

FCC Riser: Setup and Analysis

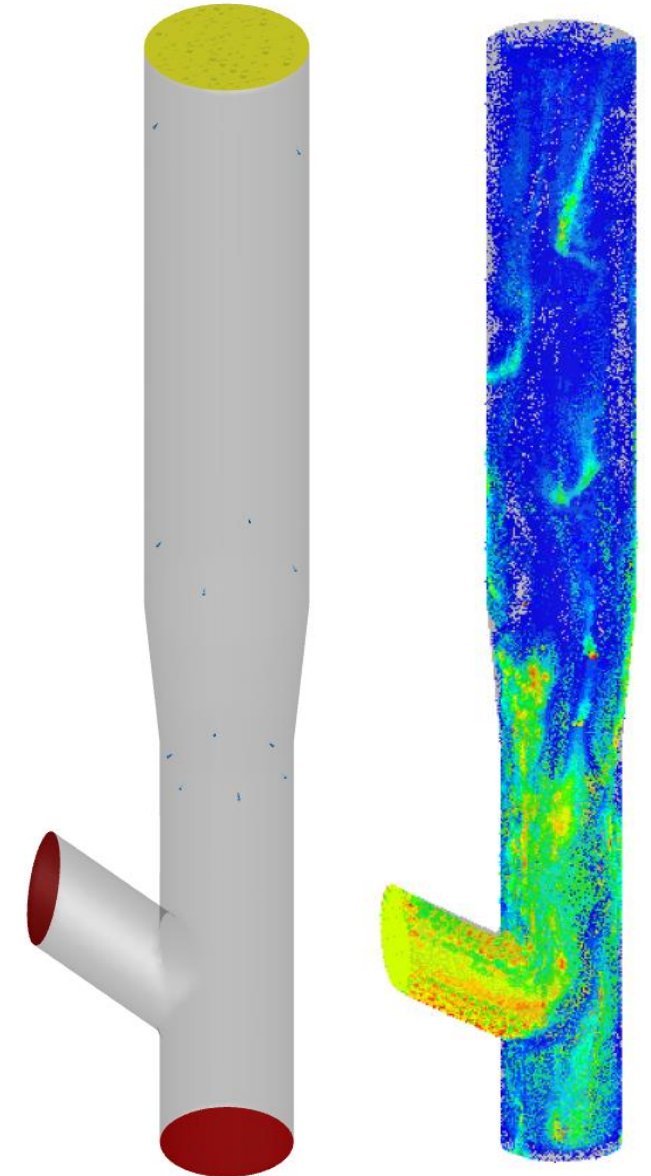
CPFD Software

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.

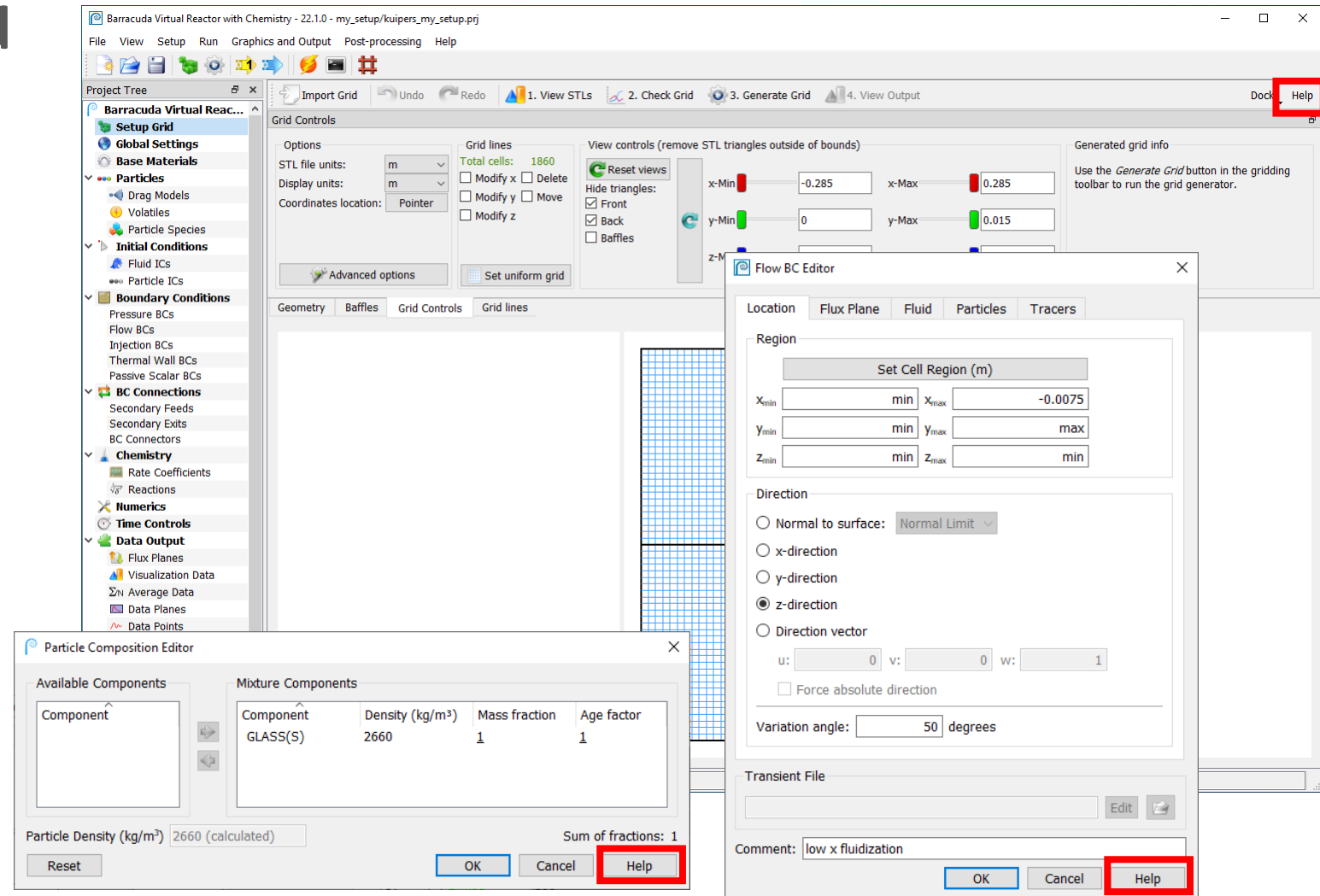
This is a thermal and reacting system with a four-lump model in which the hydrocarbons present are divided into four groups: heavy gas compounds, product gas compounds, light gas compounds, and solid carbon.



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.



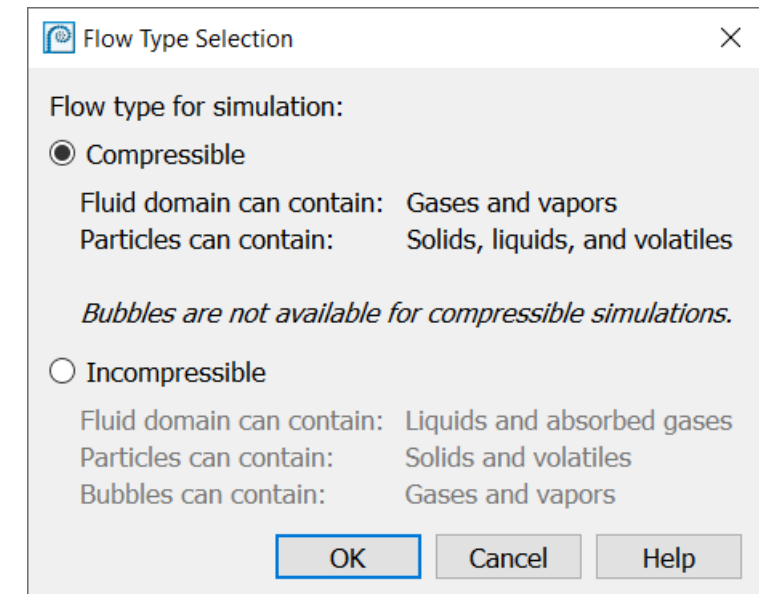
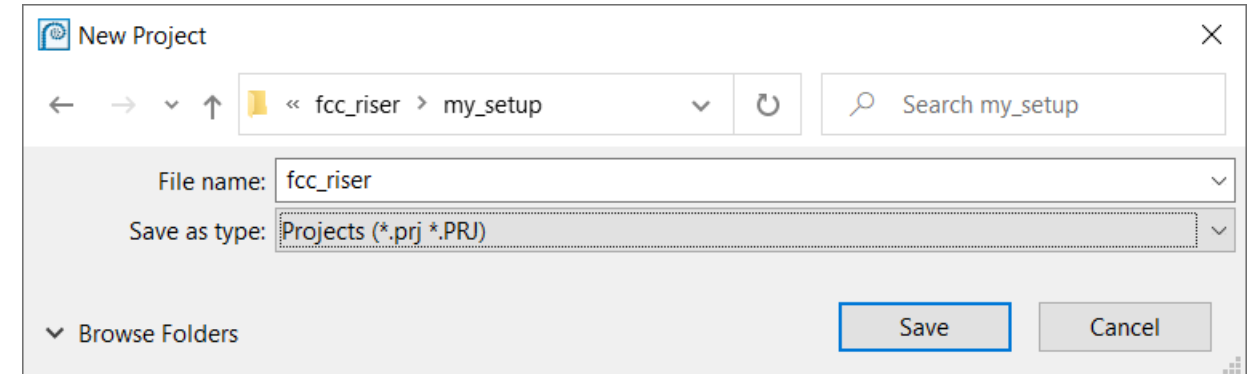
Project File

