# 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 µm diameter coal particles
- Mass of coal particles = 100 kg
- Coal is assumed to be 90% carbon and 10% ash (SiO_2)
- Initial temperature = 975 K
- Initial pressure = 10 atm
- Initial gas composition (mole basis)
  - 50% H_2O
  - 25% H_2
  - 25% CO
- No inlets or outlets for gas or particles
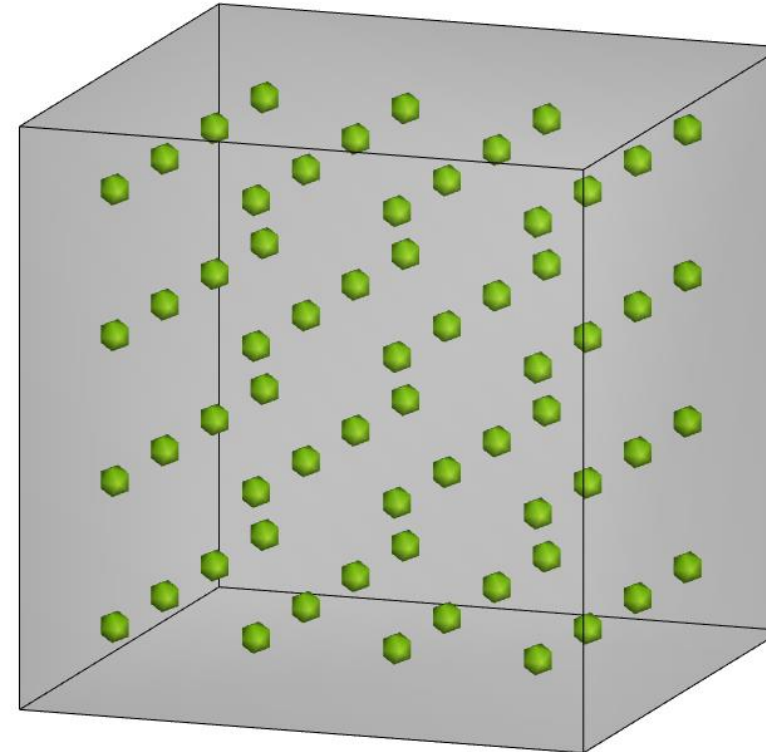
Model will be set up with volume average chemistry

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

Volume Average Project File

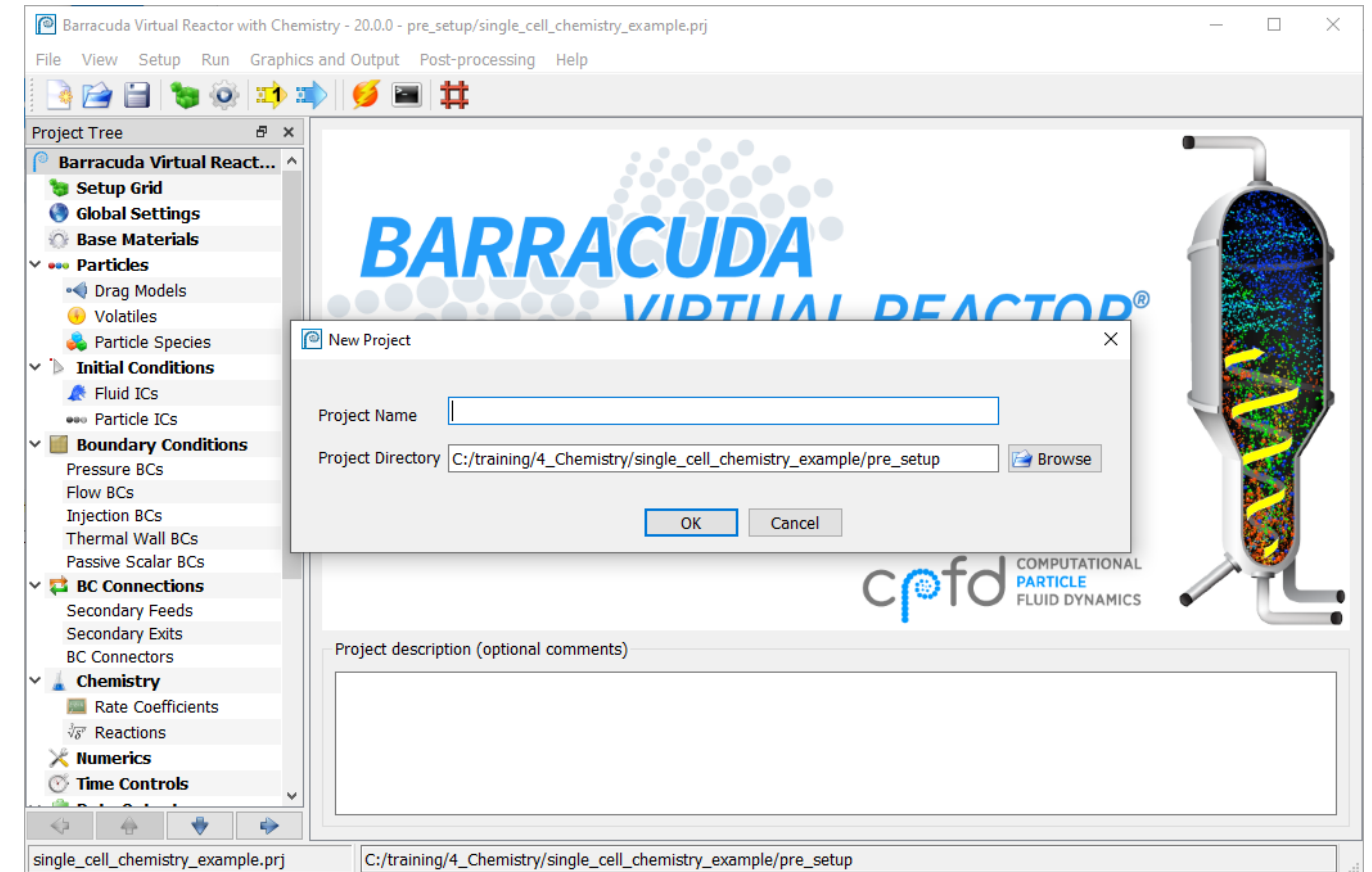**Create a new project file under the directory:**

- 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

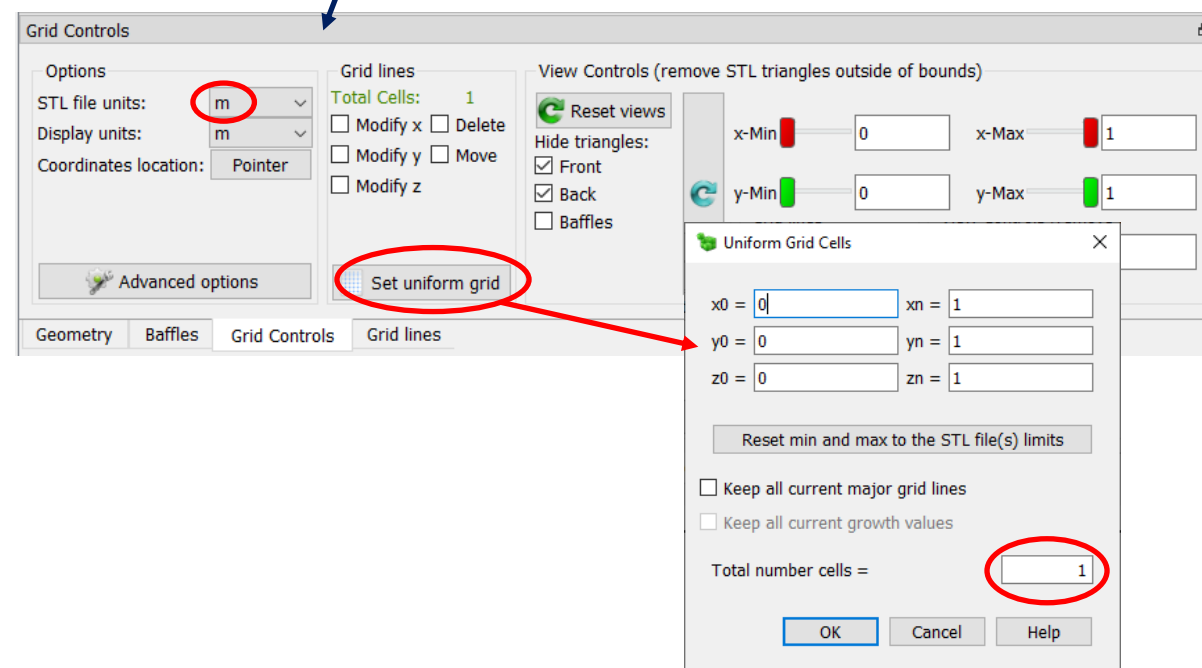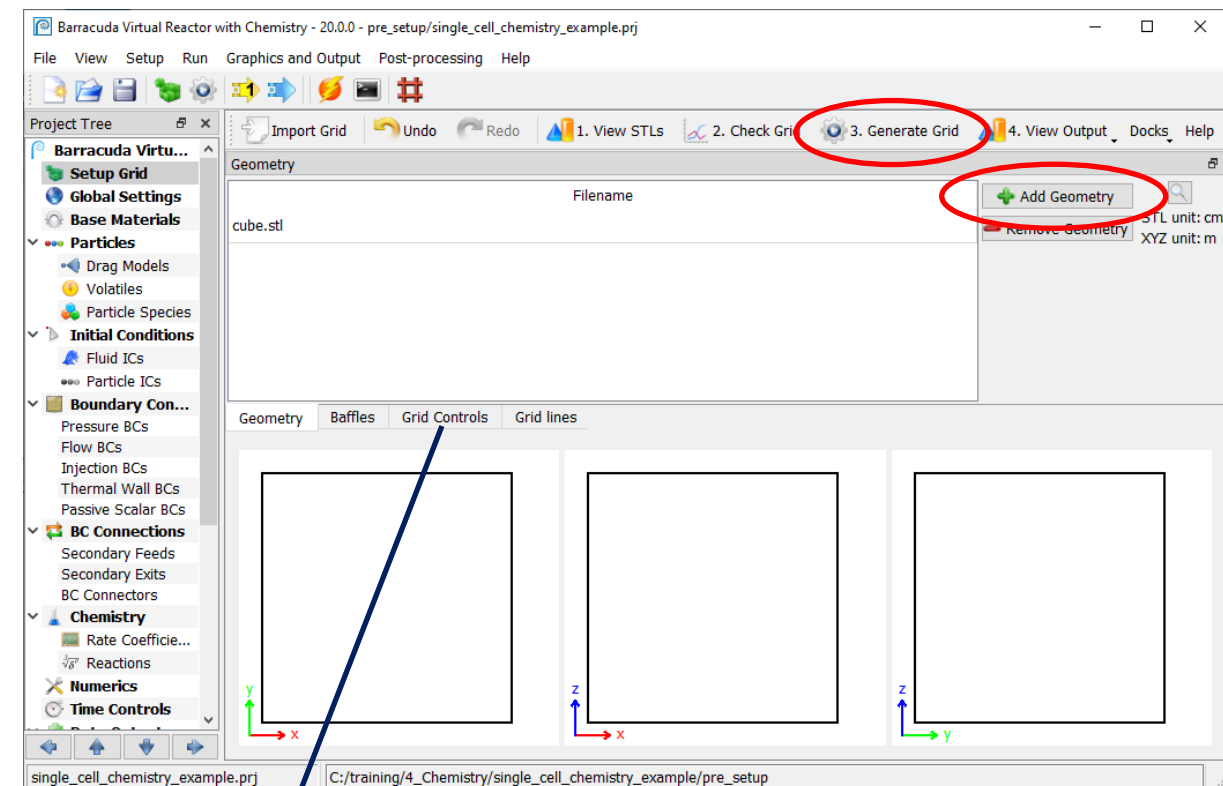**An STL file is included in your project directory, named cube.stl**

