

Single-Cell Chemistry: Setup and Analysis

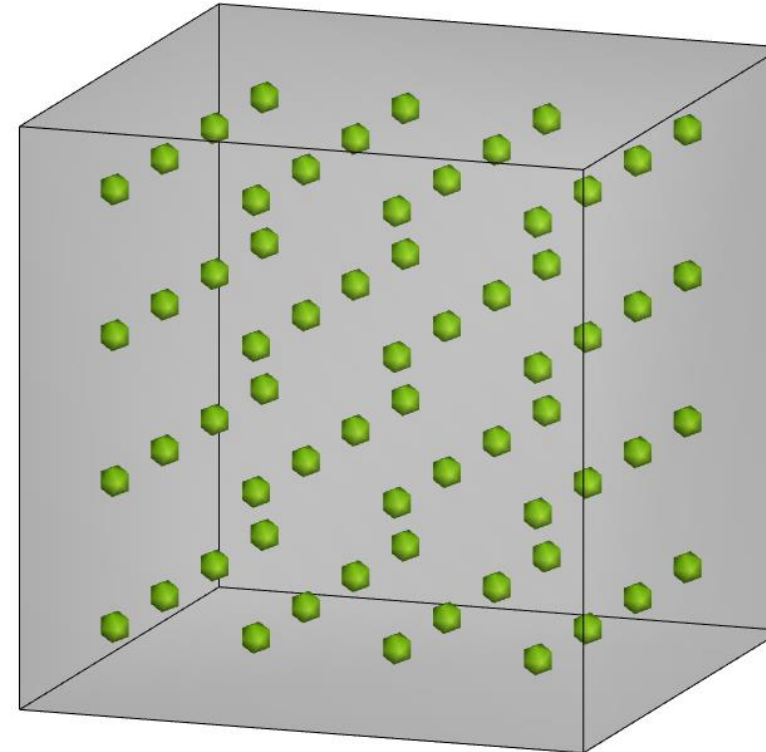
CPFD Software

www.cdfd-software.com

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



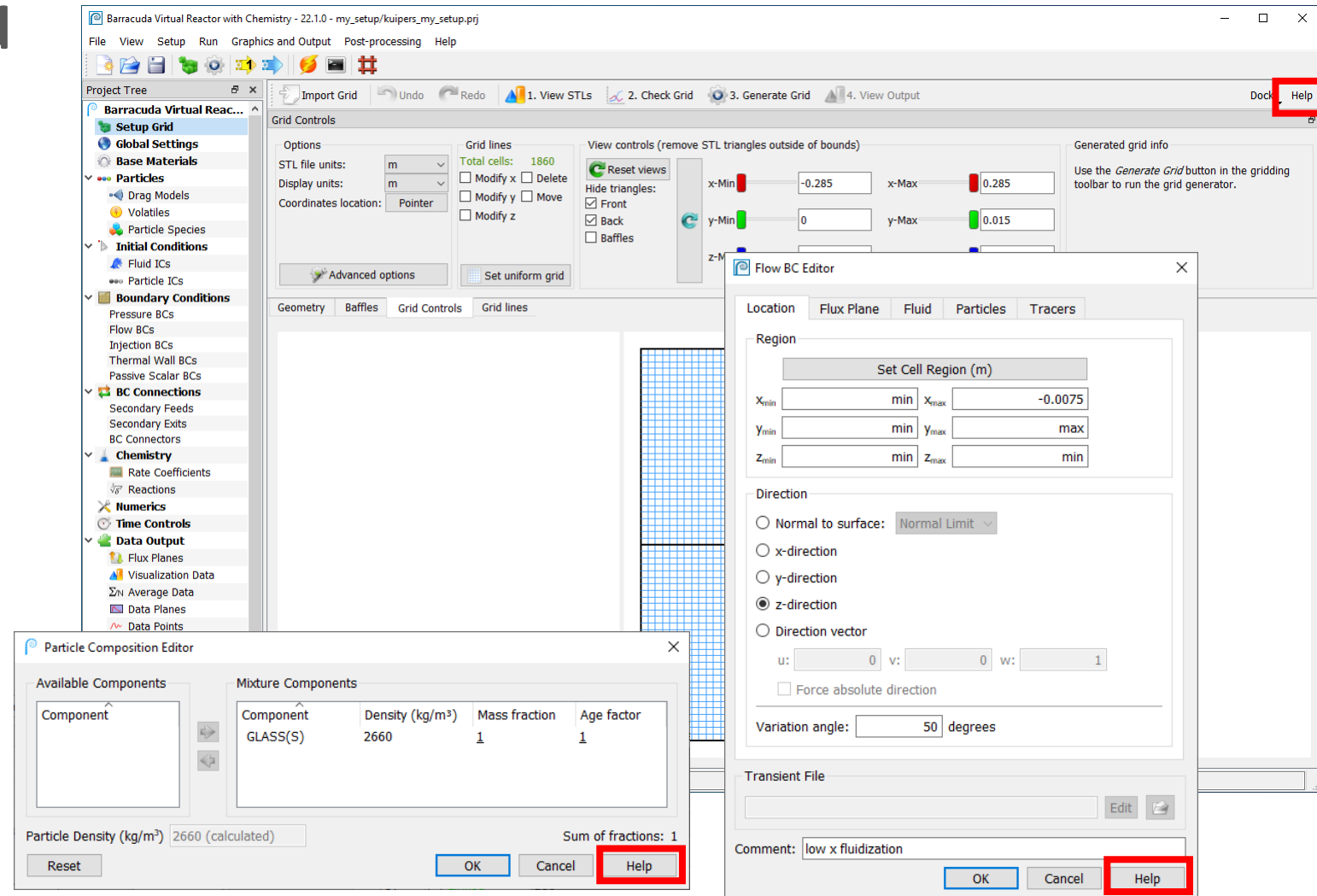
Model will be set up with volume average chemistry

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

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.



