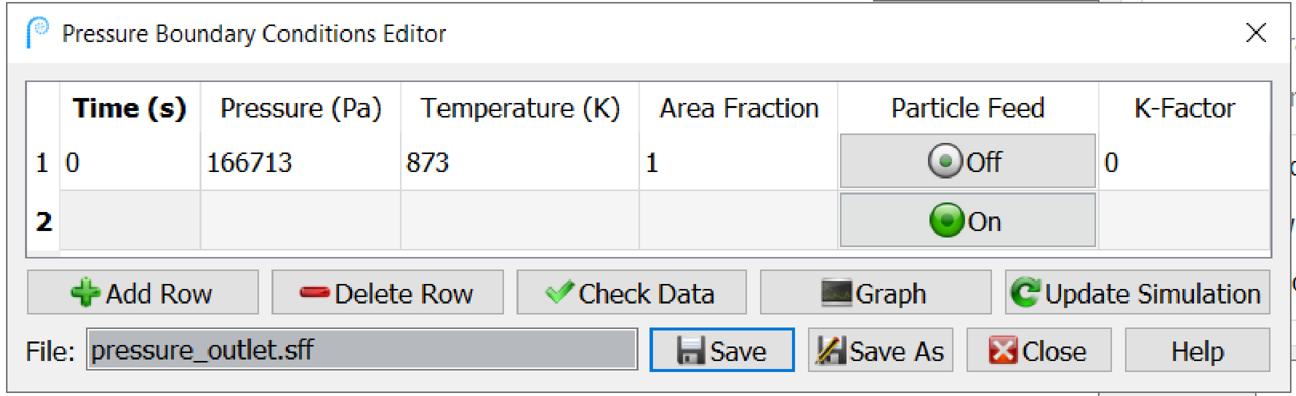


Pressure BC

Add a pressure BC with information shown here for the outlet

Use 100% N2 for Applied Fluids

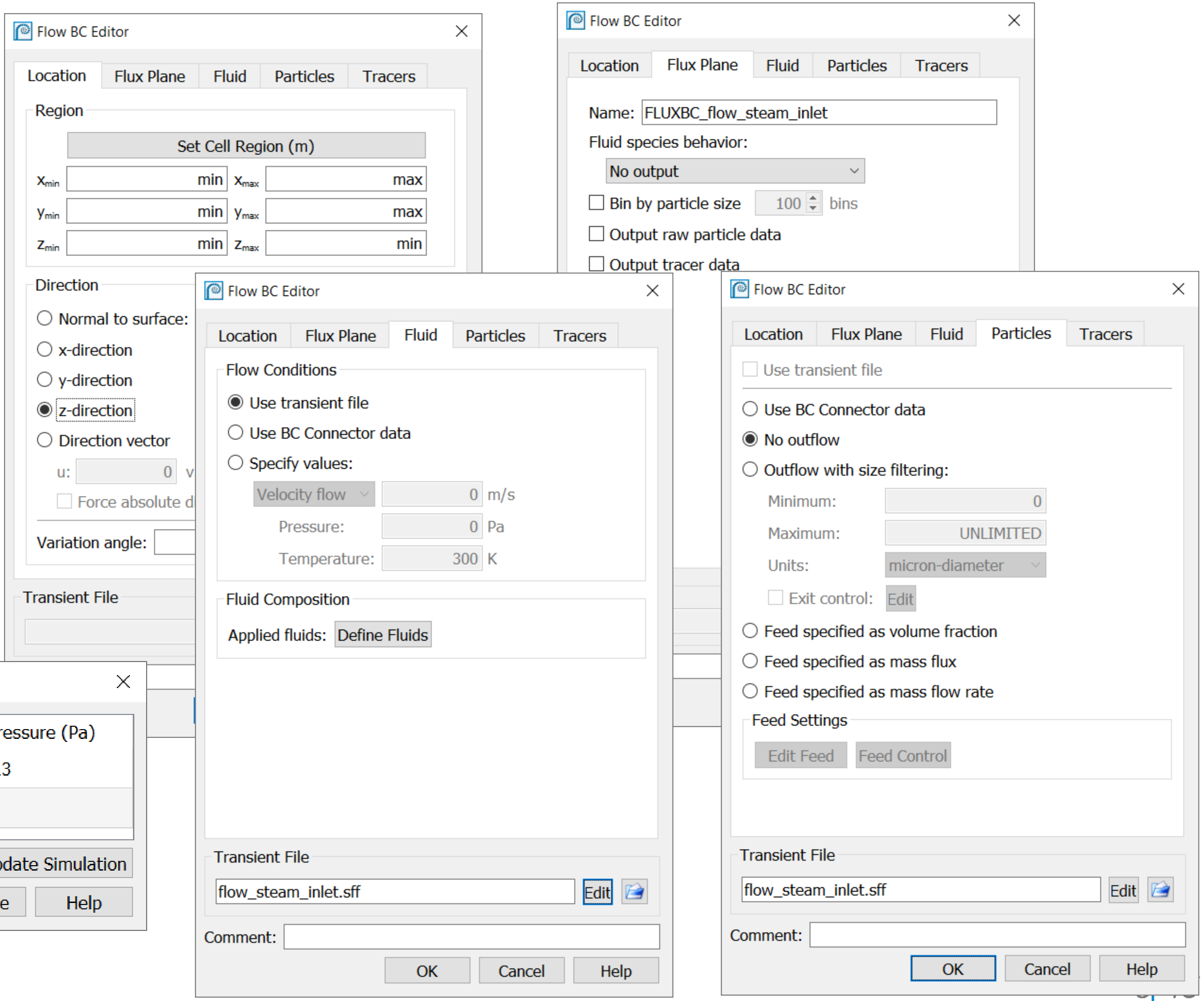


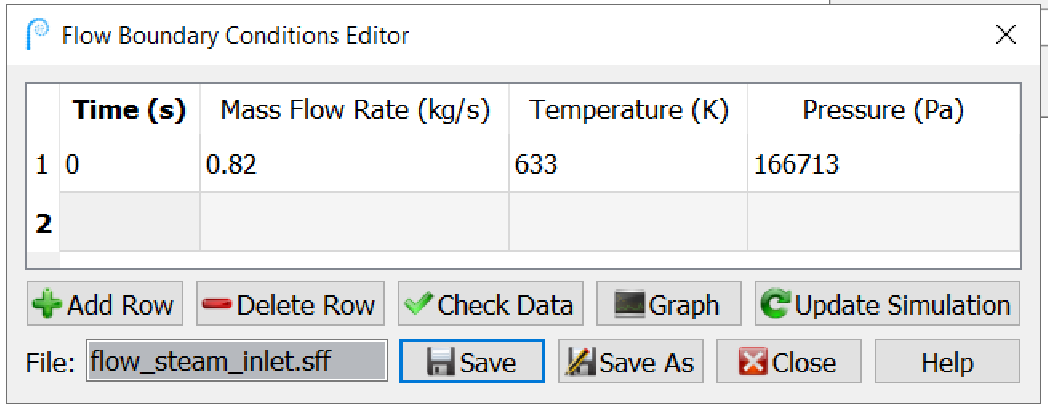


Flow BCs

Add flow BC with information shown here for bottom steam

Use 100% H_2O for Applied fluids



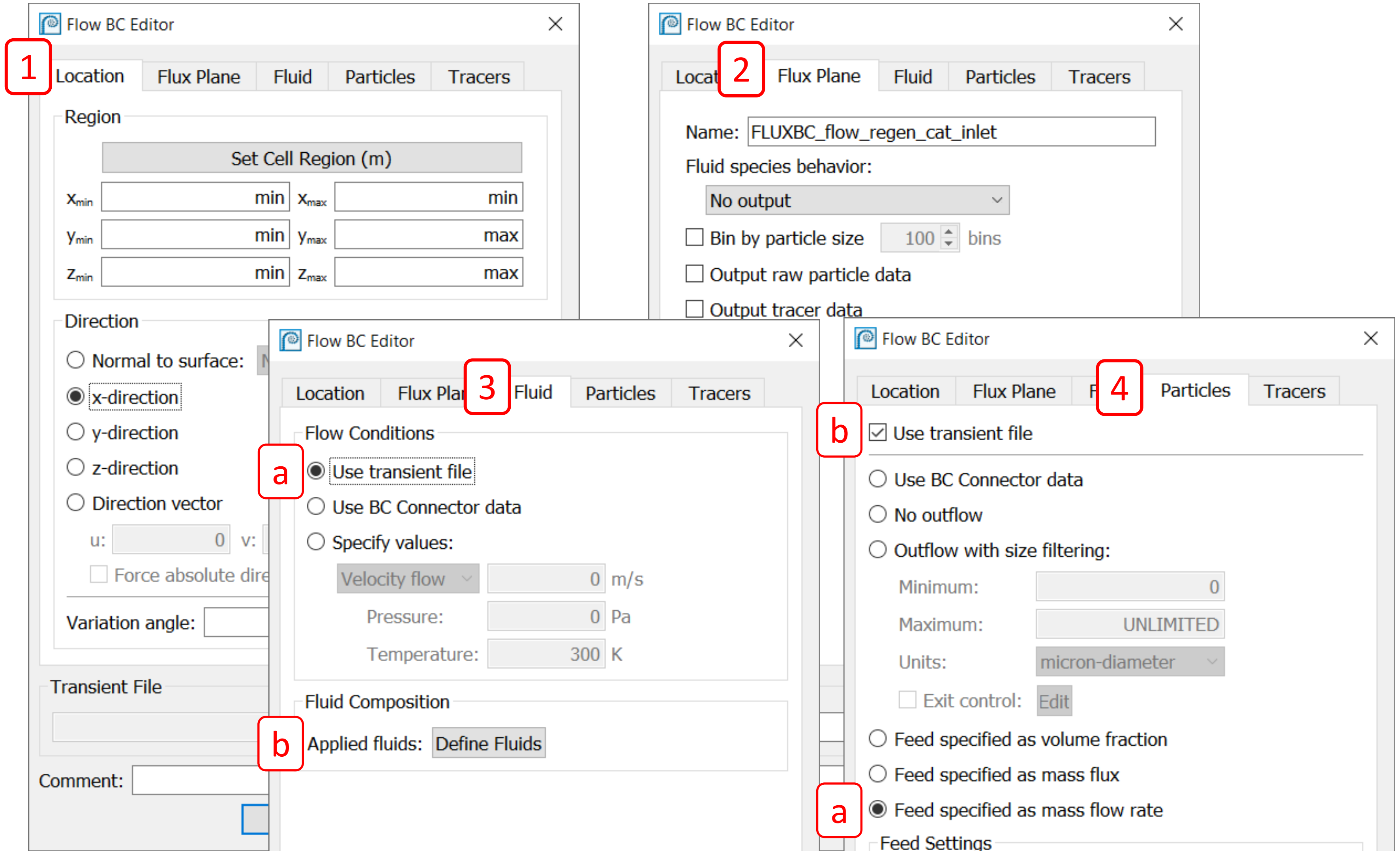


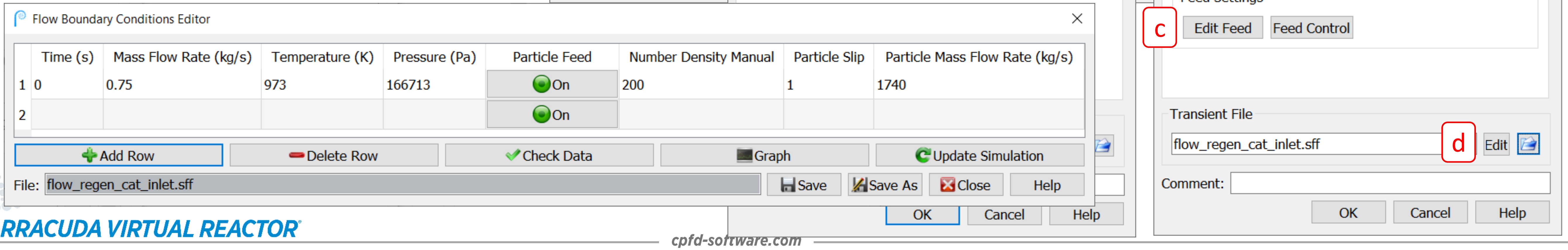
Flow BCs

Add flow BC with information shown here for steam and catalyst feed

Use 100% H2O for Applied fluids

Use 100% FCC for particle feed





Injection BC – Feed Oil

Add Feed Oil injection BC

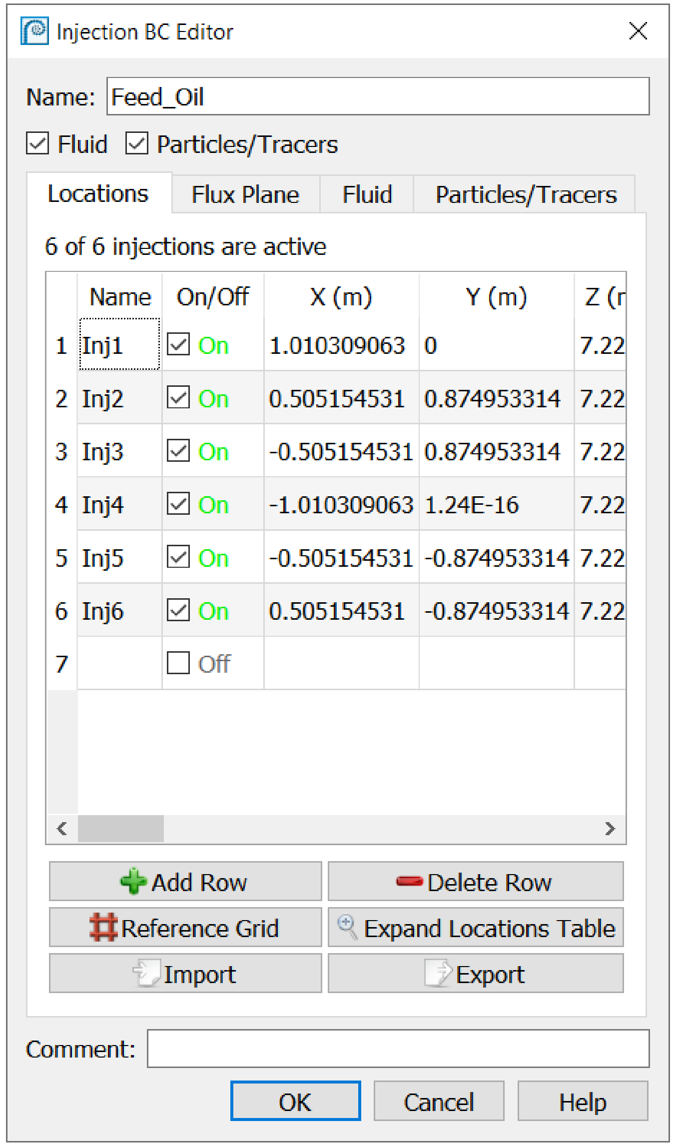
- Name = Feed_Oil
- Select Fluid and Particles/Tracers