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

`\fcc_riser\my_setup\`

With the project name:

`fcc_riser.prj`



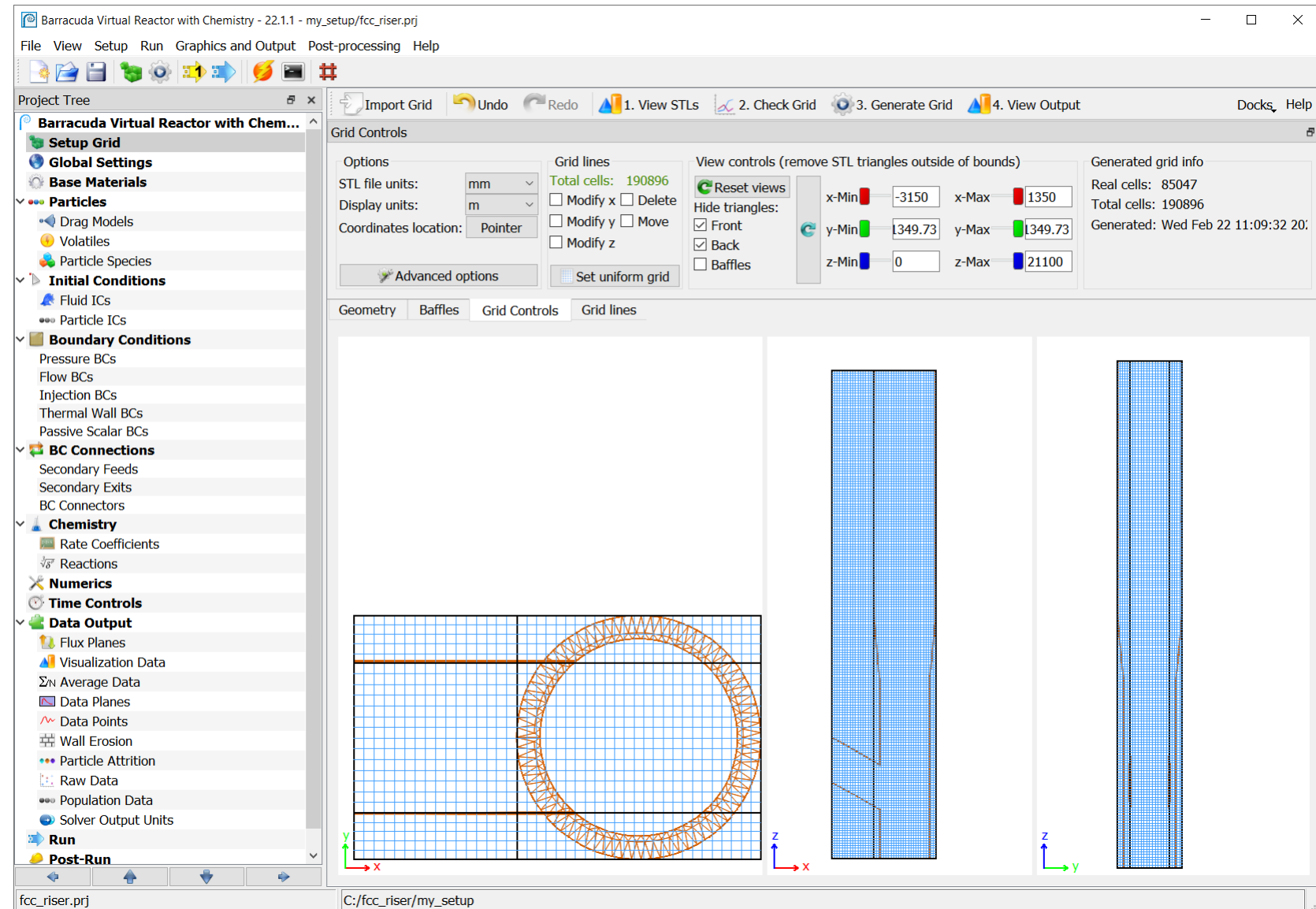
Setup Grid

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

Global Settings

Flow Type: Compressible

Fluid domain can contain: Gases and vapors

Particles can contain: Solids, liquids, and volatiles

Bubbles are not available for compressible simulations.

Gravity Settings

x-direction: m/s² y-direction: m/s² z-direction: m/s²

Thermal Settings

☐ Isothermal

Temperature: K

☒ Thermal

Heat Transfer Coefficients

Radiation Model

☒ None ☐ Near wall

Temperature Warning Limits

Minimum: K Maximum: K

☐ Record minimum and maximum temperature

Simulation Start Options

Heat Transfer Coefficients

Fluid-to-wall heat transfer coefficient

$$h = h_i + f_d h_d$$
$$h_i = (c_0 \text{Re}^{n_1} \text{Pr}^{n_2} + c_1) k_f / L + c_2 \text{ (J/m}^2\text{sK)}$$

c0= c1= c2= J/m²sK

n1= n2=

$$\text{Re}_L = \rho_f U_f L / \mu_f$$
$$\text{Pr} = C_p \mu_f / k_f$$

Dense phase heat transfer coefficient

$$h_d = (c_0 \text{Re}_p^{n_1}) k_f / d_p \text{ (J/m}^2\text{sK)}$$

c0= n1=

$$\text{Re}_p = \rho_f U_f d_p / \mu_f$$

Fluid-to-particle heat transfer coefficient

$$h = (c_0 \text{Re}^{n_1} \text{Pr}^{0.33} + c_1) k_f / D_p + c_2 \text{ (J/m}^2\text{sK)}$$

c0= c1= c2= J/m²sK

n1=

$$\text{Re} = |U_f - U_p| D_p / \nu_f$$
$$\text{Pr} = C_p \mu_f / k_f$$

OK Cancel Help

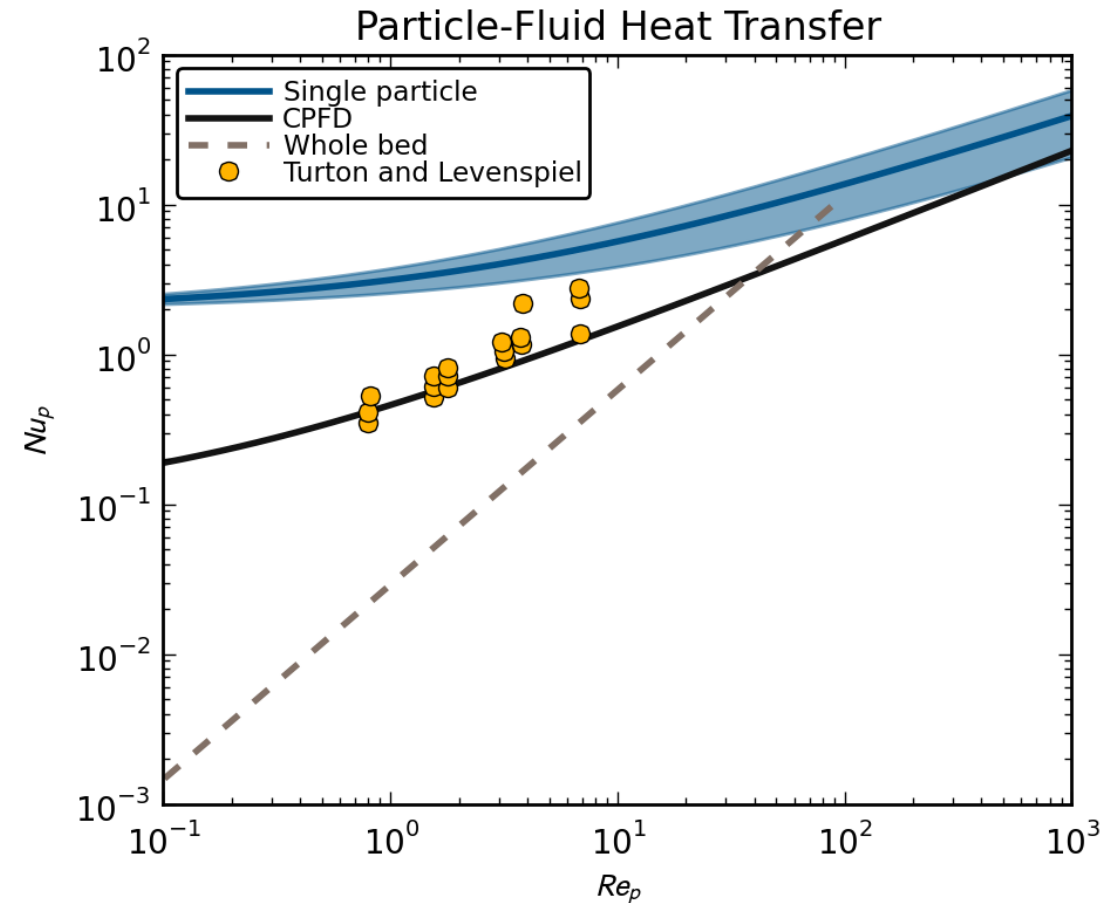
Heat Transfer Coefficients

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

Project Material List		
Material name	Phase(s)	Description
Cat_base	S	FCC CATALYST (EQUILIBRIUM).
Coke	S	FCC CATALYST (EQUILIBRIUM).
Gas	G	
GasOil	L/V	
Gasoline	G	
H2O	G	H2O STEAM
N2	G	N2 NITROGEN. REF ELEMENT

