

# Chemistry Training Problem Part 2: Project

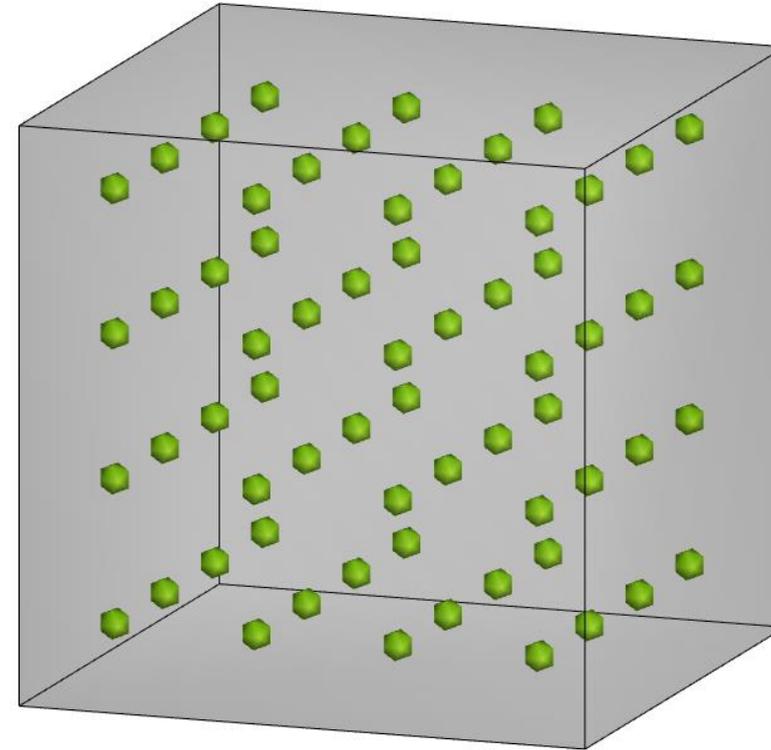
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# Single-Cell Example Problem Setup

## Model parameters

- Unit cube geometry (1 m x 1 m x 1 m)
- Cube is filled with 200  $\mu\text{m}$  diameter coal particles
- Mass of coal particles = 100 kg
- Coal is assumed to be 90% carbon and 10% ash ( $\text{SiO}_2$ )
- Initial temperature = 975 K
- Initial pressure = 10 atm
- Initial gas composition (mole basis)
  - 50%  $\text{H}_2\text{O}$
  - 25%  $\text{H}_2$
  - 25%  $\text{CO}$
- No inlets or outlets for gas or particles



## Model will be set up with volume average chemistry

- Steam gasification reaction
- Both forward and reverse reaction directions considered

# Volume Average Project File

Create a new project file under the directory:

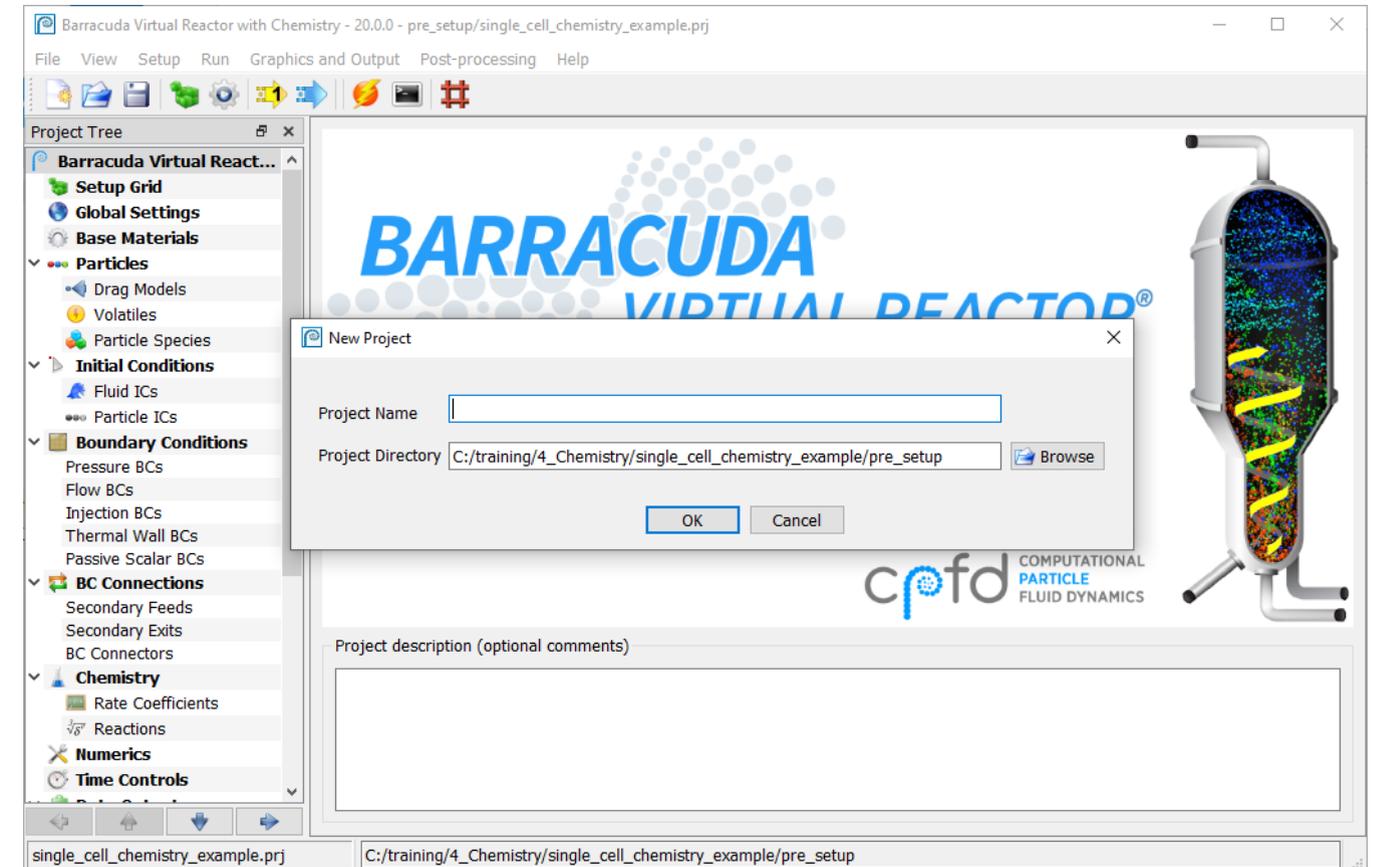
- Linux:

~/barracuda\_training/4\_Chemistry/my\_setup

- Windows:

C:\barracuda\_training\4\_Chemistry\ my\_setup

Enter an appropriate project name



# Generate the Grid

In the Geometry tab, click Add Geometry

An STL file is included in your project directory, named cube.stl

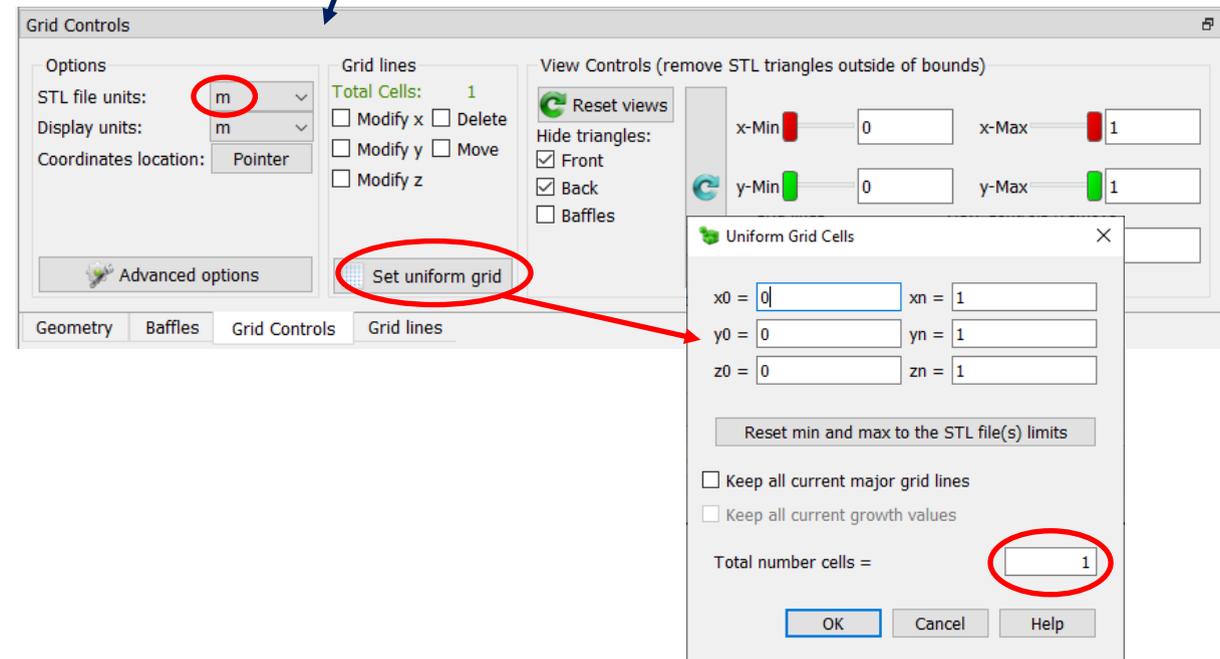
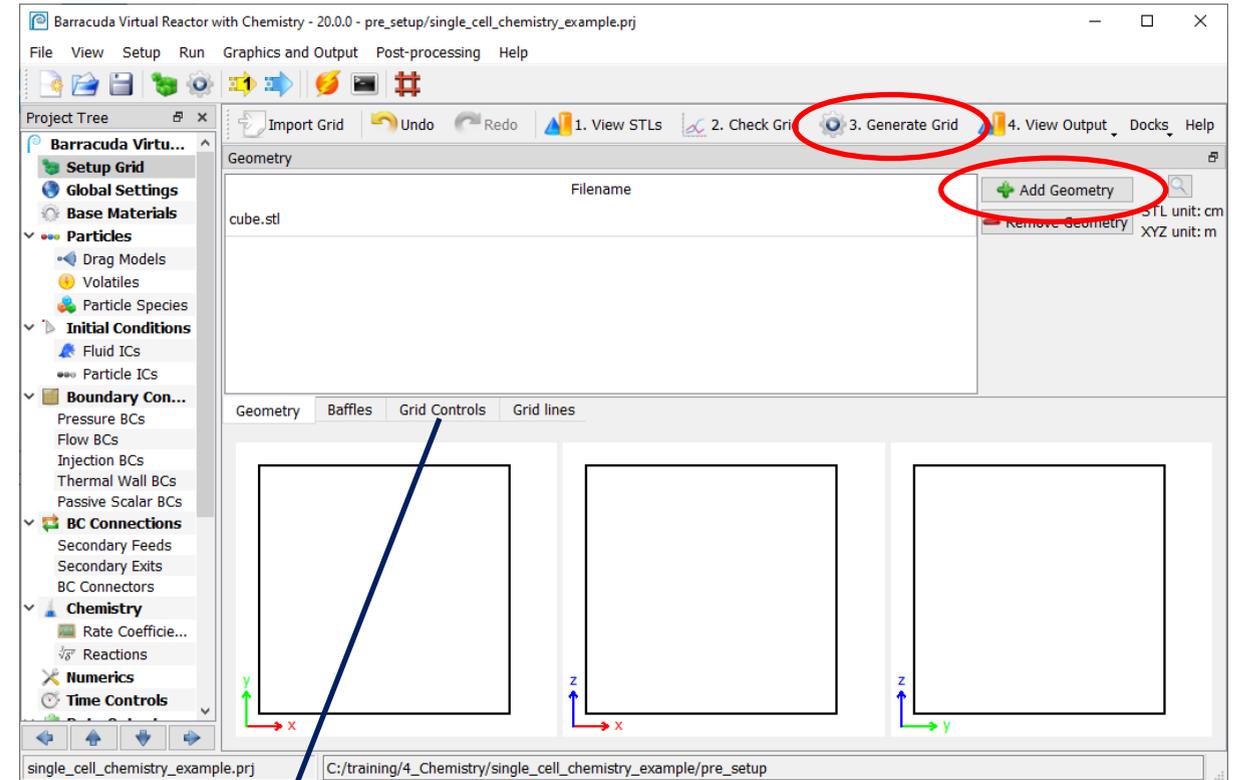
- Each side-length = 1 m