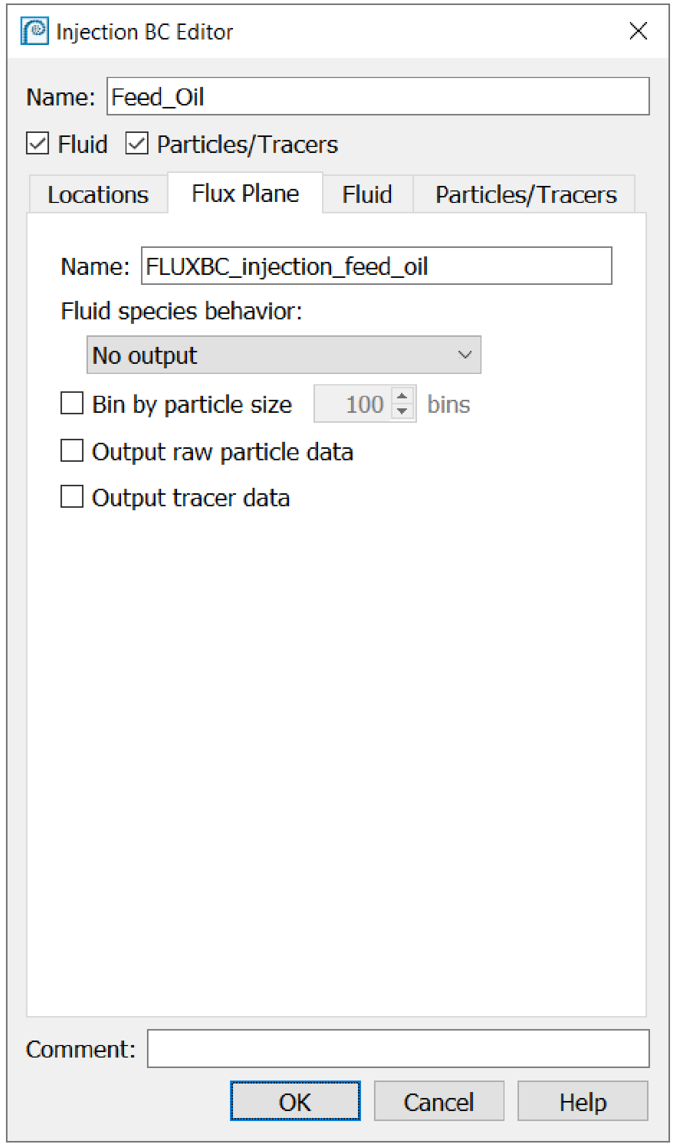
Locations tab

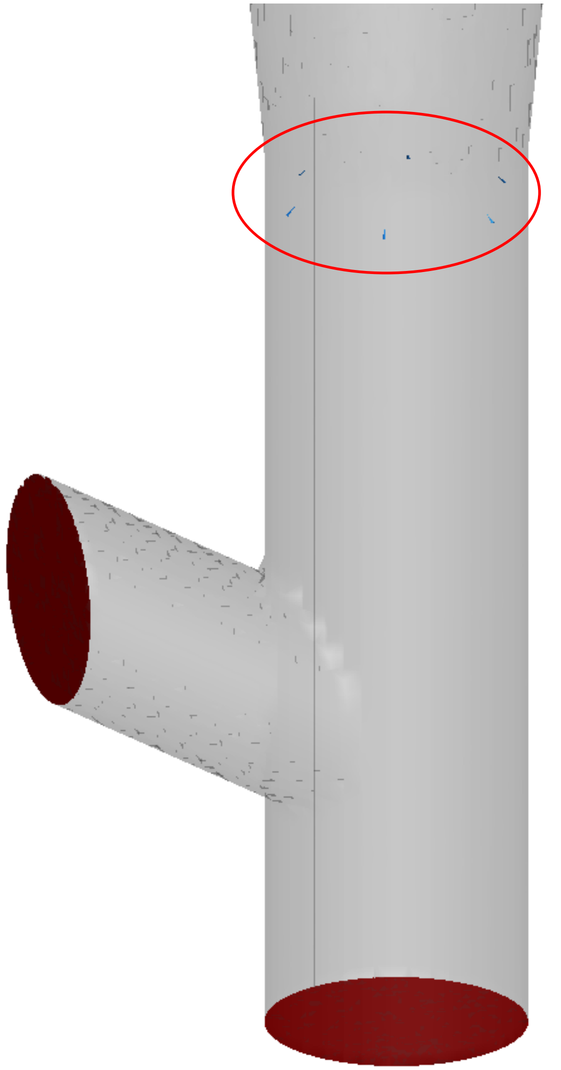
- Import feed_oil_locations.csv

Flux Plane tab

- Add a flux plane name



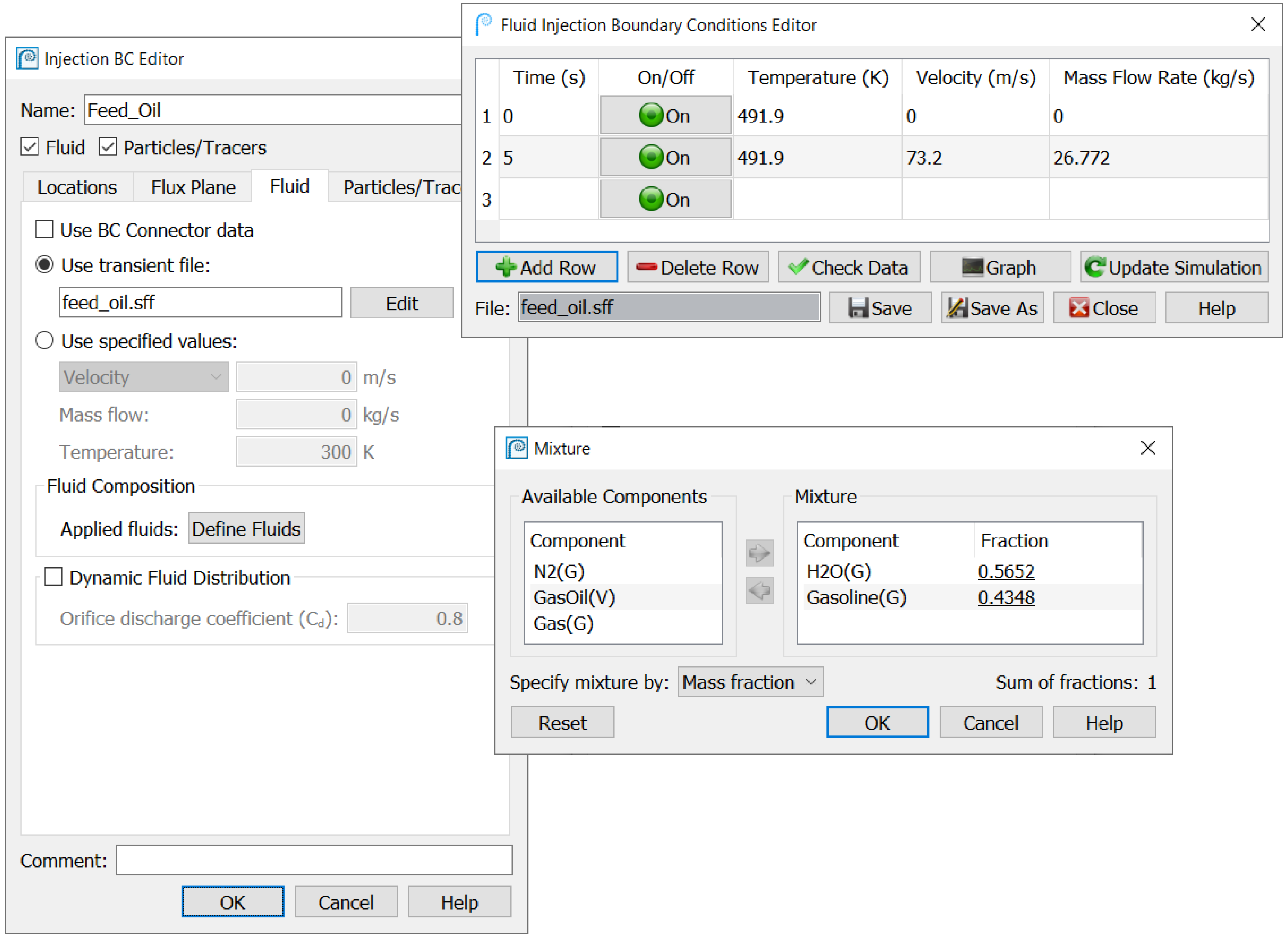




Injection BC – Feed Oil

Fluid tab

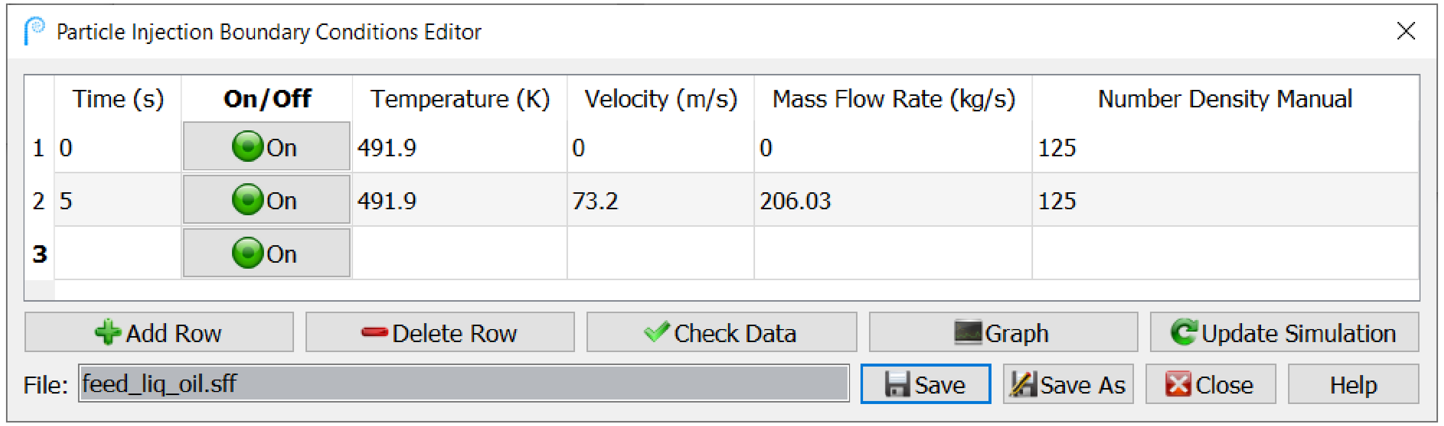
- Set up transient file as shown ramping the fluid velocity and mass flow rate over the first 5 seconds
- Applied fluids
  - 0.5652 H2O(G)
  - 0.4348 Gasoline(G)

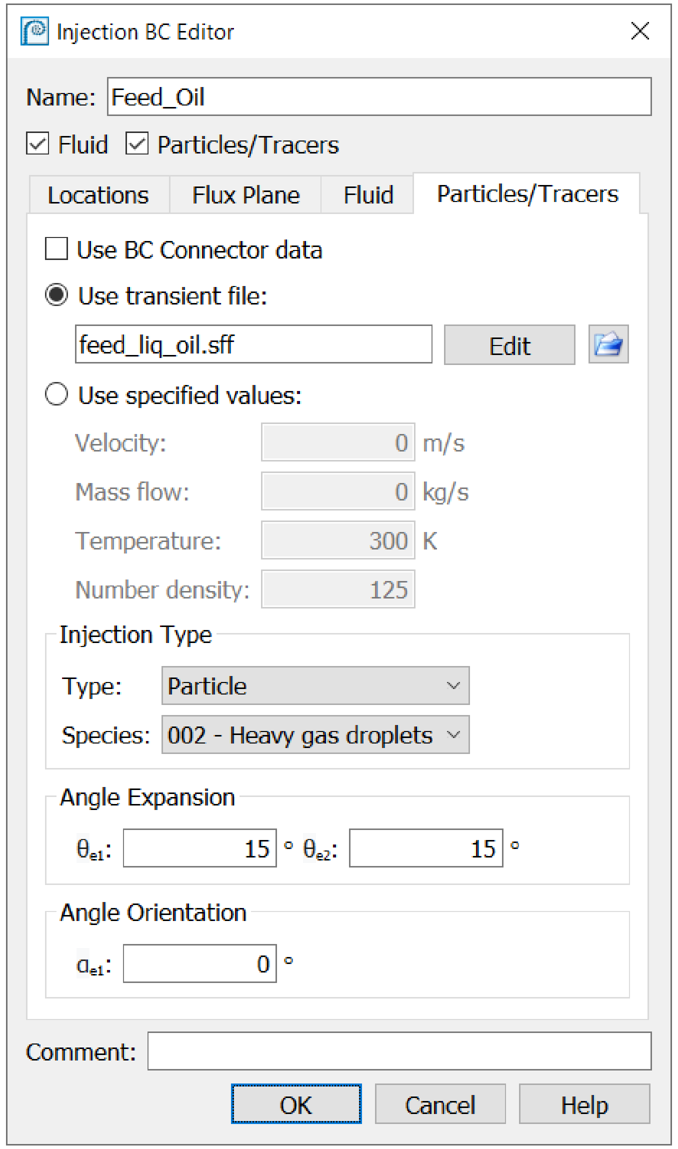


Injection BC – Feed Oil

Particles/Tracers tab

- Set up transient file as shown, ramping up particle velocity and mass flow rate over the first 5 seconds
- Select Heavy gas droplets for the particle species
- Set the Angle Expansion to 15˚

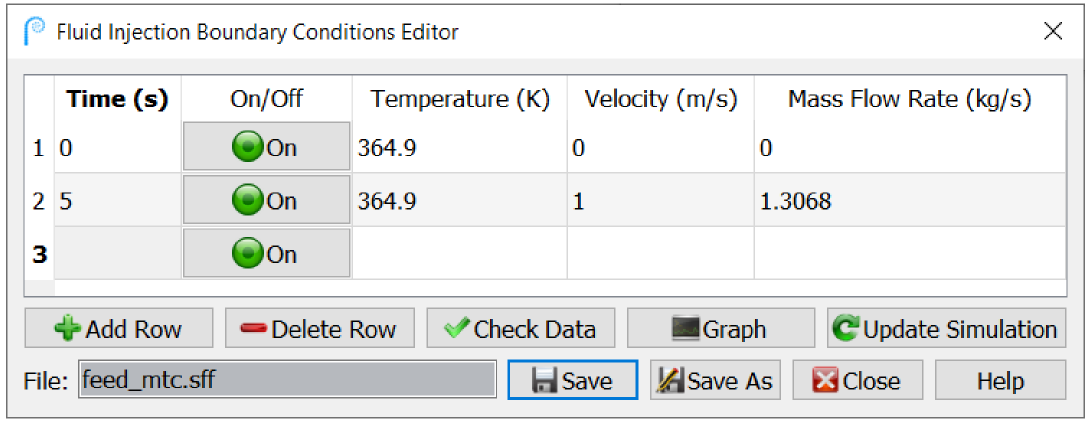




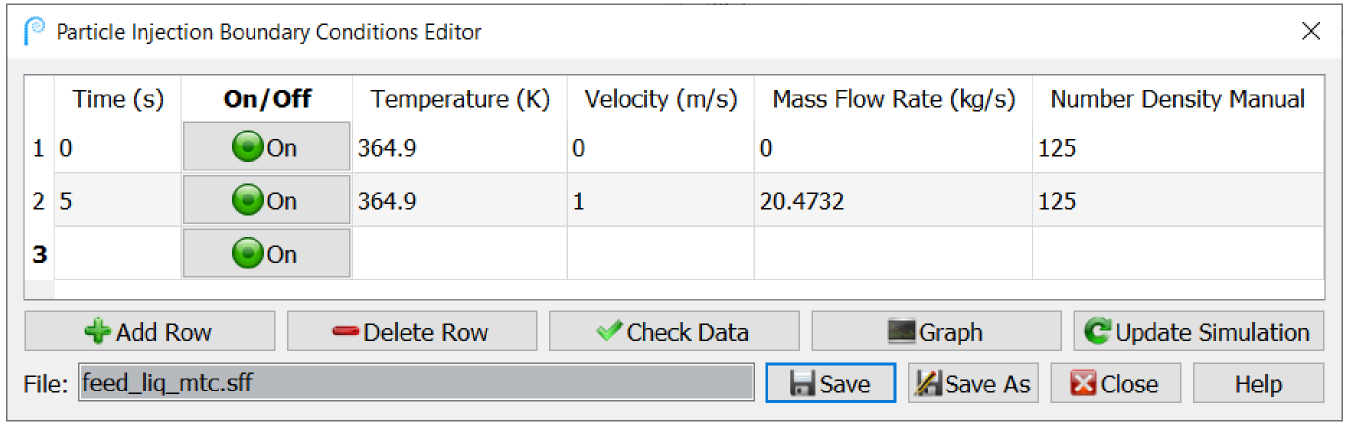
Injection BC - MTC

Add MTC Injection BC:

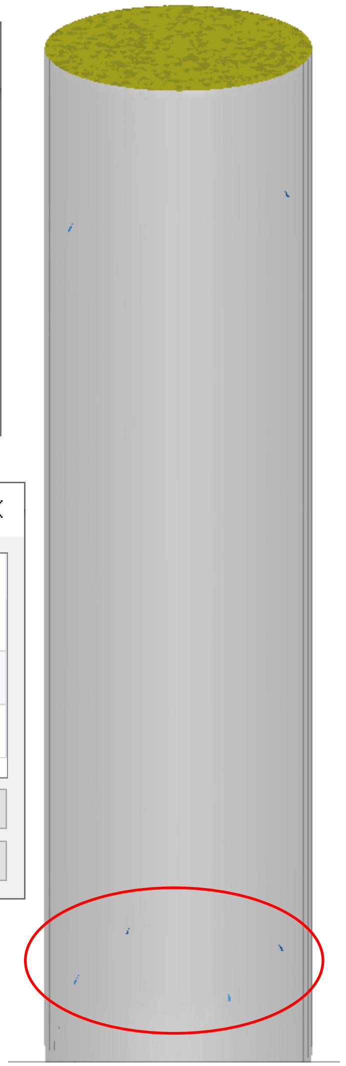
- Name = MTC
- Select Fluid and Particle/Tracers
- Locations tab
  - Import MTC_nozzle_locations.csv
- Flux Plane tab
  - FLUXBC_injection_mtc
- Fluid tab
  - Use transient file shown here
  - Applied fluids – 100% Gasoline
- Particles/Tracers tab
  - Use transient file shown here
  - Use Heavy gas droplets particle species
  - Angle Expansion of 15˚



	Time (s)	On/Off	Temperature (K)	Velocity (m/s)	Mass Flow Rate (kg/s)
1	0	On	364.9	0	0
2	5	On	364.9	1	1.3068
3		On			



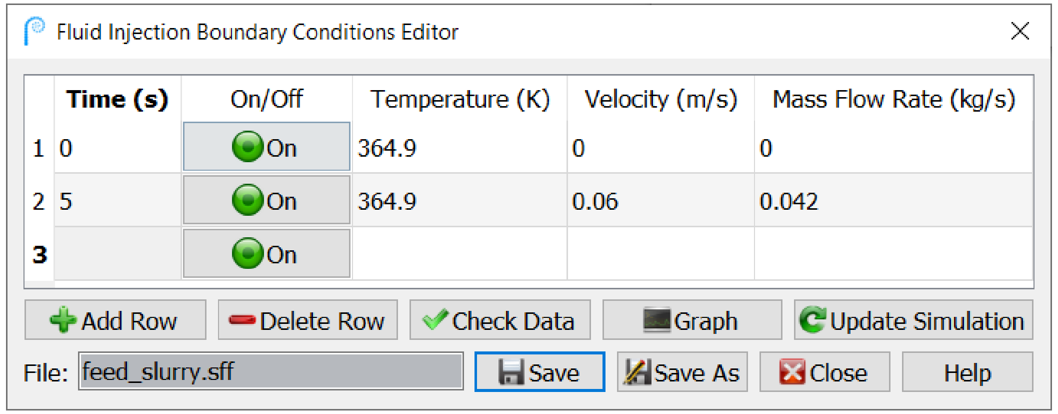
	Time (s)	On/Off	Temperature (K)	Velocity (m/s)	Mass Flow Rate (kg/s)	Number Density Manual
1	0	On	364.9	0	0	125
2	5	On	364.9	1	20.4732	125
3		On				



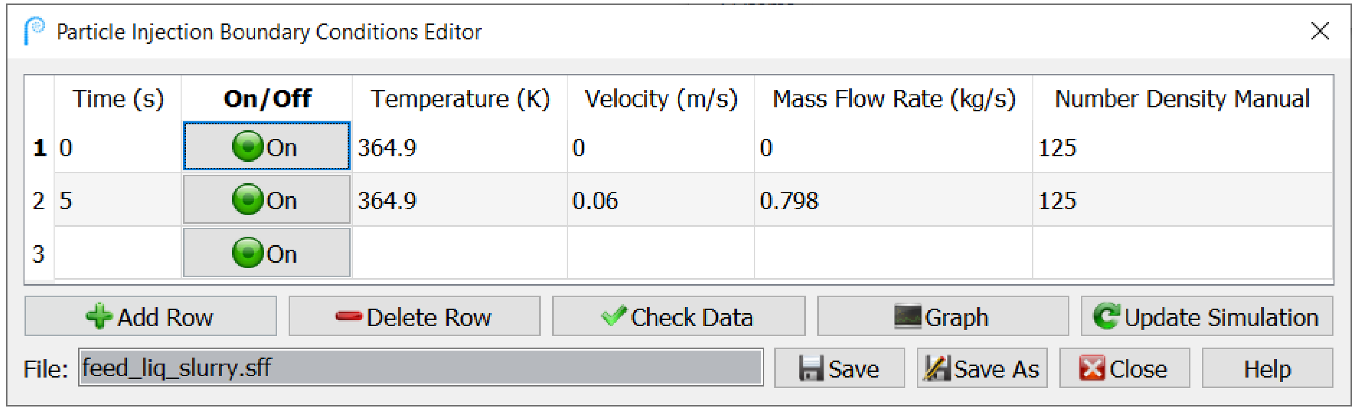
Injection BC – Slurry Back Wash

Add Slurry Back Wash Injection BC :

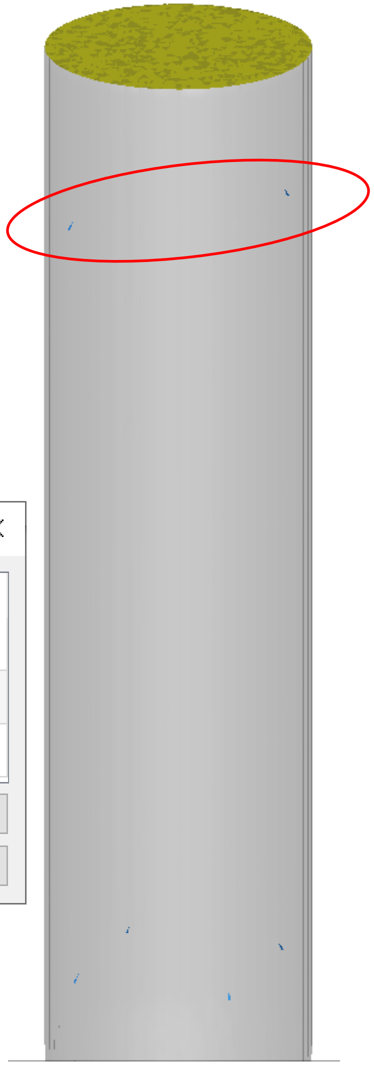
- Name = Slurry_Back_Wash
- Select Fluid and Particles/Tracers
- Locations tab
  - Import slurry_nozzle_locations.csv
- Flux Plane tab
  - FLUXBC_injection_slurry
- Fluid tab
  - Use transient file shown here
  - Applied fluids – 100% H_2O
- Particles/Tracers tab
  - Use transient file shown here
  - Use Heavy gas droplets particle species
  - Angle Expansion of 15˚



	Time (s)	On/Off	Temperature (K)	Velocity (m/s)	Mass Flow Rate (kg/s)
1	0	On	364.9	0	0
2	5	On	364.9	0.06	0.042
3		On			



	Time (s)	On/Off	Temperature (K)	Velocity (m/s)	Mass Flow Rate (kg/s)	Number Density Manual
1	0	On	364.9	0	0	125
2	5	On	364.9	0.06	0.798	125
3		On				



Reaction Chemistry

A four lump cracking model is being used in this work. The kinetics have been adapted from the kinetics used by [Nayak et al (2005)](). The four-lump model assumes that there are four hydrocarbon components in the system: Gas oil, Gasoline, Gas, and Coke:

$$\text{GasOil} \xrightarrow{r_1} 4\ \text{Gasoline} \qquad r_1 = \frac{3.589\times10^{6}\,s^{-1}\cdot RT\theta_{\text{Cat}}}{P\theta_f}\exp\left(-\frac{8222.3\ \text{K}}{T}\right)[\text{GasOil}]^2\varphi$$

$$\text{GasOil} \xrightarrow{r_2} 8\ \text{Gas} \qquad r_2 = \frac{2.541\times10^{7}\,s^{-1}\cdot RT\theta_{\text{Cat}}}{P\theta_f}\exp\left(-\frac{10748.1\ \text{K}}{T}\right)[\text{GasOil}]^2\varphi$$

$$\text{GasOil} \xrightarrow{r_3} 32\ \text{Coke} \qquad r_3 = \frac{6.791\times10^{4}\,s^{-1}\cdot RT\theta_{\text{Cat}}}{P\theta_f}\exp\left(-\frac{7779.65\ \text{K}}{T}\right)[\text{GasOil}]^2\varphi$$

$$\text{Gasoline} \xrightarrow{r_4} 2\ \text{Gas} \qquad r_4 = 885.72\,s^{-1}\theta_{\text{Cat}}\theta_f^{-1}\exp\left(-\frac{6350.7\ \text{K}}{T}\right)[\text{Gasoline}]\varphi$$

$$\text{Gasoline} \xrightarrow{r_5} 8\ \text{Coke} \qquad r_5 = 5.3198\times10^{7}\,s^{-1}\theta_{\text{Cat}}\theta_f^{-1}\exp\left(-\frac{13910.3\ \text{K}}{T}\right)[\text{Gasoline}]\varphi$$

Where R = 8.3145 kg·m^{2}·s^{-2}·K^{-1}·mol^{-1} and φ is the catalyst deactivation function (next slide)

Nayak, S., Joshi, S., and Ranade, V. (2005). Modeling of vaporization and cracking of liquid oil injected in a gas-solid riser. *Chemical Engineering Science*. 60: 6049-6066.