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/ Vapor	400	900	5.00E-02	-692000	2798	0.15
		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:

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

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

The image displays three overlapping software windows from the cpfd software:

- Base Materials Editor - GasOil (L/V)**: Shows the material name "GasOil", phase "Liquid/Vapor", molecular weight "400 g/mol", and the "Specify enthalpy as" dropdown set to "Liquid enthalpy and vapor entha". The "Heat of vaporization" is set to "Edit expression". The "Enable evaporation model" checkbox is checked. The "Vapor pressure" and "Vapor mass diffusivity" are both set to "Edit expression".
- Material Property Editor** (top right): Shows the material "GasOil (L/V)", property "Vapor pressure", units "Pa", and temperature units "K". The expression is set to "Antoine equation" with the formula $32.5 \cdot 10^{(7.825 - 2301.41 / (65.45965 + T))}$. The "Temperature Limits" and "Value Limits" checkboxes are unchecked.
- Material Property Editor** (bottom): Shows the material "GasOil (V)", property "Mass diffusivity", units "cm²/s", and temperature units "K". The expression is set to "Polynomial (4th order)" with the formula $0.01 + 0 \cdot T + 5e-08 \cdot T^2 + 0 \cdot T^3 + 0 \cdot T^4$. The "Temperature Limits" and "Value Limits" checkboxes are unchecked. The "Verification" section shows "Display units as" set to "Specified" with a preview of $T = 300 \text{ K}$ and $\text{Expression} = 0.0145 \text{ cm}^2/\text{s}$. The "Messages" section shows "Expression is valid".

Particles

Close pack volume fraction: 0.58

Normal-to-wall momentum retention: 0.9

Tangent-to-wall momentum retention: 0.9

Diffuse bounce: 5

Particles

Contact and Collision Models

Close pack volume fraction:

Maximum momentum redirection from collision:

☐ Blended acceleration model for the contact force

☒ Transfer liquid mass on collision

Stress Model Options

Wall Interactions

Normal-to-wall momentum retention:

Tangent-to-wall momentum retention:

Diffuse bounce:

Cloud Options

☒ Allow clouds to represent fractional particles

Dense Fluid Forces

☐ Enable virtual mass force

☐ Enable lift force

Help

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

Species-ID	Comment	Materials	Size	Sphericity	Emissivity	Drag model	Agglomeration
001	FCC	Cat_base, Coke	psd_fcc.sff	1	1	WenYu-Ergun	Off
002	Heavy gas droplets	GasOil	50 to 500 micron-diameter	1	1	WenYu-Ergun	Off

Add Edit Copy Delete

Particle Species Editor

Species-ID: 001
Comment: FCC
Materials: Applied Materials
Size Distribution: File: psd_fcc.sff
Import Preset Distribution:
Size Range: Minimum: Maximum: micron-diameter
Surface and Shape: Sphericity: 1.0, Emissivity: 1.0, Scattering Factor: 0.0

Drag Model: Model Name: WenYu-Ergun

Name	Link To Default	Value
c0	Linked	1
c1	Linked	0.15
c2	Linked	0.44
c3	Linked	2

Particle Composition Editor

Component	Density (kg/m³)	Mass fraction	Age factor
Cat_base(S)	1620	0.999	1
Coke(S)	1200	0.001	1

Particle Density (kg/m³) 1619.43 (calculated)
Sum of fractions: 1

Particle Species Editor

Species-ID: 002
Comment: Heavy gas droplets
Materials: Applied Materials
Size Distribution: Size Range: Minimum: 50 Maximum: 500 micron-diameter
Surface and Shape: Sphericity: 1.0, Emissivity: 1.0, Scattering Factor: 0.0

Drag Model: Model Name: WenYu-Ergun

Name	Link To Default	Value
c0	Linked	1
c1	Linked	0.15
c2	Linked	0.44
c3	Linked	2
c4	Linked	180

Particle Composition Editor

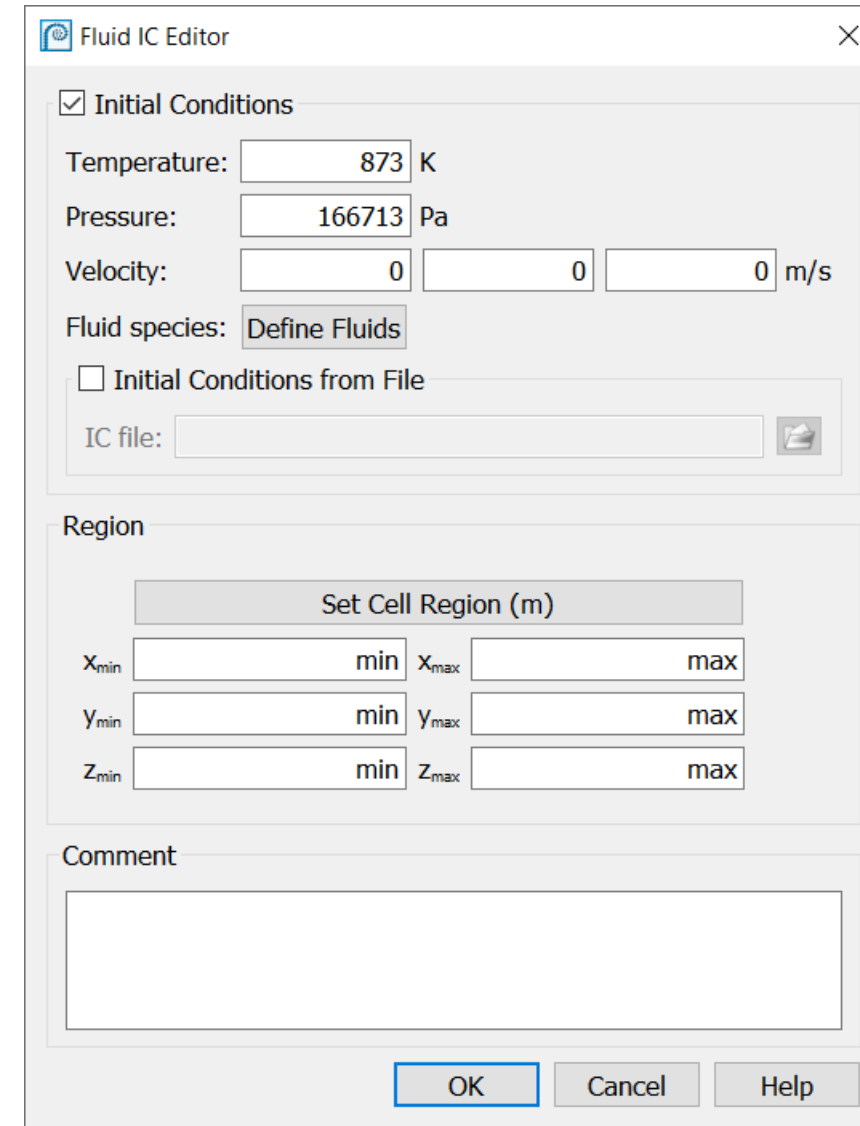
Component	Density (kg/m³)	Mass fraction	Age factor
GasOil(L)	900	1	1

Particle Density (kg/m³) 900 (calculated)
Sum of fractions: 1

Fluid ICs

Fluid IC

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



The image shows a screenshot of the 'Fluid IC Editor' dialog box. The 'Initial Conditions' section is checked, and the values are: Temperature: 873 K, Pressure: 166713 Pa, Velocity: 0 0 0 m/s, and Fluid species: Define Fluids. The 'Initial Conditions from File' section is unchecked, and the 'IC file' field is empty. The 'Region' section has a 'Set Cell Region (m)' button and fields for X_{min}, X_{max}, Y_{min}, Y_{max}, Z_{min}, and Z_{max}, all with 'min' and 'max' labels. The 'Comment' section has a large text area. At the bottom are 'OK', 'Cancel', and 'Help' buttons.

Fluid IC Editor

☒ Initial Conditions

Temperature: 873 K

Pressure: 166713 Pa

Velocity: 0 0 0 m/s

Fluid species: Define Fluids

☐ Initial Conditions from File

IC file:

Region

Set Cell Region (m)

X_{min} min X_{max} max

Y_{min} min Y_{max} max

Z_{min} min Z_{max} max

Comment

OK Cancel Help

Pressure BC

Add a pressure BC with information shown here for the outlet

Use 100% N2 for Applied Fluids

The image displays four overlapping screenshots of the 'Pressure BC Editor' window, illustrating the configuration steps for a pressure boundary condition.