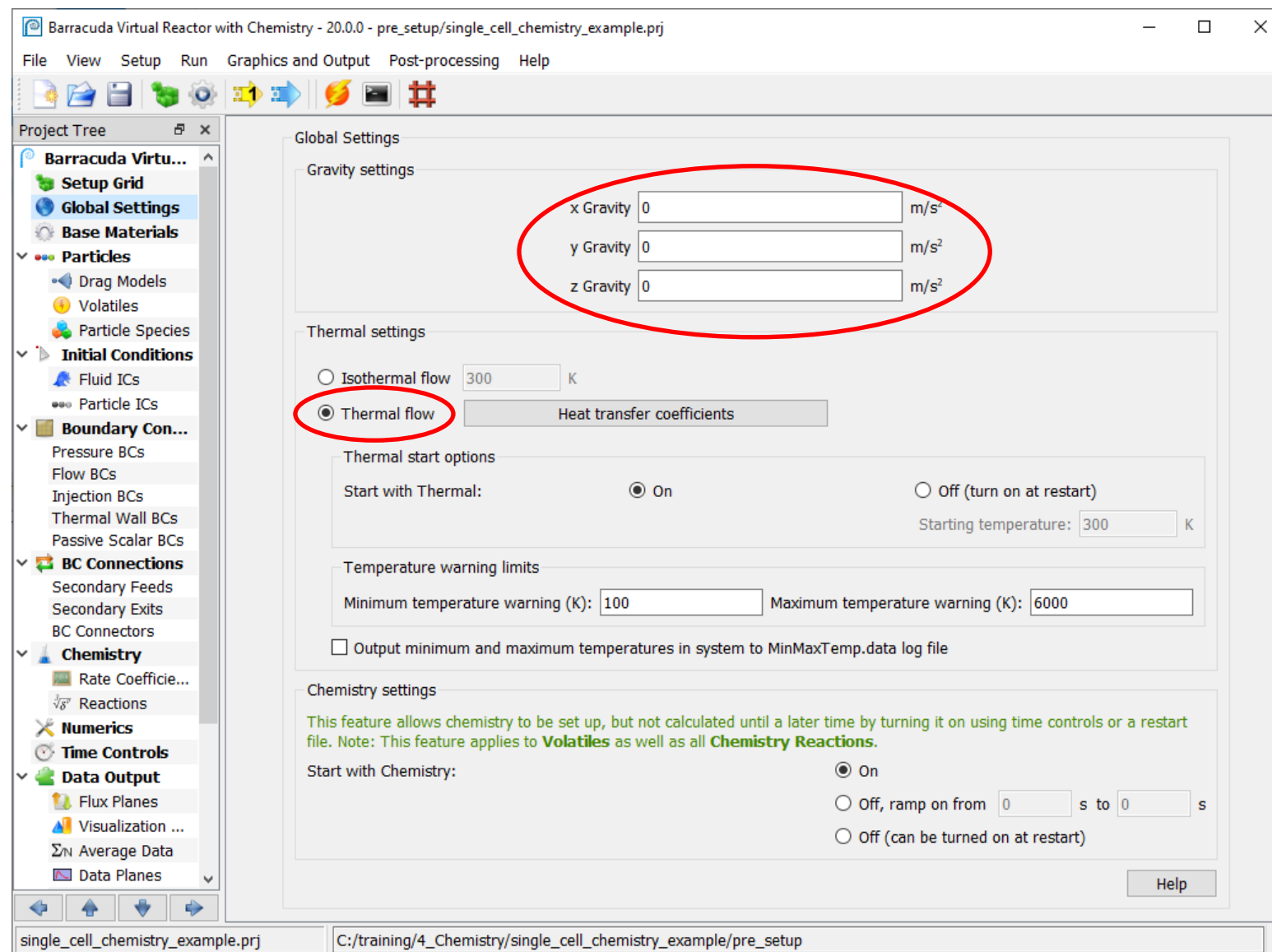- Each side-length = 1 m

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

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
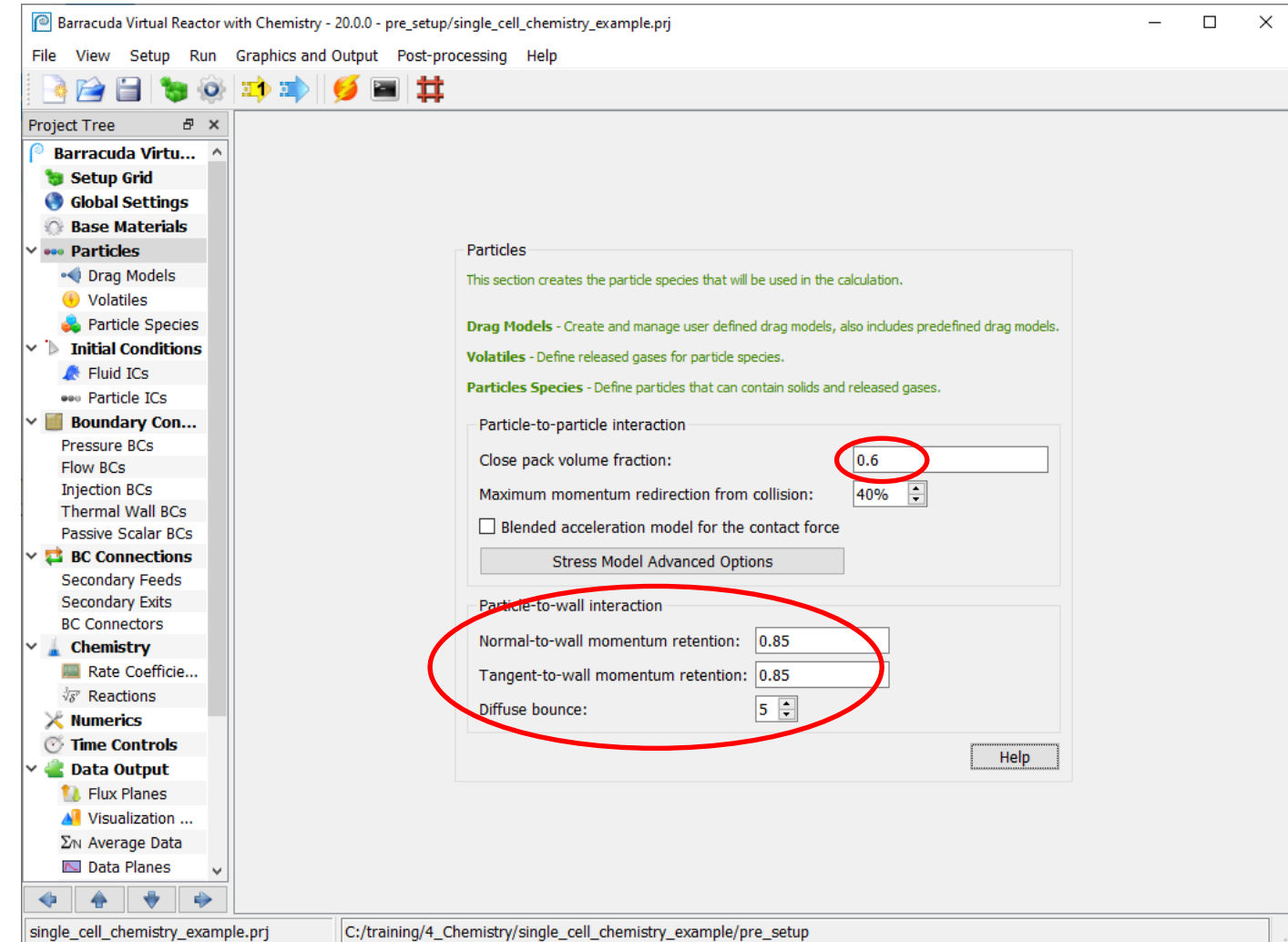
- Import SiO2_2 QUARTZ (HQZ), then select it on the Project material list, click Edit, and rename it ASH
- Import C_1 and rename it C

Choose Compressible Flow to add multiple fluids
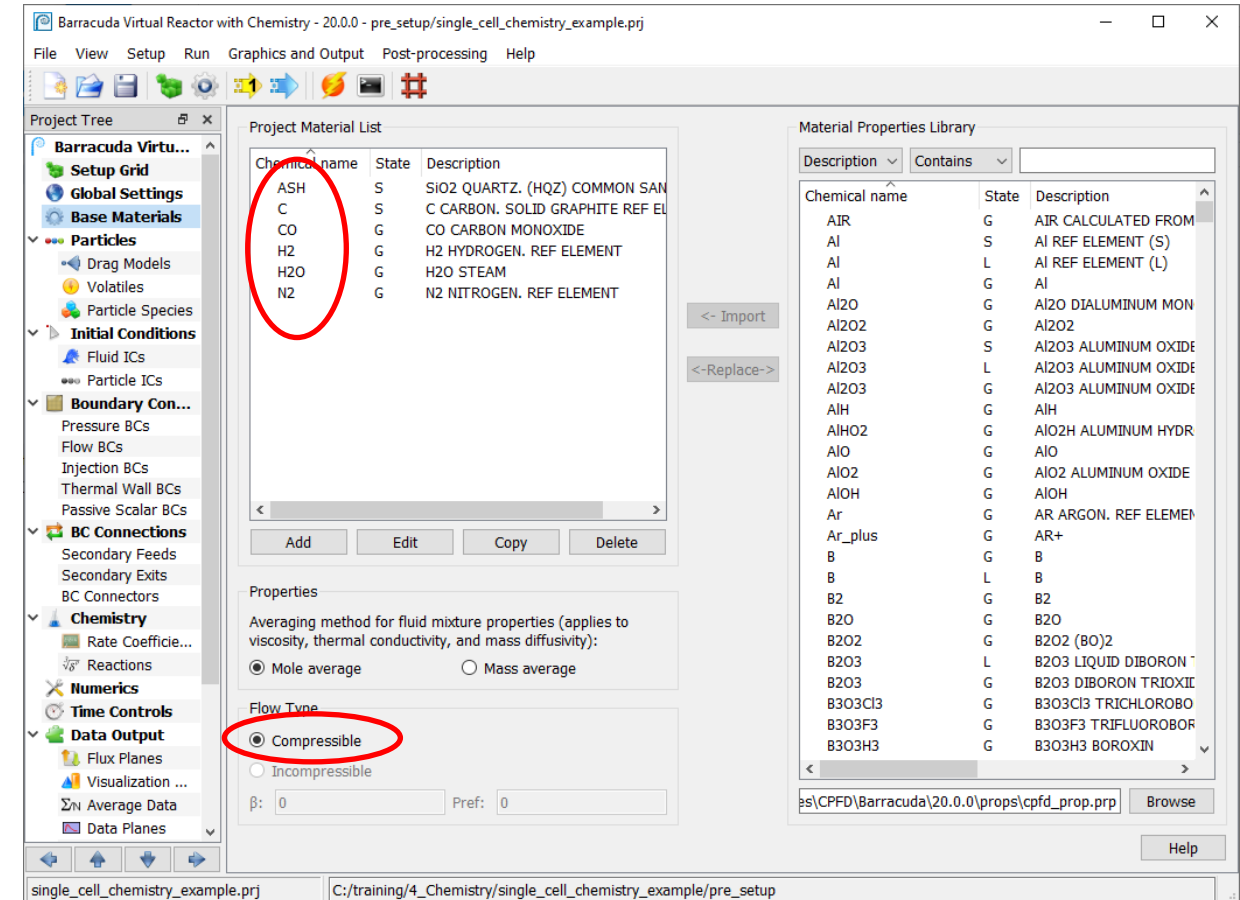
Particles

