

FCC Riser: Setup and Analysis

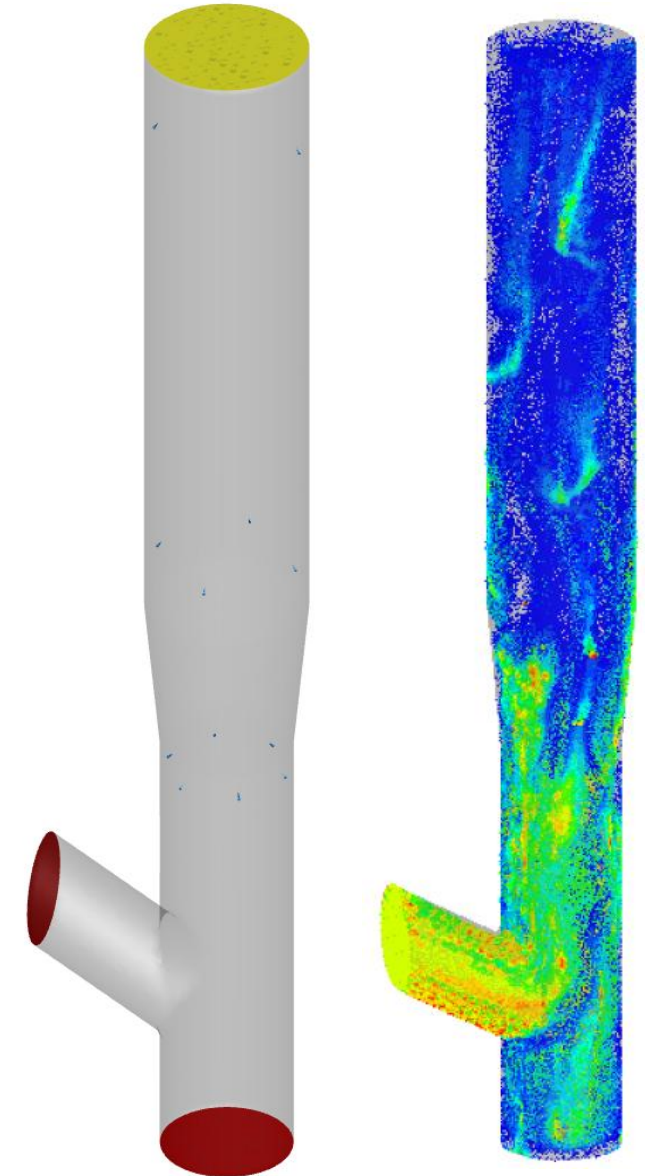
CPFD Software

www.cdfd-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.

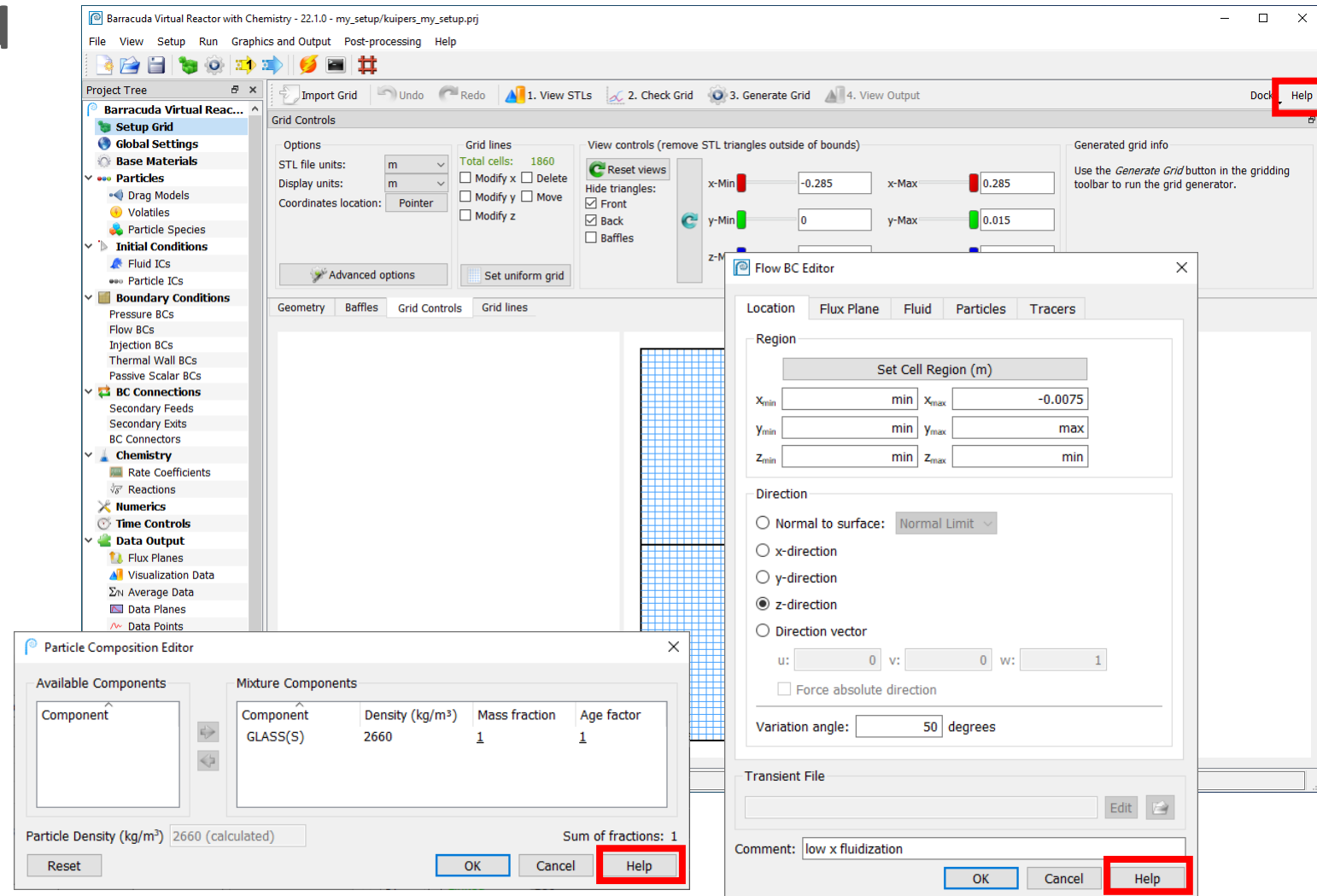
This is a thermal and reacting system with a four-lump model in which the hydrocarbons present are divided into four groups: heavy gas compounds, product gas compounds, light gas compounds, and solid carbon.



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.



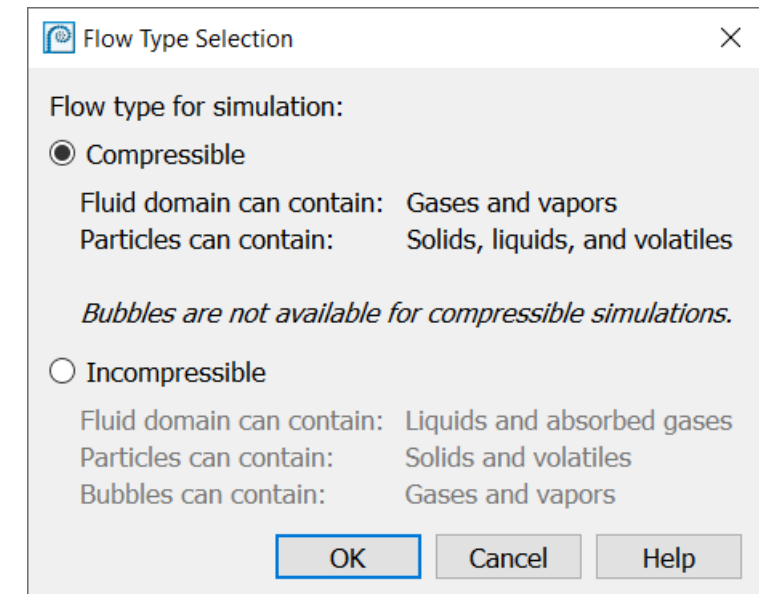
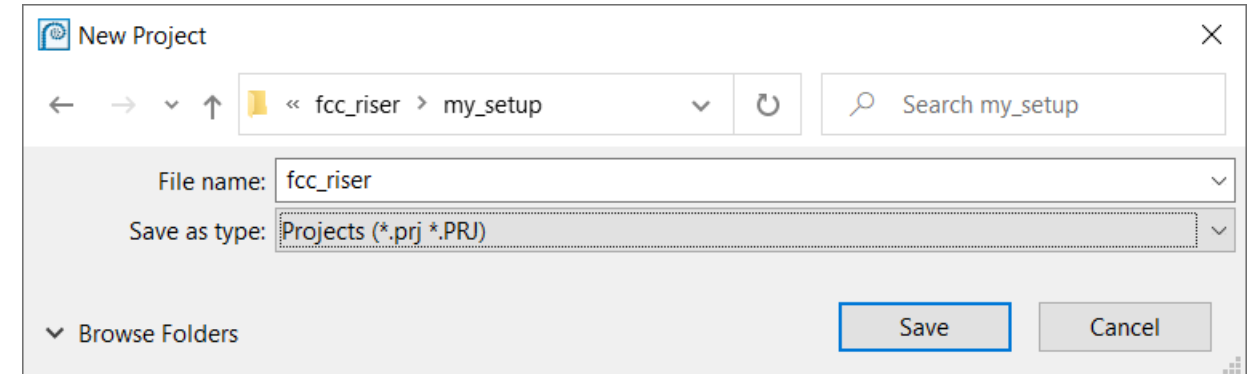
Project File

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

`\fcc_riser\my_setup\`

With the project name:

`fcc_riser.prj`



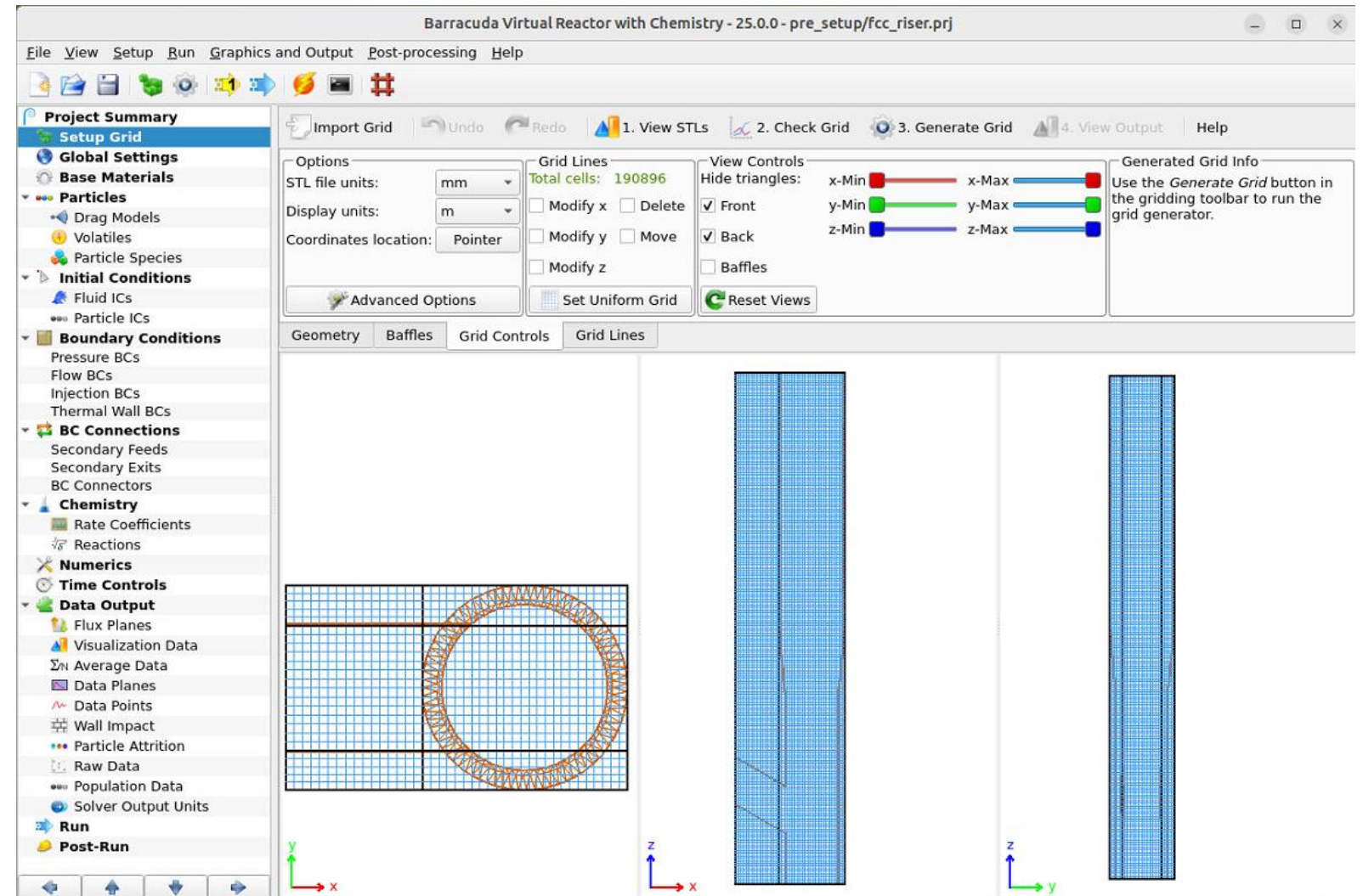
Setup Grid

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

☒ Use specified values: x-direction: m/s² y-direction: m/s² z-direction: m/s²

☐ Rotate about major axis: X Rotation velocity: rad/s

☐ Use transient file:

Thermal Settings

☐ Isothermal

Temperature: K

☒ Thermal

Convection

Conduction

☐ Enable particle-to-particle heat conduction

Radiation

☒ None ☐ Near wall ☐ P-1 ☒ Cap ex

Temperature Warning Limits

Minimum: K

☐ Record minimum and maximum temperature

Simulation Start Options

Heat Transfer Coefficients

Fluid-to-wall heat transfer coefficient

$$h = h_l + f_d h_d$$
$$h_l = (c_0 Re^{n_1} Pr^{n_2} + c_1) k_f / L + c_2 \text{ (J/m}^2\text{sK)}$$
$$h_d = (c_0 Re_p^{n_1}) k_f / d_p \text{ (J/m}^2\text{sK)}$$
$$Re_L = \rho_f U_f L / \mu_f$$
$$Pr = C_p \mu_f / k_f$$
$$Re_p = \rho_f U_f d_p / \mu_f$$

Fluid-to-particle heat transfer coefficient

$$h = (c_0 Re^{n_1} Pr^{0.33} + c_1) k_f / D_p + c_2 \text{ (J/m}^2\text{sK)}$$
$$Re = |U_f - U_p| D_p / \nu_f$$
$$Pr = C_p \mu_f / k_f$$

Parameters for Fluid-to-wall:

c0 = c1 = c2 = J/m²sK

n1 = n2 =

Parameters for Fluid-to-particle:

c0 = c1 = c2 = J/m²sK

n1 =

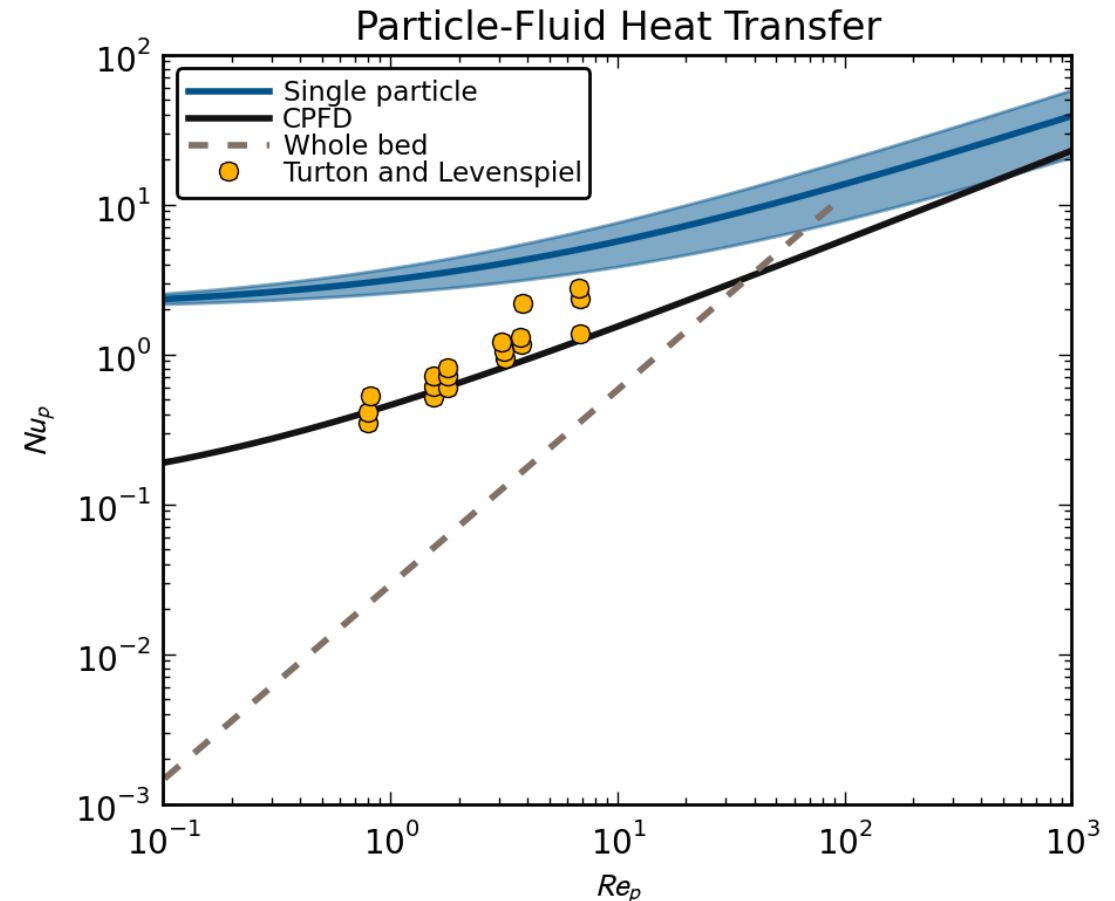
Heat Transfer Coefficients

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 suite, illustrating the configuration of a material named 'GasOil'.

- Base Materials Editor - GasOil (L/V)**: This window is used to define the material's basic properties. It shows 'Name: GasOil' and 'Phase(s): Liquid/Vapor'. Under the 'Liquid Phase' tab, 'Molecular weight' is set to '400 g/mol'. The 'Specify enthalpy as:' dropdown is set to 'Liquid enthalpy and vapor entha'. The 'Heat of vaporization:' field has an 'Edit expression' button. The 'Enable evaporation model' checkbox is checked. 'Vapor pressure:' and 'Vapor mass diffusivity:' both have 'Edit expression' buttons.
- Material Property Editor (Top)**: This window is used to define the vapor pressure. It shows 'Material: GasOil (L/V)' and 'Property: Vapor pressure'. The 'Property units:' are set to 'Pa' and 'Temperature units:' are set to 'K'. The 'Expression' dropdown is set to 'Antoine equation', and the expression field contains the Antoine equation: $32.5 \cdot 10^{(7.825 - 2301.41 / (65.45965 + T))}$. There are checkboxes for 'Temperature Limits' and 'Value Limits'.
- Material Property Editor (Bottom)**: This window is used to define the mass diffusivity. It shows 'Material: GasOil (V)' and 'Property: Mass diffusivity'. The 'Property units:' are set to 'cm²/s' and 'Temperature units:' are set to 'K'. The 'Expression' dropdown is set to 'Polynomial (4th order)', and the expression field contains the polynomial equation: $0.01 + 0 \cdot T + 5e-08 \cdot T^2 + 0 \cdot T^3 + 0 \cdot T^4$. There are checkboxes for 'Temperature Limits' and 'Value Limits'. The 'Verification' section shows 'Display units as: Specified' and a verification result of 'T = 300 K Expression = 0.0145 cm²/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

The screenshot shows the 'Particles' settings window. It is divided into several sections: 'Contact and Collision Models' with fields for 'Close pack volume fraction' (0.58), 'Momentum redirection model' (Directional), and 'Maximum momentum redirection from collision' (40%); a checkbox for 'Blended acceleration model for the contact force' (unchecked) and 'Transfer liquid mass on collision' (checked); a 'Stress Model Options' button; 'Wall Interactions' with fields for 'Normal-to-wall momentum retention' (0.9), 'Tangent-to-wall momentum retention' (0.9), and 'Diffuse bounce' (5); a 'Help' button; 'Cloud Options' with 'Global cloud resolution' set to 'Automatic' (slider at Medium) and 'Specify resolution' set to 'Clouds per cell' (125); and 'Dense Fluid Forces' with checkboxes for 'Enable virtual mass force' and 'Enable lift force' (both unchecked).