- Top Left Screenshot (Region Tab):** Shows the 'Region' tab with a 'Select region (m)' button and input fields for X_{min}, X_{max}, Y_{min}, Y_{max}, Z_{min}, and Z_{max}. The 'Direction' section has radio buttons for x-direction, y-direction, and z-direction (selected).
- Top Right Screenshot (Name/Fluid species behavior Tab):** Shows the 'Name' field set to 'FLUXBC_pressure_outlet'. Under 'Fluid species behavior', 'Mass flow rate' is selected. Other options include 'Bin by particle size' (100 bins), 'Output raw particle data', and 'Output tracer data'.
- Middle Screenshot (Flow Conditions Tab):** Shows the 'Flow Conditions' tab. 'Transient file' is selected with the file 'pressure_outlet.sff'. Other options include 'Specify values' with fields for Area fraction (1), Pressure (0 Pa), and Temperature (300 K).
- Bottom Screenshot (Behavior at Boundary Tab):** Shows the 'Behavior at Boundary' tab. 'Outflow with size filtering' is selected. Fields include 'Minimum' (0), 'Maximum' (UNLIMITED), and 'Units' (micron-diameter). Other options include 'Feed specified as volume fraction', 'Feed specified as mass flux', and 'Feed specified as mass flow rate'. The 'Feed Settings' section has 'Edit Feed' and 'Feed Control' buttons.

At the bottom, a 'Pressure Boundary Conditions Editor' window shows a table with two rows of data:

	Time (s)	Pressure (Pa)	Temperature (K)	Area Fraction	Particle Feed	K-Factor
1	0	166713	873	1	Off	0
2					On	

Below the table are buttons: '+ Add Row', '- Delete Row', '✓ Check Data', 'Graph', and 'Update Simulation'. At the bottom are 'File: pressure_outlet.sff', 'Save', 'Save As', 'Close', and 'Help' buttons.

Flow BCs

Add flow BC with information shown here for bottom steam

Use 100% H2O for Applied fluids

Flow Boundary Conditions Editor

	Time (s)	Mass Flow Rate (kg/s)	Temperature (K)	Pressure (Pa)
1	0	0.82	633	166713
2				

+ Add Row - Delete Row ✓ Check Data 📊 Graph ↻ Update Simulation

File: flow_steam_inlet.sff Save Save As Close Help

Flow BC Editor

Location Flux Plane Fluid Particles Tracers

Region

Set Cell Region (m)

X_{min} min X_{max} max

Y_{min} min Y_{max} max

Z_{min} min Z_{max} min

Direction

☐ Normal to surface:

☐ x-direction

☐ y-direction

☒ z-direction

☐ Direction vector

u: 0 v: 0

☐ Force absolute d

Variation angle: 0

Transient File

Flow BC Editor

Location Flux Plane Fluid Particles Tracers

Flow Conditions

☒ Use transient file

☐ Use BC Connector data

☐ Specify values:

Velocity flow 0 m/s

Pressure: 0 Pa

Temperature: 300 K

Fluid Composition

Applied fluids: Define Fluids

Transient File

flow_steam_inlet.sff Edit

Comment:

OK Cancel Help

Flow BC Editor

Location Flux Plane Fluid Particles Tracers

Name: FLUXBC_flow_steam_inlet

Fluid species behavior:

No output

☐ Bin by particle size 100 bins

☐ Output raw particle data

☐ Output tracer data

Flow BC Editor

Location Flux Plane Fluid Particles Tracers

☐ Use transient file

☐ Use BC Connector data

☒ No outflow

☐ Outflow with size filtering:

Minimum: 0

Maximum: UNLIMITED

Units: micron-diameter

☐ Exit control: Edit

☐ Feed specified as volume fraction

☐ Feed specified as mass flux

☐ Feed specified as mass flow rate

Feed Settings

Edit Feed Feed Control

Transient File

flow_steam_inlet.sff Edit

Comment:

OK Cancel Help

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

The image displays four screenshots of the Flow BC Editor interface, illustrating the configuration of a flow boundary condition. The screenshots are labeled with red boxes and letters:

- 1**: Location tab, showing the Region (Set Cell Region (m)) and Direction (x-direction selected).
- 2**: Location tab, showing the Name (FLUXBC_flow_regen_cat_inlet) and Fluid species behavior (No output).
- 3**: Fluid tab, showing Flow Conditions (Use transient file selected) and Fluid Composition (Applied fluids: Define Fluids).
- 4**: Particles tab, showing Use transient file selected, Feed specified as mass flow rate selected, and Transient File (flow_regen_cat_inlet.sff).

Additional labels and settings visible in the screenshots include:

- a**: x-direction selected in Direction.
- a**: Use transient file selected in Flow Conditions.
- b**: Use transient file selected in Flow Conditions.
- b**: Applied fluids: Define Fluids.
- c**: Edit Feed button in Feed Settings.
- d**: Edit button in Transient File.

The main Flow Boundary Conditions Editor window shows a table with the following data:

	Time (s)	Mass Flow Rate (kg/s)	Temperature (K)	Pressure (Pa)	Particle Feed	Number Density Manual	Particle Slip	Particle Mass Flow Rate (kg/s)
1	0	0.75	973	166713	On	200	1	1740
2					On			

Buttons at the bottom include: Add Row, Delete Row, Check Data, Graph, Update Simulation, Save, Save As, Close, Help, OK, Cancel, and Help.

Injection BC – Feed Oil

Add Feed Oil injection BC

- Name = Feed_Oil
- Select Fluid and Particles/Tracers

Locations tab

- Import feed_oil_locations.csv

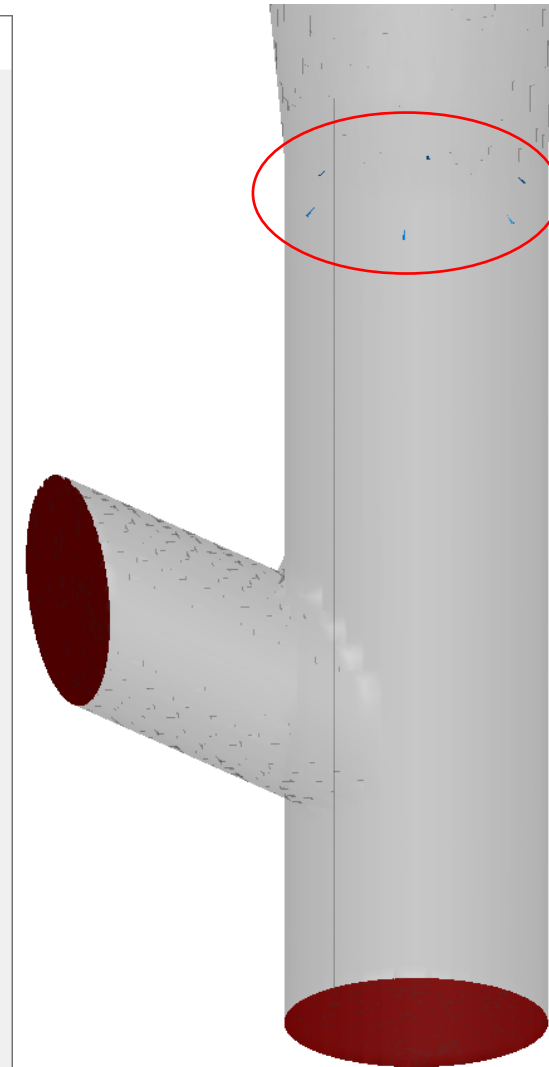
Flux Plane tab

- Add a flux plane name

The screenshot shows the 'Injection BC Editor' dialog box with the 'Locations' tab selected. The 'Name' field is set to 'Feed_Oil'. Both 'Fluid' and 'Particles/Tracers' checkboxes are checked. A table lists 6 active injections. Below the table are buttons for 'Add Row', 'Delete Row', 'Reference Grid', 'Expand Locations Table', 'Import', and 'Export'. A 'Comment' field and 'OK', 'Cancel', and 'Help' buttons are at the bottom.

	Name	On/Off	X (m)	Y (m)	Z (m)
1	Inj1	<input checked="" type="checkbox"/> On	1.010309063	0	7.22
2	Inj2	<input checked="" type="checkbox"/> On	0.505154531	0.874953314	7.22
3	Inj3	<input checked="" type="checkbox"/> On	-0.505154531	0.874953314	7.22
4	Inj4	<input checked="" type="checkbox"/> On	-1.010309063	1.24E-16	7.22
5	Inj5	<input checked="" type="checkbox"/> On	-0.505154531	-0.874953314	7.22
6	Inj6	<input checked="" type="checkbox"/> On	0.505154531	-0.874953314	7.22
7		<input type="checkbox"/> Off			

The screenshot shows the 'Injection BC Editor' dialog box with the 'Flux Plane' tab selected. The 'Name' field is set to 'Feed_Oil'. Both 'Fluid' and 'Particles/Tracers' checkboxes are checked. The 'Name' field for the flux plane is set to 'FLUXBC_injection_feed_oil'. The 'Fluid species behavior' dropdown is set to 'No output'. There are checkboxes for 'Bin by particle size' (100 bins), 'Output raw particle data', and 'Output tracer data'. A 'Comment' field and 'OK', 'Cancel', and 'Help' buttons are at the bottom.



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)

The image shows two software windows from the Barracuda Virtual Reactor. The 'Injection BC Editor' window is in the background, showing the 'Fluid' tab. It has a 'Name' field set to 'Feed_Oil'. Under 'Use transient file:', the file 'feed_oil.sff' is selected. The 'Fluid Composition' section shows 'Applied fluids' as 'Define Fluids'. The 'Mixture' window is in the foreground, showing a table of components and their fractions. The 'Available Components' list includes N2(G), GasOil(V), and Gas(G). The 'Mixture' table shows H2O(G) with a fraction of 0.5652 and Gasoline(G) with a fraction of 0.4348. The 'Specify mixture by:' dropdown is set to 'Mass fraction'.