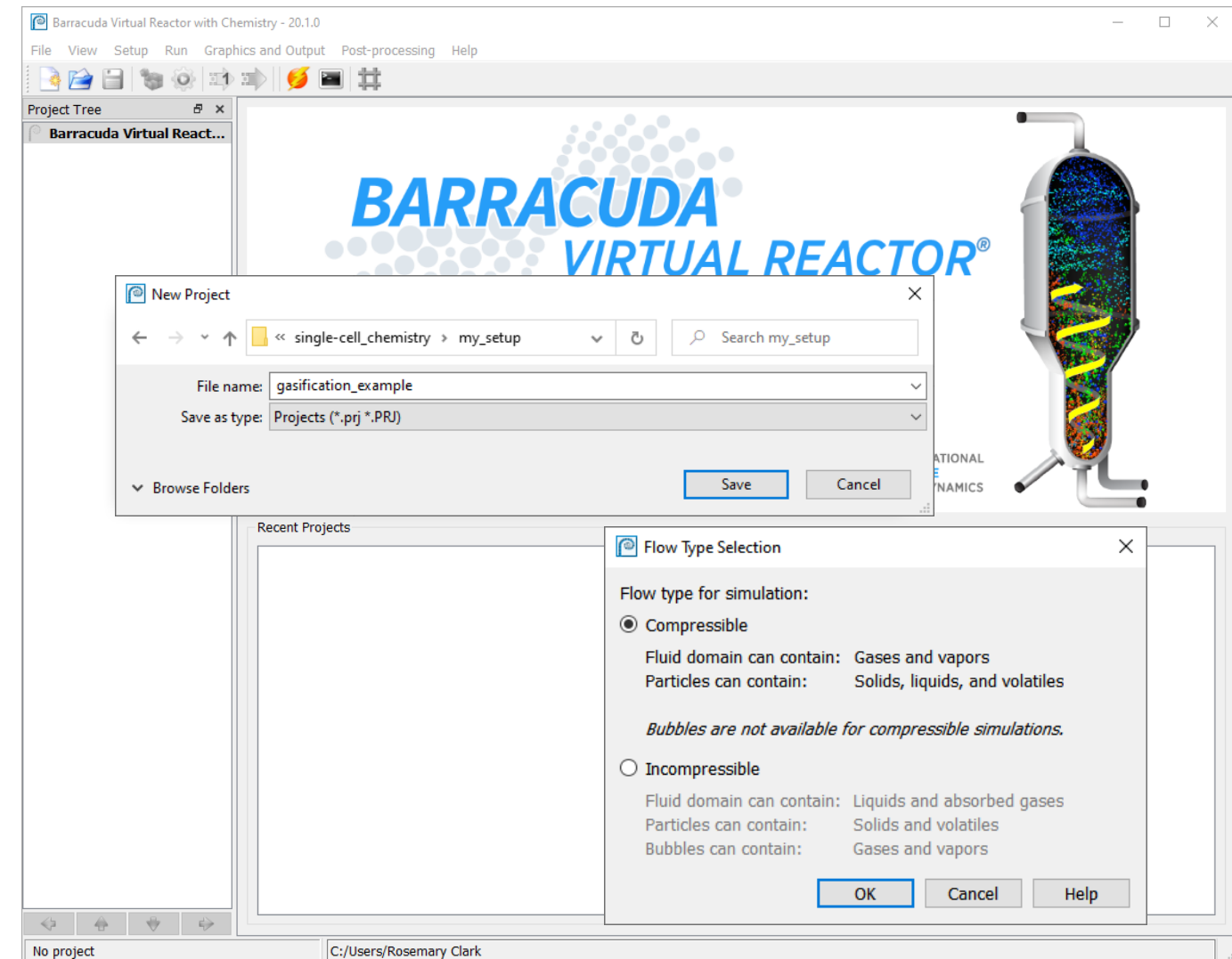
Volume Average Project File

Create a new project file in the directory:

- Linux:
~/single-cell_chemistry/my_setup
- Windows:
C:\single-cell_chemistry\my_setup