Chemistry Implementation Notes

Take note of the following when defining your chemistry:

- Volume average chemistry will need to be used for each reaction. Units are mol/m^3 for concentration and mol/m^3/s for the reaction rate.
- Reactions of this nature are possible to implement in Barracuda but can be challenging at times.

Hint: the rate expression for the Gas Oil to Gasoline reaction can be implemented as:

$$R00 = \left((k_0)[GasOil]^2\right)*\left((k_5)\right)$$

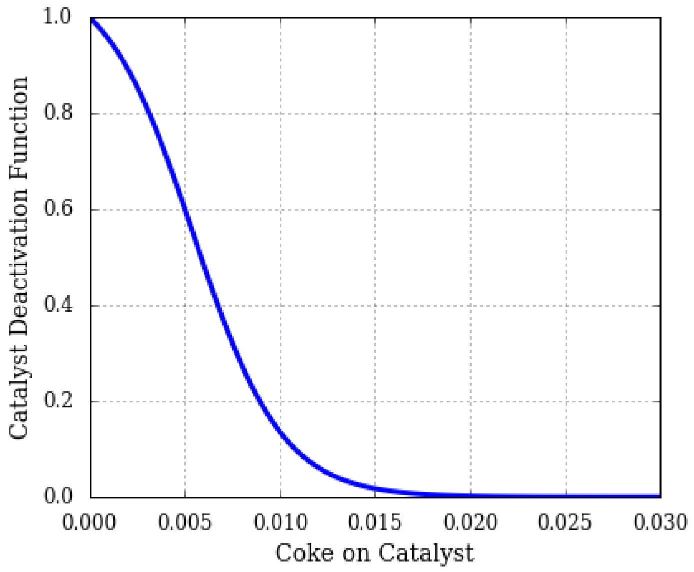
where k0 and k5 are appropriate rate coefficients

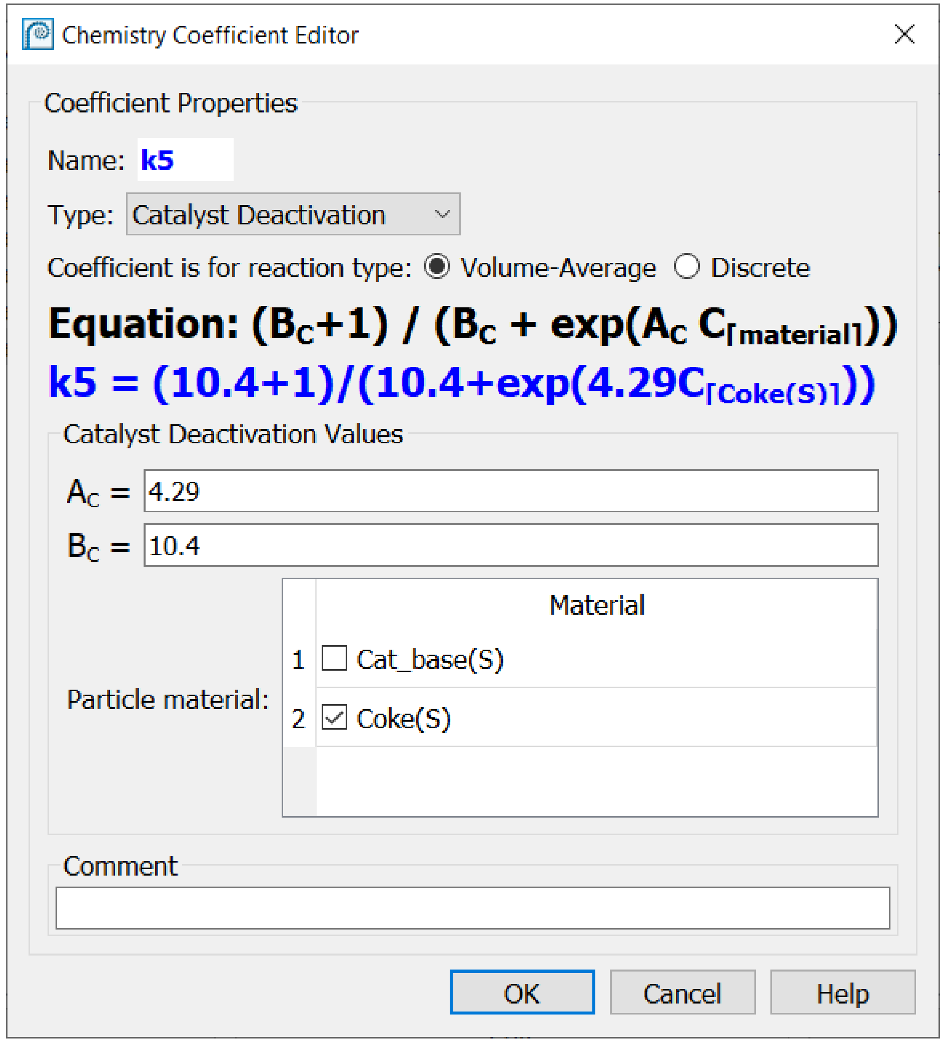
Catalyst deactivation function

The catalyst deactivation function is given in the following form:

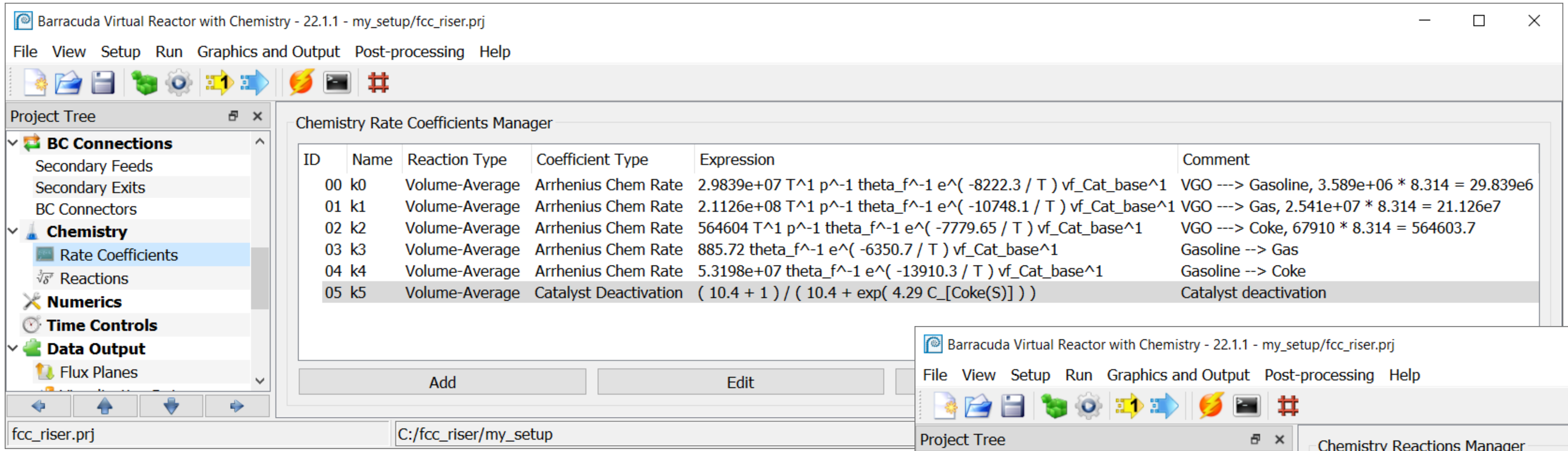
$$\varphi = \frac{11.4}{10.4 + \exp(4.29 w_c)}$$

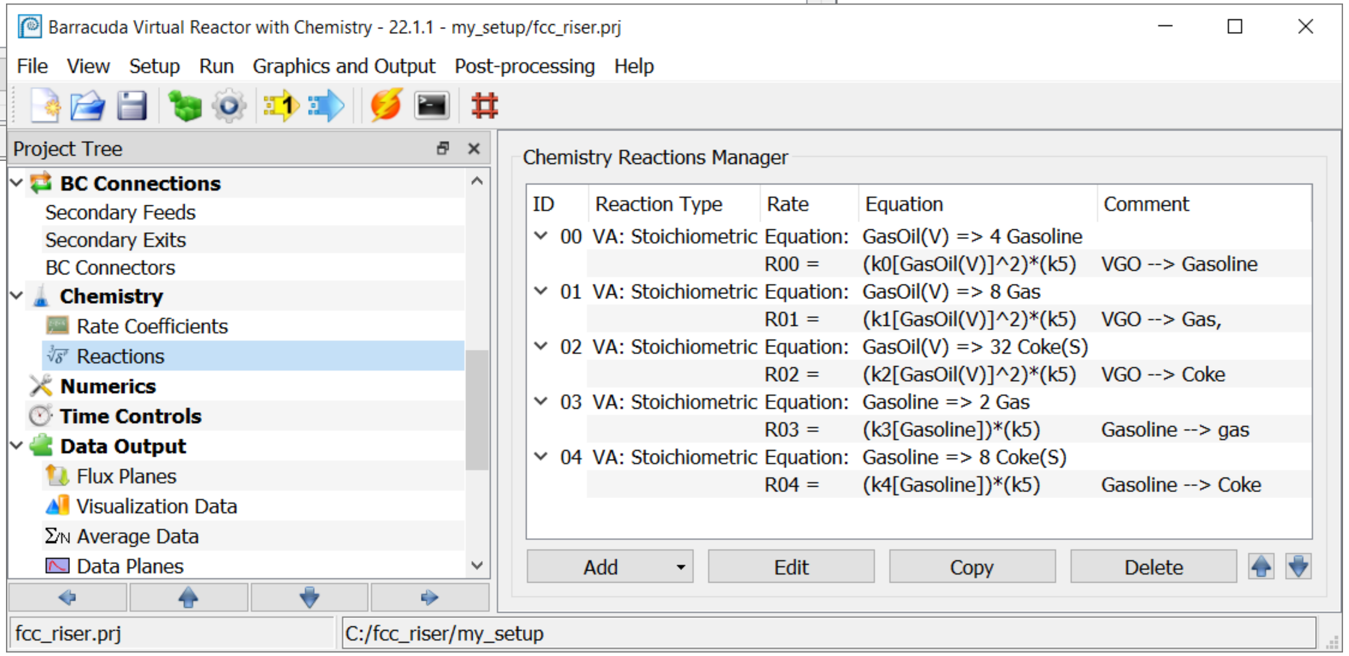
where w_C is the weight fraction of coke on the particle.