Injection BC Editor

Name: Feed_Oil

☒ Fluid ☒ Particles/Tracers

Locations Flux Plane Fluid Particles/Tracers

☐ Use BC Connector data

☒ Use transient file:
feed_oil.sff Edit

☐ Use specified values:
Velocity: 0 m/s
Mass flow: 0 kg/s
Temperature: 300 K

Fluid Composition

Applied fluids: Define Fluids

☐ Dynamic Fluid Distribution
Orifice discharge coefficient (C_d): 0.8

Comment:

OK Cancel Help

Fluid Injection Boundary Conditions Editor

	Time (s)	On/Off	Temperature (K)	Velocity (m/s)	Mass Flow Rate (kg/s)
1	0	On	491.9	0	0
2	5	On	491.9	73.2	26.772
3		On			

+ Add Row - Delete Row ✓ Check Data Graph ↻ Update Simulation

File: feed_oil.sff Save Save As Close Help

Mixture

Component	Fraction
H2O(G)	0.5652
Gasoline(G)	0.4348

Specify mixture by: Mass fraction Sum of fractions: 1

Reset OK Cancel Help

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°

Particle Injection Boundary Conditions Editor

	Time (s)	On/Off	Temperature (K)	Velocity (m/s)	Mass Flow Rate (kg/s)	Number Density Manual
1	0	On	491.9	0	0	125
2	5	On	491.9	73.2	206.03	125
3		On				

Add Row Delete Row Check Data Graph Update Simulation

File: feed_liq_oil.sff Save Save As Close Help

Injection BC Editor

Name: Feed_Oil

☒ Fluid ☒ Particles/Tracers

Locations Flux Plane Fluid **Particles/Tracers**

☐ Use BC Connector data

☒ Use transient file:
feed_liq_oil.sff

☐ Use specified values:
Velocity: 0 m/s
Mass flow: 0 kg/s
Temperature: 300 K
Number density: 125

Injection Type
Type: Particle
Species: 002 - Heavy gas droplets

Angle Expansion
 θ_{e1} : 15° θ_{e2} : 15°

Angle Orientation
 α_{e1} : 0°

Comment:

OK Cancel Help

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°

Fluid Injection Boundary Conditions Editor

	Time (s)	On/Off	Temperature (K)	Velocity (m/s)	Mass Flow Rate (kg/s)
1	0	<input checked="" type="radio"/> On	364.9	0	0
2	5	<input checked="" type="radio"/> On	364.9	1	1.3068
3		<input checked="" type="radio"/> On			

+ Add Row - Delete Row ✓ Check Data 📊 Graph ↻ Update Simulation

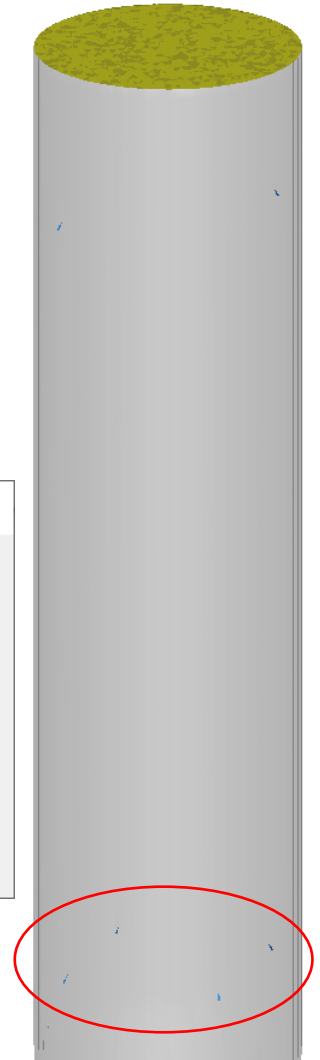
File: feed_mtc.sff 💾 Save 📁 Save As 🗑 Close ? Help

Particle Injection Boundary Conditions Editor

	Time (s)	On/Off	Temperature (K)	Velocity (m/s)	Mass Flow Rate (kg/s)	Number Density Manual
1	0	<input checked="" type="radio"/> On	364.9	0	0	125
2	5	<input checked="" type="radio"/> On	364.9	1	20.4732	125
3		<input checked="" type="radio"/> On				

+ Add Row - Delete Row ✓ Check Data 📊 Graph ↻ Update Simulation

File: feed_liq_mtc.sff 💾 Save 📁 Save As 🗑 Close ? Help



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% H2O
- Particles/Tracers tab
 - Use transient file shown here
 - Use Heavy gas droplets particle species
 - Angle Expansion of 15°

Fluid Injection Boundary Conditions Editor

	Time (s)	On/Off	Temperature (K)	Velocity (m/s)	Mass Flow Rate (kg/s)
1	0	<input checked="" type="radio"/> On	364.9	0	0
2	5	<input checked="" type="radio"/> On	364.9	0.06	0.042
3		<input checked="" type="radio"/> On			

+ Add Row - Delete Row ✓ Check Data 📊 Graph ↻ Update Simulation

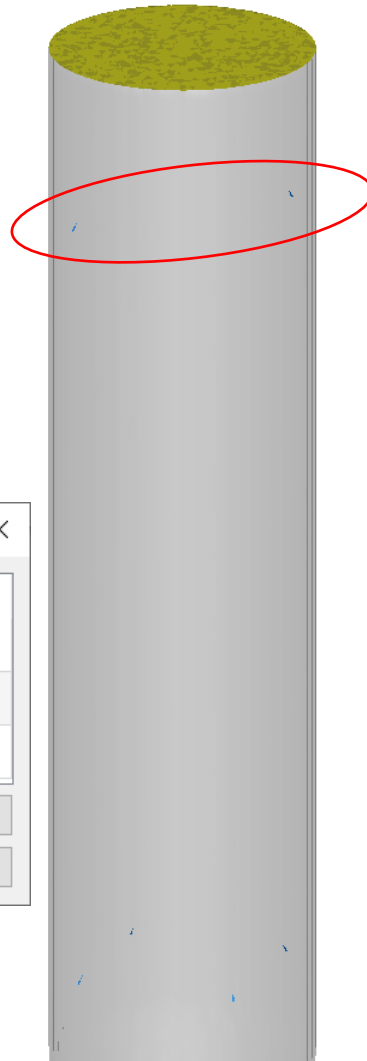
File: feed_slurry.sff 💾 Save 📁 Save As 🗑 Close ? Help

Particle Injection Boundary Conditions Editor

	Time (s)	On/Off	Temperature (K)	Velocity (m/s)	Mass Flow Rate (kg/s)	Number Density Manual
1	0	<input checked="" type="radio"/> On	364.9	0	0	125
2	5	<input checked="" type="radio"/> On	364.9	0.06	0.798	125
3		<input checked="" type="radio"/> On				

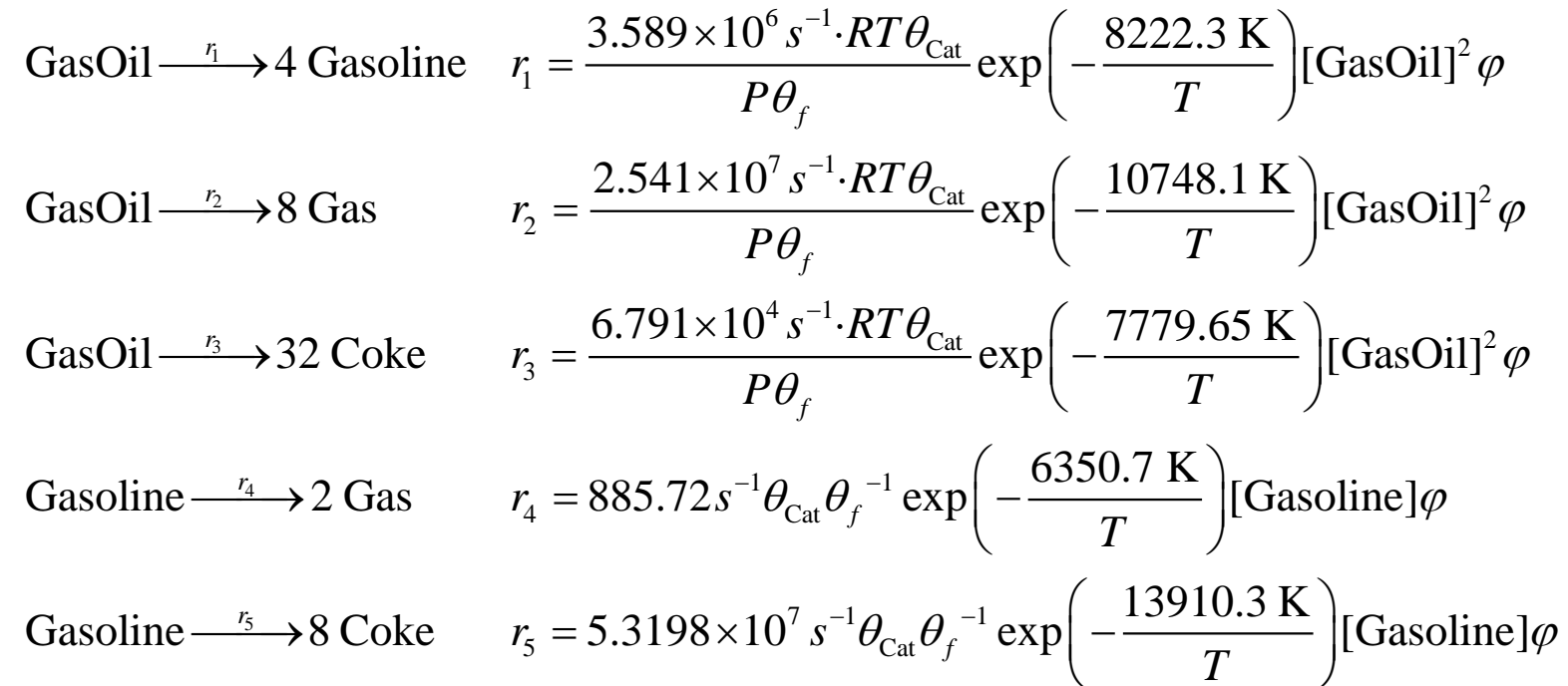
+ Add Row - Delete Row ✓ Check Data 📊 Graph ↻ Update Simulation