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

| Particle Species Manager | | | | | | | |
|--------------------------|--------------------|----------------|---------------------------|------------|------------|-------------|---------------|
| 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 |

AddEditCopyDelete

Particle Species Editor

Species-ID: 1

Comment: FCC

Materials: Applied Materials

Size Distribution

☒ File: psd_fcc.sff Edit

☐ Size Range:

Minimum: Maximum: micron-diameter

Close Pack Volume Fraction

☒ Use global value:

Surface and Shape

Sphericity: 1

Emissivity: 1

Scattering Factor: 0

Particle Density (kg/m³): 1619.43 (calculated)

Sum of fractions: 1

Reset OK Cancel Help

Drag Model

Model Name: WenYu-Ergun

| Name | Link To Default | Value |
|------|--|-------|
| c0 | <input checked="" type="checkbox"/> Linked | 0.85 |
| c1 | <input checked="" type="checkbox"/> Linked | 0.75 |
| c2 | <input checked="" type="checkbox"/> Linked | 2 |
| c3 | <input checked="" type="checkbox"/> Linked | 180 |

Particle Species Editor

Species-ID: 2

Comment: Heavy gas droplets

Materials: Applied Materials

Size Distribution

☐ File:

☒ Size Range:

Minimum: 50 Maximum: 500 micron-diameter

Close Pack Volume Fraction

☒ Use global value: 0.58

Surface and Shape

Sphericity: 1

Emissivity: 1

Scattering Factor: 0

Particle Density (kg/m³): 900 (calculated)

Sum of fractions: 1

Reset OK Cancel Help

Drag Model

Model Name: WenYu-Ergun

| Name | Link To Default | Value |
|------|--|-------|
| c0 | <input checked="" type="checkbox"/> Linked | 0.85 |
| c1 | <input checked="" type="checkbox"/> Linked | 0.75 |
| c2 | <input checked="" type="checkbox"/> Linked | 2 |
| c3 | <input checked="" type="checkbox"/> Linked | 180 |

Particle Composition Editor

| Component | Density (kg/m ³) | 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

Reset OK Cancel Help

Particle Composition Editor

| Component | Density (kg/m ³) | Mass fraction | Age factor |
|-----------|------------------------------|---------------|------------|
| GasOil(L) | 900 | 1 | 1 |

Particle Density (kg/m³): 900 (calculated)

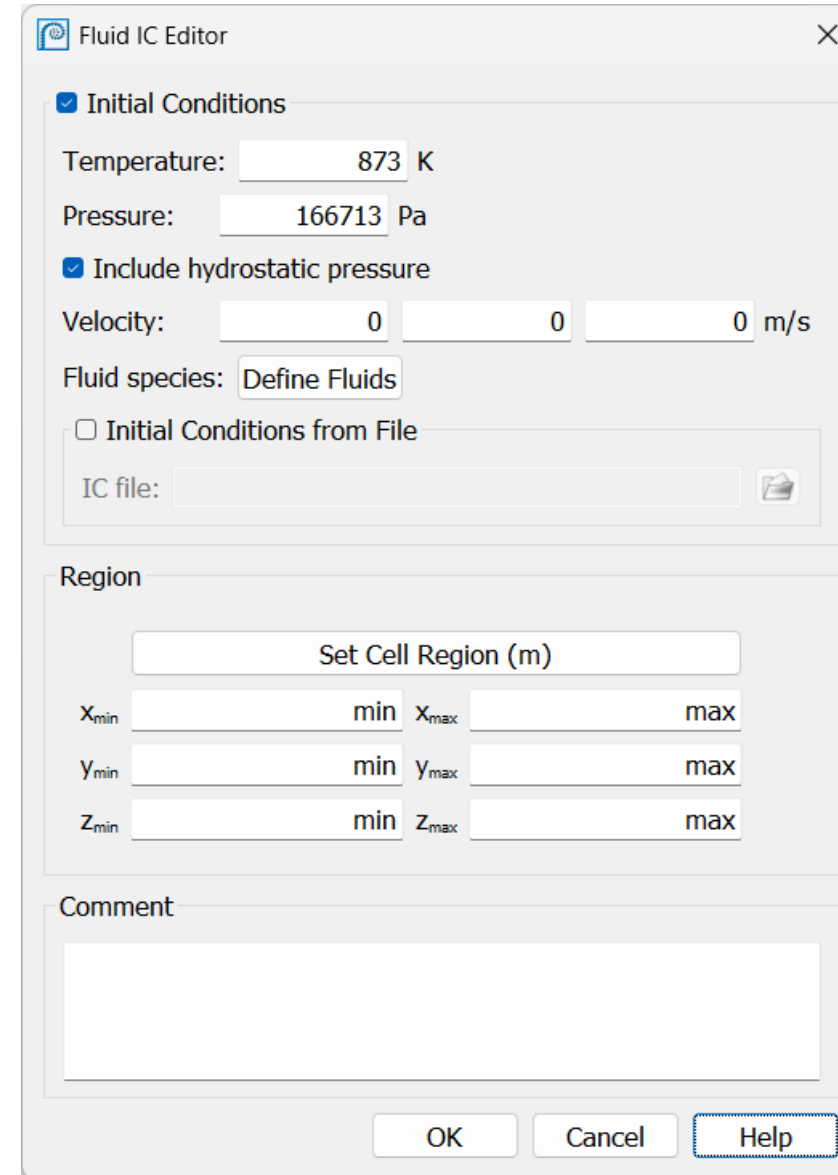
Sum of fractions: 1

Reset OK Cancel Help

Fluid ICs

Fluid IC

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



The image shows a software dialog box titled "Fluid IC Editor". It contains several sections for configuring initial conditions. The "Initial Conditions" section is active, showing fields for Temperature (873 K), Pressure (166713 Pa), and Velocity (0, 0, 0 m/s). There is a checkbox for "Include hydrostatic pressure" which is checked. Below this is a "Fluid species" dropdown menu set to "Define Fluids". There is also an unchecked checkbox for "Initial Conditions from File" with an "IC file:" input field and a folder icon. The "Region" section has a "Set Cell Region (m)" button and three rows of input fields for x, y, and z coordinates, each with "min" and "max" labels. At the bottom is a "Comment" text area and three buttons: "OK", "Cancel", and "Help".

Fluid IC Editor

☒ Initial Conditions

Temperature: 873 K

Pressure: 166713 Pa

☒ Include hydrostatic pressure

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 screenshots of the Pressure BC Editor dialog box, illustrating the configuration steps for a pressure boundary condition. The dialog box has tabs for Location, Flux Plane, Fluid, Particles, and Tracers.

- Step 1:** The Location tab is selected. The Region section shows 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).
- Step 2:** The Name field is set to "FLUXBC_pressure_outlet". The Fluid species behavior is set to "Mass flow rate".
- Step 3:** The Fluid tab is selected. The Flow Conditions section has radio buttons for "Transient file:" (selected) and "Specify values:". The "Transient file:" field is set to "pressure_outlet.sff". The Fluid Composition section has "Fluid inflow properties" set to "Interior cell values" and "Applied fluids" set to "Define Fluids".
- Step 4:** The Particles tab is selected. The Behavior at Boundary section has radio buttons for "No outflow" and "Outflow with size filtering:" (selected). The "Outflow with size filtering:" section has input fields for Minimum (0), Maximum (UNLIMITED), and Units (micron-diameter). The Feed Settings section has buttons for "Edit Feed" and "Feed Control".

Additional annotations include a red box labeled 'a' around the Direction section in the first screenshot, and a red box labeled 'b' around the "pressure_outlet.sff" field in the third screenshot.

The screenshot shows the Pressure Boundary Conditions Editor dialog box. It contains a table with columns: Time (s), Pressure (Pa), Temperature (K), Area Fraction, Particle Feed, and K-Factor. The table has two rows. Below the table are buttons for "Add Row", "Delete Row", "Check Data", "Graph", and "Update Simulation". At the bottom, there is a "File:" field set to "pressure_outlet.sff" and buttons for "Save", "Save As", "Close", and "Help".

| | Time (s) | Pressure (Pa) | Temperature (K) | Area Fraction | Particle Feed | K-Factor |
|---|----------|---------------|-----------------|---------------|-------------------------------------|----------|
| 1 | 0 | 166713 | 873 | 1 | <input type="radio"/> Off | 0 |
| 2 | | | | | <input checked="" type="radio"/> On | |

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 **a** **4** Save Save As Close Help

Flow BC Editor

1 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

a ☒ z-direction

☐ Direction vector

u: 0 v: 0

☐ Force absolute direction

Variation angle: 0

Transient File

Flow BC Editor

Location Flux Plane **3** 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 **b** Edit

Comment:

OK Cancel Help

Flow BC Editor

Location **2** 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 **5** Particles Tracers

☐ Use transient file

☐ Use BC Connector data

a ☒ 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 steps for a flow boundary condition.

Screenshot 1 (Region Tab): Shows the 'Region' tab with 'Set Cell Region (m)' fields for x_{min} , x_{max} , y_{min} , y_{max} , z_{min} , and z_{max} . The 'Direction' section has 'x-direction' selected.

Screenshot 2 (Fluid Tab): Shows the 'Fluid' tab with 'Name: FLUXBC_flow_regen_cat_inlet' and 'Fluid species behavior: No output'. The 'Bin by particle size' checkbox is checked with 100 bins.

Screenshot 3 (Fluid Tab): Shows the 'Fluid' tab with 'Flow Conditions' set to 'Use transient file'. The 'Fluid Composition' section shows 'Applied fluids: Define Fluids'.

Screenshot 4 (Particles Tab): Shows the 'Particles' tab with 'Use transient file' checked. The 'Feed Settings' section shows 'Feed specified as mass flow rate' selected. The 'Transient File' section shows 'flow_regen_cat_inlet.sff'.

Screenshot 5 (Summary Table): Shows the 'Flow Boundary Conditions Editor' summary table.

| | Time (s) | Mass Flow Rate (kg/s) | Temperature (K) | Pressure (Pa) | Particle Feed | Cloud Resolution (clouds/cell) | Particle Slip | Particle Mass Flow Rate (kg/s) |
|---|----------|-----------------------|-----------------|---------------|---------------|--------------------------------|---------------|--------------------------------|
| 1 | 0 | 0.75 | 973 | 166713 | On | 200 | 1 | 1740 |
| 2 | | | | | On | | | |

Buttons: Add Row, Delete Row, Check Data, Graph, Update Simulation, Edit, Save, Save As, Close, Help, OK, Cancel, Help.