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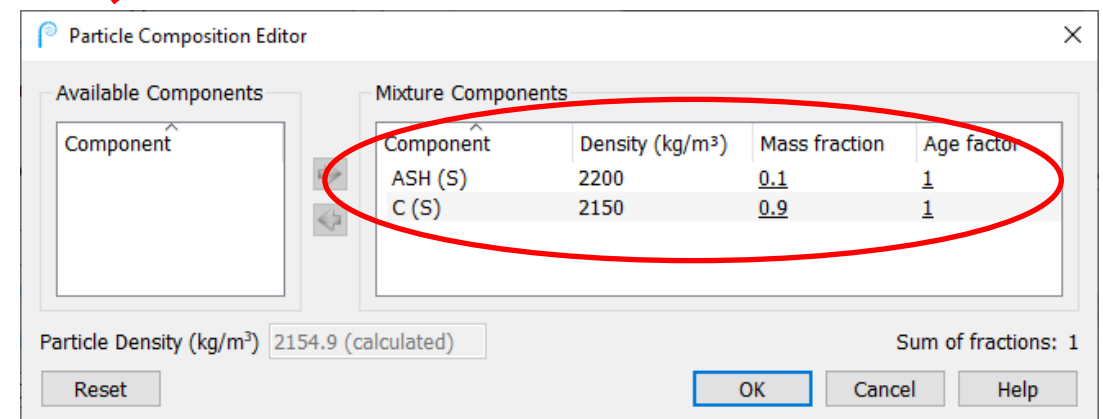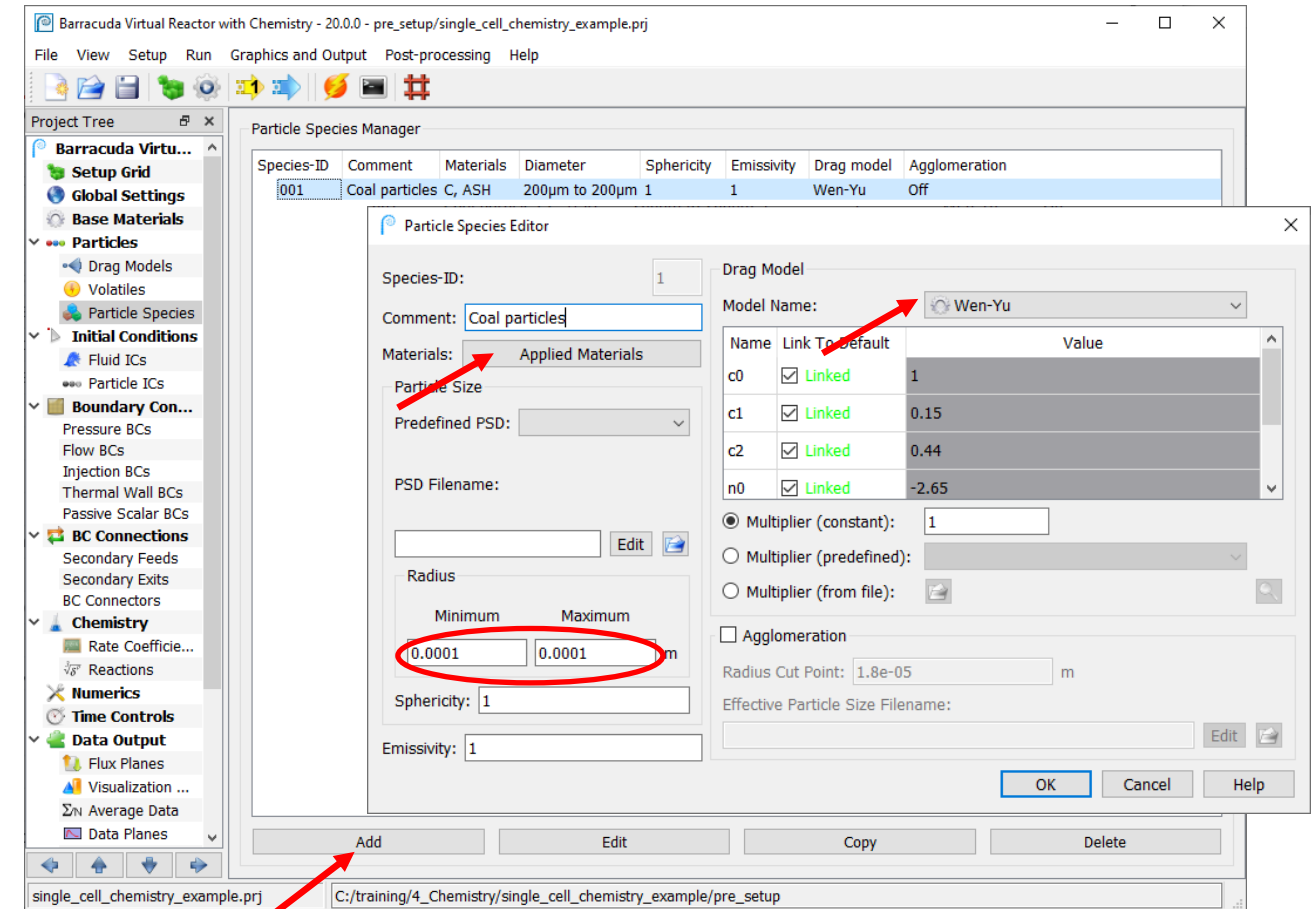
Particle Species

Click on the Particle Species tab

- Click Add
- Enter a comment
- Click Applied Materials
  - 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.
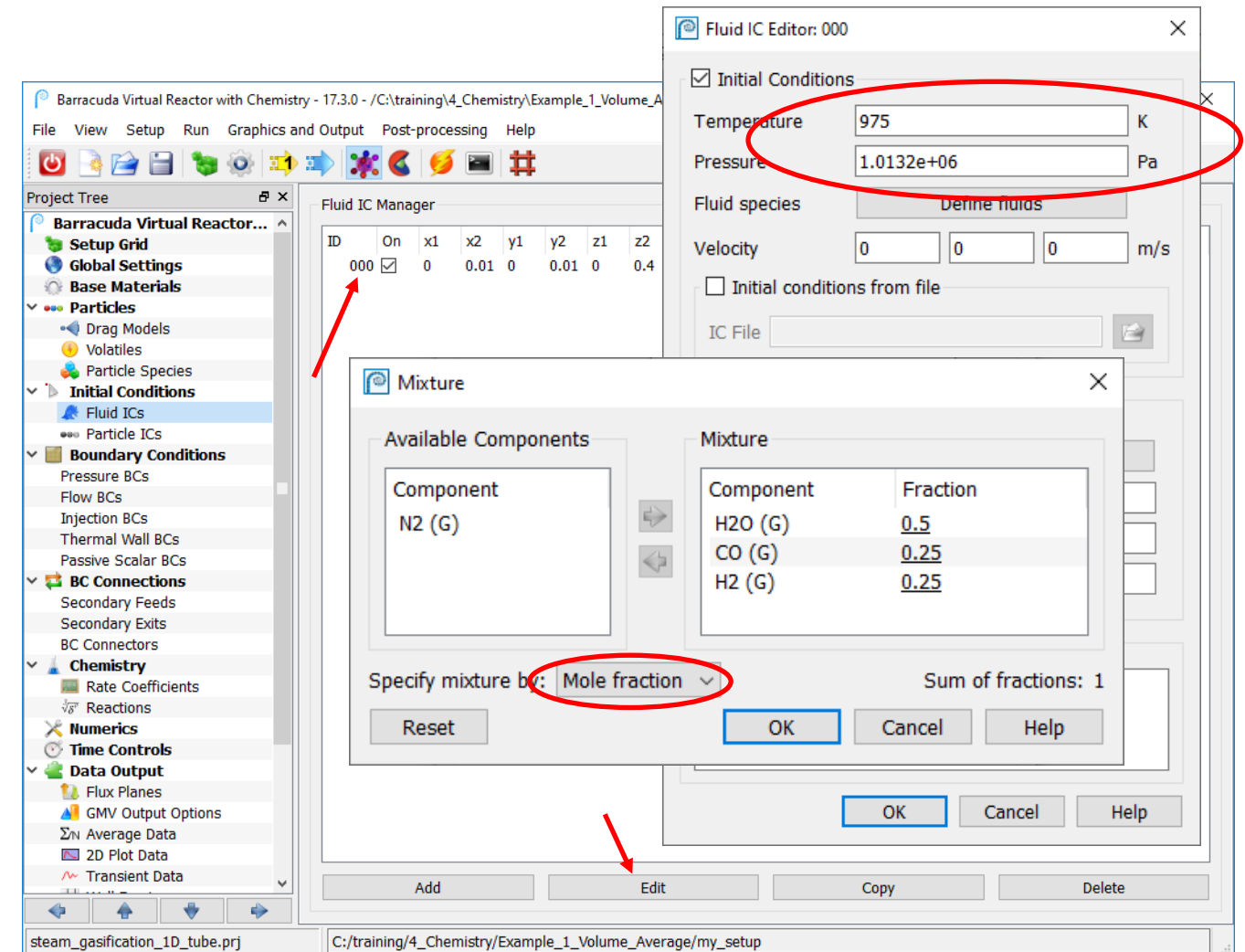
Use Wen-Yu drag model

Fluid Initial Conditions

For the fluid initial condition:

- 975 K
- 10 atm
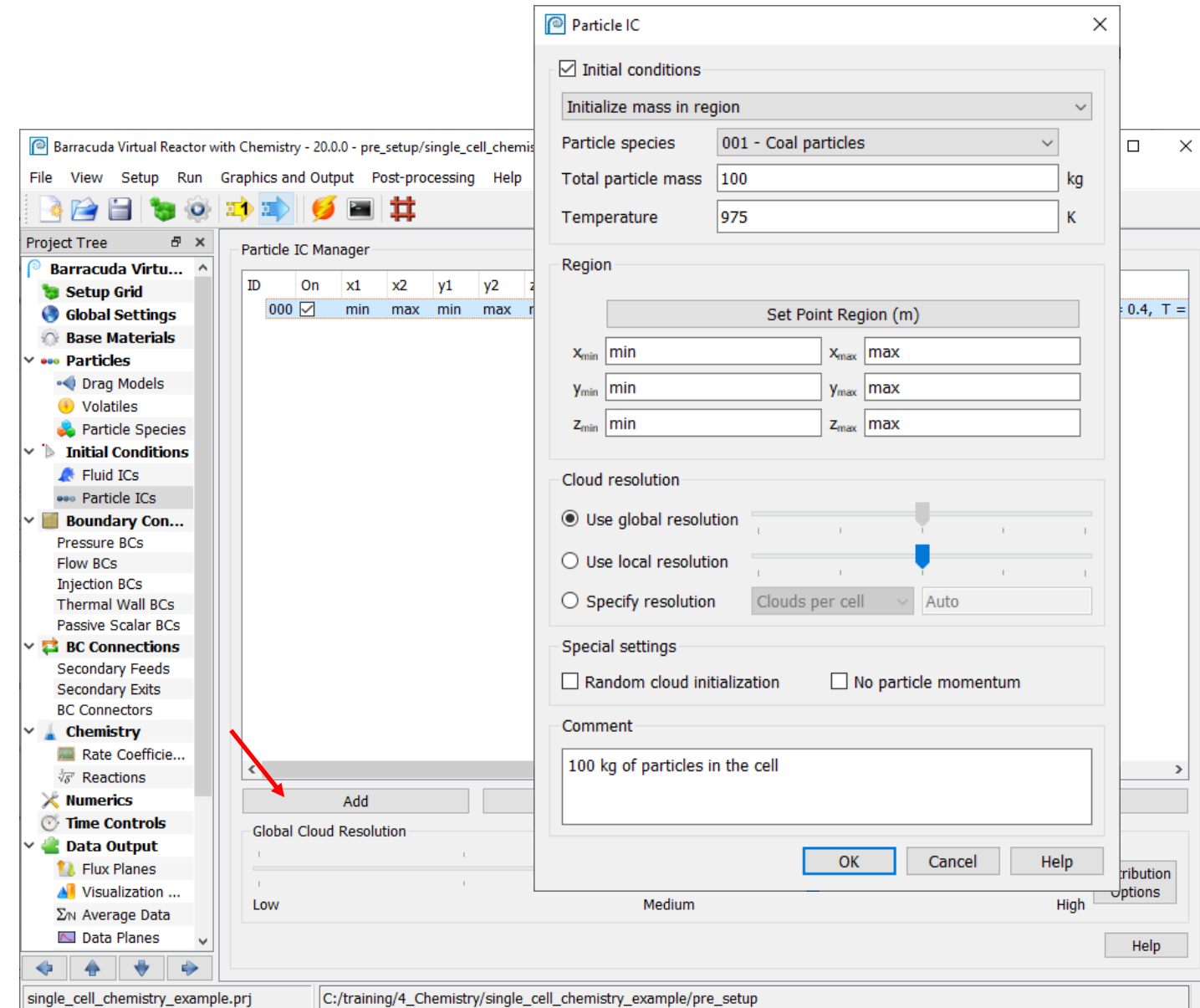- 0.50 H2O
- 0.25 H2
- 0.25 CO

The mixture should be specified by Mole fraction
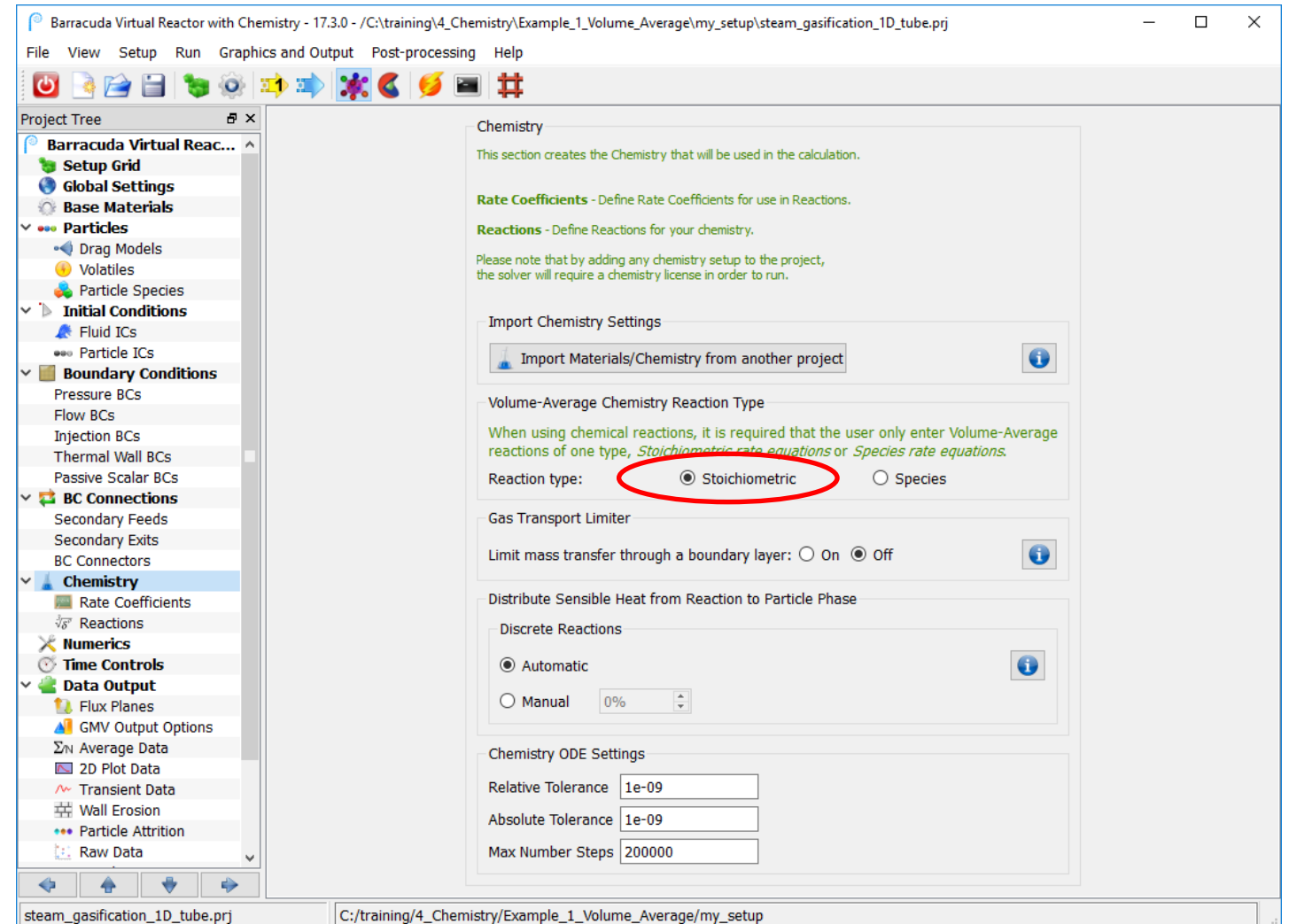
Particle Initial Conditions

Click Add

- Initialize mass in region
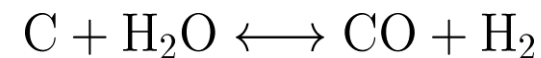- Initial mass of 100 kg of coal particles
- T = 975 K

Chemistry

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

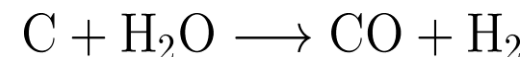**In this example, reactions will be entered in the Stoichiometric form**

Steam Gasification Reaction

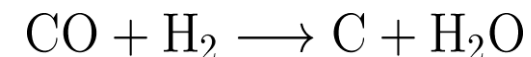Steam gasification is a reaction that converts solid carbon and water into carbon monoxide and hydrogen.

$$C + H_2O \longleftrightarrow CO + H_2$$

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

Forward Reaction	Reverse Reaction
$C + H_2O \longrightarrow CO + H_2$	$CO + H_2 \longrightarrow C + H_2O$
$\frac{d[CO]}{dt} = \left(219 \, \frac{m^3}{kg\,K\,s}\right) T \exp\left(\frac{-22645K}{T}\right) \rho_C \, [H_2O]$	$\frac{d[H_2O]}{dt} = \left(15.7 \, \frac{m^6}{kg\,mol\,K^2\,s}\right) T^2 \exp\left(\frac{-33190\,K}{T}\right) \rho_C \, [H_2] \, [CO]$

Note: If gas concentration units are mol/m³, the reaction rate units will be mol/m³/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:

$$C + H_2O \longrightarrow CO + H_2$$
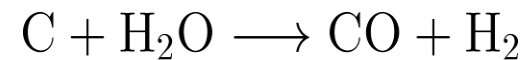
A Rate Coefficient will be used to specify the forward reaction rate.

$$r_{\text{forward}} = \frac{d[CO]}{dt} = \left(219 \, \frac{\text{m}^3}{\text{kg K s}}\right) T \exp\left(\frac{-22645\text{K}}{T}\right) \rho_C \, [H_2O]$$

In Barracuda:

> **Reaction rate expression:** $\quad r_{\text{forward}} = k_0 \, [H_2O]$
>
> **Reaction rate units:** mol/m³/s **Gas concentration units:** mol/m³
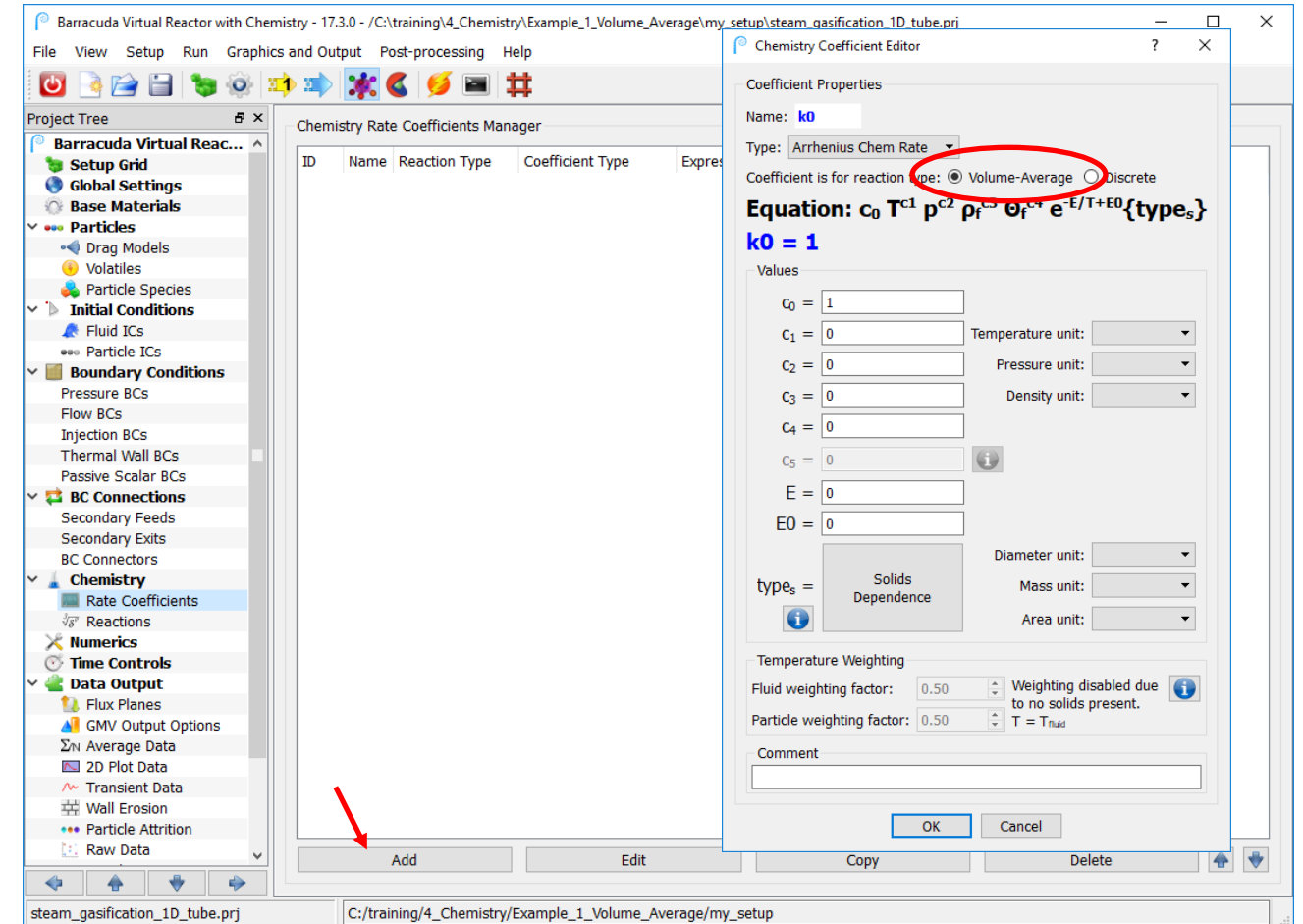>
> **Rate coefficient:** $\quad k_0 = 219T \exp\left(\frac{-22645}{T}\right) \rho_C$
>
> **Temperature units:** K **Solid Mass units:** kg/m³