File: feed_liq_slurry.sff 💾 Save 📁 Save As 🗑 Close ? Help



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:



Where $R = 8.3145 \text{ kg} \cdot \text{m}^2 \cdot \text{s}^{-2} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ 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/m³ for concentration and mol/m³/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:

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

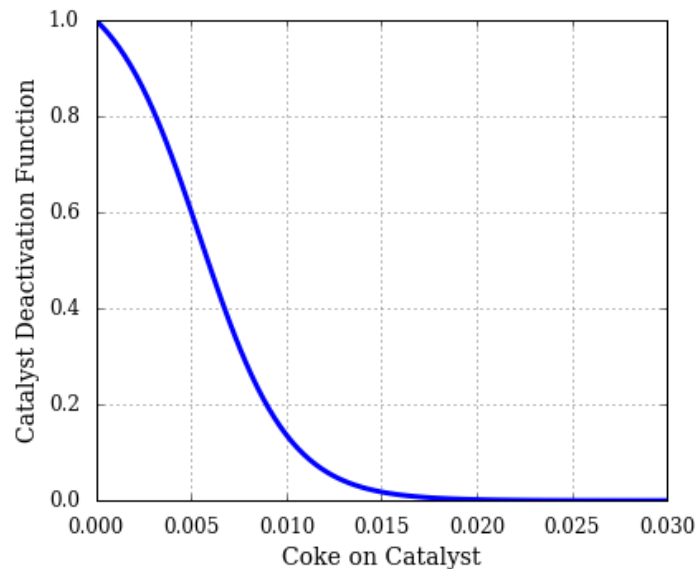
where k0 and k5 are appropriate rate coefficients

Catalyst deactivation function

The catalyst deactivation function is given in the following form:

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

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



Chemistry Coefficient Editor

Coefficient Properties

Name: **k5**

Type: Catalyst Deactivation

Coefficient is for reaction type: ☒ Volume-Average ☐ Discrete

Equation: $(B_C + 1) / (B_C + \exp(A_C C_{[material]}))$

k5 = $(10.4 + 1) / (10.4 + \exp(4.29 C_{[Coke(S)]})$

Catalyst Deactivation Values

$A_C = 4.29$

$B_C = 10.4$

Particle material:

	Material
1	<input type="checkbox"/> Cat_base(S)
2	<input checked="" type="checkbox"/> Coke(S)

Comment

OK Cancel Help

Chemistry Rate Coefficients and Reactions

Chemistry Rate Coefficients Manager

ID	Name	Reaction Type	Coefficient Type	Expression	Comment
00	k0	Volume-Average	Arrhenius Chem Rate	$2.9839e+07 T^{p-1} \theta_{f^{-1}} e^{(-8222.3 / T)} v_{f_Cat_base}^{v1}$	VGO --> Gasoline, $3.589e+06 * 8.314 = 29.839e6$
01	k1	Volume-Average	Arrhenius Chem Rate	$2.1126e+08 T^{p-1} \theta_{f^{-1}} e^{(-10748.1 / T)} v_{f_Cat_base}^{v1}$	VGO --> Gas, $2.541e+07 * 8.314 = 21.126e7$
02	k2	Volume-Average	Arrhenius Chem Rate	$564604 T^{p-1} \theta_{f^{-1}} e^{(-7779.65 / T)} v_{f_Cat_base}^{v1}$	VGO --> Coke, $67910 * 8.314 = 564603.7$
03	k3	Volume-Average	Arrhenius Chem Rate	$885.72 \theta_{f^{-1}} e^{(-6350.7 / T)} v_{f_Cat_base}^{v1}$	Gasoline --> Gas
04	k4	Volume-Average	Arrhenius Chem Rate	$5.3198e+07 \theta_{f^{-1}} e^{(-13910.3 / T)} v_{f_Cat_base}^{v1}$	Gasoline --> Coke
05	k5	Volume-Average	Catalyst Deactivation	$(10.4 + 1) / (10.4 + \exp(4.29 C_{[Coke(S)]}))$	Catalyst deactivation

Chemistry Reactions Manager

ID	Reaction Type	Rate	Equation	Comment
00	VA: Stoichiometric	Equation: $GasOil(V) \Rightarrow 4 Gasoline$ R00 = $(k0[GasOil(V)]^2)*(k5)$	VGO --> Gasoline	
01	VA: Stoichiometric	Equation: $GasOil(V) \Rightarrow 8 Gas$ R01 = $(k1[GasOil(V)]^2)*(k5)$	VGO --> Gas,	
02	VA: Stoichiometric	Equation: $GasOil(V) \Rightarrow 32 Coke(S)$ R02 = $(k2[GasOil(V)]^2)*(k5)$	VGO --> Coke	
03	VA: Stoichiometric	Equation: $Gasoline \Rightarrow 2 Gas$ R03 = $(k3[Gasoline])*(k5)$	Gasoline --> gas	
04	VA: Stoichiometric	Equation: $Gasoline \Rightarrow 8 Coke(S)$ R04 = $(k4[Gasoline])*(k5)$	Gasoline --> Coke	

Time Controls

Set Time step and End time

Time Controls

This section allows configuration of the time step size to take during a period of time for the calculation. Only the first row is required. Subsequent rows can be entered to have different time steps for different time periods. For example, starting the calculation at a smaller time step is recommended, and then increasing the time step for rows 2-5 over simulation time.

Time step and duration settings

	Time step		End time	
1.	<input type="text" value="0.01"/>	s	<input type="text" value="30"/>	s
2.	<input type="text"/>	s	<input type="text"/>	s
3.	<input type="text"/>	s	<input type="text"/>	s
4.	<input type="text"/>	s	<input type="text"/>	s
5.	<input type="text"/>	s	<input type="text"/>	s

Advanced time step settings

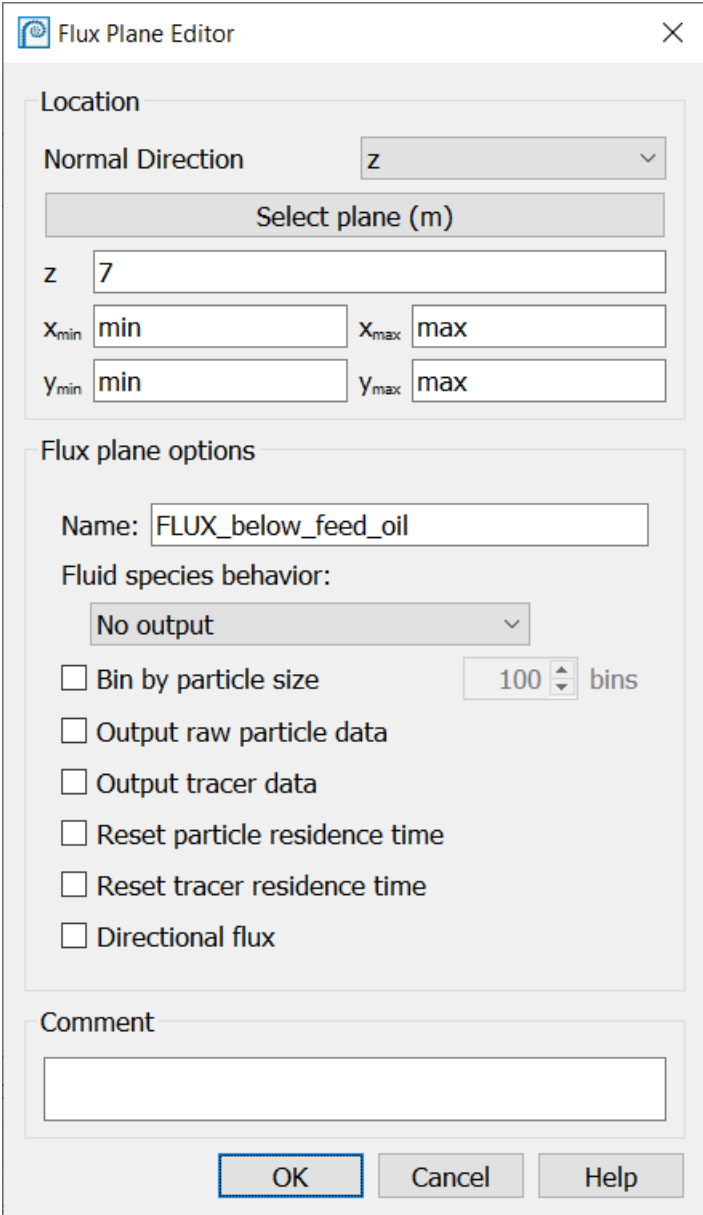
Restart file intervals

Restart interval (IC_###)	<input type="text" value="100"/>	simulation seconds
Backtrack interval (IC_)	<input type="text" value="120"/>	realtime minutes