Injection BC – Feed Oil

Add Feed Oil injection BC

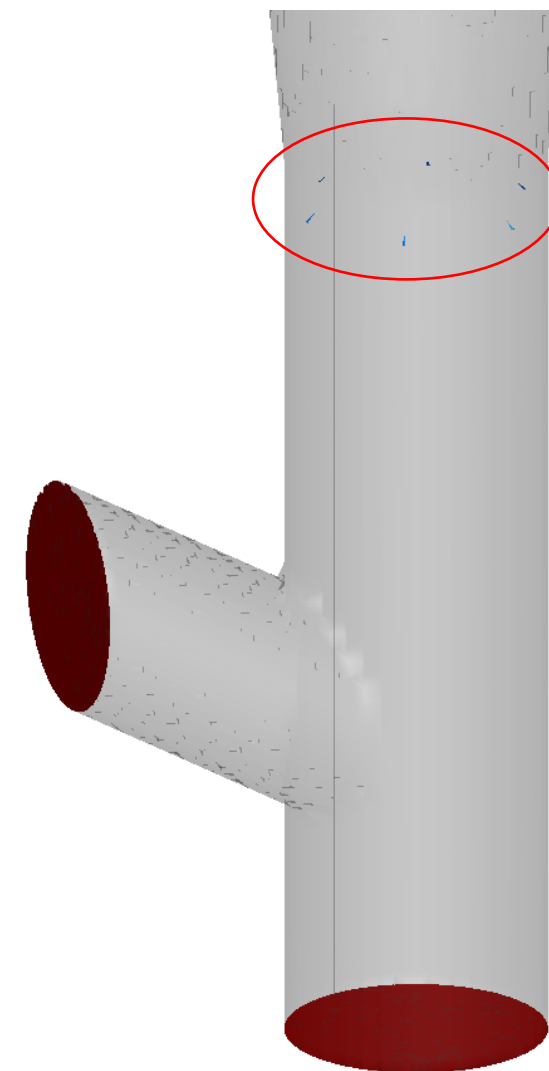
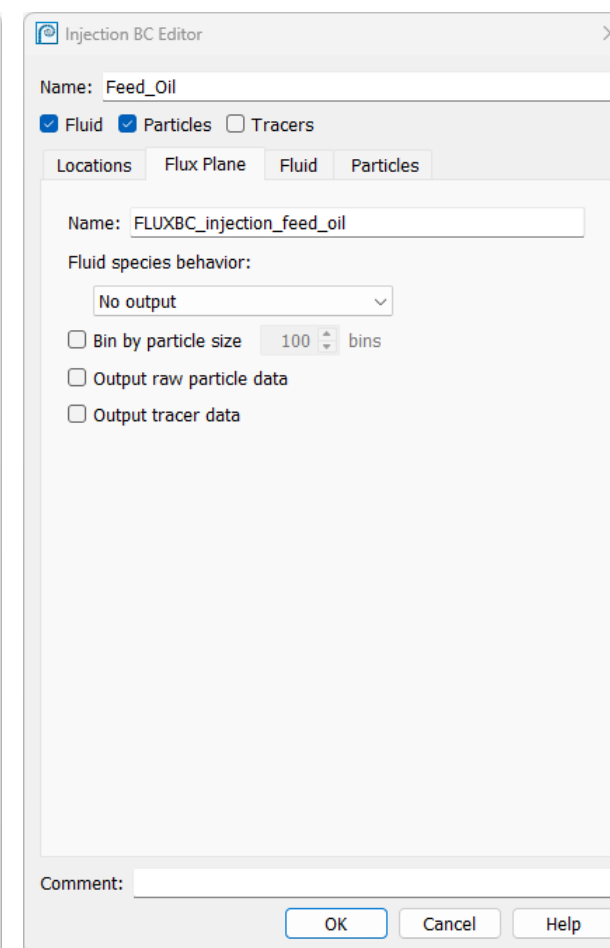
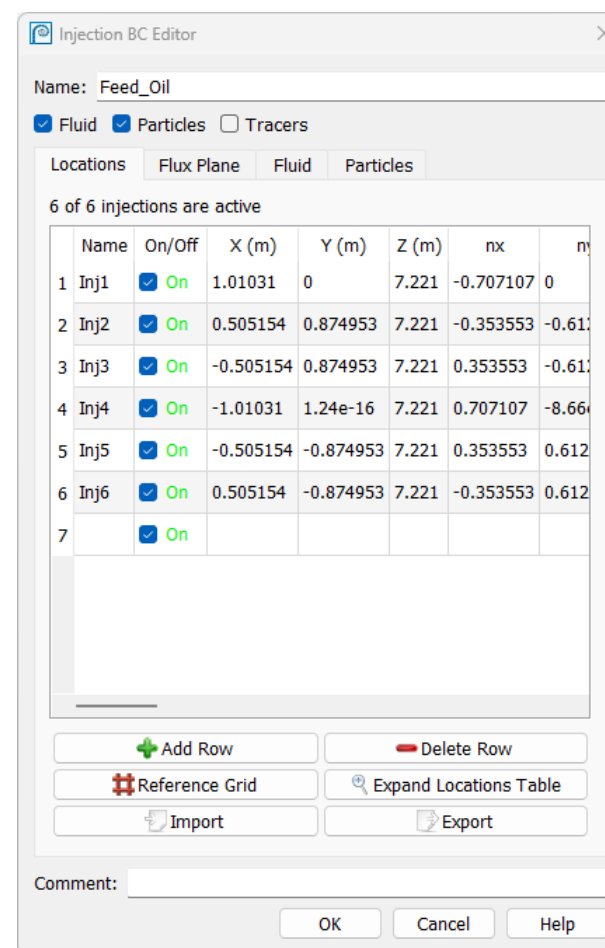
- Name = Feed_Oil
- Select Fluid and Particles/Tracers

Locations tab

- Import feed_oil_locations.csv

Flux Plane tab

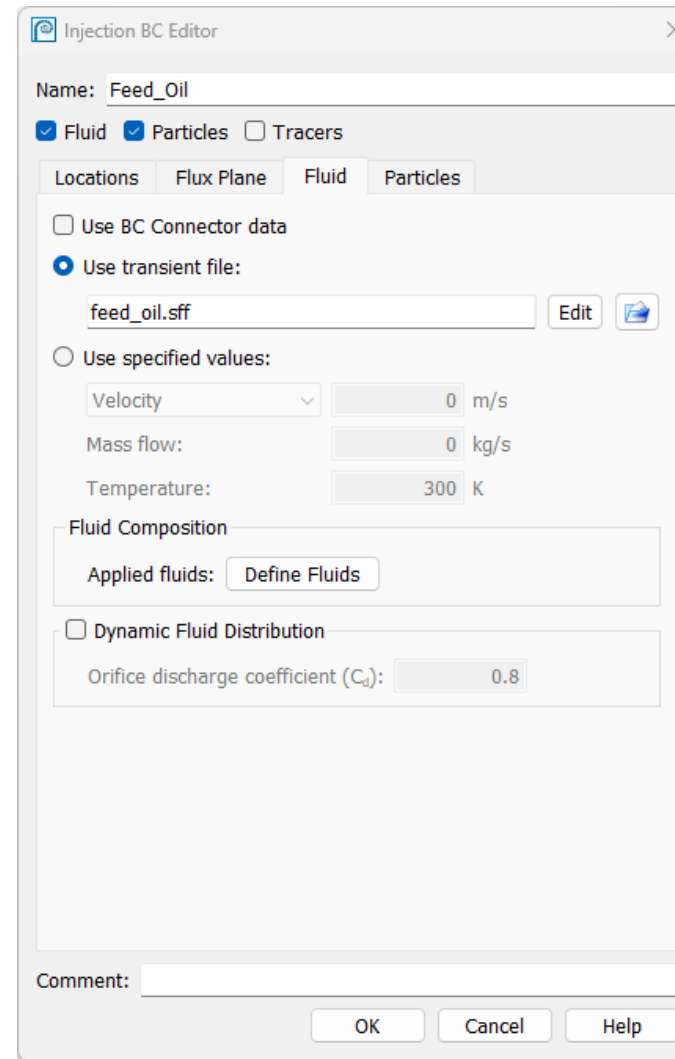
- Add a flux plane name



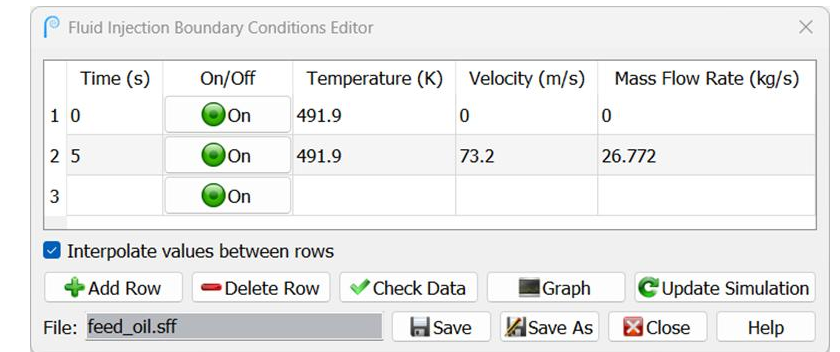
Injection BC – Feed Oil

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)

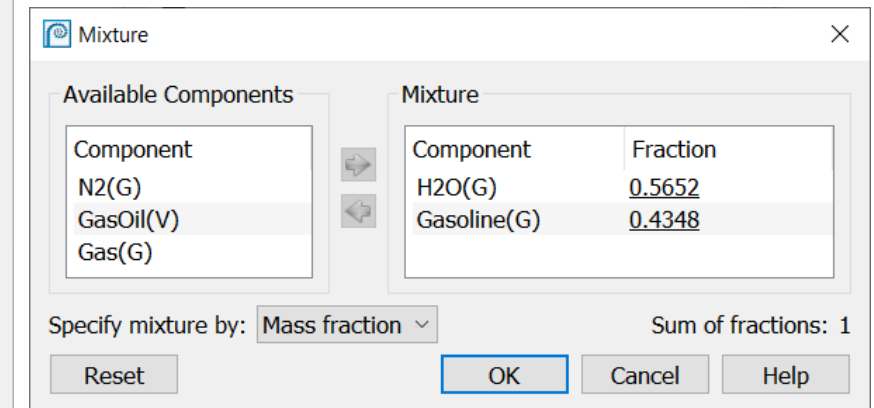


The Injection BC Editor dialog box is shown with the 'Fluid' tab selected. The 'Name' field is set to 'Feed_Oil'. The 'Fluid' and 'Particles' checkboxes are checked, while 'Tracers' is unchecked. Under the 'Locations' tab, 'Use BC Connector data' is unchecked, and 'Use transient file:' is selected with the file 'feed_oil.sff'. Under 'Use specified values:', 'Velocity' is set to 0 m/s, 'Mass flow' is 0 kg/s, and 'Temperature' is 300 K. The 'Fluid Composition' section shows 'Applied fluids' with a 'Define Fluids' button. 'Dynamic Fluid Distribution' is unchecked, and the 'Orifice discharge coefficient (C_d)' is 0.8. A 'Comment' field is at the bottom.



The Fluid Injection Boundary Conditions Editor dialog box shows a table with 5 columns: Time (s), On/Off, Temperature (K), Velocity (m/s), and Mass Flow Rate (kg/s). The table has 3 rows. The 'On/Off' column has green circles with 'On' text. The 'Interpolate values between rows' checkbox is checked. Buttons for 'Add Row', 'Delete Row', 'Check Data', 'Graph', and 'Update Simulation' are present. The file 'feed_oil.sff' is shown in the 'File' field.

| | 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 | | | |



The Mixture dialog box shows 'Available Components' on the left and 'Mixture' on the right. The 'Available Components' list includes N2(G), GasOil(V), and Gas(G). The 'Mixture' table has 2 columns: Component and Fraction. The 'Specify mixture by:' dropdown is set to 'Mass fraction', and the 'Sum of fractions' is 1. Buttons for 'Reset', 'OK', 'Cancel', and 'Help' are at the bottom.