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

Forward Rate Coefficients

Enter the equation for k0 as follows:

c_0 c_1 E   solids dependence

$$k0 = 219\ T^1\ \exp^{(-22645/T)} m_C$$

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

Chemistry Coefficient Editor

Coefficient Properties

Name: **k0**

Type: Arrhenius Chem Rate

Coefficient is for reaction type: ⦿ Volume-Average   ◯ Discrete

Equation: $c_0\ T^{c1}\ p^{c2}\ \rho_f{}^{c3}\ \Theta_f{}^{c4}\ e^{-E/T+E0}\{type_s\}$

$k0 = 219\ T^1\ e^{-22645/T}\ m_C{}^1$

Values

c_0 =	219	
c_1 =	1	Temperature unit: K
c_2 =	0	Pressure unit: Pa
c_3 =	0	Density unit: kg/m^3
c_4 =	0	
c_5 =	0	
E =	22645	
E0 =	0	

Diameter unit:

$type_s$ =   Solids Dependence   Mass unit: kg/m^3

Area unit:

Temperature Weighting

Fluid weighting factor: 0.50

Particle weighting factor: 0.50

Comment

OK   Cancel   Help

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
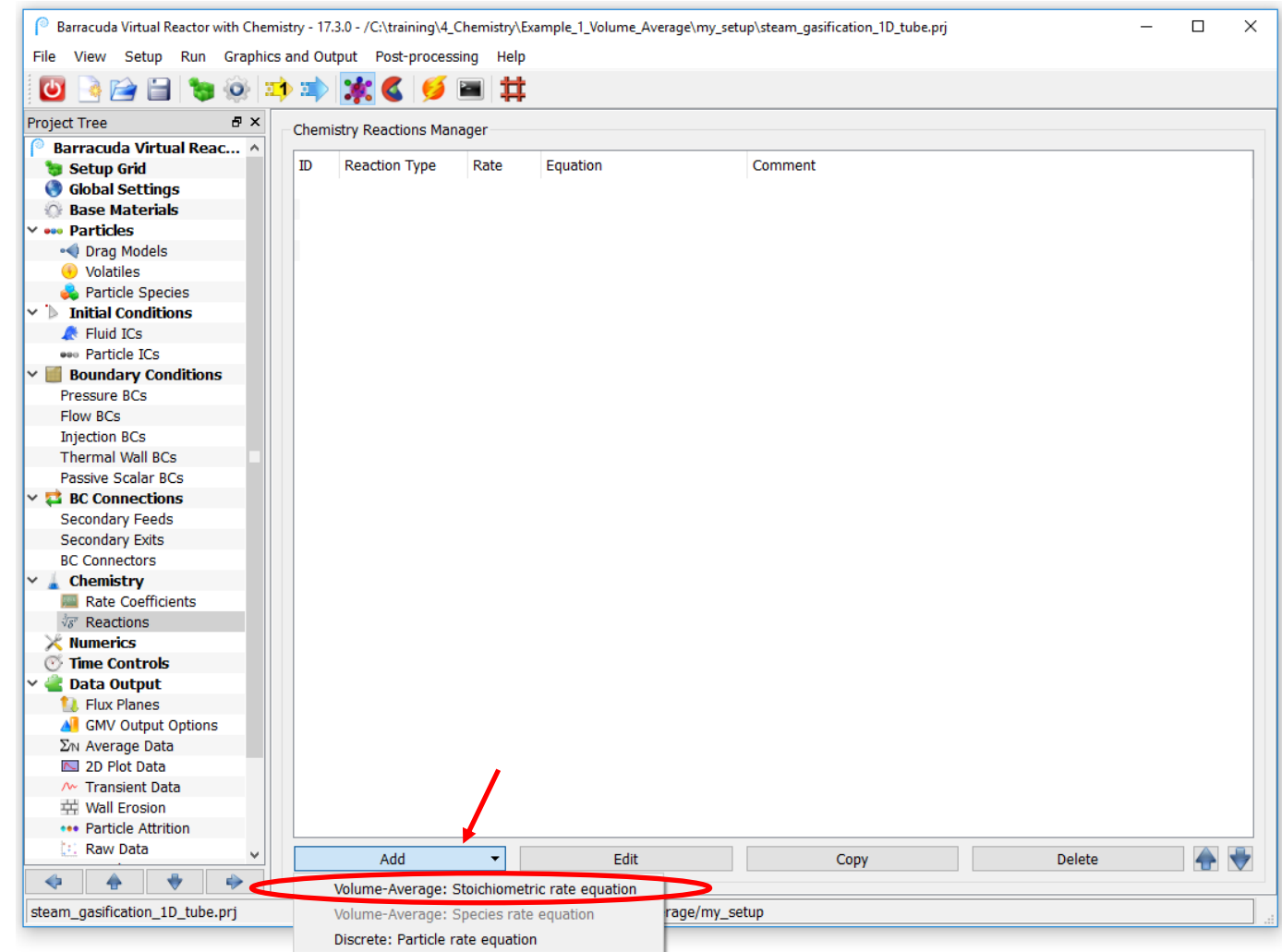- Click OK in the Chemistry Coefficient Editor window
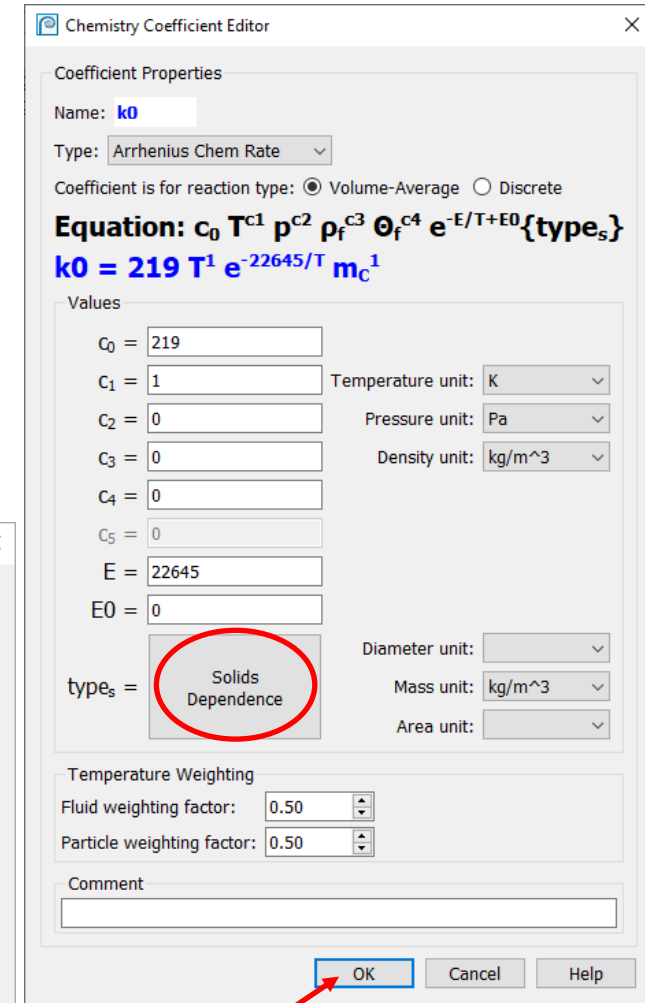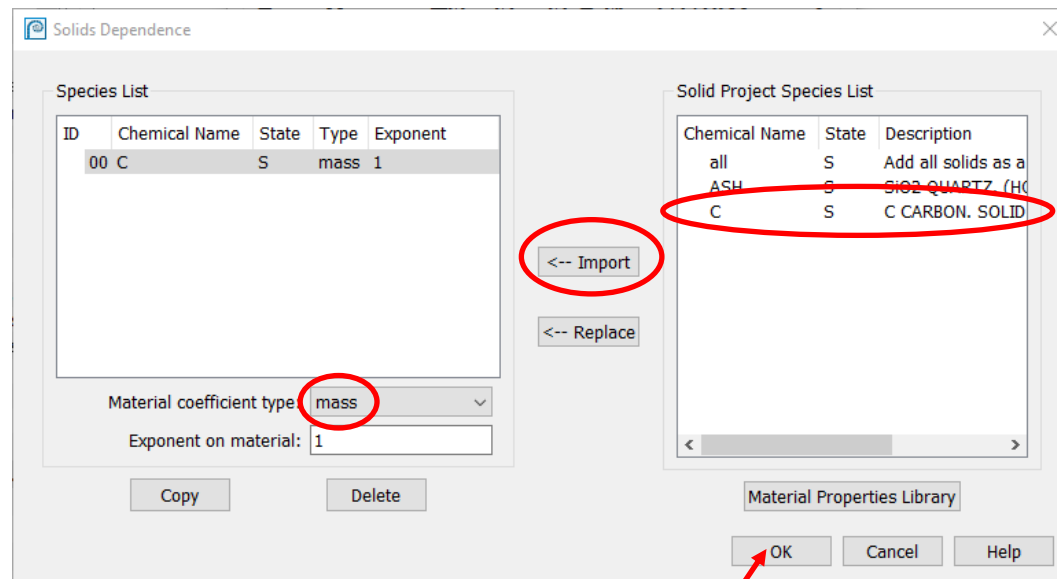
Creating the Forward Reaction

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

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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