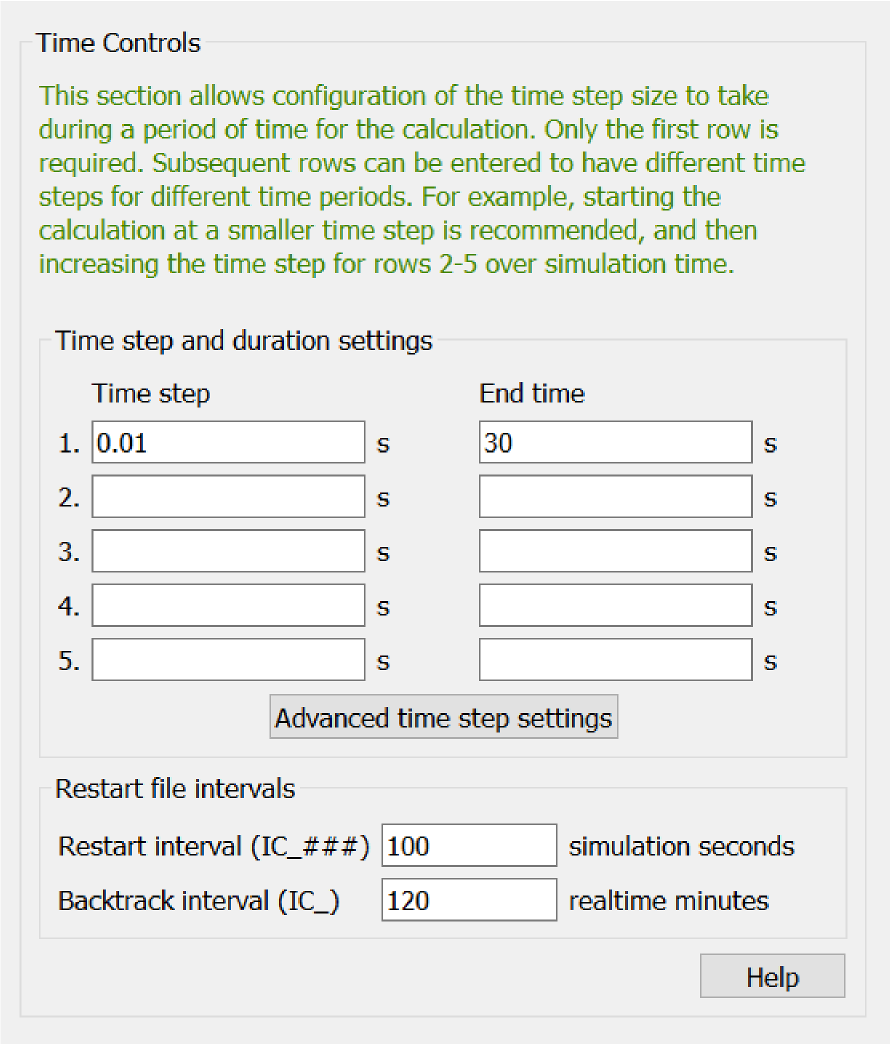
Chemistry Rate Coefficients and Reactions