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

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) | Cloud Resolution (clouds/cell) |
|---|----------|-------------------------------------|-----------------|----------------|-----------------------|--------------------------------|
| 1 | 0 | <input checked="" type="radio"/> On | 491.9 | 0 | 0 | 125 |
| 2 | 5 | <input checked="" type="radio"/> On | 491.9 | 73.2 | 206.03 | 125 |
| 3 | | <input checked="" type="radio"/> On | | | | |

☒ Interpolate values between rows ☒ Use species cloud resolution

File:

Injection BC Editor

Name:

☒ Fluid ☒ Particles ☐ Tracers

Locations Flux Plane Fluid **Particles**

☐ Use BC Connector data

☒ Use transient file:

☐ Use specified values:

Velocity: m/s

Mass flow: kg/s

Temperature: K

Cloud Resolution

☐ Use species cloud resolution

☐ Automatic:

☒ Specify resolution: Clouds per cell

Injection Properties

Mixture:

Expansion angle: θ_{e1} : ° θ_{e2} : °

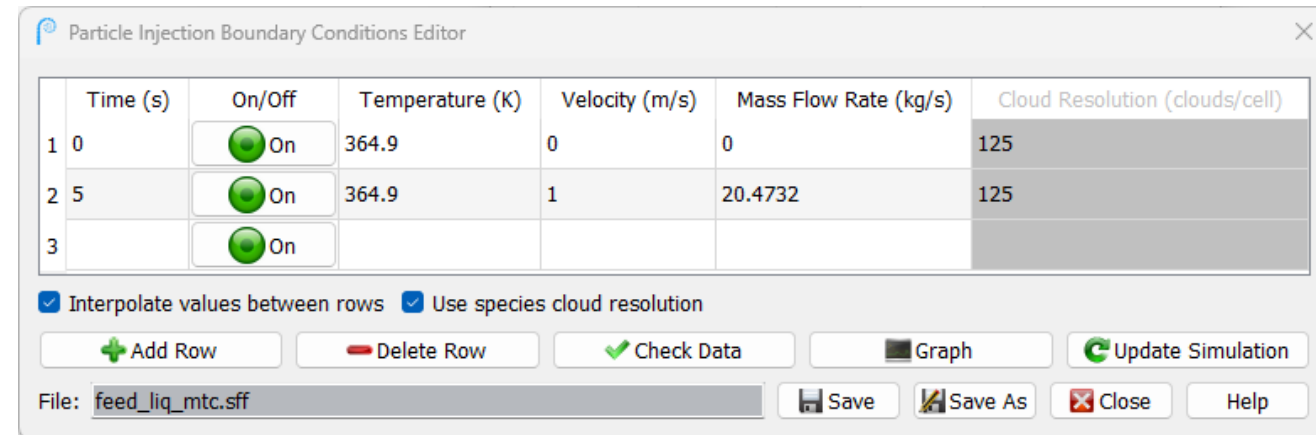
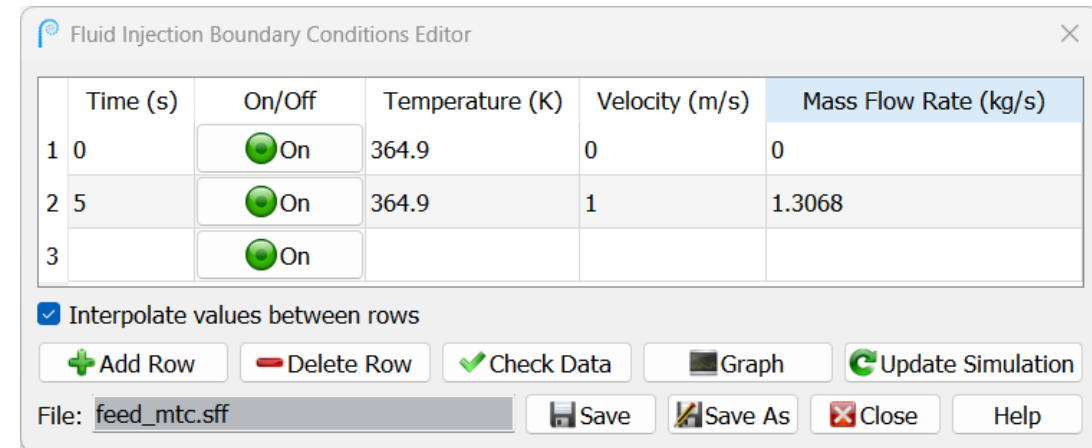
Orientation angle: α_{e1} : °

Comment:

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°



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 | | | |

☒ Interpolate values between rows

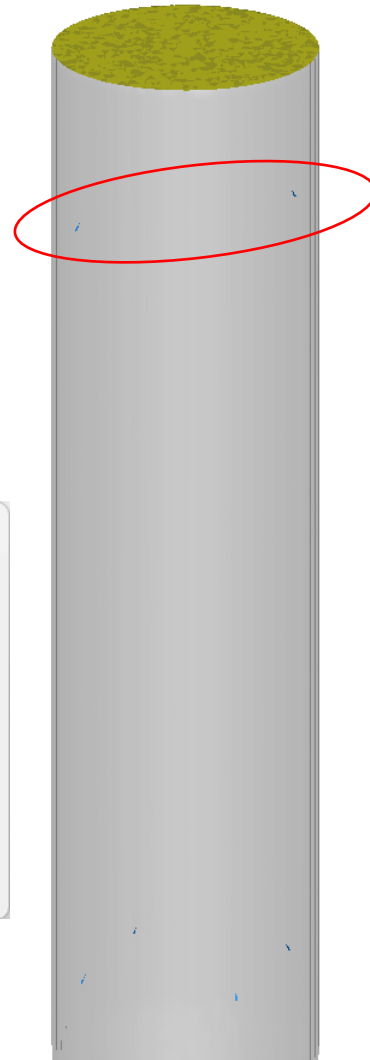
File:

Particle Injection Boundary Conditions Editor

| | Time (s) | On/Off | Temperature (K) | Velocity (m/s) | Mass Flow Rate (kg/s) | Cloud Resolution (clouds/cell) |
|---|----------|-------------------------------------|-----------------|----------------|-----------------------|--------------------------------|
| 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 | | | | |

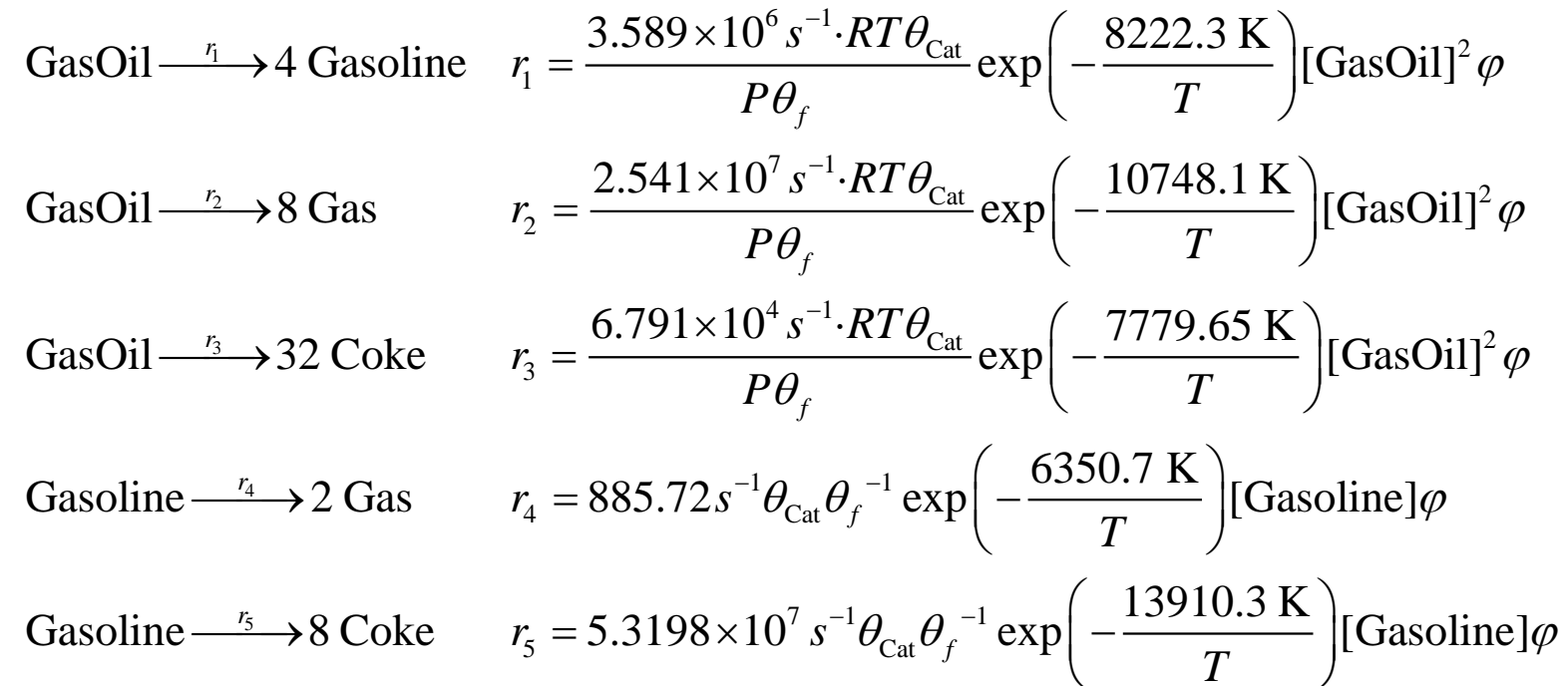
☒ Interpolate values between rows ☒ Use species cloud resolution

File:



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 and discrete chemistry will be used
- Volume average units
 - Reaction rate: mol/m³/s
 - Fluid species: mol/m³
- Discrete units
 - Reaction rate: mol/s
 - Fluid species: mol/m³
- Two catalyst deactivation rate coefficients will be needed, one volume average and one discrete

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

$$R_{00} = ((k_0)[GasOil]^2) * ((k_5))$$

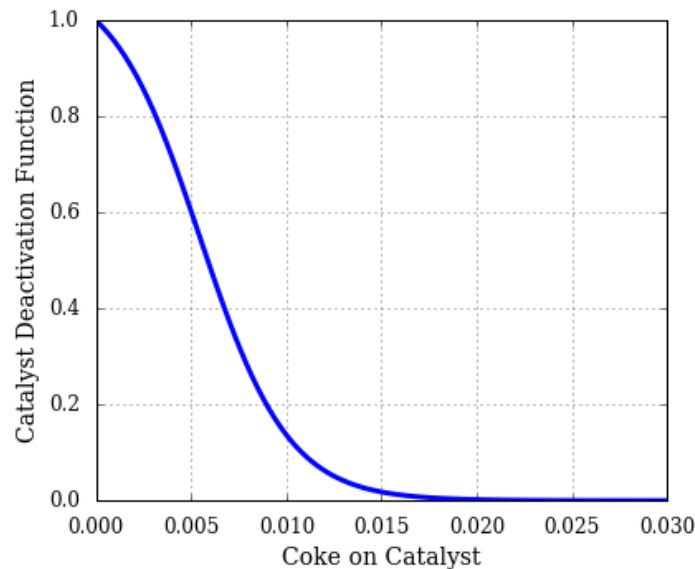
where k0 and k5 are appropriate rate coefficients

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

Barracuda Virtual Reactor with Chemistry - 25.0.0 - pre_setup/fcc_riser.prj

File View Setup Run Graphics and Output Post-processing Help

Secondary Exits
BC Connectors
Chemistry
Rate Coefficients
Reactions
Numerics
Time Controls
Data Output
Flux Planes
Visualization Data
Average Data

Chemistry Rate Coefficients Manager

| ID | Name | Reaction Type | Coefficient Type | Expression | Comment |
|----|------|----------------|-----------------------|--|---|
| 00 | k0 | Volume-Average | Arrhenius Chem Rate | $2.9839e+07 T^{-1} p^{-1} \theta_f^{-1} e^{(-8222.3 / T)} v_{f_Cat_base}^1$ | VGO → Gasoline, $3.589e+06 * 8.314 = 29.839e6$ |
| 01 | k1 | Volume-Average | Arrhenius Chem Rate | $2.1126e+08 T^{-1} p^{-1} \theta_f^{-1} e^{(-10748.1 / T)} v_{f_Cat_base}^1$ | VGO → Gas, $2.541e+07 * 8.314 = 21.126e7$ |
| 02 | k2 | Discrete | Arrhenius Chem Rate | $348.5 T^{-1} p^{-1} e^{(-7779.65 / T)} m_{Cat_base}^1$ | VGO → Coke, $67910 * 8.314 = 564603.7 / 1620 = 348.5$ |
| 03 | k3 | Volume-Average | Arrhenius Chem Rate | $885.72 \theta_f^{-1} e^{(-6350.7 / T)} v_{f_Cat_base}^1$ | Gasoline → Gas |
| 04 | k4 | Discrete | Arrhenius Chem Rate | $32838 e^{(-13910.3 / T)} m_{Cat_base}^1$ | Gasoline → Coke |
| 05 | k5 | Volume-Average | Catalyst Deactivation | $(10.4 + 1) / (10.4 + \exp(4.29 C_{Coke(S)}))$ | Catalyst deactivation |
| 06 | k6 | Discrete | Catalyst Deactivation | $(10.4 + 1) / (10.4 + \exp(4.29 C_{Coke(S)}))$ | Catalyst deactivation |