In the Grid Controls tab:

- Set STL units to “m”
- Click Set uniform grid
- Set Total number of cells to “1”

Make sure to click on Generate Grid when finished with the previous steps

This type of single-cell system is useful when first exploring a set of chemical reactions



# Global Settings

The screenshot displays the 'Global Settings' window in the Barracuda Virtual Reactor software. The interface includes a menu bar (File, View, Setup, Run, Graphics and Output, Post-processing, Help), a toolbar, and a Project Tree on the left. The Project Tree lists various setup categories: Setup Grid, Global Settings, Base Materials, Particles, Initial Conditions, Boundary Con..., BC Connections, Chemistry, Numerics, Time Controls, and Data Output. The main panel is titled 'Global Settings' and contains several sections:

- Gravity settings:** Three input fields for x Gravity, y Gravity, and z Gravity, all set to 0 m/s<sup>2</sup>. These fields are circled in red.
- Thermal settings:** Two radio buttons: 'Isothermal flow' (set to 300 K) and 'Thermal flow' (selected and circled in red). A 'Heat transfer coefficients' button is also present.
- Thermal start options:** A radio button for 'Start with Thermal' is set to 'On'. An 'Off (turn on at restart)' option is also available, with a 'Starting temperature' field set to 300 K.
- Temperature warning limits:** Two input fields for 'Minimum temperature warning (K)' (set to 100) and 'Maximum temperature warning (K)' (set to 6000). A checkbox for 'Output minimum and maximum temperatures in system to MinMaxTemp.data log file' is present.
- Chemistry settings:** A text box explaining that chemistry can be set up but not calculated until a later time. A radio button for 'Start with Chemistry' is set to 'On'. Other options include 'Off, ramp on from 0 s to 0 s' and 'Off (can be turned on at restart)'. A 'Help' button is located at the bottom right.

The status bar at the bottom shows the file name 'single\_cell\_chemistry\_example.prj' and the path 'C:/training/4\_Chemistry/single\_cell\_chemistry\_example/pre\_setup'.

# Base Materials

For each species that you want to use in your project, highlight it in the Material Properties Library pane, then click Import to add it to the Project Material List

- Import SiO<sub>2</sub>\_2 QUARTZ (HQZ), then select it on the Project material list, click Edit, and rename it ASH
- Import C\_1 and rename it C

Choose Compressible Flow to add multiple fluids

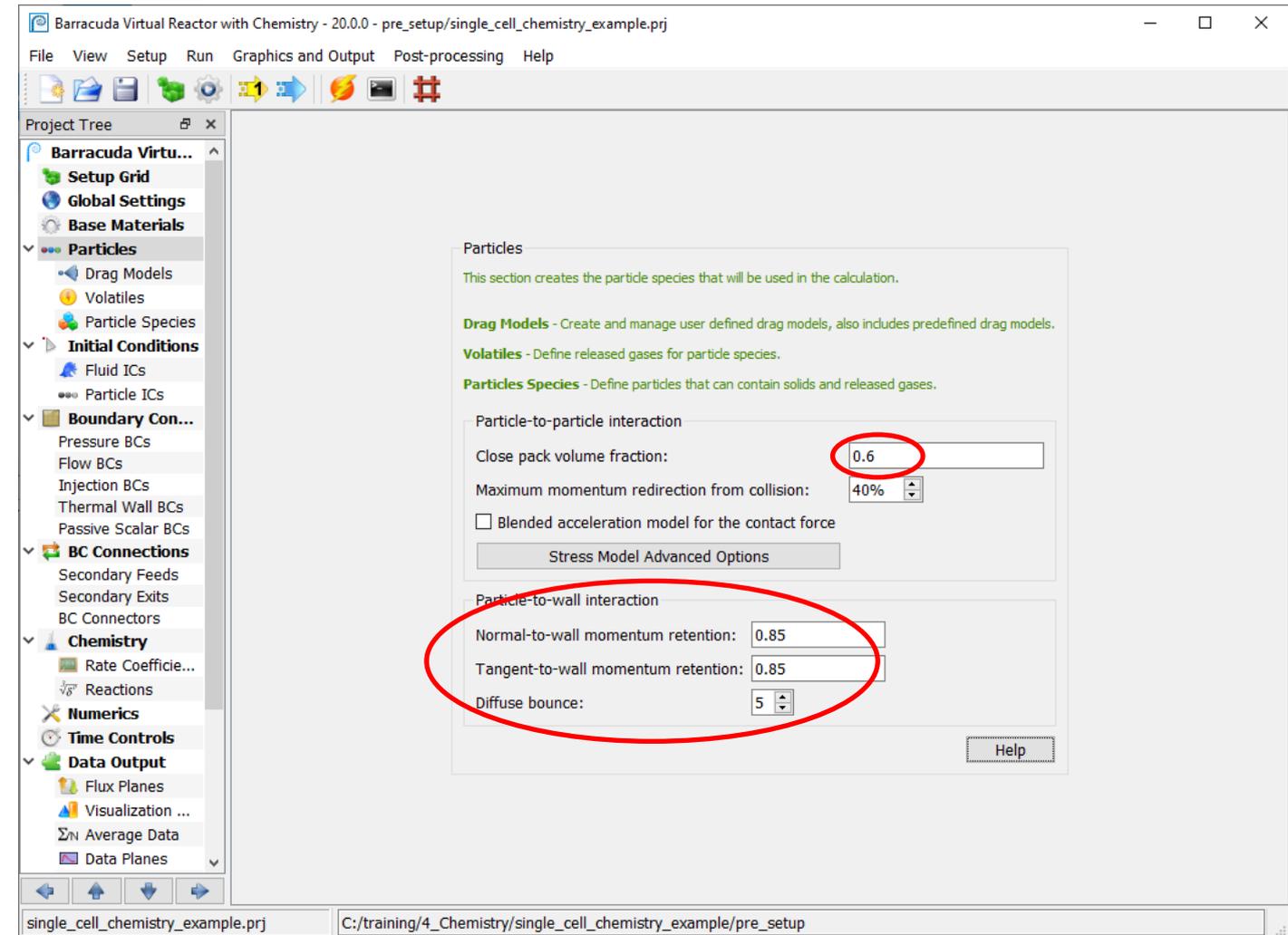
The screenshot shows the Barracuda Virtual Reactor software interface. The Project Tree on the left lists various settings, with 'Base Materials' selected. The Project Material List pane in the center displays a table of materials:

Chemical name	State	Description
ASH	S	SiO2 QUARTZ. (HQZ) COMMON SAN
C	S	C CARBON. SOLID GRAPHITE REF EL
CO	G	CO CARBON MONOXIDE
H2	G	H2 HYDROGEN. REF ELEMENT
H2O	G	H2O STEAM
N2	G	N2 NITROGEN. REF ELEMENT

The 'ASH' and 'C' entries are circled in red. Below the table are buttons for 'Add', 'Edit', 'Copy', and 'Delete'. The Material Properties Library pane on the right shows a list of materials with columns for 'Chemical name', 'State', and 'Description'. The 'Compressible' radio button under 'Flow Type' is also circled in red.

# Particles

Set the Close pack volume fraction to 0.6 and the Particle-to-wall interaction as shown below