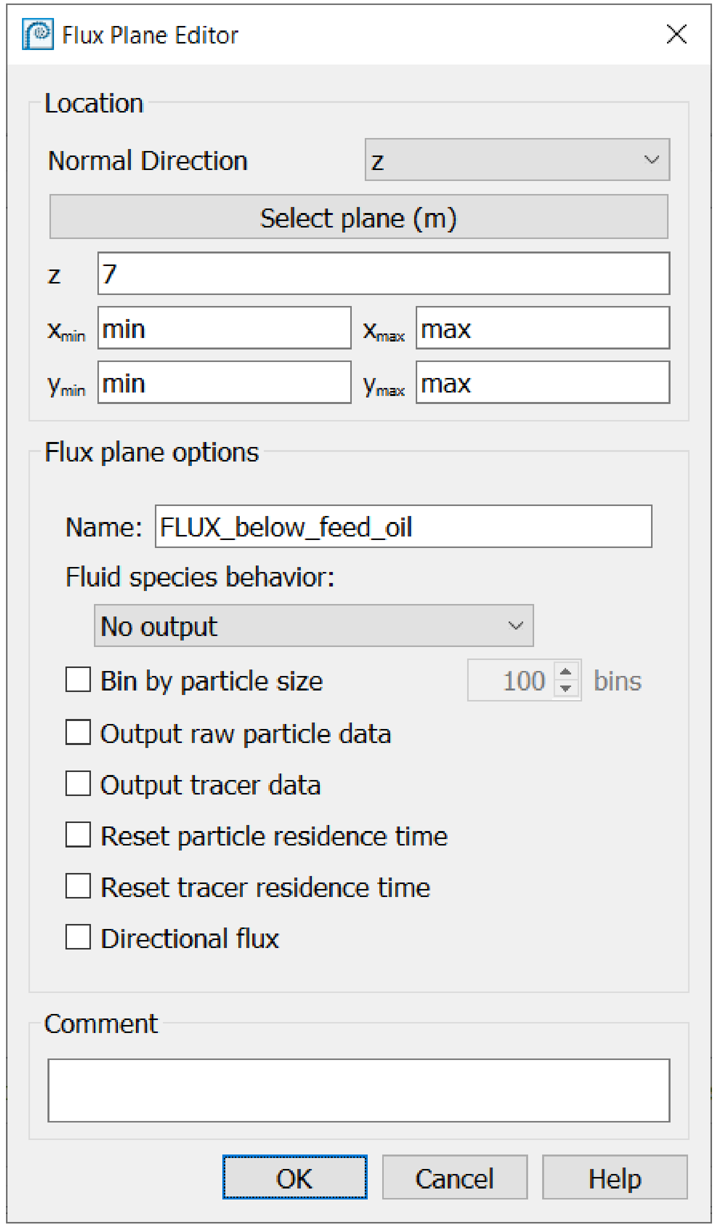
Time Controls

Set Time step and End time



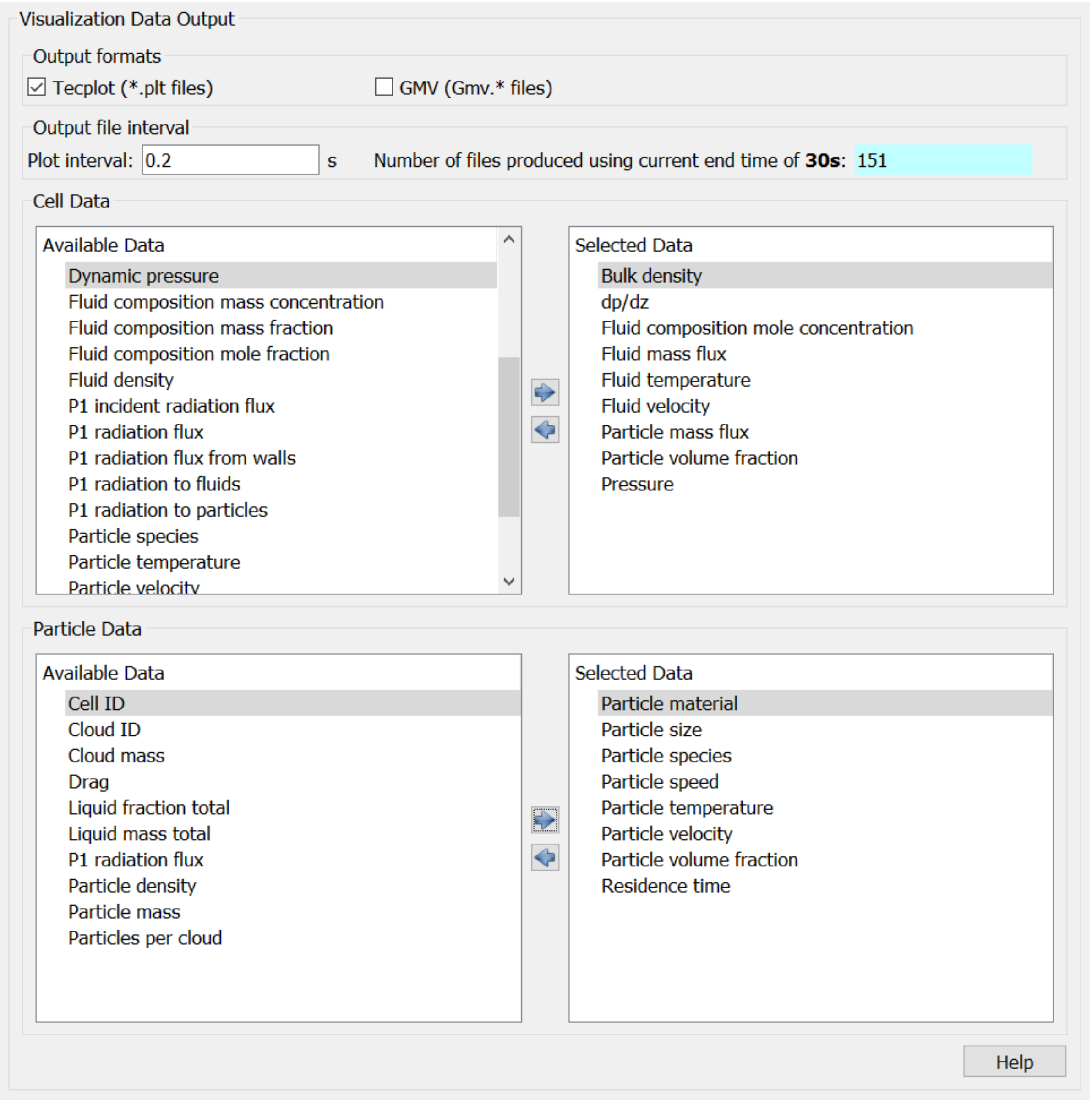
Flux Planes

Define a flux plane below the feed oil nozzles



Visualization Data Output

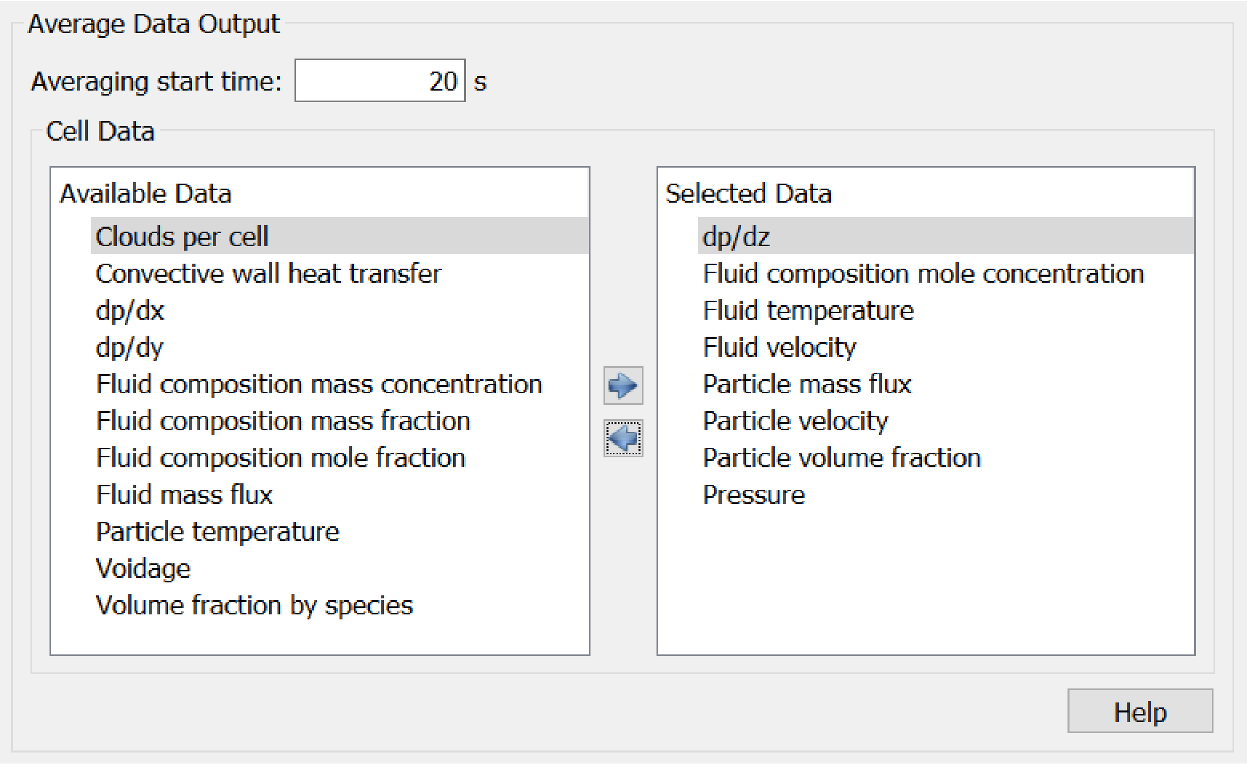
Set Output file interval and select options shown for Visualization Data Output



Average Data