Specifying the Forward Reaction Rate

To enter the rate equation for the reaction,

- Click Add Volume-Average Coefficient and select k0 ,

- Click Add Chemical and select H2O

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

Click OK

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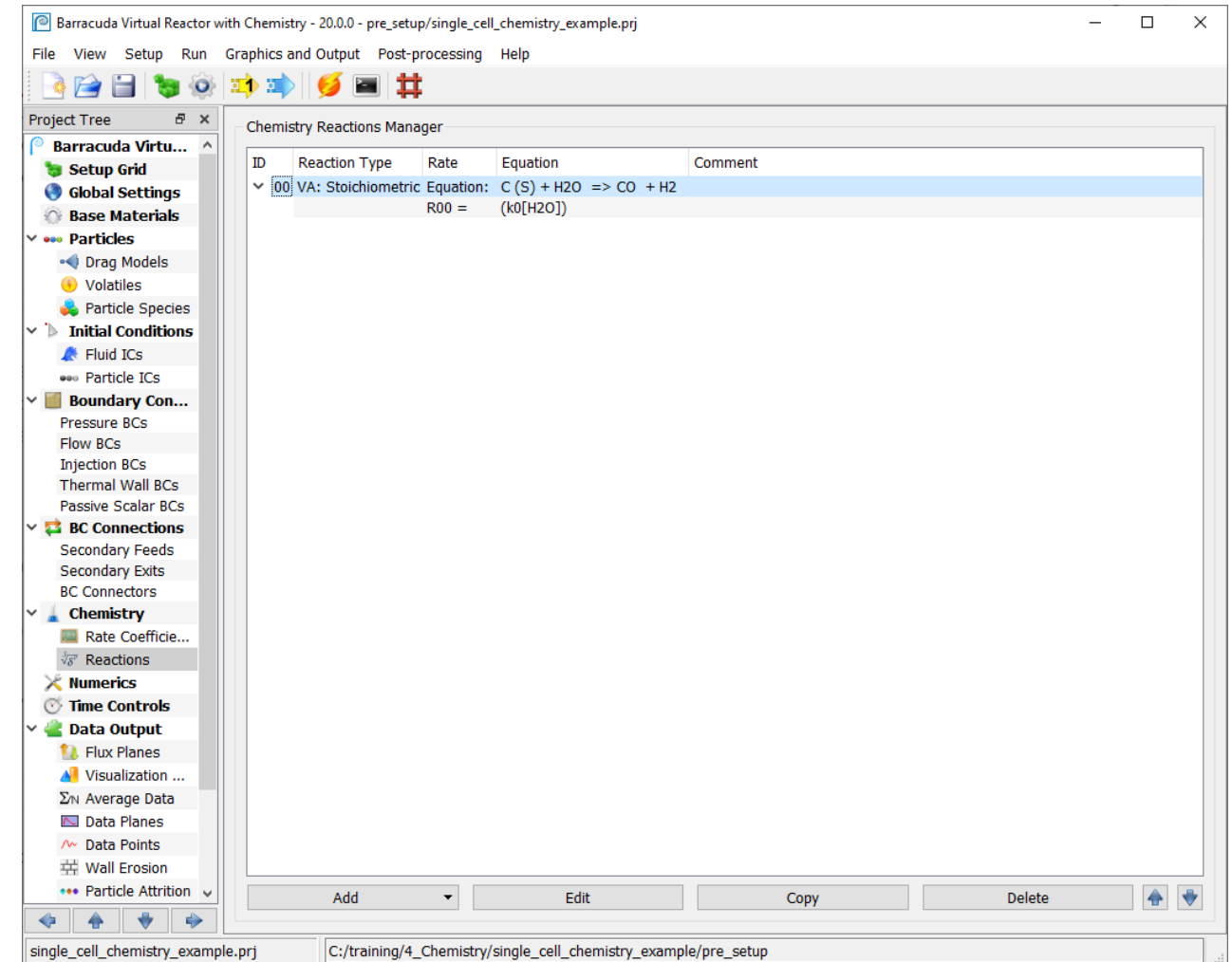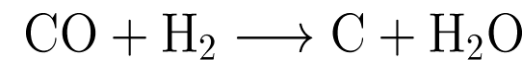
Forward Reaction Rate

The forward reaction rate equation is now complete:

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

Reverse Reaction Rate

We will specify the reverse reaction by the stoichiometric equation:

$$\mathrm{CO} + \mathrm{H}_2 \longrightarrow \mathrm{C} + \mathrm{H}_2\mathrm{O}$$

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

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

In Barracuda:

> **Reaction rate expression:** $\quad r_\mathrm{reverse} = k_1\,[\mathrm{H}_2]\,[\mathrm{CO}]$
>
> **Reaction rate units:** mol/m³/s   **Gas concentration units:** mol/m³
>
> **Rate coefficient:** $\quad k_1 = 15.7 T^2 \exp\left(\frac{-33190}{T} \right) \rho_\mathrm{C}$
>
> **Temperature units:** K   **Solid Mass units:** kg/m³

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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:

c_0 c_1 E   solids dependence

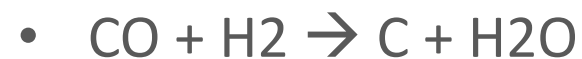$$k1 = 15.7 \; T^2 \; \exp^{(-33190/T)} m_C$$

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
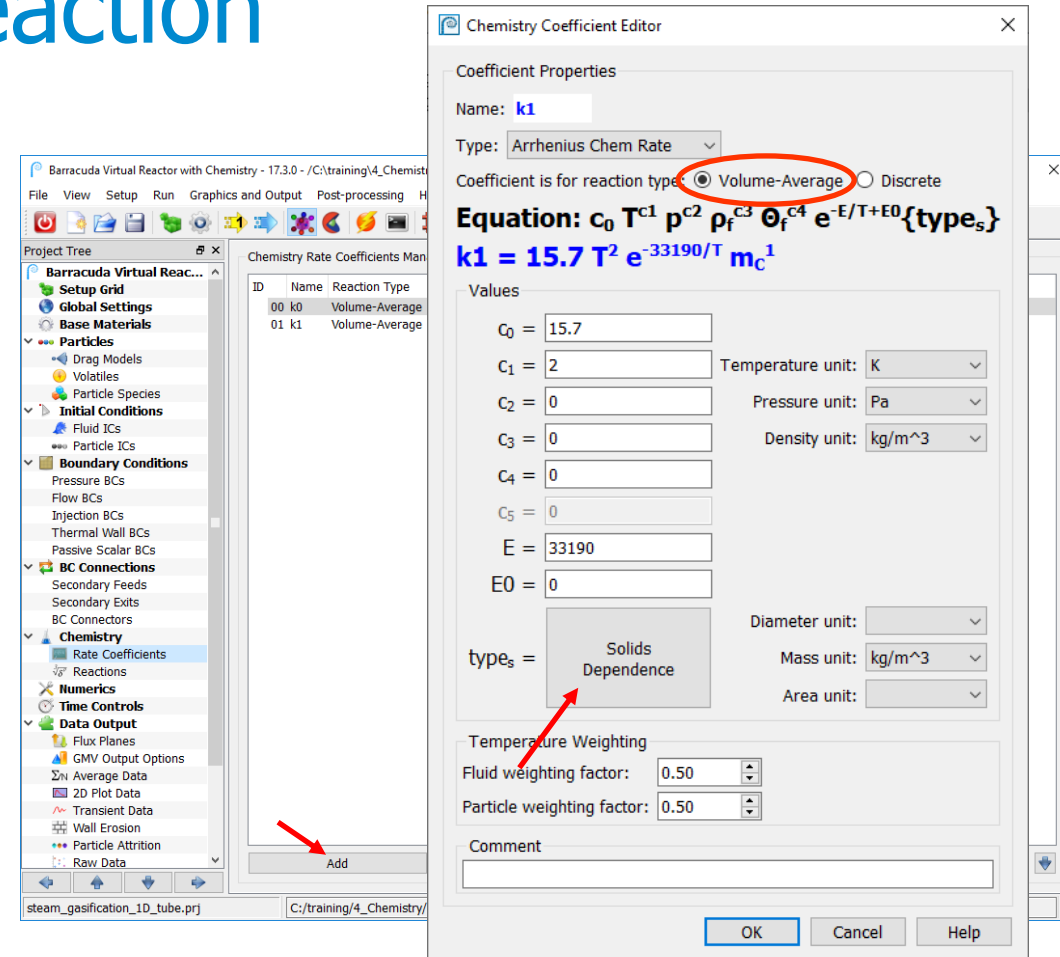
Chemical Equations: Reverse Reaction

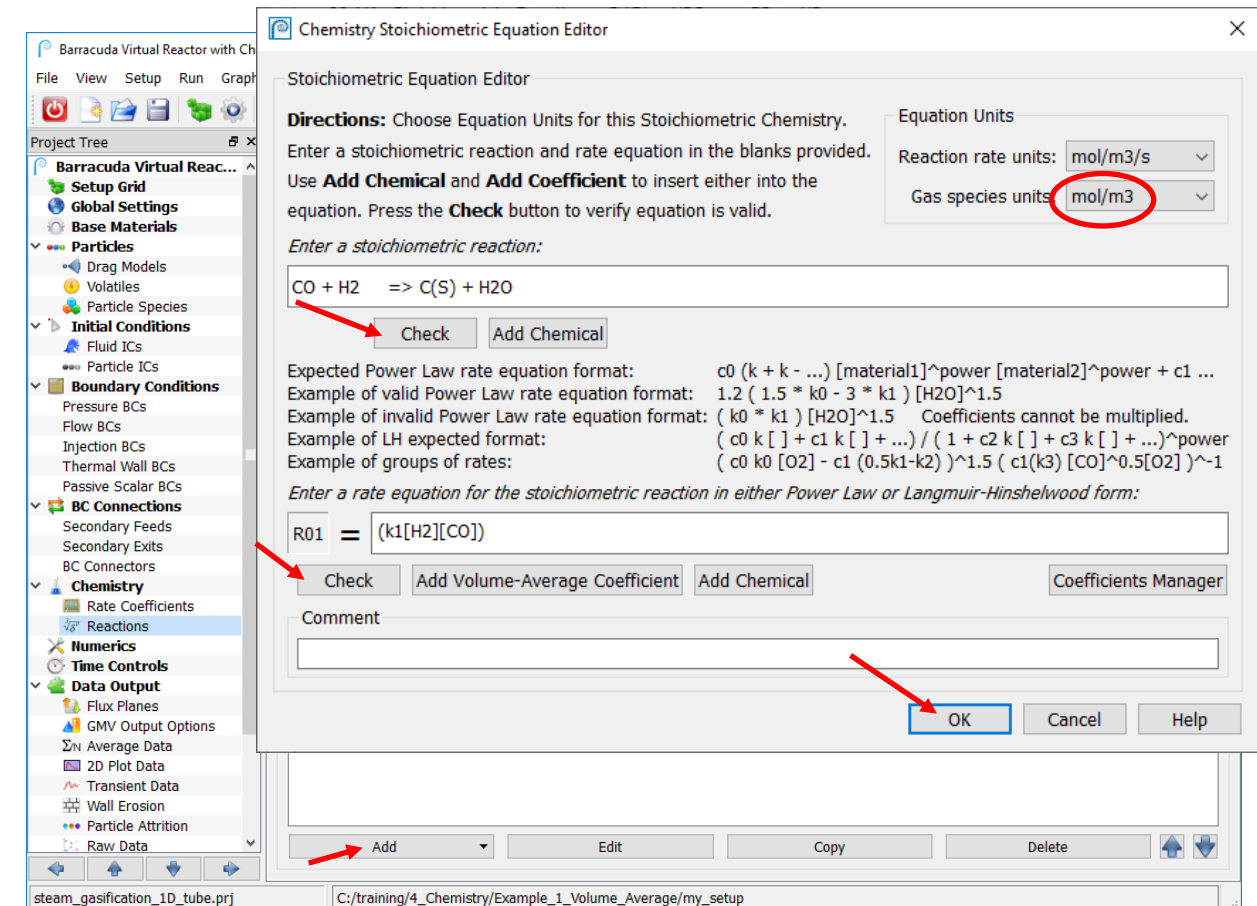**Define the stoichiometric equation for the reverse reaction:**

- CO + H2 $\rightarrow$ C + H2O

Enter the rate equation for the reverse reaction as follows:

- R01 = k1[H2][CO]