Enter an appropriate project name

Select Compressible as the Flow Type and click OK



Generate the Grid

In the Geometry tab, click Add Geometry

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

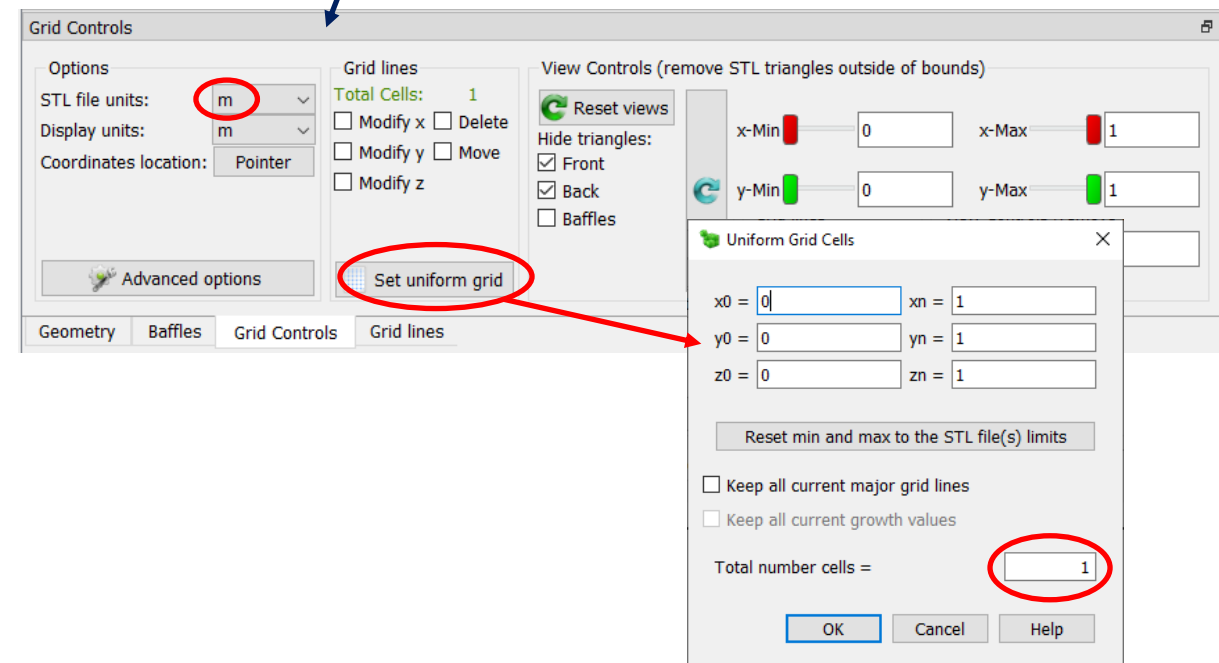
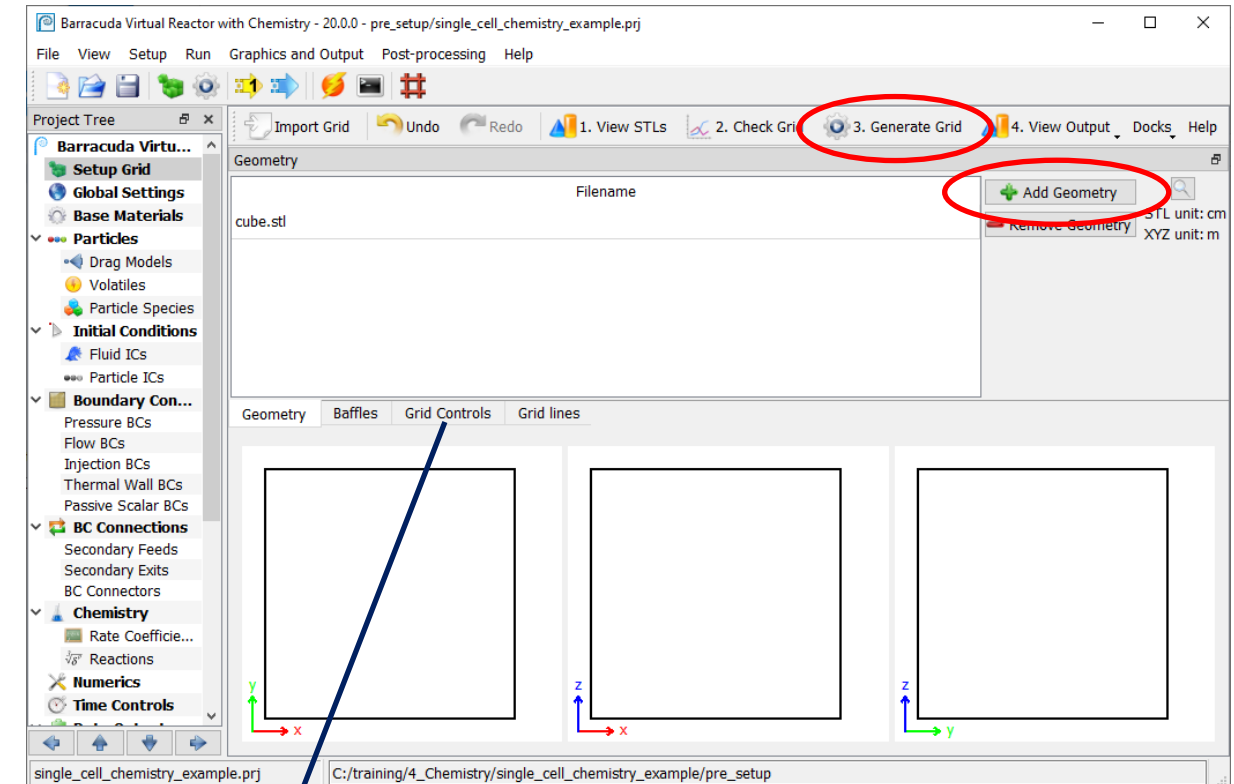
- Each side-length = 1 m