Add Edit Copy Delete

Barracuda Virtual Reactor with Chemistry - 25.0.0 - pre_setup/fcc_riser.prj

File View Setup Run Graphics and Output Post-processing Help

Secondary Exits
BC Connectors
Chemistry
Rate Coefficients
Reactions
Numerics
Time Controls
Data Output
Flux Planes
Visualization Data
Average Data
Data Planes
Data Points
Wall Impact

Chemistry Reactions Manager

| ID | Reaction Type | Rate | Equation | Comment |
|----|--------------------|---------------------|--------------------------|----------------------------------|
| 00 | VA: Stoichiometric | Equation: | GasOil(V) => 4 Gasoline | |
| | | R00 = | $(k0[GasOil(V)]^2)(k5)$ | VGO → Gasoline |
| 01 | VA: Stoichiometric | Equation: | GasOil(V) => 8 Gas | |
| | | R01 = | $(k1[GasOil(V)]^2)(k5)$ | VGO → Gas |
| 02 | VA: Stoichiometric | Equation: | Gasoline => 2 Gas | |
| | | R02 = | $(k3[Gasoline])(k5)$ | Gasoline → gas |
| 00 | Discrete | $d[Coke(S)]/dt =$ | $(k2[GasOil(V)]^2)(k6)$ | VGO → Coke on catalyst particles |
| | | $d[GasOil(V)]/dt =$ | $-0.03125 d[Coke(S)]/dt$ | |
| 01 | Discrete | $d[Coke(S)]/dt =$ | $(k4[Gasoline])(k6)$ | |
| | | $d[Gasoline]/dt =$ | $-0.125 d[Coke(S)]/dt$ | |

Add Edit Copy Delete

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

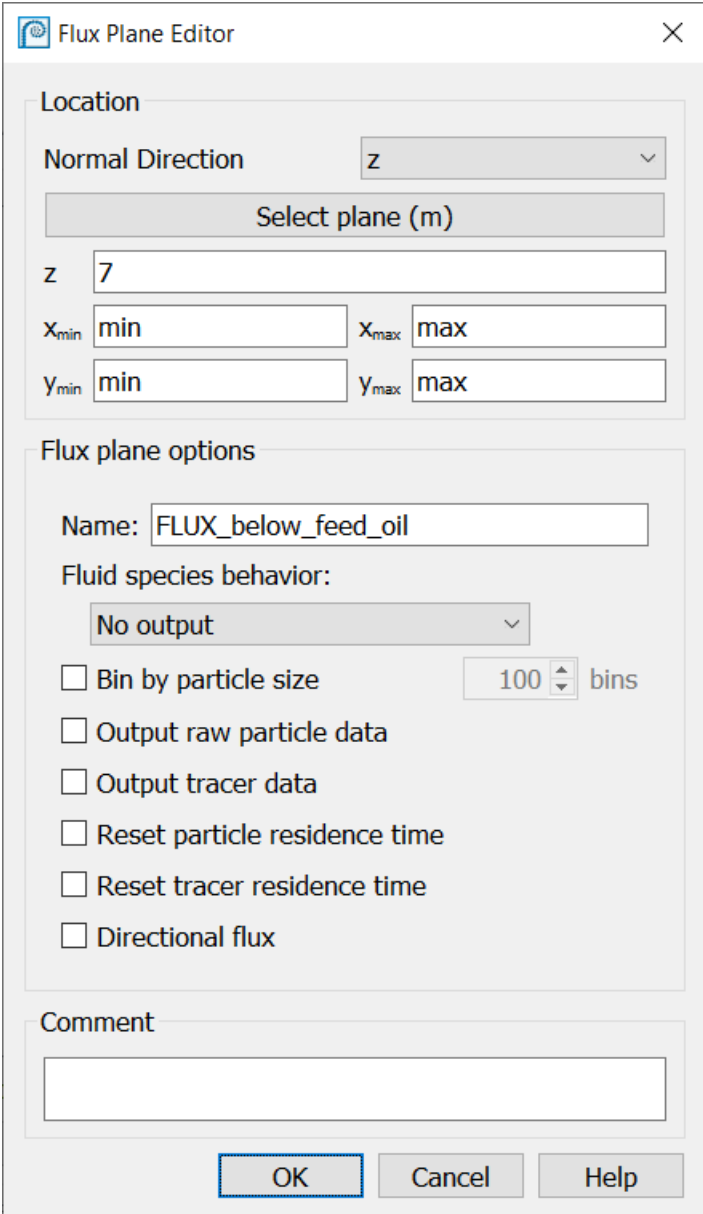
Restart interval (IC_###) simulation seconds

Backtrack interval (IC_) realtime minutes

Help

Flux Planes

Define a flux plane below the feed oil nozzles



The image shows a 'Flux Plane Editor' dialog box with the following fields and options:

- 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 file format
☒ Tecplot (*.plt files) ☐ GMV (Gmv.* files)

Output file interval
☒ Constant: s End time: 30s Number of output files: 151
☐ Time-varying: Edit 

Cell Data

| Available Data | | Selected Data |
|--------------------------------------|---|--------------------------------------|
| Cell ID |  | Bulk density |
| Cell indices | | Chemical Reaction Rates |
| Cell volume | | dp/dz |
| CFL |  | Fluid composition mole concentration |
| Clouds per cell | | Fluid mass flux |
| Convective wall heat transfer | | Fluid temperature |
| dp/dx | | Fluid velocity |
| dp/dy | | Particle mass flux |
| Dynamic pressure | | Particle volume fraction |
| Fluid composition mass concentration | | Pressure |
| Fluid composition mass fraction | | |
| Fluid composition mole fraction | | |

Particle Data

| Available Data | | Selected Data |
|-----------------------|---|--------------------------|
| Cell ID |  | Chemical Reaction Rates |
| Cloud ID | | Particle density |
| Cloud mass | | Particle material |
| Drag | | Particle size |
| Liquid fraction total |  | Particle speed |
| Liquid mass total | | Particle temperature |
| P1 radiation flux | | Particle velocity |
| Particle mass | | Particle volume fraction |
| Particles per cloud | | Residence time |
| | | Species |

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 | | Chemical Reaction Rates |
| Convective wall heat transfer | | dp/dz |
| dp/dx | | Fluid composition mole concentration |
| dp/dy | | Fluid temperature |
| Fluid composition mass concentration | | Fluid velocity |
| Fluid composition mass fraction | → | Particle mass flux |
| Fluid composition mole fraction | ← | Particle velocity |
| Fluid mass flux | | Particle volume fraction |
| Fluid velocity fluctuations | | Pressure |
| Particle temperature | | |
| Voidage | | |
| Volume fraction by species | | |

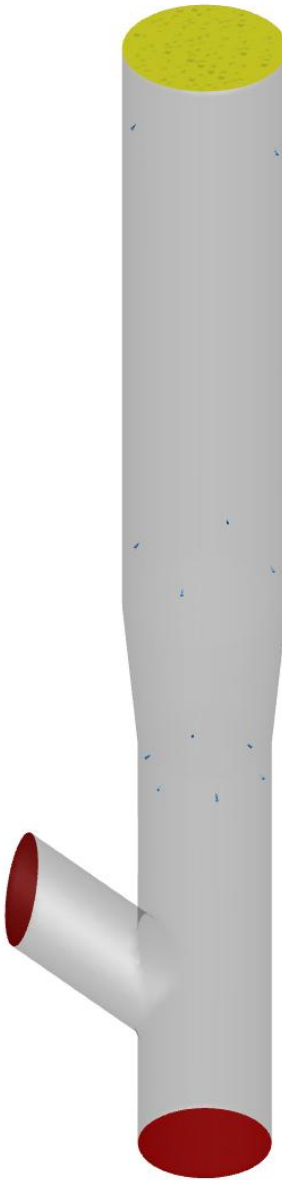
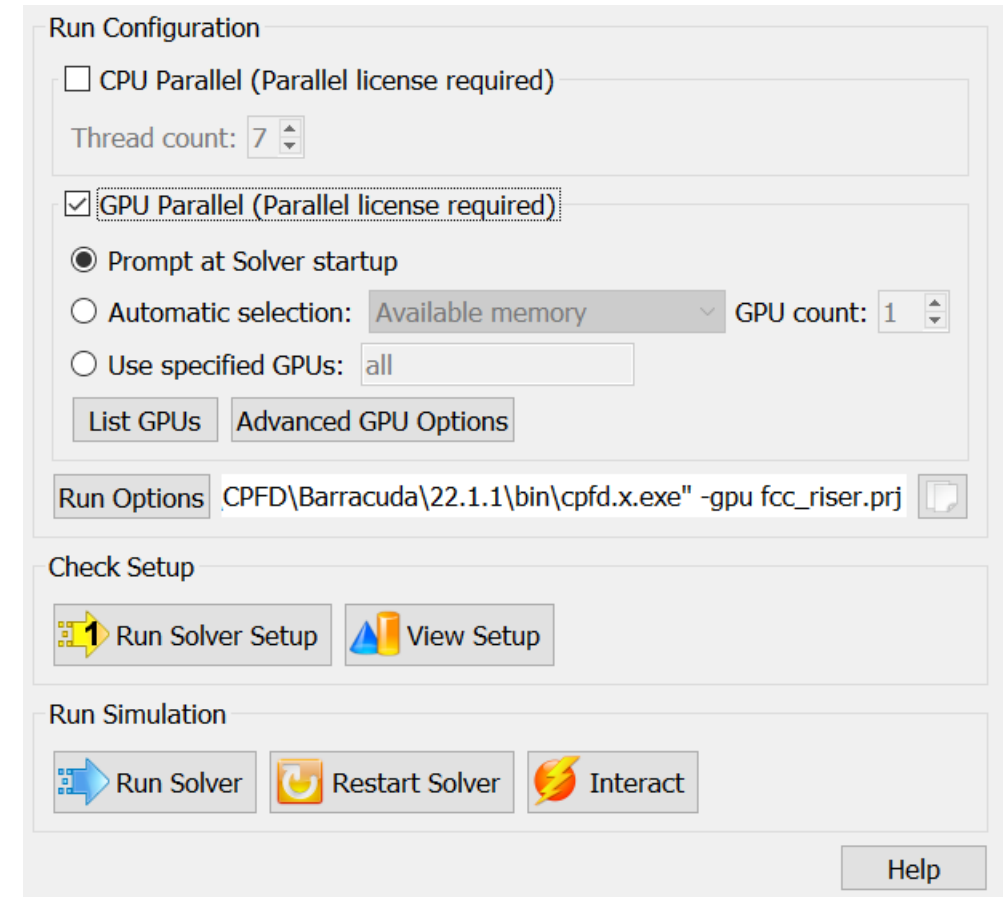
Help