Set Averaging start time to 20 s

Select the Average Data Output shown

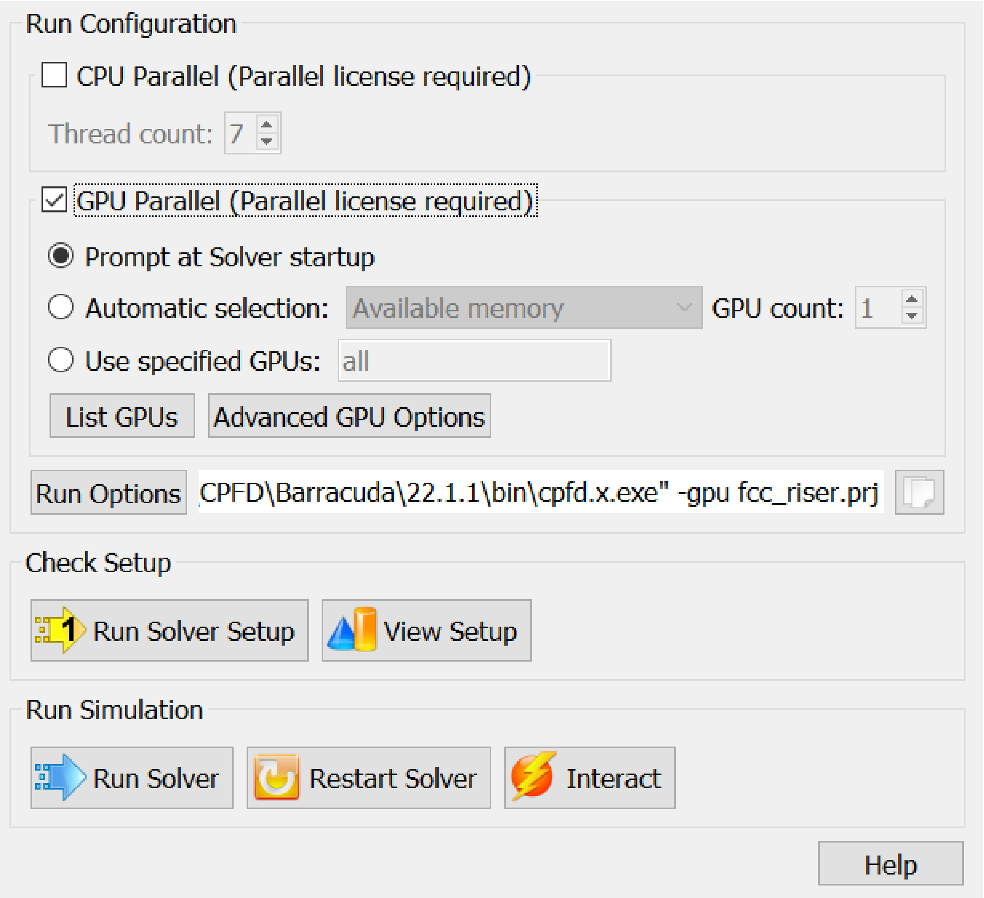


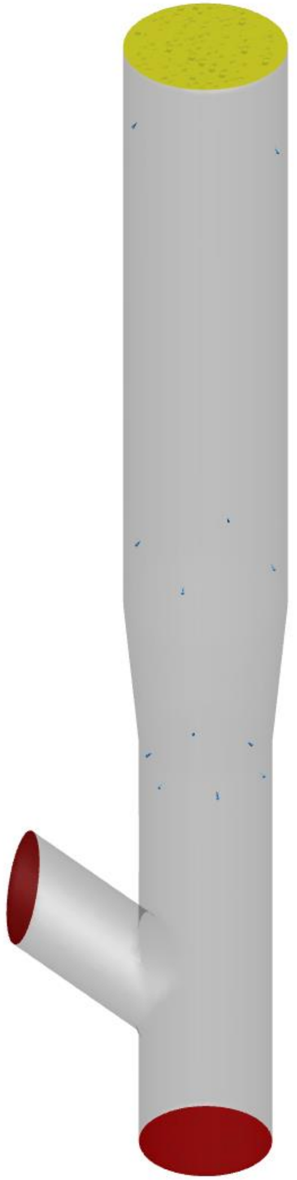
Run

If NVIDIA GPU card is available, select GPU Parallel

Run Solver Setup and View Setup

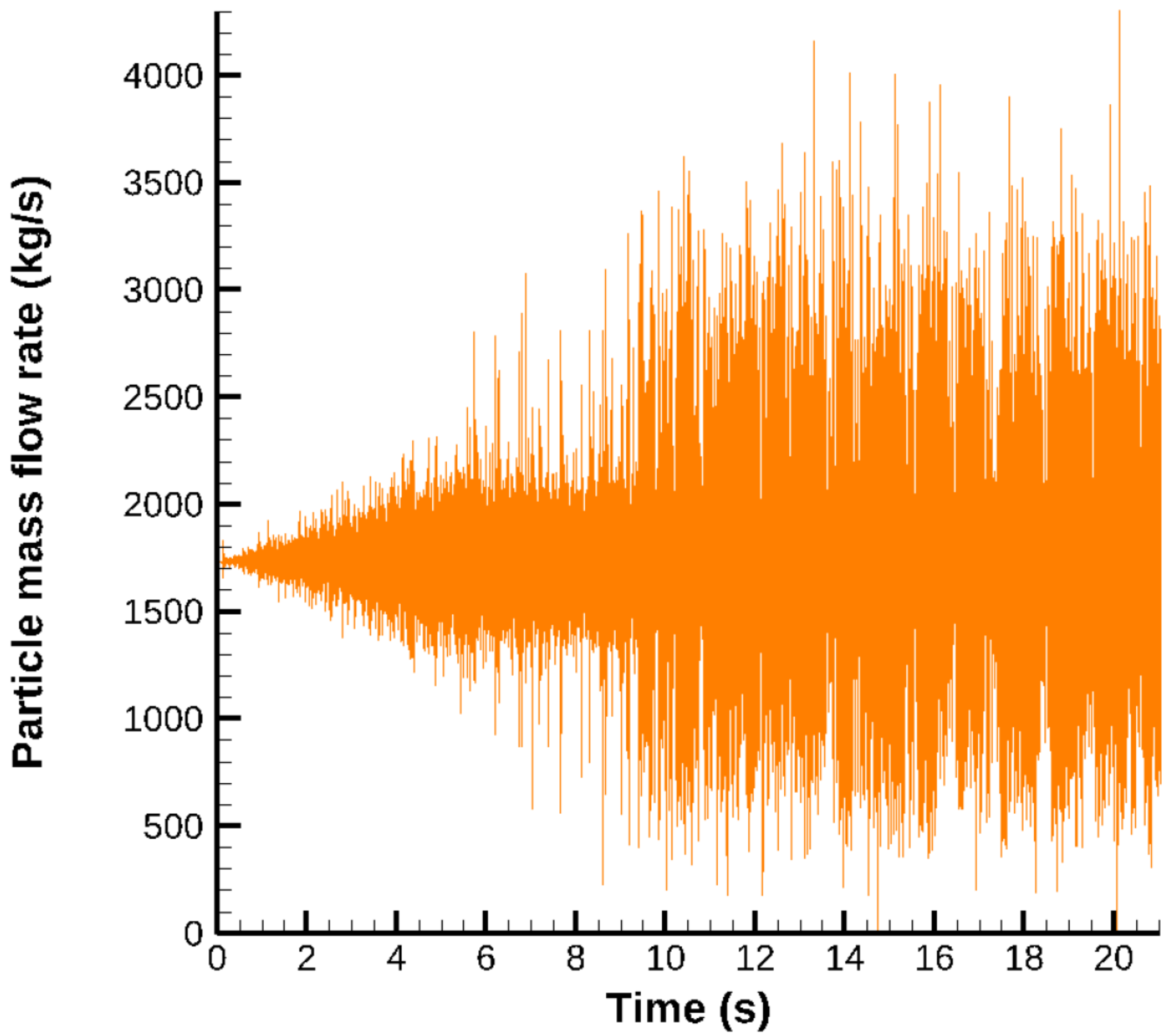
Once you have checked the setup, Run Solver to start the simulation