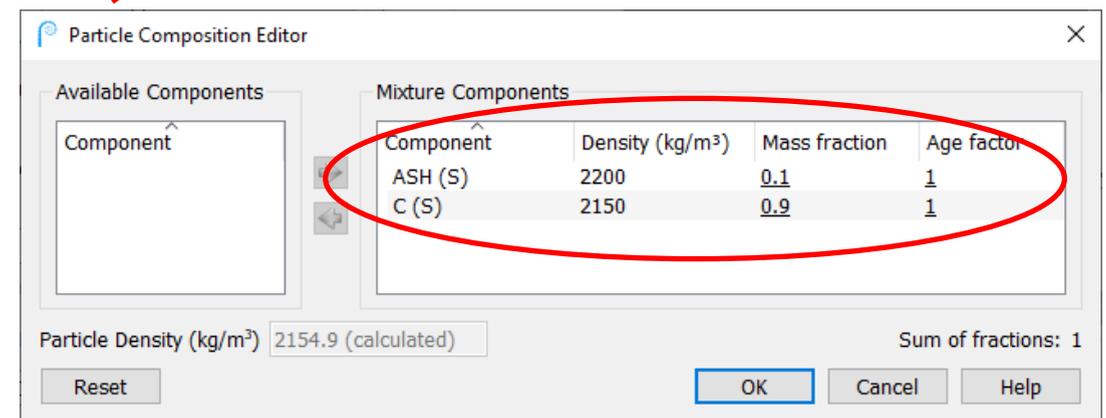
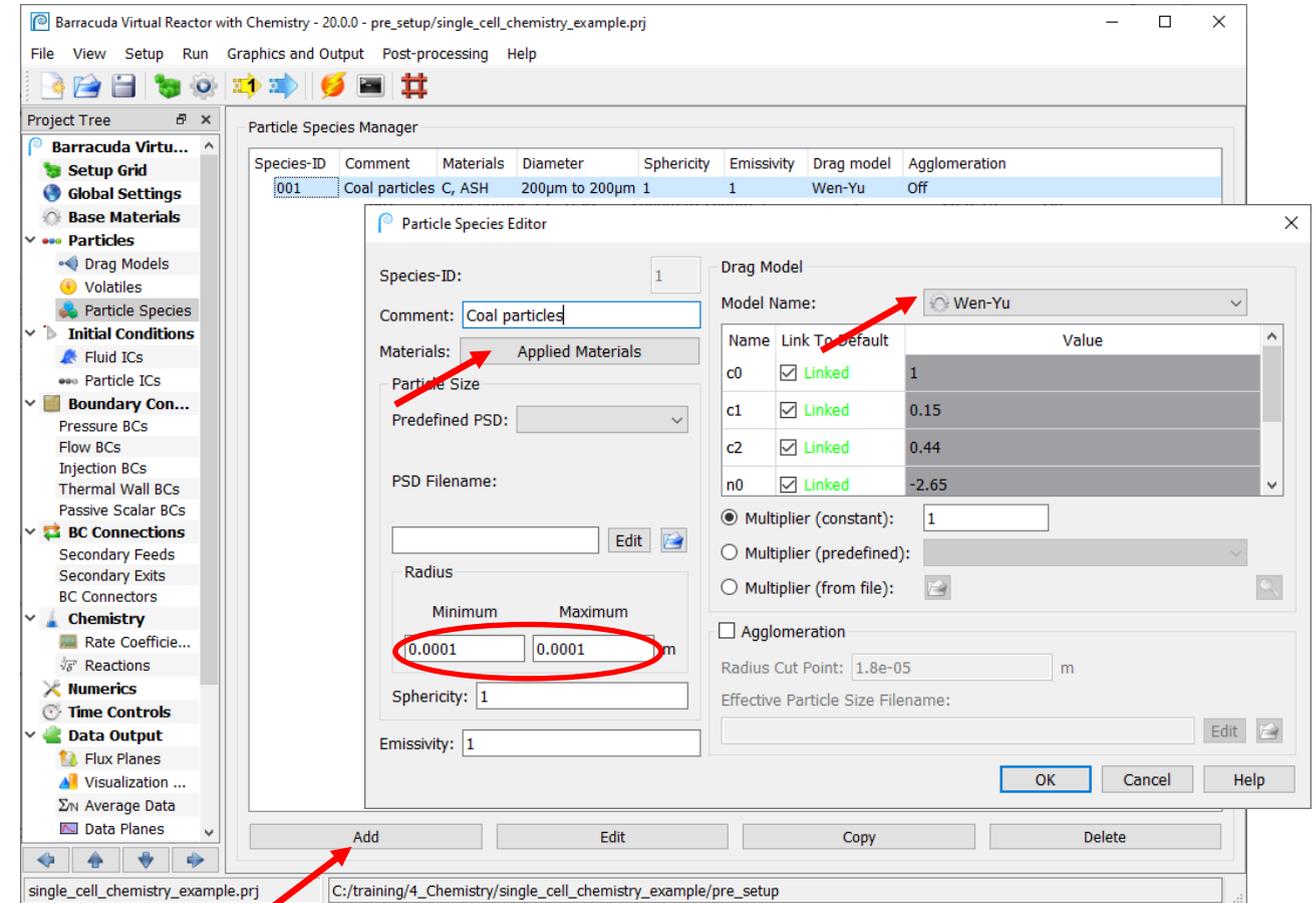
# Particle Species

Click on the Particle Species tab

- Click Add
- Enter a comment
  - 0.9 C
  - 0.1 ASH

A mono-sized particle will be used with a diameter of 200 microns. Remember that particle size is entered by radius in Barracuda.

Use Wen-Yu drag model

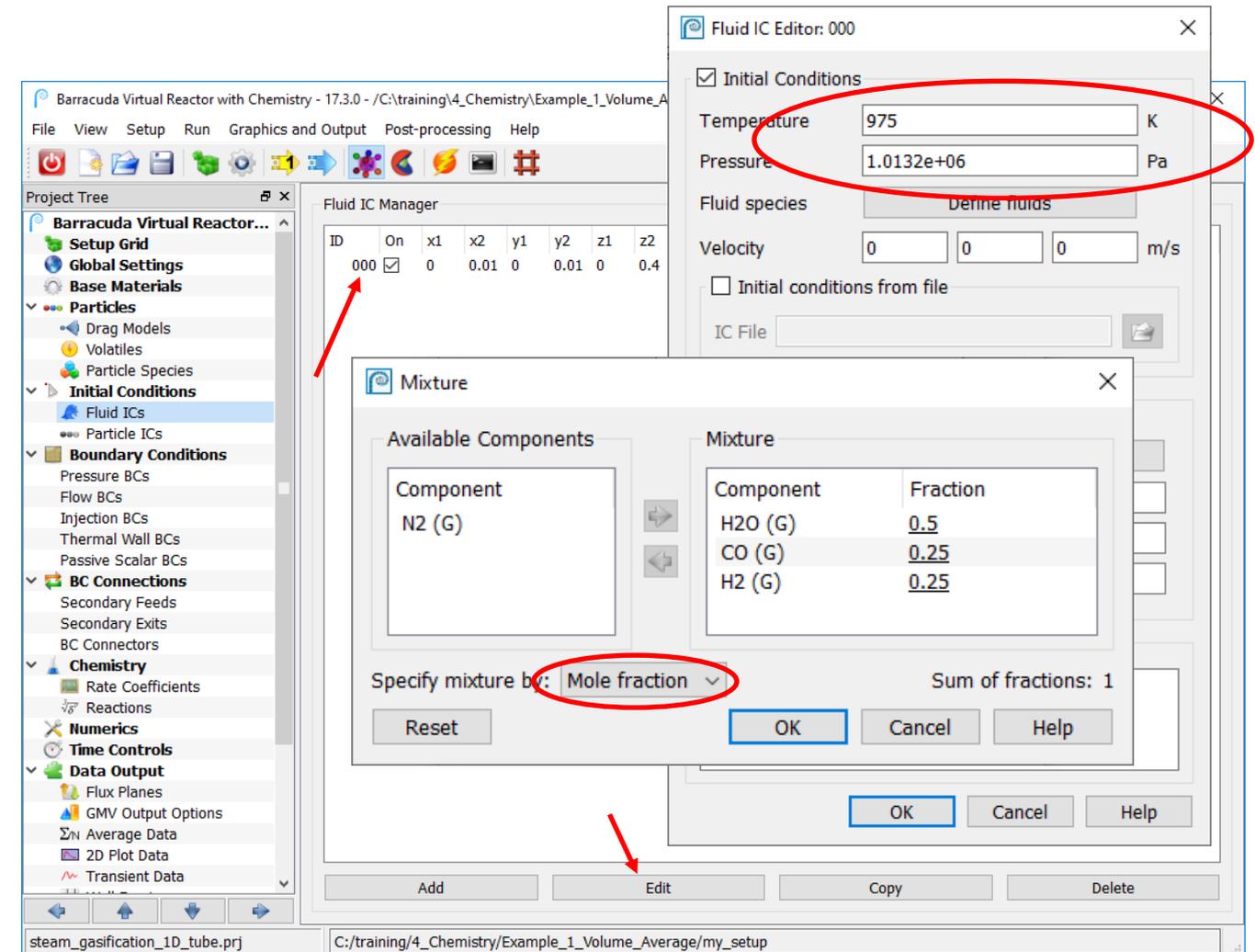


# Fluid Initial Conditions

For the fluid initial condition:

- 975 K
- 10 atm
- 0.50 H<sub>2</sub>O
- 0.25 H<sub>2</sub>
- 0.25 CO

The mixture should be specified by Mole fraction



# Particle Initial Conditions

## Click Add

- Initialize mass in region
- Initial mass of 100 kg of coal particles
- $T = 975 \text{ K}$

The screenshot displays the Barracuda Virtual Reactor interface. The Project Tree on the left shows the 'Initial Conditions' folder expanded to 'Particle ICs'. The 'Particle IC Manager' window shows a table with one entry: ID 000, On checked, and x1, x2, y1, y2 set to min and max. A red arrow points to the 'Add' button. The 'Particle IC' dialog box is open, showing the following settings:

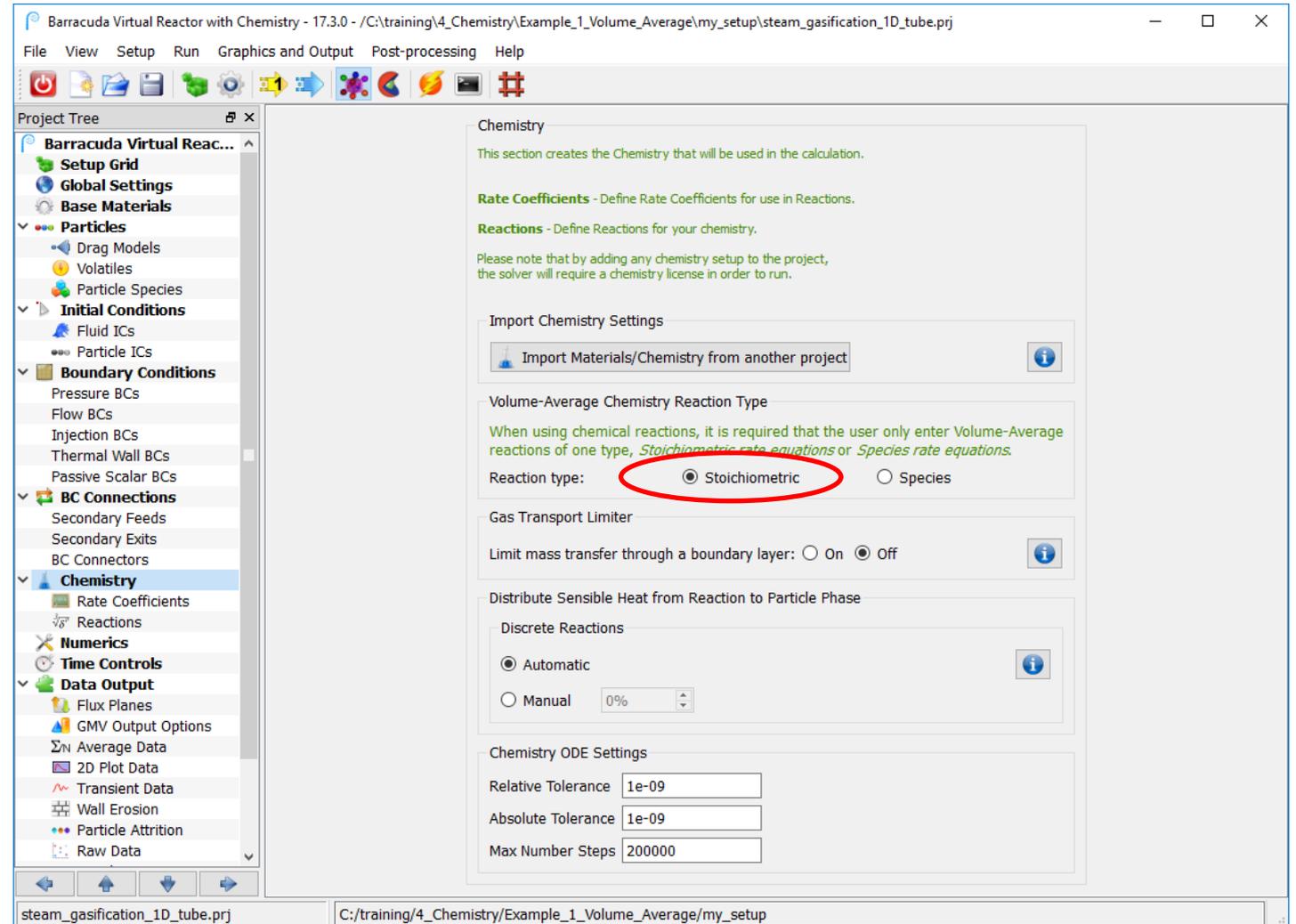
- Initial conditions
- Initialize mass in region (dropdown)
- Particle species: 001 - Coal particles
- Total particle mass: 100 kg
- Temperature: 975 K
- Region: Set Point Region (m) with x<sub>min</sub>, x<sub>max</sub>, y<sub>min</sub>, y<sub>max</sub>, z<sub>min</sub>, z<sub>max</sub> fields.
- Cloud resolution:  Use global resolution,  Use local resolution,  Specify resolution (Clouds per cell, Auto).
- Special settings:  Random cloud initialization,  No particle momentum.
- Comment: 100 kg of particles in the cell

Buttons: OK, Cancel, Help.