Help

Flux Planes

Define a flux plane below the feed oil nozzles



The Flux Plane Editor dialog box is used to define a flux plane. It contains the following sections:

- Location:**
 - Normal Direction: **z** (dropdown)
 - Select plane (m): **7** (text input)
 - x_{min} : **min** (text input), x_{max} : **max** (text input)
 - y_{min} : **min** (text input), y_{max} : **max** (text input)
- Flux plane options:**
 - Name: **FLUX_below_feed_oil** (text input)
 - Fluid species behavior: **No output** (dropdown)
 - ☐ Bin by particle size: **100** (spin box) bins
 - ☐ Output raw particle data
 - ☐ Output tracer data
 - ☐ Reset particle residence time
 - ☐ Reset tracer residence time
 - ☐ Directional flux
- Comment:**
 - (Empty text input area)

Buttons: **OK**, **Cancel**, **Help**

Visualization Data Output

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

Visualization Data Output

Output formats
☒ Tecplot (*.plt files) ☐ GMV (Gmv.* files)

Output file interval
Plot interval: s Number of files produced using current end time of **30s**:

Cell Data

Available Data		Selected Data
Dynamic pressure		Bulk density
Fluid composition mass concentration		dp/dz
Fluid composition mass fraction		Fluid composition mole concentration
Fluid composition mole fraction		Fluid mass flux
Fluid density		Fluid temperature
P1 incident radiation flux		Fluid velocity
P1 radiation flux		Particle mass flux
P1 radiation flux from walls		Particle volume fraction
P1 radiation to fluids		Pressure
P1 radiation to particles		
Particle species		
Particle temperature		
Particle velocity		

Particle Data

Available Data		Selected Data
Cell ID		Particle material
Cloud ID		Particle size
Cloud mass		Particle species
Drag		Particle speed
Liquid fraction total		Particle temperature
Liquid mass total		Particle velocity
P1 radiation flux		Particle volume fraction
Particle density		Residence time
Particle mass		
Particles per cloud		

Help

Average Data

Set Averaging start time to 20 s

Select the Average Data Output shown

Average Data Output

Averaging start time: s

Cell Data

Available Data		Selected Data
Clouds per cell		dp/dz
Convective wall heat transfer		Fluid composition mole concentration
dp/dx		Fluid temperature
dp/dy		Fluid velocity
Fluid composition mass concentration	→	Particle mass flux
Fluid composition mass fraction	←	Particle velocity
Fluid composition mole fraction		Particle volume fraction
Fluid mass flux		Pressure
Particle temperature		
Voidage		
Volume fraction by species		

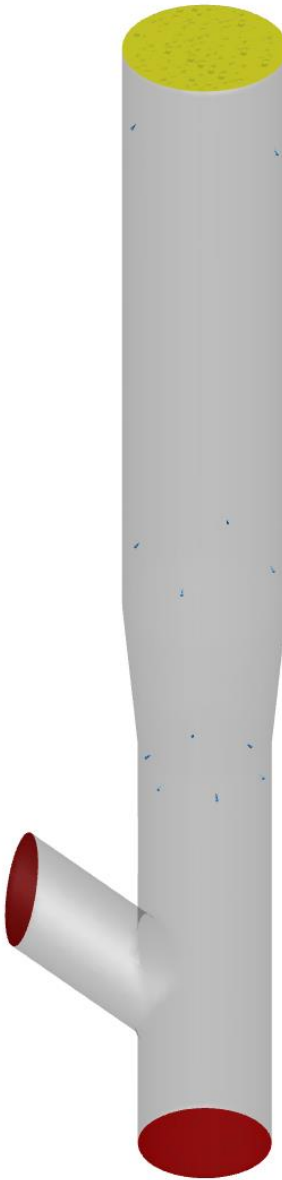
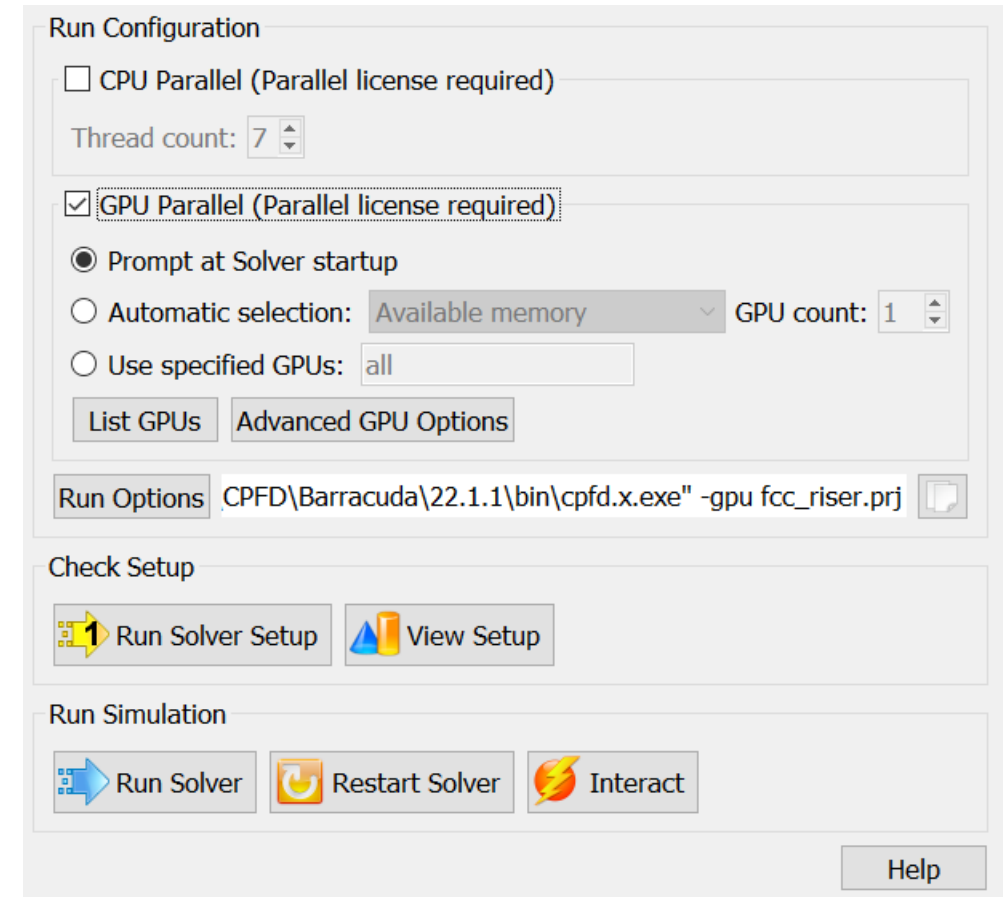
Help