Set Gas species units to mol/m3

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

Click OK

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Reverse Reaction

The reverse reaction is now complete

Time Controls

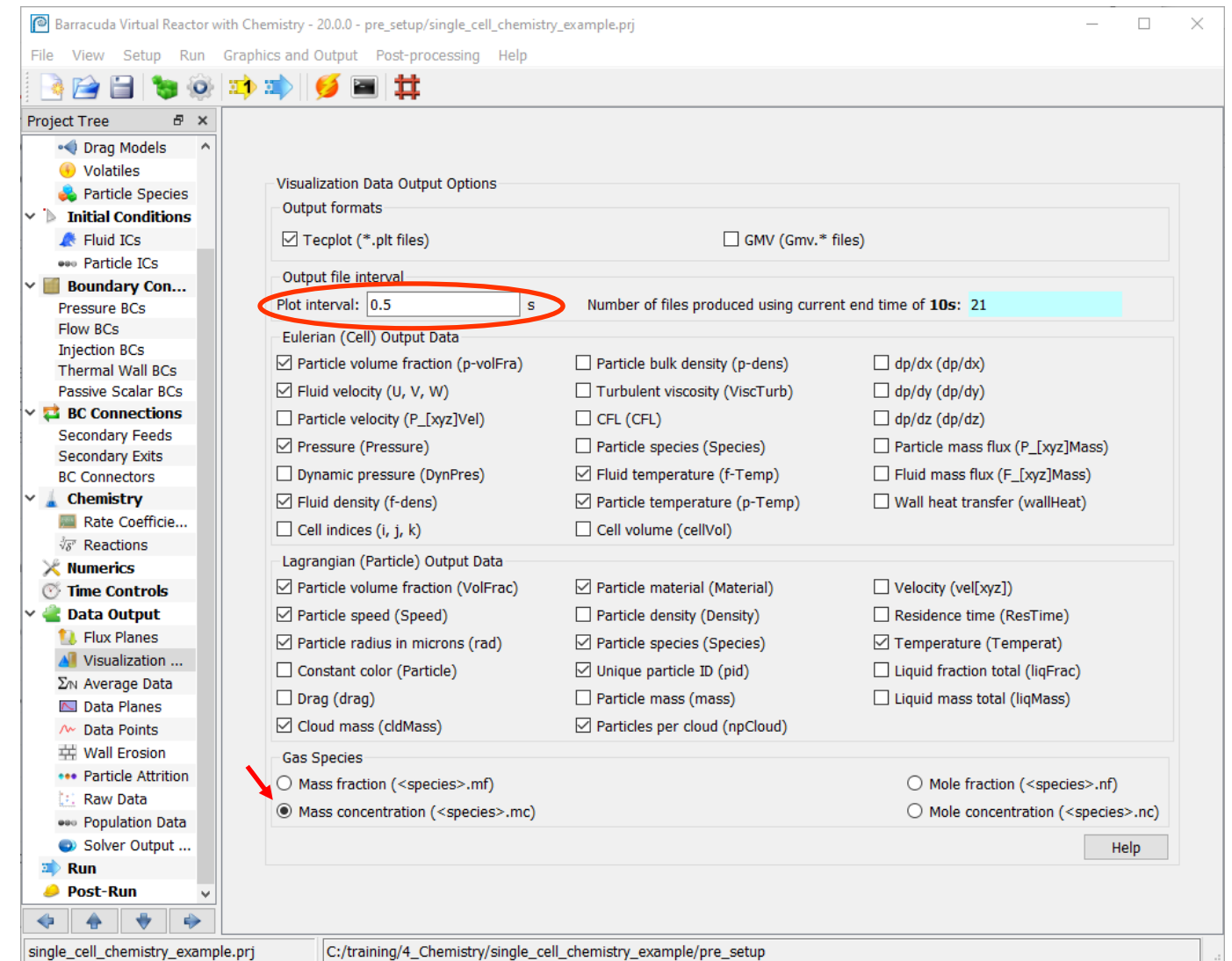**Enter Time step and End time as shown:**
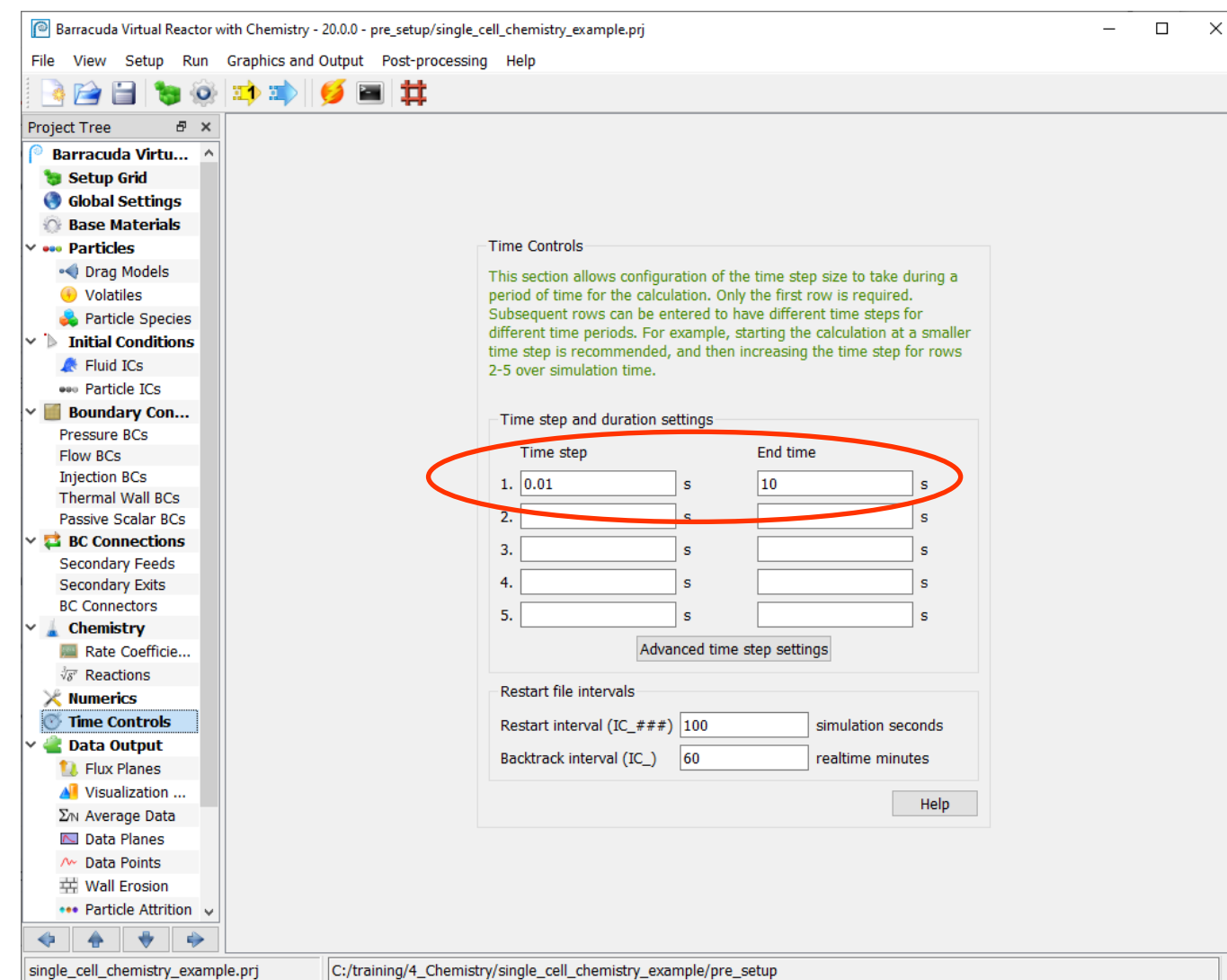
Visualization Output Options