# Chemistry

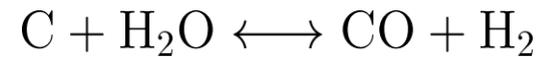
For volume average chemistry, the Stoichiometric and Species forms cannot be mixed.

In this example, reactions will be entered in the Stoichiometric form



# Steam Gasification Reaction

Steam gasification is a reaction that converts solid carbon and water into carbon monoxide and hydrogen.



Reaction is reversible, meaning that full reaction consists of a forward reaction and a reverse reaction.

## Forward Reaction



$$\frac{d[\text{CO}]}{dt} = \left( 219 \frac{\text{m}^3}{\text{kg K s}} \right) T \exp \left( \frac{-22645 \text{K}}{T} \right) \rho_{\text{C}} [\text{H}_2\text{O}]$$

## Reverse Reaction

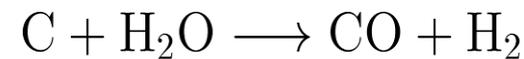


$$\frac{d[\text{H}_2\text{O}]}{dt} = \left( 15.7 \frac{\text{m}^6}{\text{kg mol K}^2 \text{s}} \right) T^2 \exp \left( \frac{-33190 \text{K}}{T} \right) \rho_{\text{C}} [\text{H}_2] [\text{CO}]$$

**Note:** If gas concentration units are mol/m<sup>3</sup>, the reaction rate units will be mol/m<sup>3</sup>/s.

# Forward Reaction Rate

Since we selected Stoichiometric on the main chemistry page, we will be able to specify the forward reaction by the stoichiometric equation:



A Rate Coefficient will be used to specify the forward reaction rate.

$$r_{\text{forward}} = \frac{d[\text{CO}]}{dt} = \left(219 \frac{\text{m}^3}{\text{kg K s}}\right) T \exp\left(\frac{-22645\text{K}}{T}\right) \rho_{\text{C}} [\text{H}_2\text{O}]$$

In Barracuda:

**Reaction rate expression:**  $r_{\text{forward}} = k_0 [\text{H}_2\text{O}]$

**Reaction rate units:** mol/m<sup>3</sup>/s    **Gas concentration units:** mol/m<sup>3</sup>

**Rate coefficient:**  $k_0 = 219T \exp\left(\frac{-22645}{T}\right) \rho_{\text{C}}$

**Temperature units:** K    **Solid Mass units:** kg/m<sup>3</sup>

# Creating the Forward Rate Coefficient

To create the rate coefficient for the forward reaction, go to the Rate Coefficients section of the tree:

- Click Add
- Check that Volume-Average is selected

The screenshot displays the Barracuda Virtual Reactor software interface. On the left, the Project Tree shows the 'Chemistry' section expanded to 'Rate Coefficients'. The 'Add' button at the bottom of the 'Rate Coefficients' section is highlighted with a red arrow. The main window shows the 'Chemistry Rate Coefficients Manager' with a table for adding coefficients. The 'Chemistry Coefficient Editor' dialog box is open, showing the 'Coefficient Properties' section. The 'Type' is set to 'Arrhenius Chem Rate', and the 'Coefficient is for reaction type' is set to 'Volume-Average' (circled in red). The 'Equation' is  $k_0 = 1$ . The 'Values' section shows  $C_0 = 1$ ,  $C_1 = 0$ ,  $C_2 = 0$ ,  $C_3 = 0$ ,  $C_4 = 0$ ,  $C_5 = 0$ ,  $E = 0$ , and  $E0 = 0$ . The 'Temperature unit', 'Pressure unit', and 'Density unit' are set to default. The 'type<sub>s</sub>' is set to 'Solids Dependence'. The 'Temperature Weighting' section shows 'Fluid weighting factor' and 'Particle weighting factor' both set to 0.50. The 'Comment' field is empty. The 'OK' button is highlighted.

# Forward Rate Coefficients

Enter the equation for k0 as follows:

$$\begin{array}{ccccccc} c_0 & c_1 & E & \text{solids dependence} & & & \\ \downarrow & \downarrow & \downarrow & \downarrow & & & \\ k_0 = 219 T^1 \exp(-22645/T) m_c^1 \end{array}$$

Parameters with values of zero will be ignored by the solver. For example, if c2 is set to zero, then the pressure term will not be evaluated by the solver during the simulation

Be sure to enter the units for temperature, pressure, density, mass, etc. as shown on the right

Note that a positive value for E is entered since the GUI already includes a negative sign in the formula for the activation energy and that it has units of (K)

There is no universal gas constant, R, in the denominator of the activation energy term

The screenshot shows the 'Chemistry Coefficient Editor' window. The 'Coefficient Properties' section includes:

- Name: k0
- Type: Arrhenius Chem Rate
- Coefficient is for reaction type: Volume-Average (selected)
- Equation:  $c_0 T^{c_1} p^{c_2} \rho_f^{c_3} \theta_f^{c_4} e^{-E/T+E0} \{type_s\}$
- Equation preview:  $k_0 = 219 T^1 e^{-22645/T} m_c^1$

The 'Values' section contains input fields for:

- c0 = 219
- c1 = 1
- c2 = 0
- c3 = 0
- c4 = 0
- c5 = 0
- E = 22645
- E0 = 0
- type\_s = Solids Dependence

Units are set to:

- Temperature unit: K
- Pressure unit: Pa
- Density unit: kg/m^3
- Mass unit: kg/m^3
- Area unit: (empty)

The 'Temperature Weighting' section has:

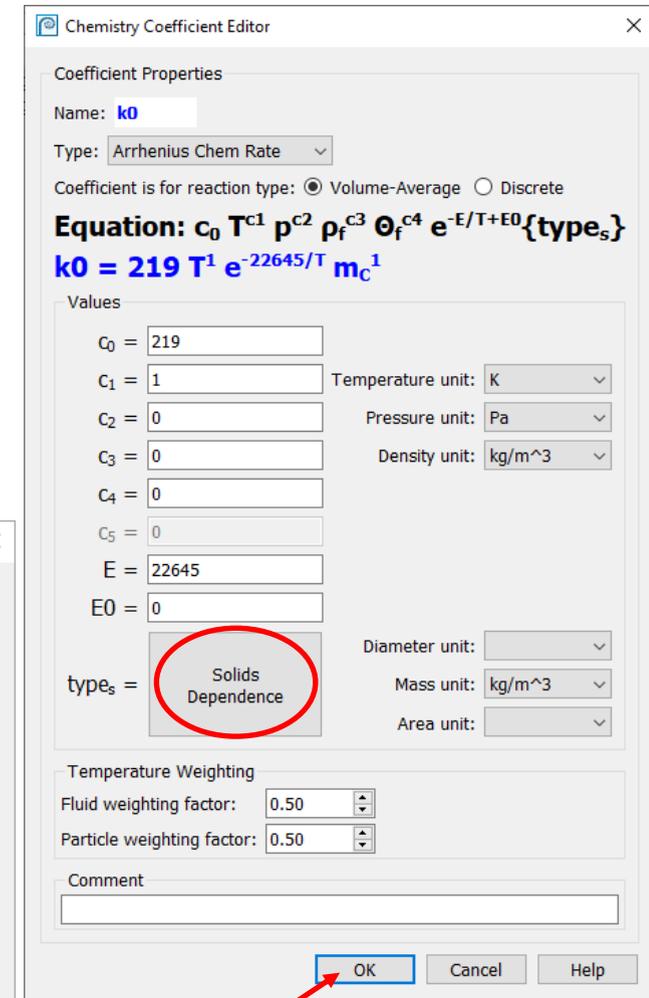
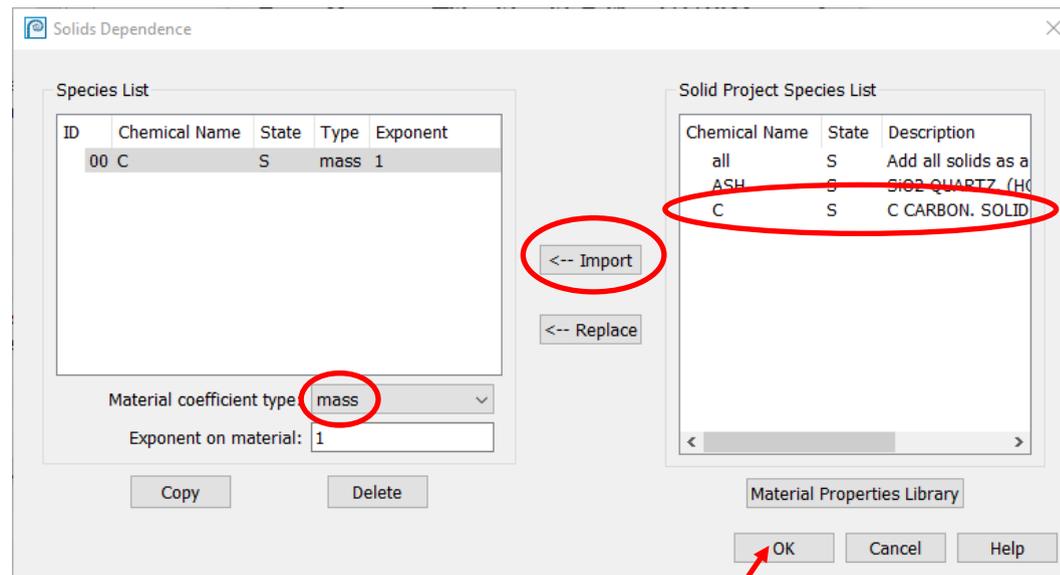
- Fluid weighting factor: 0.50
- Particle weighting factor: 0.50

A 'Comment' field is empty. Buttons for 'OK', 'Cancel', and 'Help' are at the bottom.