Run

If NVIDIA GPU card is available, select GPU Parallel

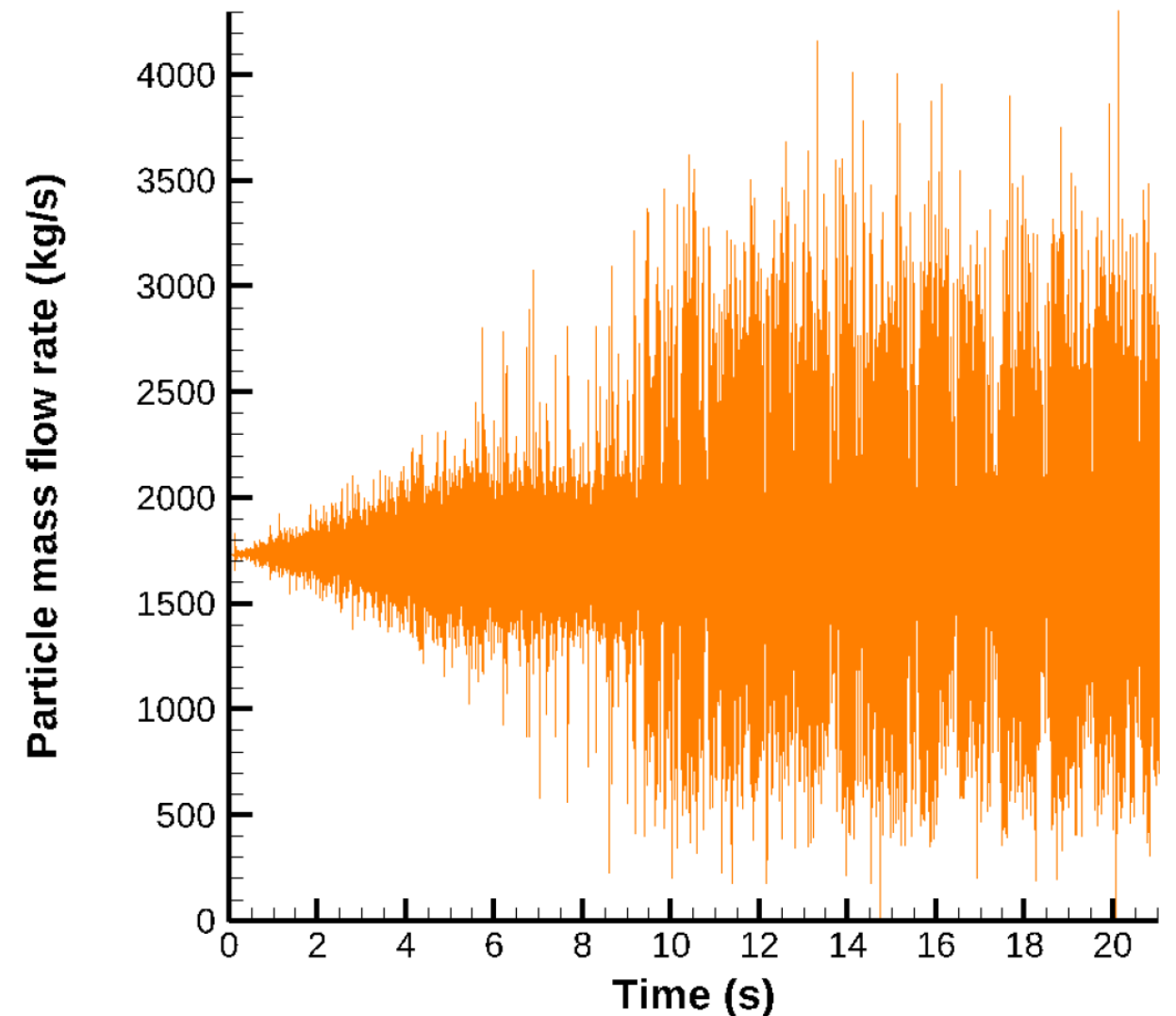
Run Solver Setup and View Setup

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.



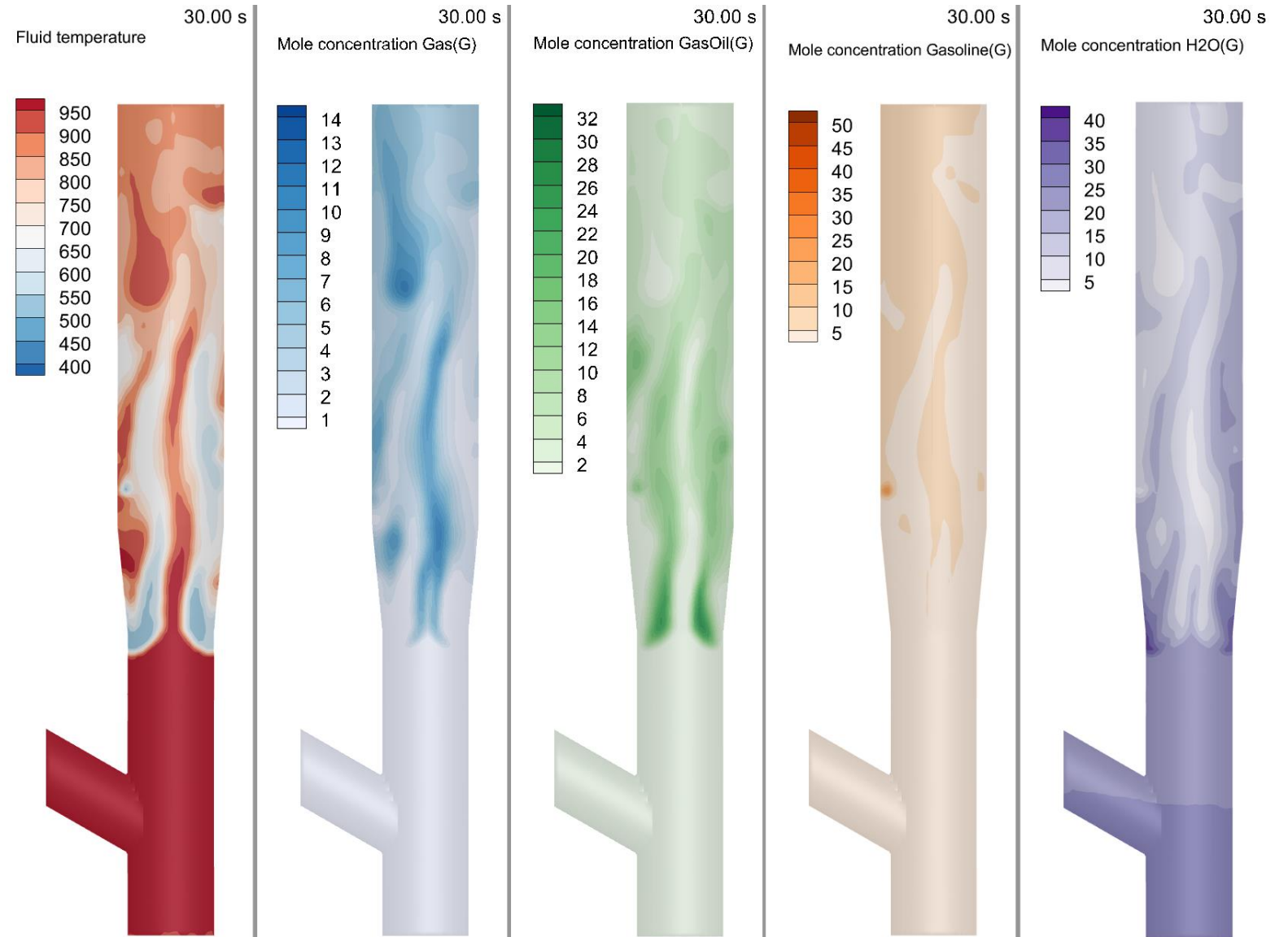
Post-Processing - Slices

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:

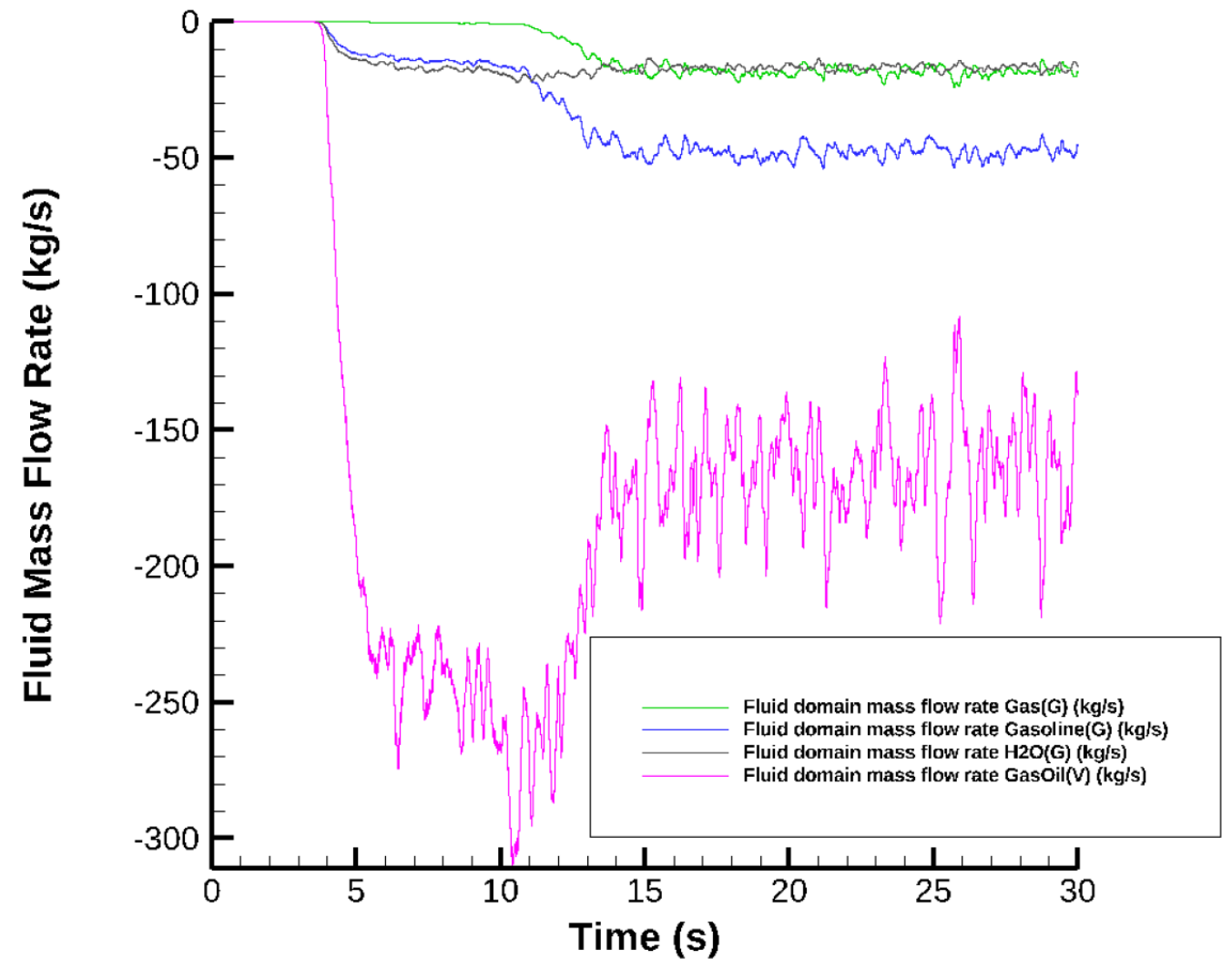
- [Frames](#)
- [Slices](#)
- [Contour legend](#)



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