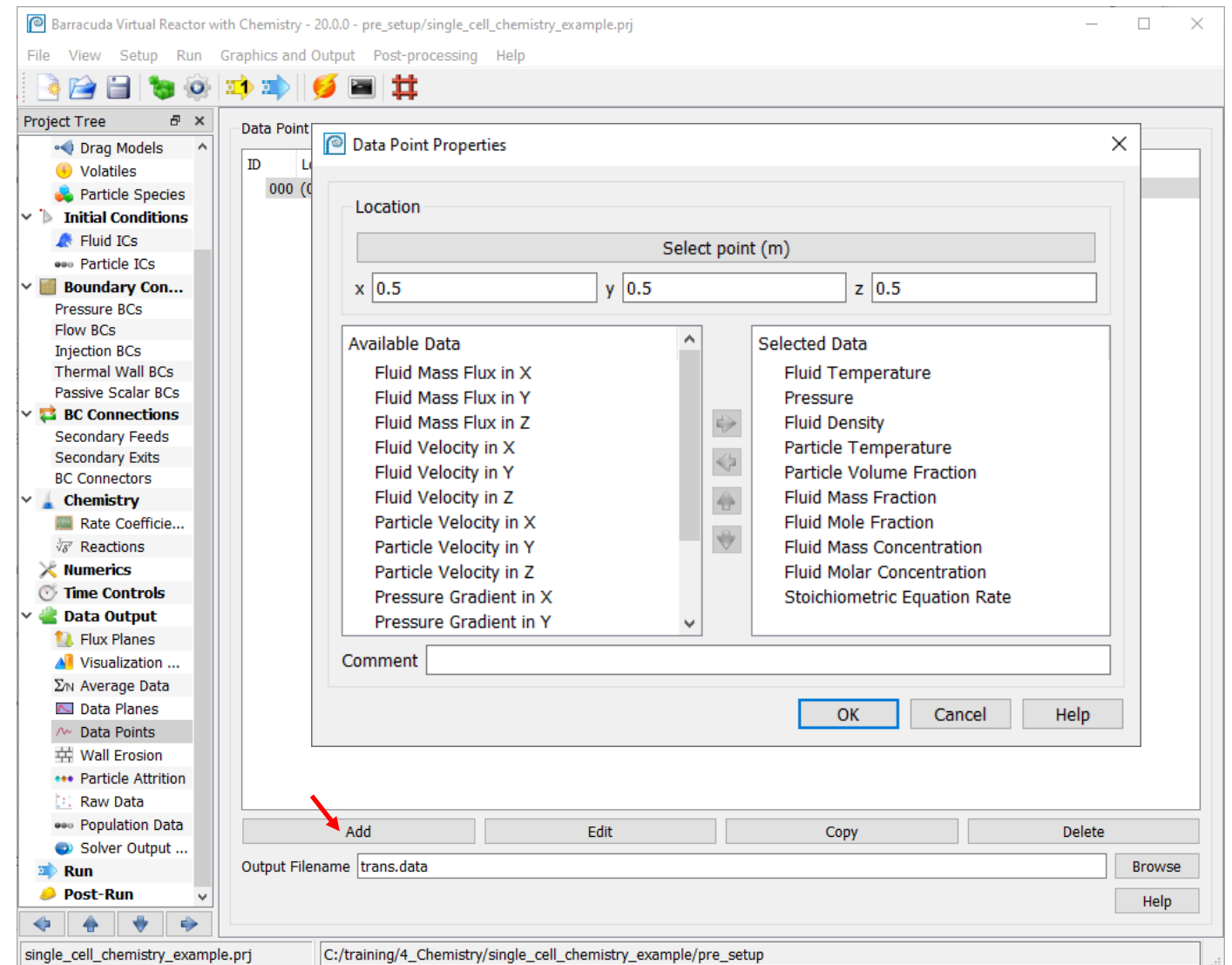**Enter a Plot interval of 0.5 s**

Choose the output variables shown on the right

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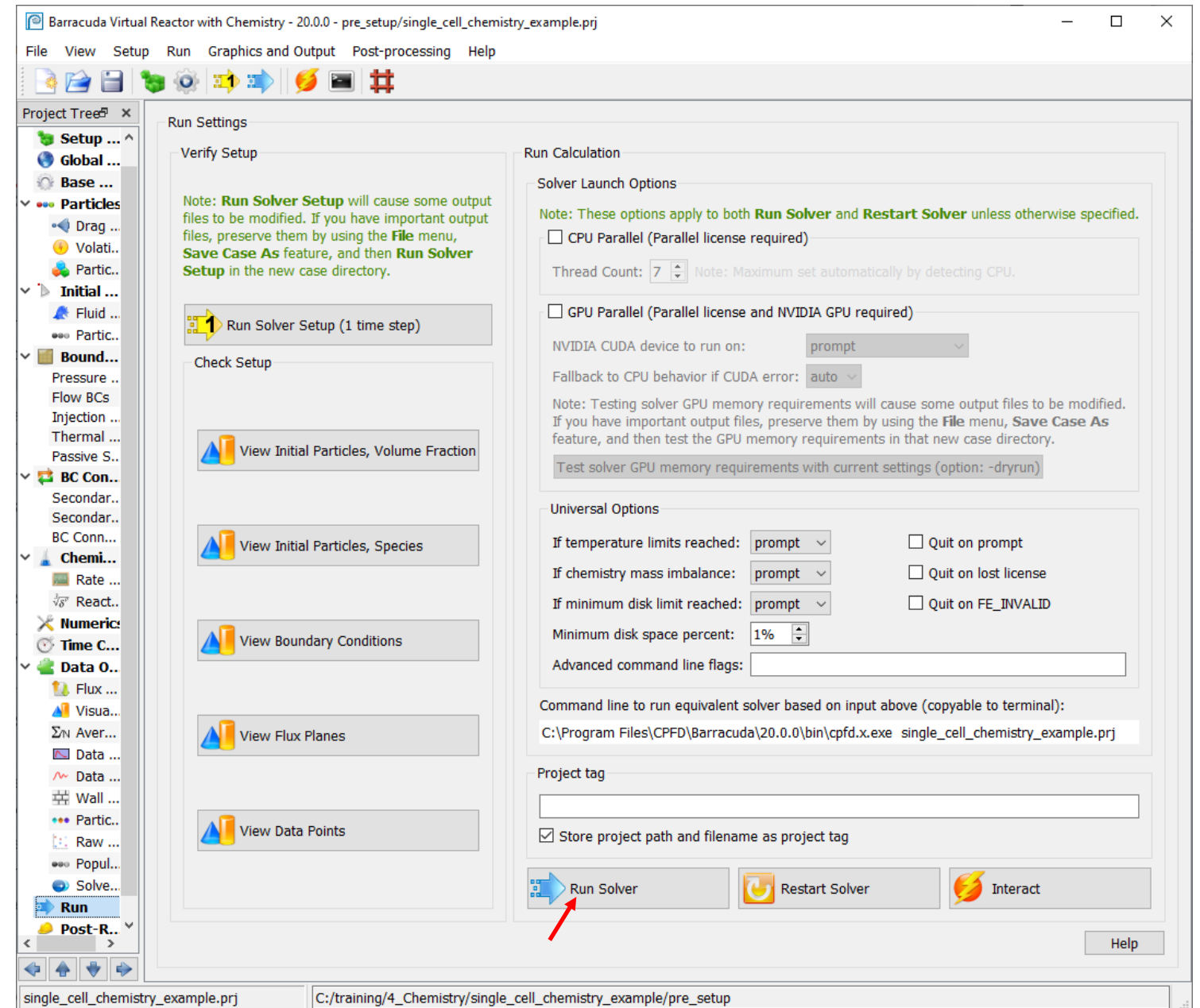
Data Points

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

Run the Simulation

Run the simulation

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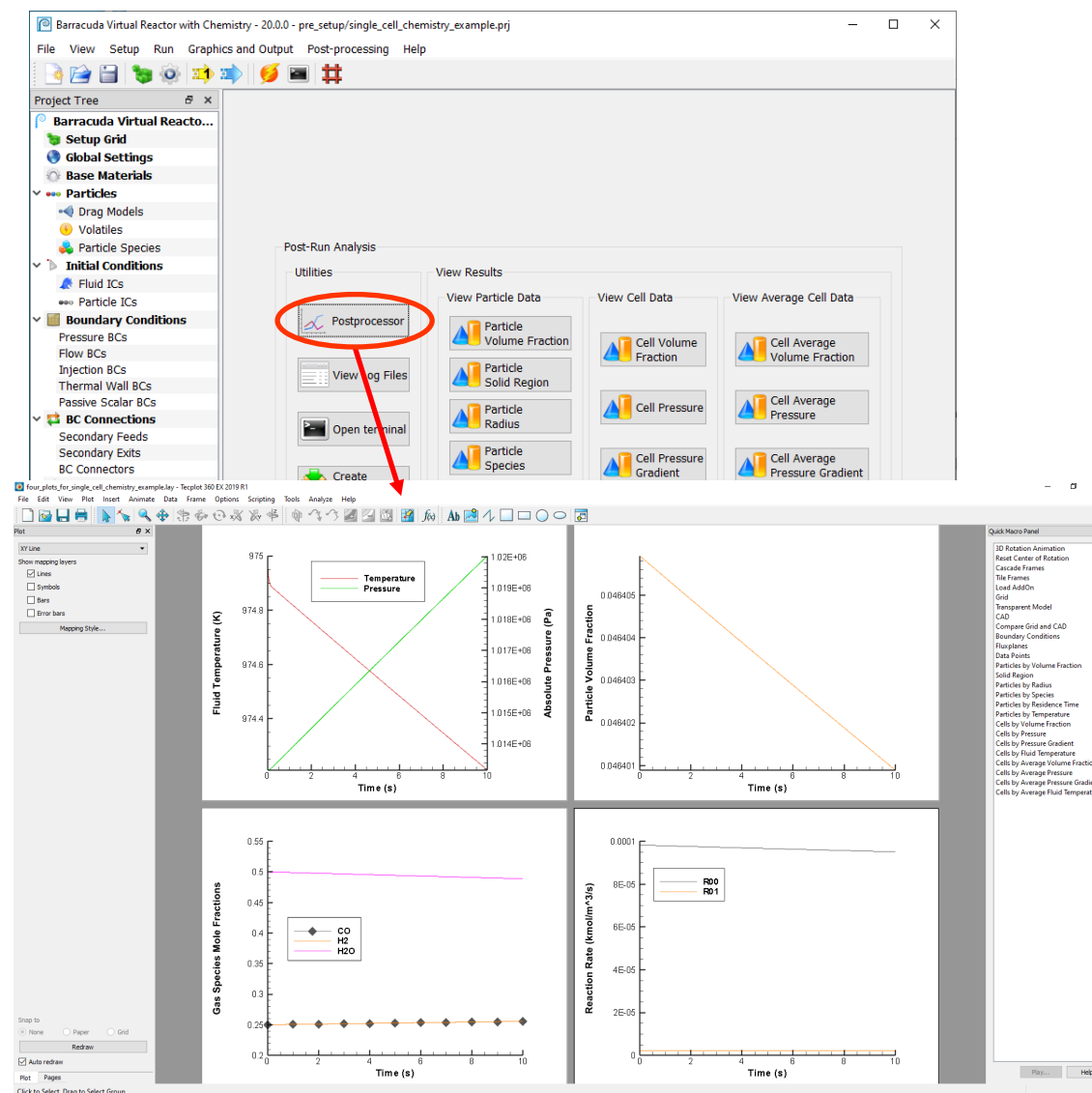
Create the following 4 plots (see next slide for larger version of final result):

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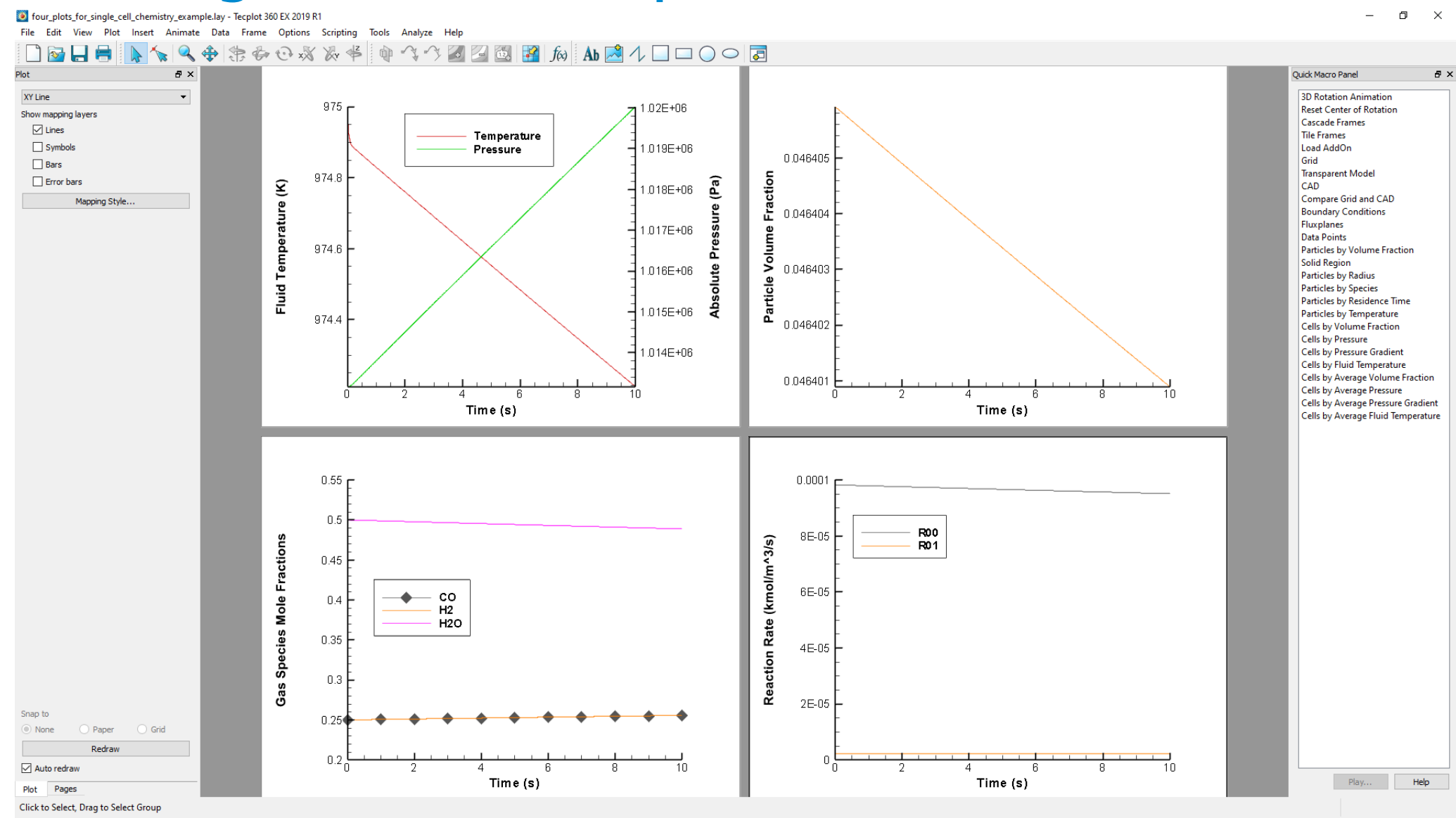- Plot 3: mole fractions of gas species vs time
- Plot 4: reaction rates vs time

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

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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	**Initial Conditions in Simulation**		
2	Volume of cell	1	m^3
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^3
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^3
13	Molar concentration of H2	3.1246E+01	mol/m^3
14	Molar concentration of CO	3.1246E+01	mol/m^3
15			
16	**Hand-calculated Reaction Rates**		
17	Forward reaction, R00	9.8344E-05	kmol/m^3/s
18	Reverse reaction, R01	2.1573E-06	kmol/m^3/s

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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.

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