# Rate Coefficients: Solids Term

## Click on Solids Dependence in the Chemistry Coefficient Editor window

- Select C then click Import, make sure that Material coefficient type is set to mass, click OK
- Click OK in the Chemistry Coefficient Editor window

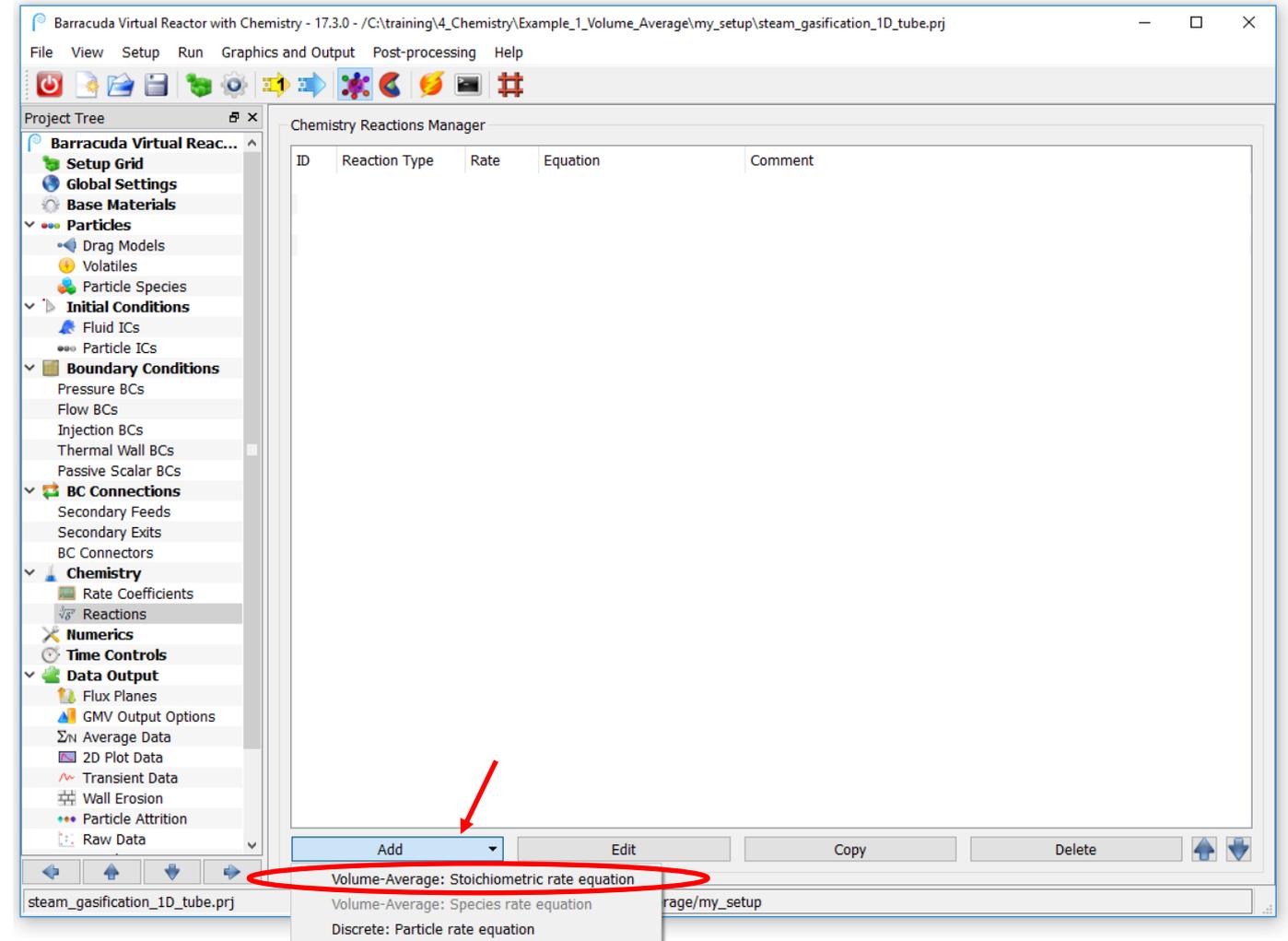


# Creating the Forward Reaction

Start by entering the chemical equation for the forward reaction

Under Reactions:

- Click Add → Volume-Average: Stoichiometric rate equation to define the chemical reaction and its reaction rate



# Specifying the Forward Reaction Stoichiometry

Define the stoichiometric reaction by either:

- Typing directly into the text box using the chemical names needed to match the name in the materials library
- Clicking in the text box to place your cursor in the appropriate position, then using the Add Chemical button

With either method, you will need to type in the “+” signs and coefficients for each species. The characters “=>” represent the forward direction for the reaction

Set the Gas species units to mol/m3

Chemistry Stoichiometric Equation Editor

Stoichiometric Equation Editor

**Directions:** Choose Equation Units for this Stoichiometric Chemistry. Enter a stoichiometric reaction and rate equation in the blanks provided. Use **Add Chemical** and **Add Coefficient** to insert either into the equation. Press the **Check** button to verify equation is valid.

Equation Units  
Reaction rate units: mol/m3/s  
Gas species units: mol/m3

Enter a stoichiometric reaction:

C(S) + H2O => CO + H2

Check Add Chemical

Expected Power Law rate equation format:  $c_0 (k + k - \dots) [\text{material1}]^{\text{power}} [\text{material2}]^{\text{power}} + c_1 \dots$   
Example of valid Power Law rate equation format:  $1.2 ( 1.5 * k_0 - 3 * k_1 ) [\text{H}_2\text{O}]^{1.5}$   
Example of invalid Power Law rate equation format:  $( k_0 * k_1 ) [\text{H}_2\text{O}]^{1.5}$  Coefficients cannot be multiplied.  
Example of LH expected format:  $( c_0 k [ ] + c_1 k [ ] + \dots ) / ( 1 + c_2 k [ ] + c_3 k [ ] + \dots )^{\text{power}}$   
Example of groups of rates:  $( c_0 k_0 [\text{O}_2] - c_1 (0.5k_1 - k_2) )^{1.5} ( c_1(k_3) [\text{CO}]^{0.5} [\text{O}_2] )^{-1}$

Enter a rate equation for the stoichiometric reaction in either Power Law or Langmuir-Hinshelwood form:

R00 = (k0[H2O])

Check Add Volume-Average Coefficient Add Chemical Coefficients Manager

Comment

OK Cancel Help

# Specifying the Forward Reaction Rate

To enter the rate equation for the reaction,

- Click Add Volume-Average Coefficient and select  $k_0$ ,
- Click Add Chemical and select H<sub>2</sub>O

Use the Check buttons to verify that both the chemical equation and the rate equation are formatted properly

Click OK

Chemistry Stoichiometric Equation Editor

Stoichiometric Equation Editor

**Directions:** Choose Equation Units for this Stoichiometric Chemistry.  
Enter a stoichiometric reaction and rate equation in the blanks provided.  
Use **Add Chemical** and **Add Coefficient** to insert either into the equation. Press the **Check** button to verify equation is valid.

Equation Units  
Reaction rate units: mol/m3/s  
Gas species units: mol/m3

Enter a stoichiometric reaction:  
C(S) + H2O => CO + H2

Check Add Chemical

Expected Power Law rate equation format:  $c_0 (k + k - \dots) [\text{material1}]^{\text{power}} [\text{material2}]^{\text{power}} + c_1 \dots$   
Example of valid Power Law rate equation format:  $1.2 ( 1.5 * k_0 - 3 * k_1 ) [\text{H}_2\text{O}]^{1.5}$   
Example of invalid Power Law rate equation format:  $( k_0 * k_1 ) [\text{H}_2\text{O}]^{1.5}$  Coefficients cannot be multiplied.  
Example of LH expected format:  $( c_0 k [ ] + c_1 k [ ] + \dots ) / ( 1 + c_2 k [ ] + c_3 k [ ] + \dots )^{\text{power}}$   
Example of groups of rates:  $( c_0 k_0 [\text{O}_2] - c_1 (0.5k_1 - k_2) )^{1.5} ( c_1(k_3) [\text{CO}]^{0.5} [\text{O}_2] )^{-1}$

Enter a rate equation for the stoichiometric reaction in either Power Law or Langmuir-Hinshelwood form:  
R00 = (k0[H2O])

Check Add Volume-Average Coefficient Add Chemical Coefficients Manager

Comment

OK Cancel Help

# Forward Reaction Rate

The forward reaction rate equation is now complete:

- Rate coefficient and units
- Stoichiometric chemical equation
- Reaction rate equation
- Reaction rate and concentration units

Barracuda Virtual Reactor with Chemistry - 20.0.0 - pre\_setup/single\_cell\_chemistry\_example.prj

File View Setup Run Graphics and Output Post-processing Help

Project Tree

- Barracuda Virtu...
- Setup Grid
- Global Settings
- Base Materials
- Particles
  - Drag Models
  - Volatiles
  - Particle Species
- Initial Conditions
  - Fluid ICs
  - Particle ICs
- Boundary Con...
  - Pressure BCs
  - Flow BCs
  - Injection BCs
  - Thermal Wall BCs
  - Passive Scalar BCs
- BC Connections
  - Secondary Feeds
  - Secondary Exits
  - BC Connectors
- Chemistry
  - Rate Coefficie...
  - Reactions
- Numerics
- Time Controls
- Data Output
  - Flux Planes
  - Visualization ...
  - Average Data
  - Data Planes
  - Data Points
  - Wall Erosion
  - Particle Attrition

Chemistry Reactions Manager

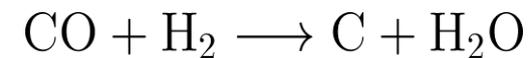
ID	Reaction Type	Rate	Equation	Comment
00	VA: Stoichiometric	Equation: R00 = (k0[H2O])	C (S) + H2O => CO + H2	

Add Edit Copy Delete

single\_cell\_chemistry\_example.prj C:/training/4\_Chemistry/single\_cell\_chemistry\_example/pre\_setup

# Reverse Reaction Rate

We will specify the reverse reaction by the stoichiometric equation:



A Rate Coefficient will be used to specify the reverse reaction rate.

$$\frac{d[\text{H}_2\text{O}]}{dt} = \left(15.7 \frac{\text{m}^6}{\text{kg mol K}^2 \text{s}}\right) T^2 \exp\left(\frac{-33190 \text{ K}}{T}\right) \rho_C [\text{H}_2] [\text{CO}]$$

In Barracuda:

**Reaction rate expression:**  $r_{\text{reverse}} = k_1 [\text{H}_2] [\text{CO}]$

**Reaction rate units:** mol/m<sup>3</sup>/s    **Gas concentration units:** mol/m<sup>3</sup>

**Rate coefficient:**  $k_1 = 15.7 T^2 \exp\left(\frac{-33190}{T}\right) \rho_C$

**Temperature units:** K    **Solid Mass units:** kg/m<sup>3</sup>

# Rate Coefficient: Reverse Reaction

In a similar manner, add the rate coefficient for the reverse reaction

Under Rate Coefficients, click Add and enter the equation for k1 as follows:

$$k_1 = 15.7 T^2 \exp(-33190/T) m_C$$

$c_0$     $c_1$     $E$    solids dependence  
 ↓   ↓   ↓   ↓

Check that Volume-Average is selected and that units are selected for temperature, pressure, density, mass, etc.