Run

If NVIDIA GPU card is available, select GPU Parallel

Run Solver Setup and View Setup

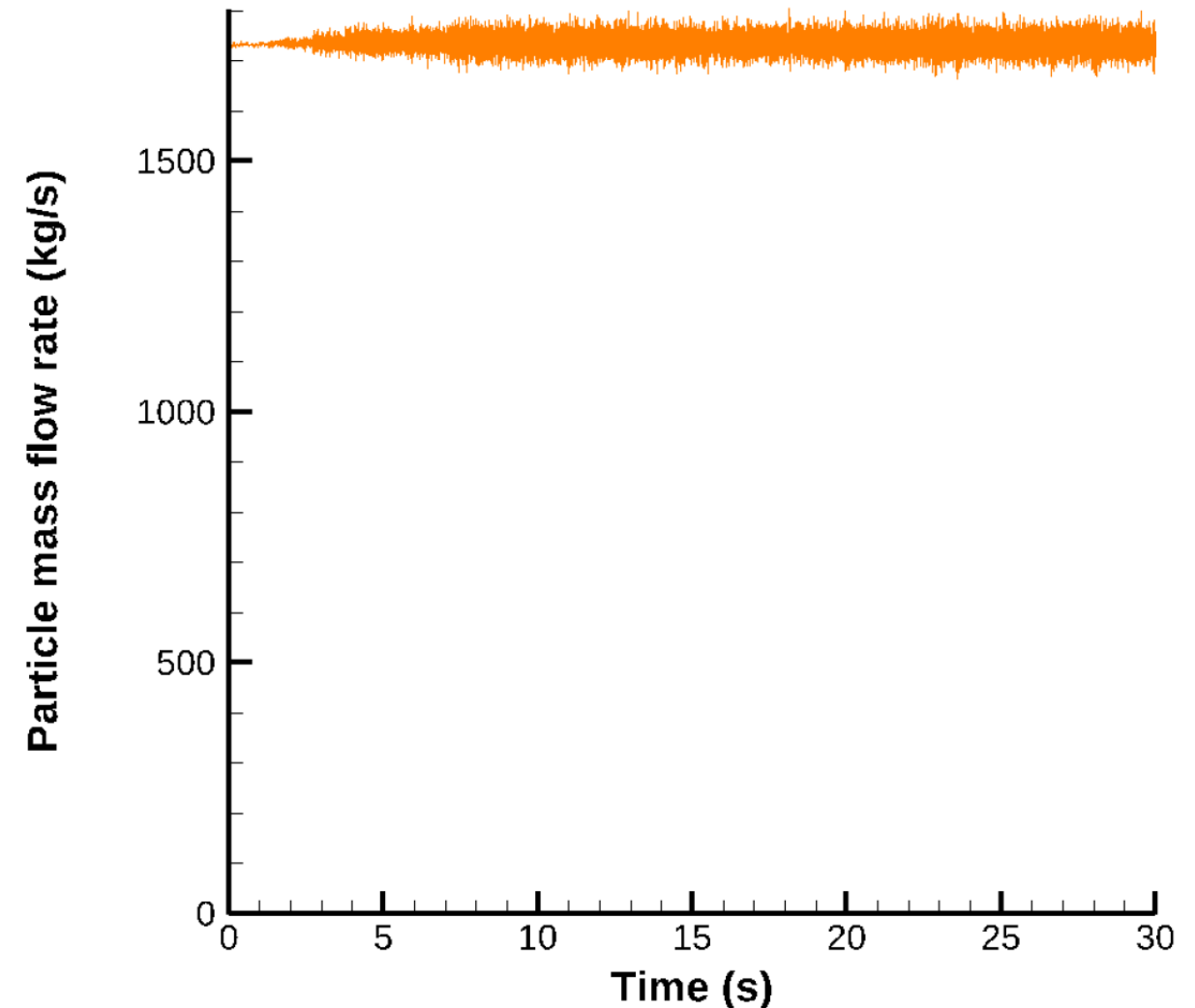
Once you have checked the setup, Run Solver to start the simulation



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 if necessary.

This [video](#) shows how to smooth the data in the xy plot if desired.



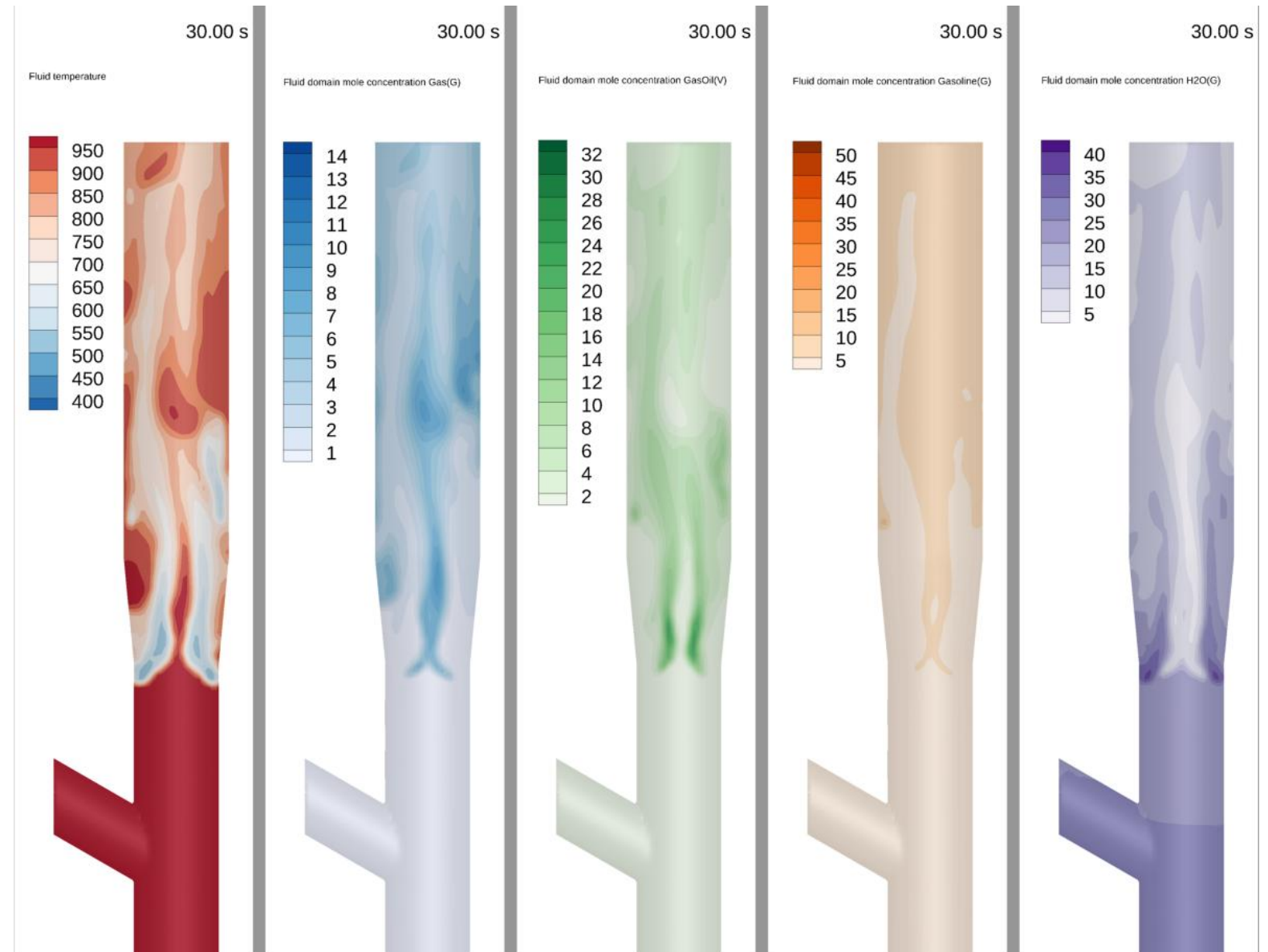
Post-Processing - Slices

Create slices of fluid temperature, fluid domain mole concentrations, and rate of volume-average stoichiometric and discrete reactions

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

See the following videos:

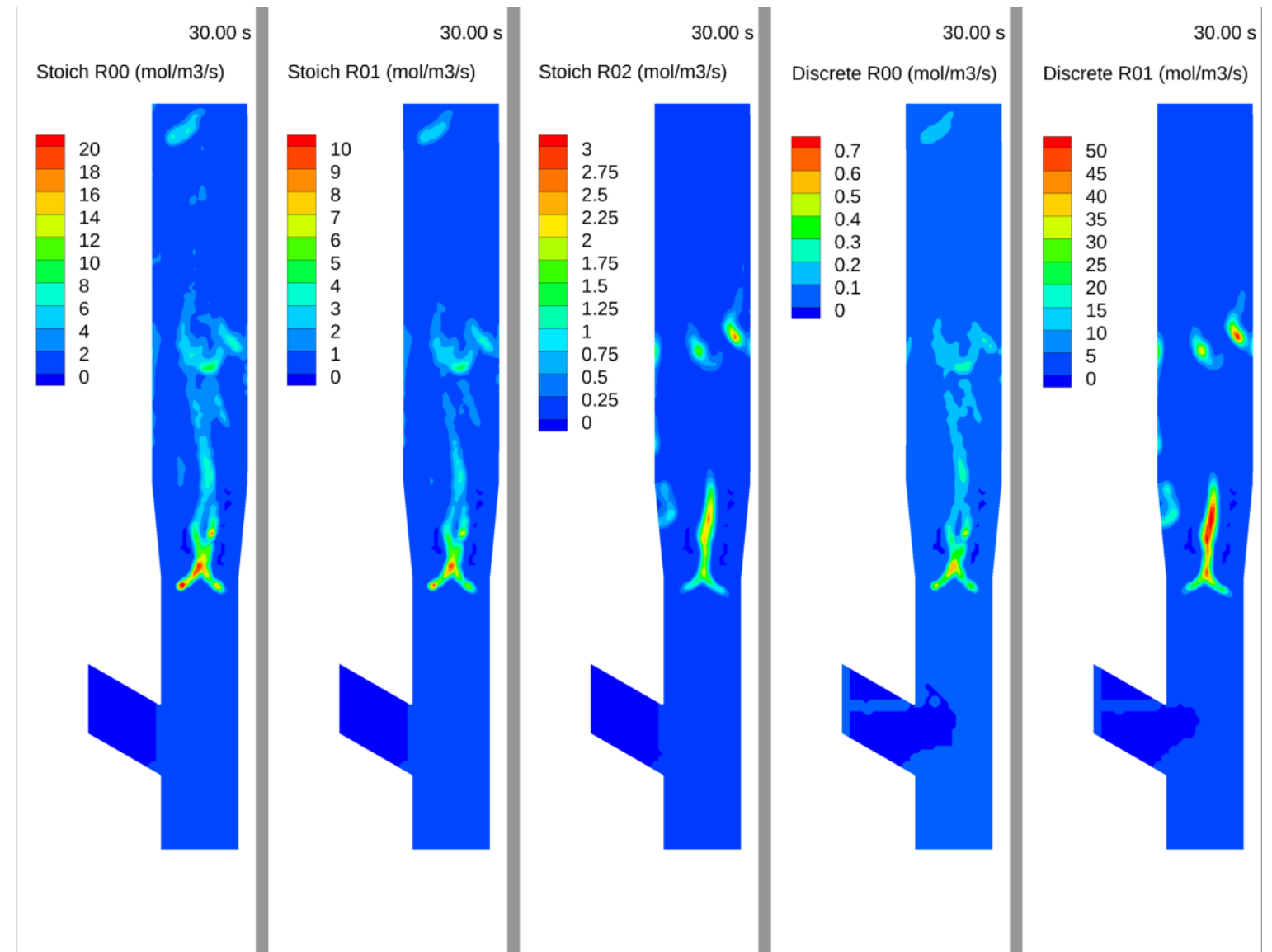
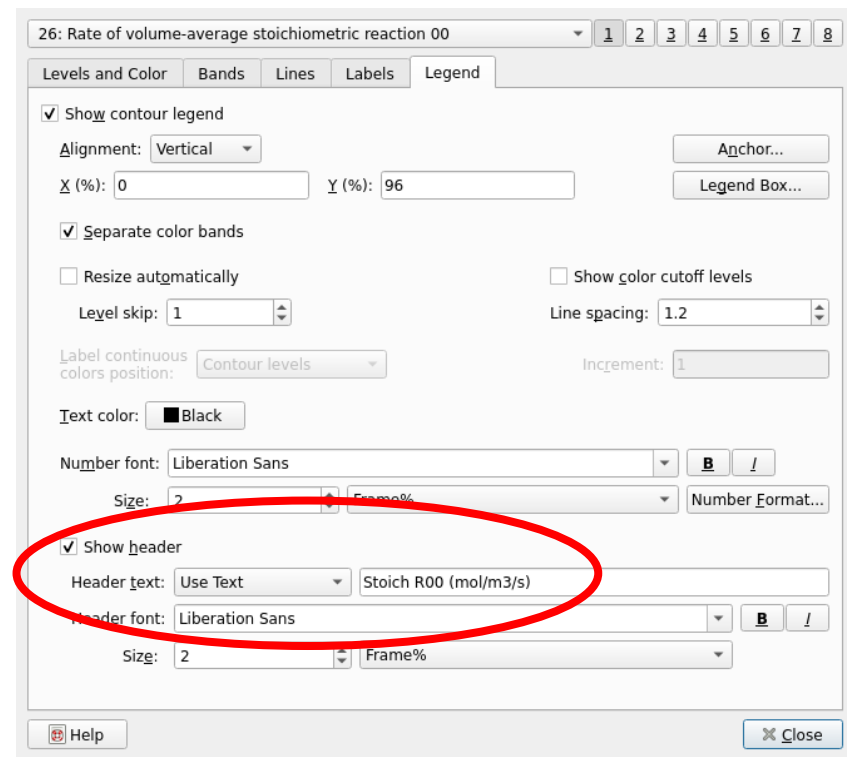
- [Frames](#)
- [Slices](#)
- [Contour legend](#)



Post-Processing – Slices of Chemical Reaction Rates

Create slices of volume-average reaction rates

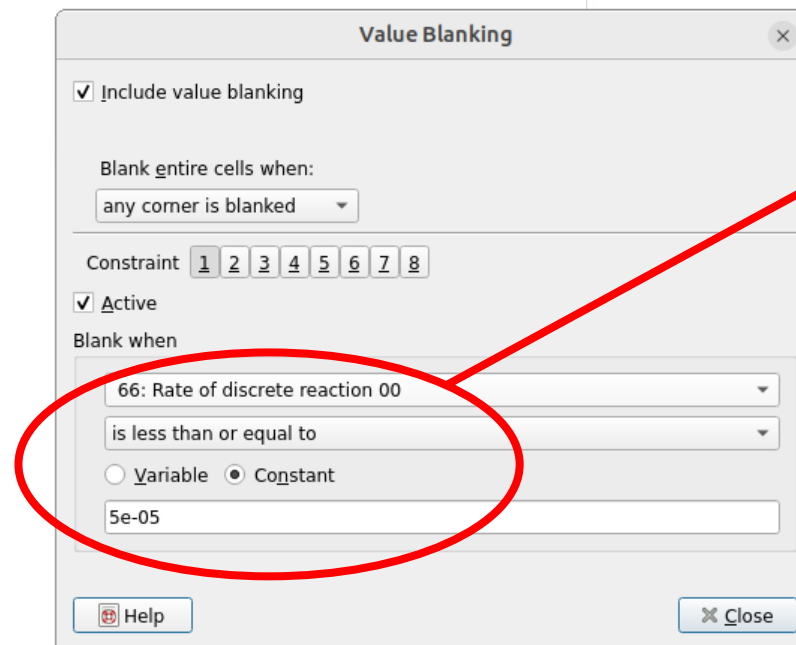
“Use Text” for custom headers



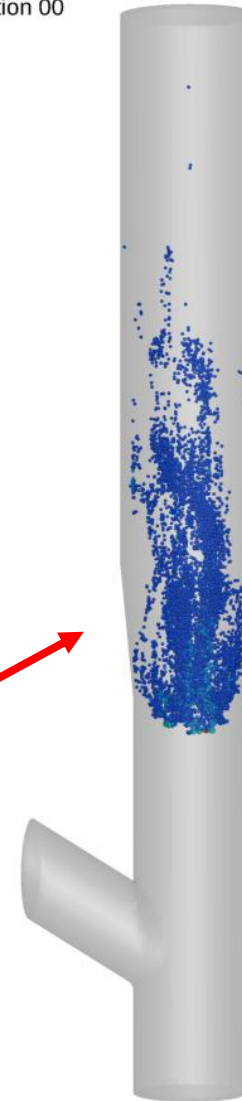
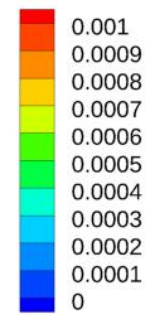
Color Particles by Discrete Reaction Rate

Color particles by discrete reaction rates

For discrete reaction 00, use value blanking to hide particles with very low reaction rates

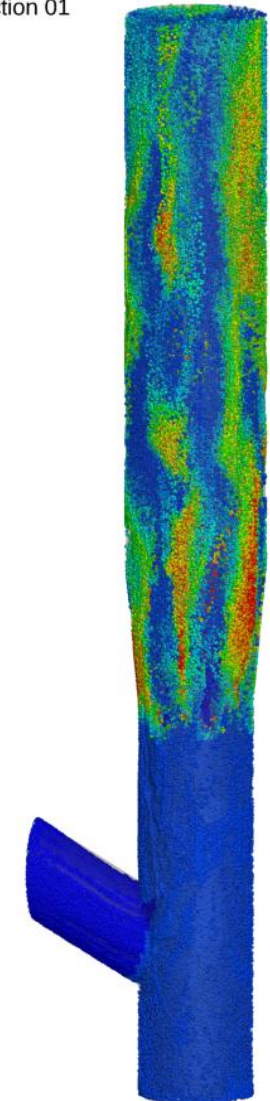
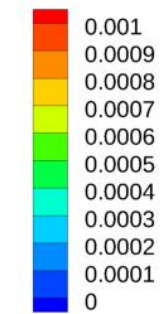


Rate of discrete reaction 00



30.00 s

Rate of discrete reaction 01

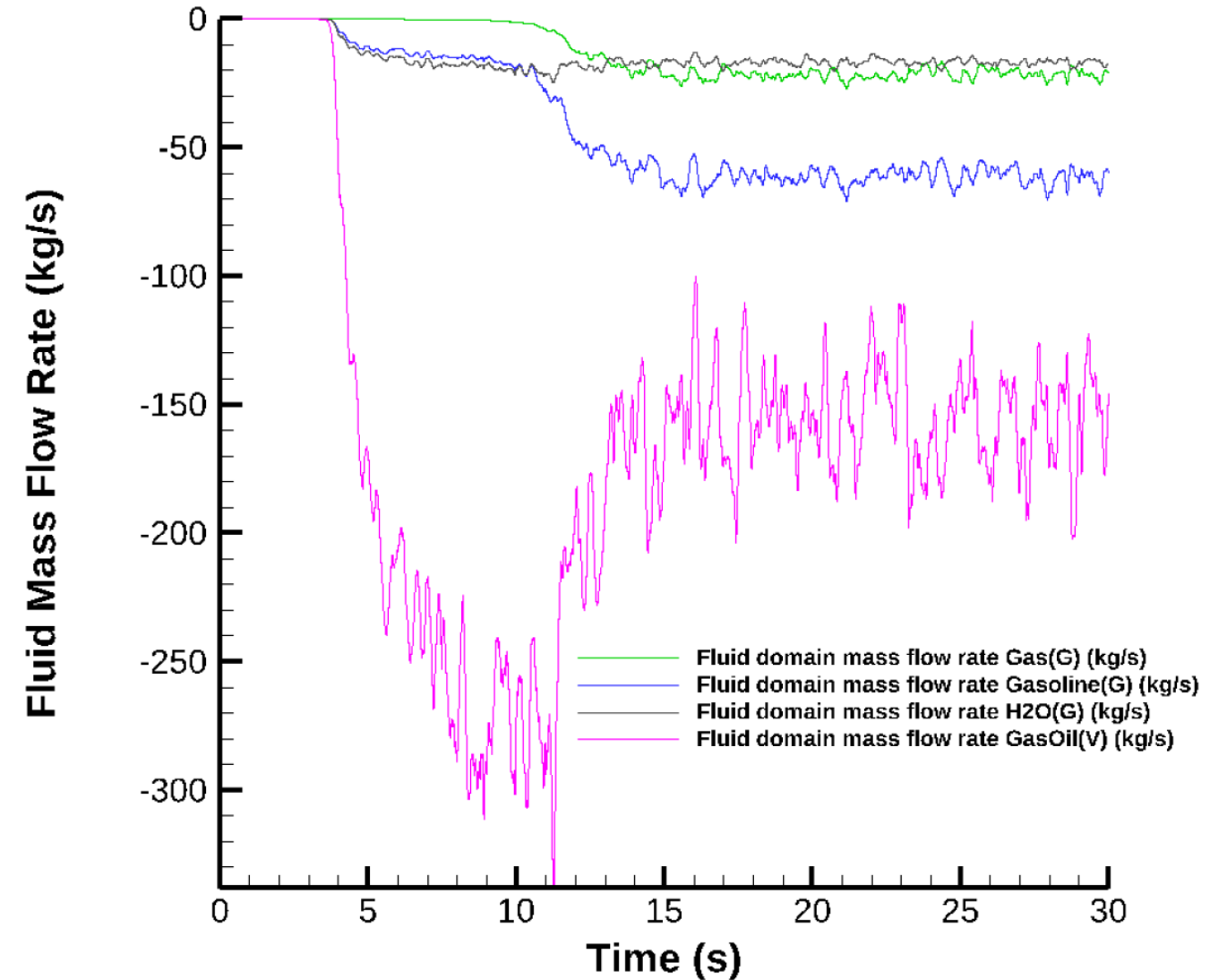


30.00 s

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