Run: Monitoring Catalyst feed

Catalyst enters at a relatively high volume fraction which can lead to particle feed deficit. Monitoring this feed rate during the simulation is recommended. This can be done by creating an xy plot of the particle mass flow rate vs. time from `FLUXBC_flow regen_cat_inlet` file and refreshing often as the simulation runs. Changes to the fluid mass flow rate can be made to the .sff file in order to help the particles flow more easily.



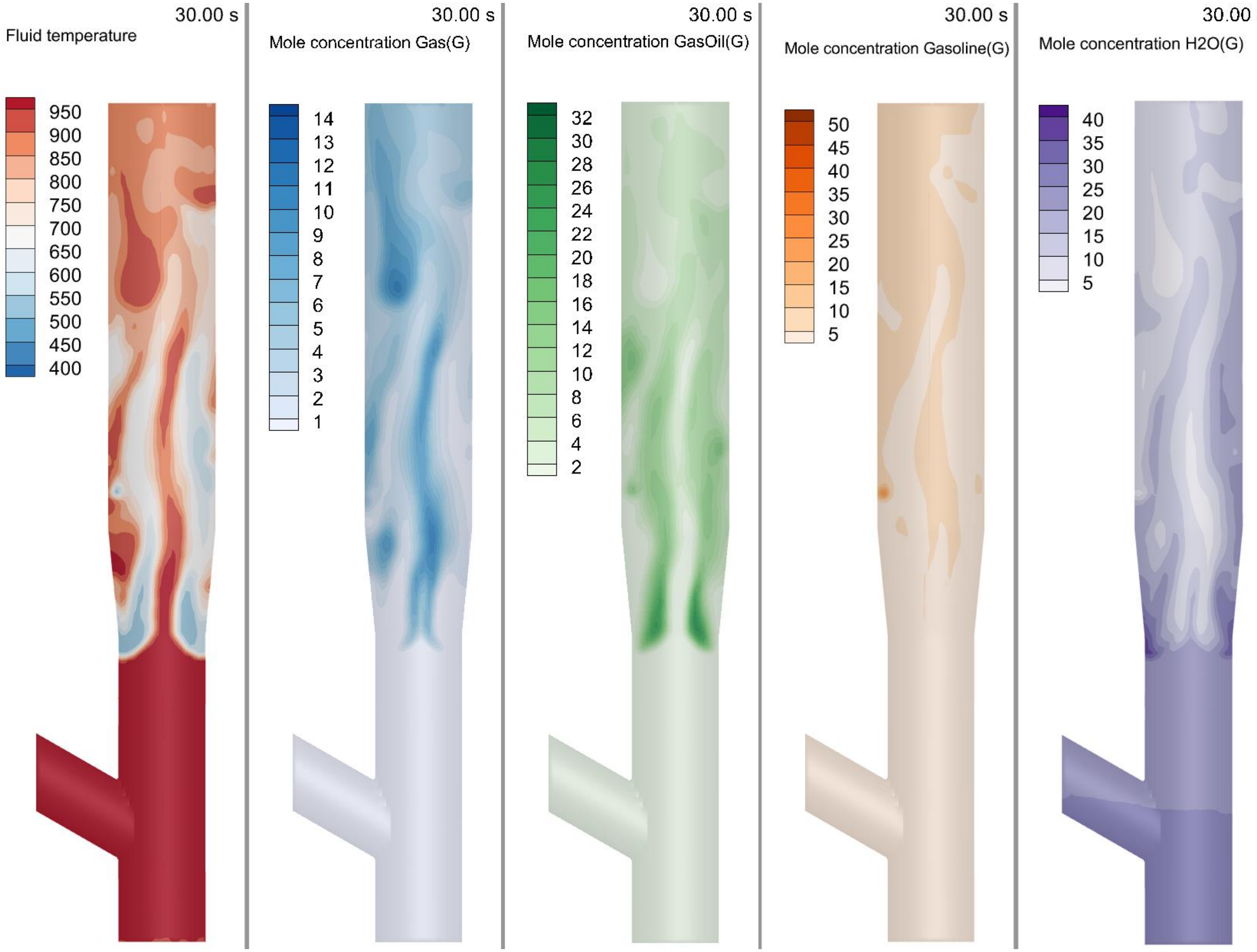
Post-Processing - Slices

Create slices of fluid temperature and fluid domain mole concentrations

Compare with time-averaged slices after the simulation reaches the averaging time

See the following videos:

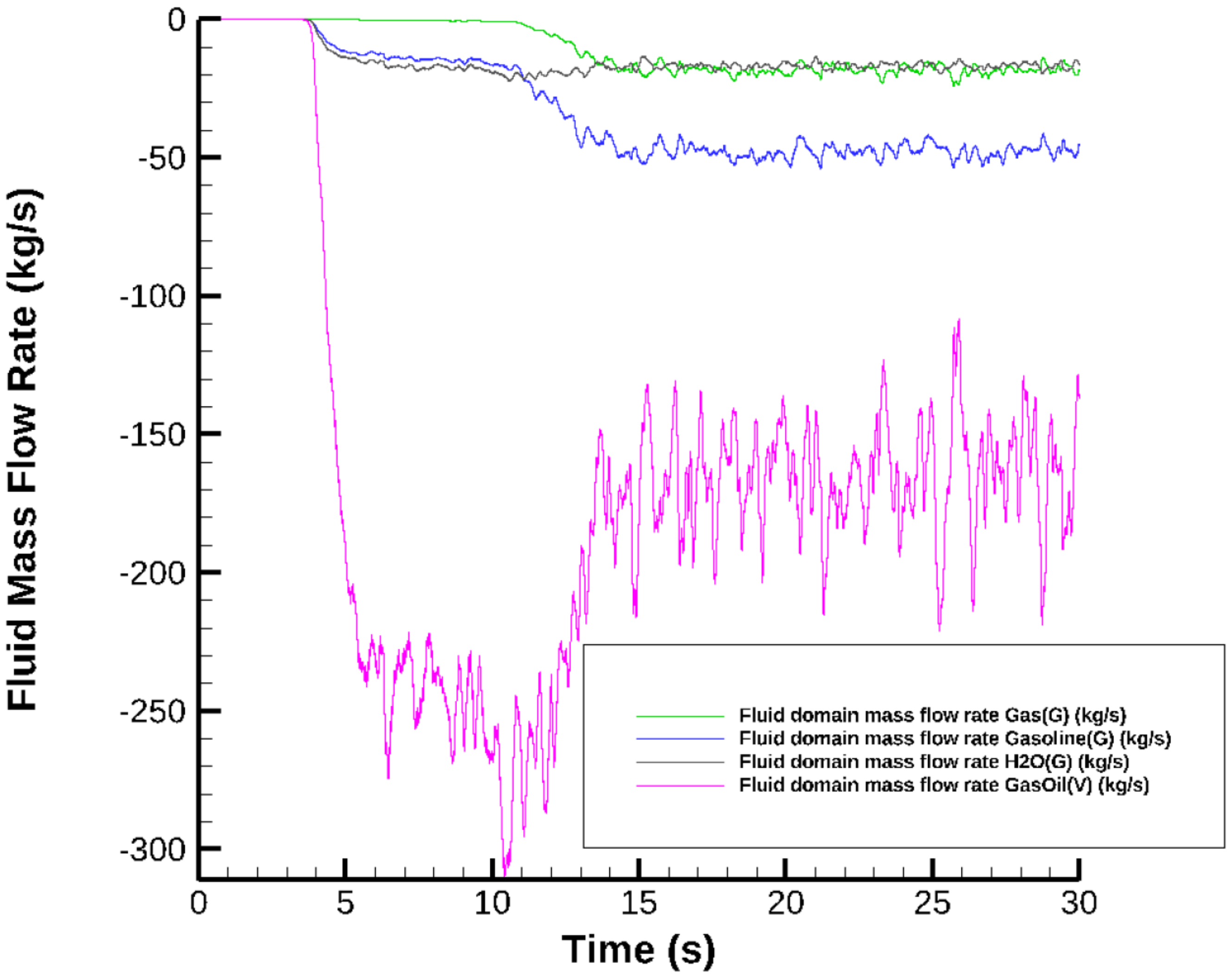
- Frames
- Slices
- Contour legend



Post-Processing: xy plot

Create an xy plot showing the fluid mass flow rate for each gas leaving through the pressure BC flux plane `FLUXBC_pressure_outlet_fluidSpecies`

This [video]() shows how to create xy plots in Tecplot for Barracuda



Post-Processing: Animation

It can be useful to create a half view animation to see the behavior of particles in the system over time

Use Value Blanking to blank when y is less than or equal to 0

Create an animation of the view over the simulation time