Remember to click on Solids Dependence to select C and set Material coefficient type to mass

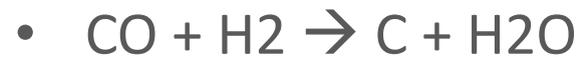
The screenshot shows the software interface with the 'Chemistry Rate Coefficients Manager' window open. The 'Add' button is highlighted with a red arrow. The 'Chemistry Coefficient Editor' dialog box is also open, showing the following details:

- Name:** k1
- Type:** Arrhenius Chem Rate
- Coefficient is for reaction type:**  Volume-Average  Discrete
- Equation:**  $c_0 T^{c_1} p^{c_2} \rho_f^{c_3} \theta_f^{c_4} e^{-E/T+E0} \{type_s\}$
- Equation for k1:**  $k_1 = 15.7 T^2 e^{-33190/T} m_C^1$
- Values:**
  - $C_0 = 15.7$
  - $C_1 = 2$
  - $C_2 = 0$
  - $C_3 = 0$
  - $C_4 = 0$
  - $C_5 = 0$
  - $E = 33190$
  - $E0 = 0$
- Units:**
  - Temperature unit: K
  - Pressure unit: Pa
  - Density unit: kg/m<sup>3</sup>
  - Diameter unit: (empty)
  - Mass unit: kg/m<sup>3</sup>
  - Area unit: (empty)
- Temperature Weighting:**
  - Fluid weighting factor: 0.50
  - Particle weighting factor: 0.50
- Comment:** (empty text box)
- Buttons:** OK, Cancel, Help

A red arrow in the dialog points to the 'Solids Dependence' dropdown menu, which is currently set to 'Solids Dependence'.

# Chemical Equations: Reverse Reaction

Define the stoichiometric equation for the reverse reaction:



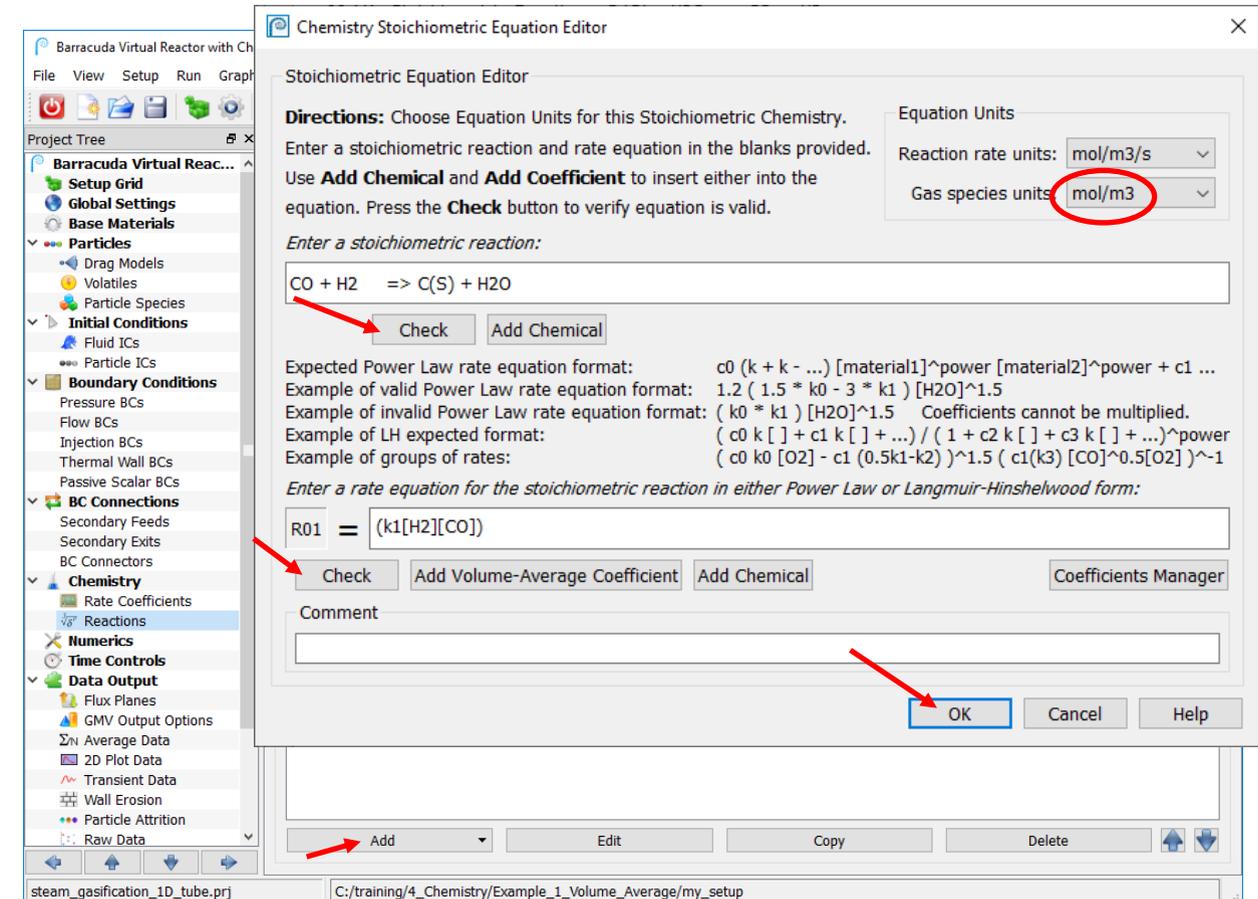
Enter the rate equation for the reverse reaction as follows:



Set Gas species units to mol/m<sup>3</sup>

Use the Check buttons to verify that both the chemical equation and the rate equation are formatted properly

Click OK



# Reverse Reaction

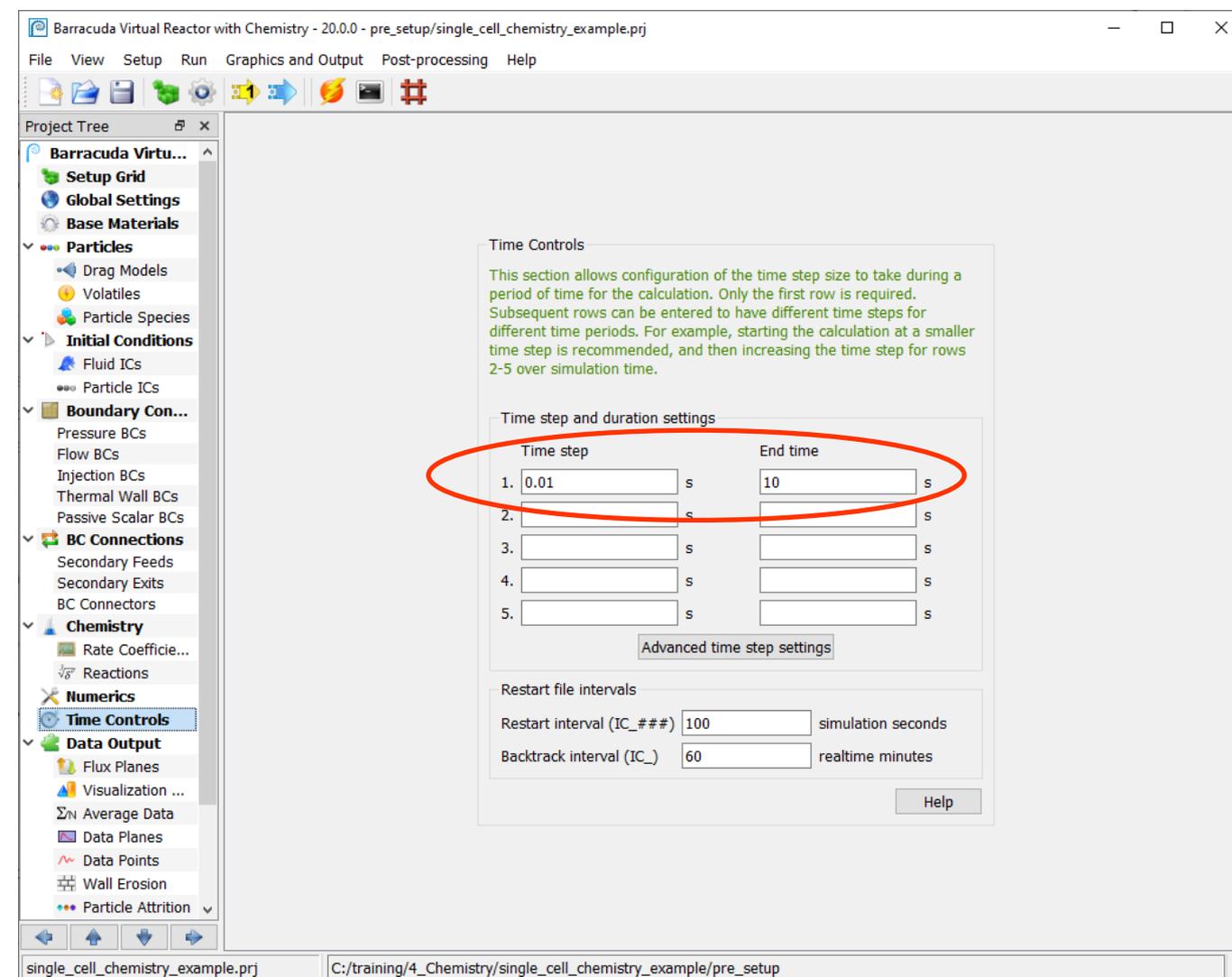
The reverse reaction is now complete

The screenshot shows the Barracuda Virtual Reactor software interface. The main window is titled "Barracuda Virtual Reactor with Chemistry - 20.0.0 - pre\_setup/single\_cell\_chemistry\_example.prj". The "Chemistry Reactions Manager" panel is open, displaying a table of reactions. The reaction ID [01] is highlighted with a red circle. The reaction is a stoichiometric reaction with the equation  $\text{CO} + \text{H}_2 \Rightarrow \text{C (S)} + \text{H}_2\text{O}$  and the rate equation  $R01 = (k1[\text{H}_2][\text{CO}])$ .