In the Grid Controls tab:

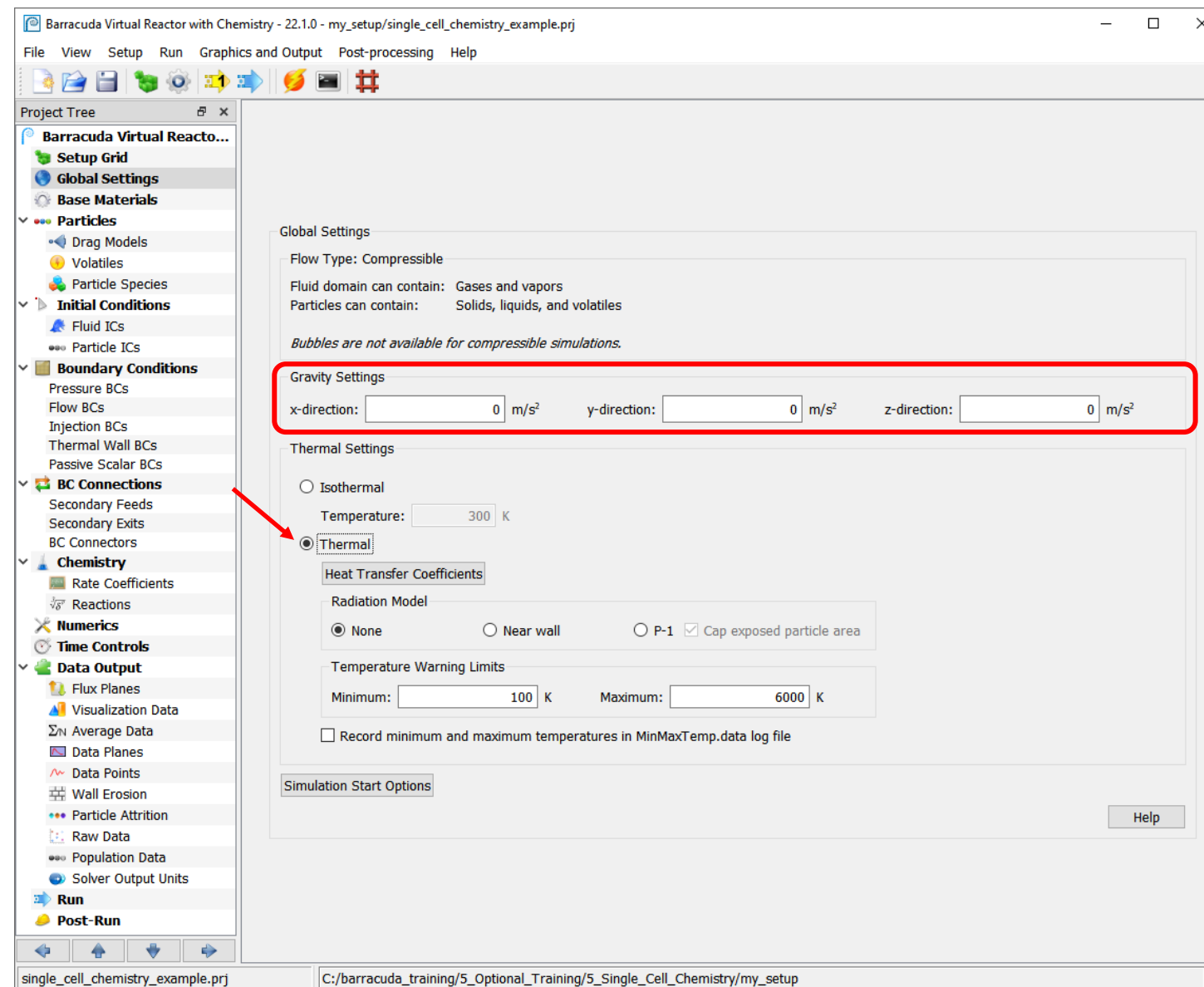
- Set STL units to “m”
- Click **Set uniform grid**
- Set **Total number of cells** to “1”