ID	Reaction Type	Rate	Equation	Comment
00	VA: Stoichiometric		Equation: $\text{C (S)} + \text{H}_2\text{O} \Rightarrow \text{CO} + \text{H}_2$ R00 = $(k0[\text{H}_2\text{O}])$	
[01]	VA: Stoichiometric		Equation: $\text{CO} + \text{H}_2 \Rightarrow \text{C (S)} + \text{H}_2\text{O}$ R01 = $(k1[\text{H}_2][\text{CO}])$	

# Time Controls

Enter Time step and End time as shown:

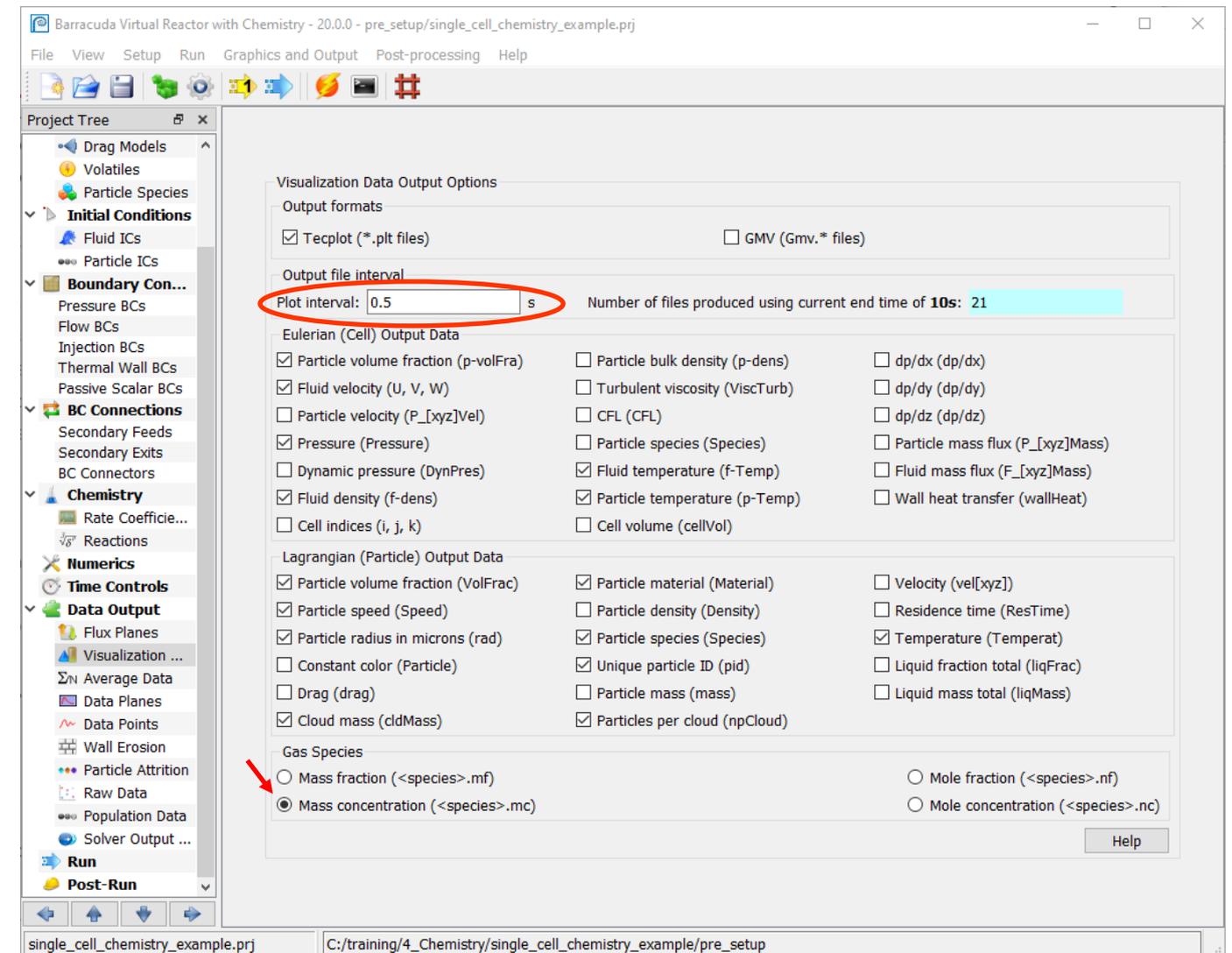


# Visualization Output Options

Enter a Plot interval of 0.5 s

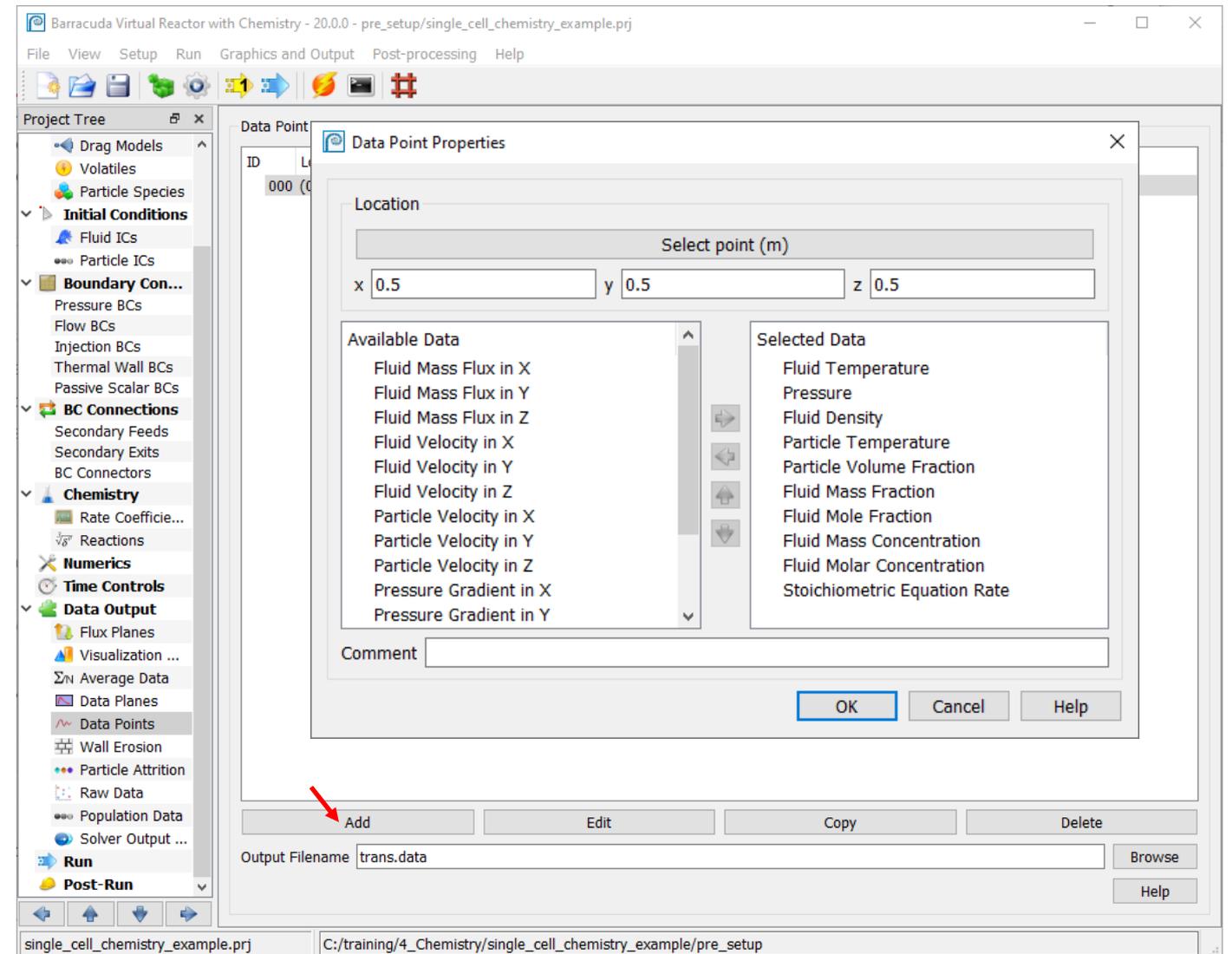
Choose the output variables shown on the right

Note that only one Gas Species option can be chosen, in this case use Mass concentration



# Data Points

Define a single Data Point at the cell center, and select the output data shown:



# Run the Simulation

## Run the simulation

The screenshot displays the Barracuda Virtual Reactor software interface. The main window is titled "Barracuda Virtual Reactor with Chemistry - 20.0.0 - pre\_setup/single\_cell\_chemistry\_example.prj". The interface includes a menu bar (File, View, Setup, Run, Graphics and Output, Post-processing, Help) and a toolbar with various icons. On the left, a "Project Tree" pane shows a hierarchical view of the simulation setup, including sections for Setup, Global, Base, Particles, Initial, Bound, BC Con, Chemi, Numeric, Time C, and Data O. The "Run" button in the Project Tree is highlighted with a blue selection box. The main area is titled "Run Settings" and is divided into two columns. The left column, "Verify Setup", contains a note about the "Run Solver Setup" button and a list of view options: "View Initial Particles, Volume Fraction", "View Initial Particles, Species", "View Boundary Conditions", "View Flux Planes", and "View Data Points". The right column, "Run Calculation", contains "Solver Launch Options" (CPU Parallel and GPU Parallel), "Universal Options" (temperature, mass imbalance, disk space limits), and a "Command line to run equivalent solver" field. At the bottom of the "Run Calculation" section, three buttons are visible: "Run Solver" (highlighted with a red arrow), "Restart Solver", and "Interact". A "Help" button is located at the bottom right of the dialog.

# Plotting Data Point Information in Tecplot for Barracuda

## Open Tecplot for Barracuda using the Postprocessor button in Post-Run

- File → Load Barracuda data... → Load Data File
- Select trans.data00
- Copy the default plotting frame, and paste it 3 times to get 4 frames total
- Tile the frames in a 2x2 grid pattern (see this [video](#) for instructions on frames and this [video](#) for instructions on xy plots)

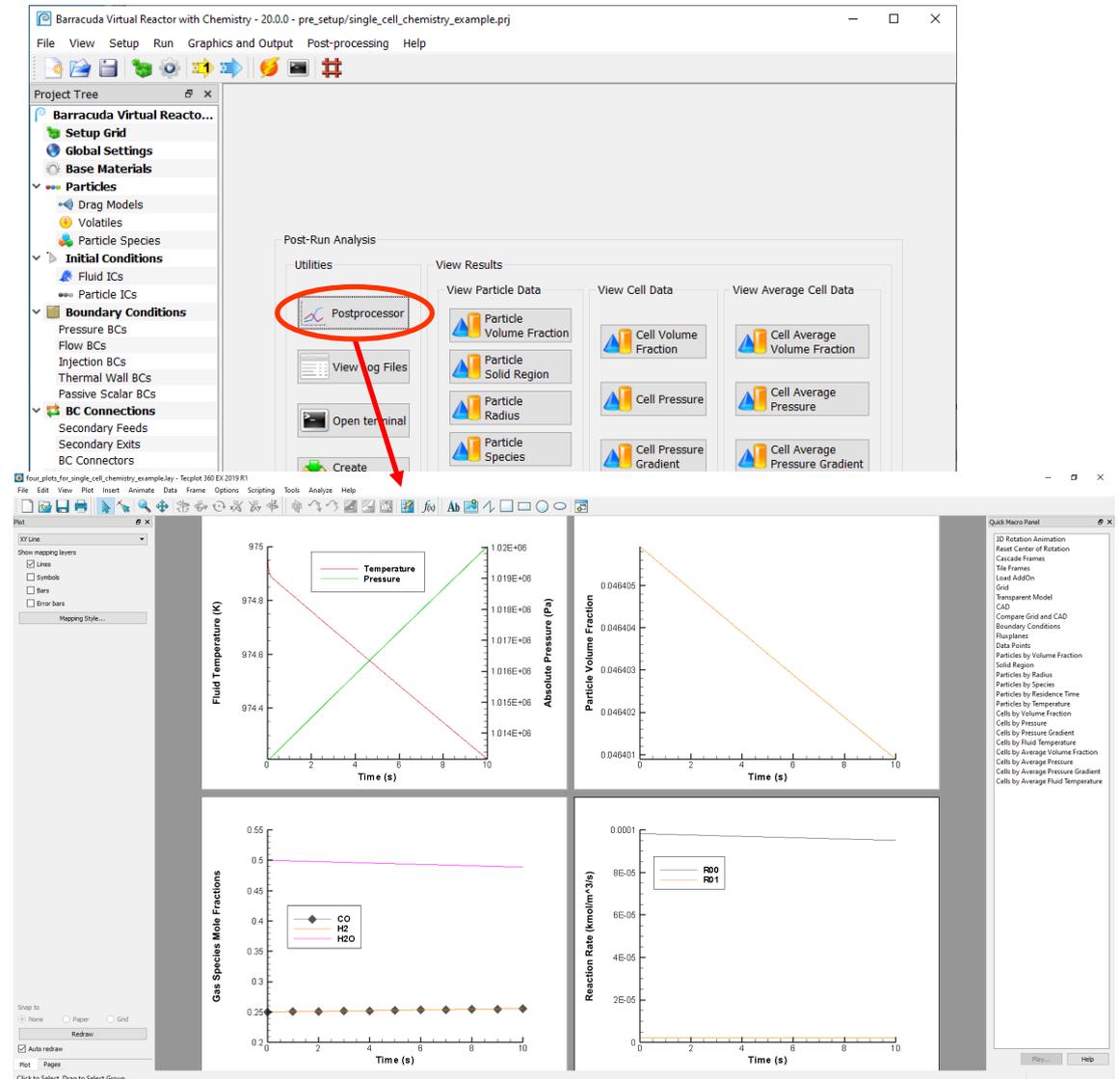
## Create the following 4 plots (see next slide for larger version of final result):

- Plot 1: fluid temperature on left axis, pressure on right axis (both plotted vs time)
- Plot 2: particle volume fraction vs time
- Plot 3: mole fractions of gas species vs time
- Plot 4: reaction rates vs time

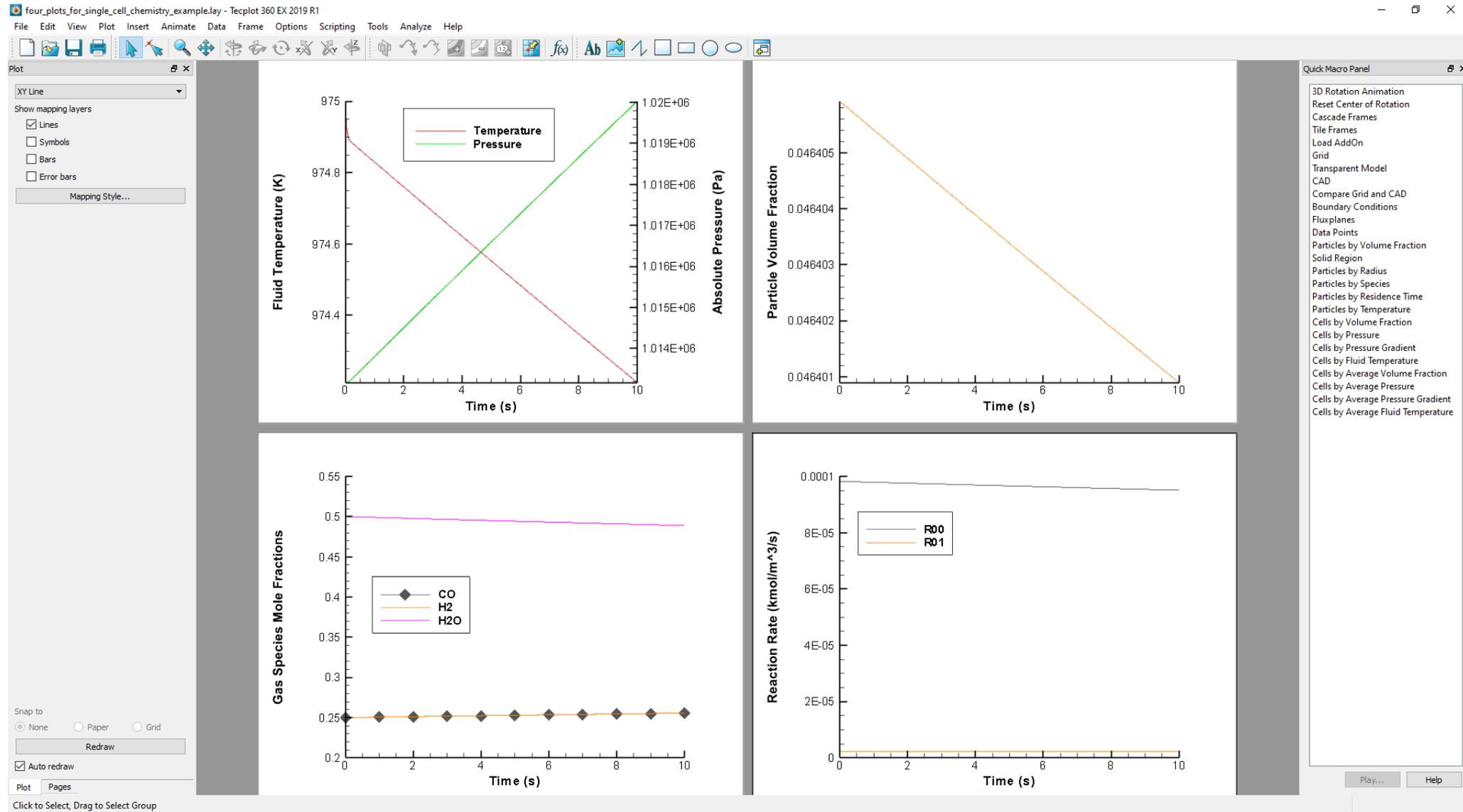
Hint: use Ctrl+F to rescale axes after selecting data or adjusting plot sizes

Export a PNG image of the array of plots

Save a layout file for this analysis



# Final Plotting Result in Tecplot for Barracuda



# Verifying Reaction Rate at t = 0 s

## Advantages of using a single-cell system:

- Easy to set up and run simulation
- Possible to hand-calculate reaction rate at t = 0 s
- Helps to ensure that chemical reaction rates have been entered correctly

## See spreadsheet containing hand calculation:

steam\_gasification\_hand\_calculation.xlsx

Verify that the first time-step result in trans.data00 matches expected reaction rate result from spreadsheet

	A	B	C
1	<b>Initial Conditions in Simulation</b>		
2	Volume of cell	1	m <sup>3</sup>
3	Fluid temperature	975	K
4	Absolute pressure	1.01E+06	Pa
5	Mass of particles	100	kg
6	Mass fraction of C in particles	0.9	
7	Mass concentration of C	90	kg/m <sup>3</sup>
8	Ideal gas constant	8.3145	J/mol/K
9	Mole fraction of H2O	0.50	
10	Mole fraction of H2	0.25	
11	Mole fraction of CO	0.25	
12	Molar concentration of H2O	6.2492E+01	mol/m <sup>3</sup>
13	Molar concentration of H2	3.1246E+01	mol/m <sup>3</sup>
14	Molar concentration of CO	3.1246E+01	mol/m <sup>3</sup>
15			
16	<b>Hand-calculated Reaction Rates</b>		
17	Forward reaction, R00	9.8344E-05	kmol/m <sup>3</sup> /s
18	Reverse reaction, R01	2.1573E-06	kmol/m <sup>3</sup> /s

```

trans.data00 (C:\training\4_Chemistry\single_cell_chemistry_example\pre_setup) - GVIM
File Edit Tools Syntax Buffers Window Help
[Icons]
28 #@ 20 "Mole concentration H2 @ (5.000e-01, 5.000e-01, 5.000e-01)" "mol/m^3" " 1 1 1" " 5.00000e-01 5.00000e-01 5.00000e-01" " "
29 #@ 21 "Mole concentration H2O @ (5.000e-01, 5.000e-01, 5.000e-01)" "mol/m^3" " 1 1 1" " 5.00000e-01 5.00000e-01 5.00000e-01" " "
30 #@ 22 "Mole concentration N2 @ (5.000e-01, 5.000e-01, 5.000e-01)" "mol/m^3" " 1 1 1" " 5.00000e-01 5.00000e-01 5.00000e-01" " "
31 #@ 23 "Stoichiometric equation rate R00 @ (5.000e-01, 5.000e-01, 5.000e-01)" "kmol/s*m^3" " 1 1 1" " 5.00000e-01 5.00000e-01 5.00000e-01" " "
32 #@ 24 "Stoichiometric equation rate R01 @ (5.000e-01, 5.000e-01, 5.000e-01)" "kmol/s*m^3" " 1 1 1" " 5.00000e-01 5.00000e-01 5.00000e-01" " "
33 0.000000e+00 9.7500000000e+02 1.0132000000e+06 2.0622429899e+00 9.7500000000e+02 4.6405919662e-02 4.2424242424e-01 3.0303030303e-02 5.4545454545e-01 0.0000000000e+00
2.5000000000e-01 2.5000000000e-01 5.0000000000e-01 0.0000000000e+00 0.0000000000e+00 0.7189096244e-01 6.2492211603e-02 1.1248598089e+00 0.0000000000e+00 3.1246105801e+01 3.1246105801e+01
01 6.2492211603e+01 0.0000000000e+00 9.8344346441e-05 2.1573151680e-06
[Icons]
30,1 2%
  
```

# Summary

This example problem introduced several important components of a typical Barracuda simulation with chemistry:

- Importing multiple materials
- Defining chemical reaction rate coefficients
- Defining stoichiometric chemical reactions
- Defining reaction rate expressions
- Defining a reversible chemical reaction by splitting the reaction into forward and reverse directions

Additionally, some specific concepts for verifying chemistry input were presented:

- A single-cell case is often the easiest and fastest way to verify that chemical reaction rates have been specified correctly in Barracuda
- For reaction sets with multiple reactions, it is best to create a single-cell simulation for each reaction

Once chemical reactions have been verified using this method, import them into the full simulation project using Import Chemistry.

Chemistry

This section creates the Chemistry that will be used in the calculation.

**Rate Coefficients** - Define Rate Coefficients for use in Reactions.

**Reactions** - Define Reactions for your chemistry.

Please note that by adding any chemistry setup to the project, the solver will require a chemistry license in order to run.

Import Chemistry Settings

Import Materials/Chemistry from another project

Volume-Average Chemistry Reaction Type

When using chemical reactions, it is required that the user only enter Volume-Average reactions of one type, *Stoichiometric rate equations* or *Species rate equations*.

Reaction type:  Stoichiometric  Species

Gas Transport Limiter

Limit mass transfer through a boundary layer:  On  Off

Distribute Sensible Heat from Reaction to Particle Phase

Discrete Reactions

Automatic

Manual 0%

Chemistry ODE Settings

Relative Tolerance 1e-09

Absolute Tolerance 1e-09

Max Number Steps 200000

Help