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

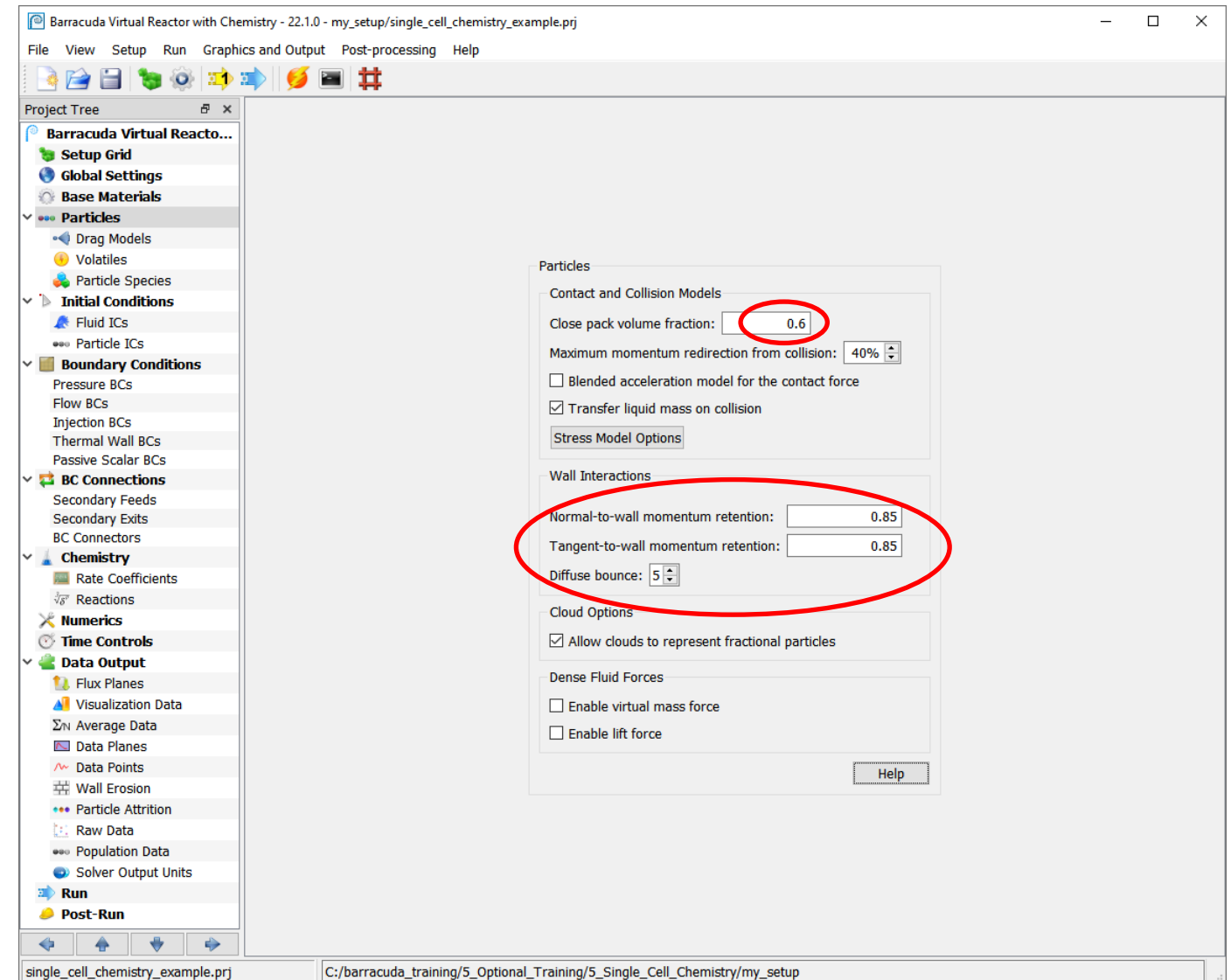
The screenshot shows the Barracuda Virtual Reactor software interface. The Project Tree on the left lists various setup options, with 'Base Materials' highlighted. The Project Material List in the center shows a table of materials, with 'Ash', 'C', 'CO', 'H2', and 'H2O' highlighted by a red circle. The Material Properties Library on the right shows a list of materials, with 'N2' selected. The 'Import' button is visible between the two panes.

Material Name	Phase(s)	Description
Ash	S	SiO2 QUARTZ. (HQZ) COMMON SAND
C	S	C CARBON. SOLID GRAPHITE REF ELE
CO	G	CO CARBON MONOXIDE
H2	G	H2 HYDROGEN. REF ELEMENT
H2O	G	H2O STEAM

Material name	Phase(s)	Description
N2	G	N2 NITROGEN. REF ELEMENT
N2D2	G	N2D2 -CIS
N2F2	G	N2F2 ISOMERS CIS AND TRA
N2F4	G	N2F4 EQUILIBRIUM MIXTURE
N2H	G	N2H (NNH)
N2H2	G	N2H2
N2H3	G	N2H3 HYDRAZINE RADICAL
N2H4	G	N2H4 HYDRAZINE
N2H4O3	L	NH4NO3 AMMONIUM NITRAT
N2H4O3_1	S	NH4NO3 SOLID AMMONIUM
N2H4O3_2	S	NH4NO3 SOLID AMMONIUM
N2H4O3_3	S	NH4NO3 SOLID AMMONIUM
N2H4O3_4	S	NH4NO3 SOLID AMMONIUM
N2H4O3_5	S	NH4NO3 SOLID AMMONIUM
N2O	L	N2O LIQUID NITROUS OXIDE
N2O	G	N2O NITROUS OXIDE. NNO
N2O_plus	G	N2O+ ION
N2O3	L	N2O3 LIQUID NITROGEN TRI
N2O3	G	N2O3 NITROGEN TRIOXIDE
N2O4	G	N2O4 STATW=1
N2O5	G	N2O5 O2N-O-NO2

Particles

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



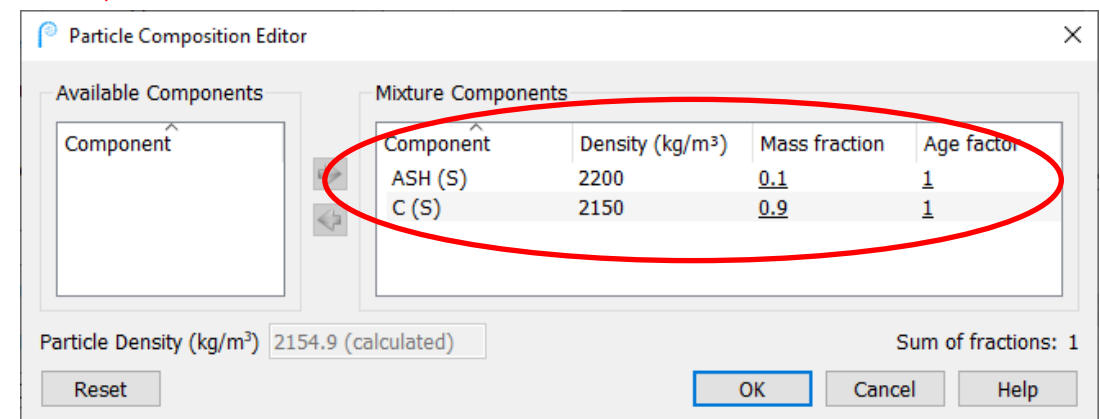
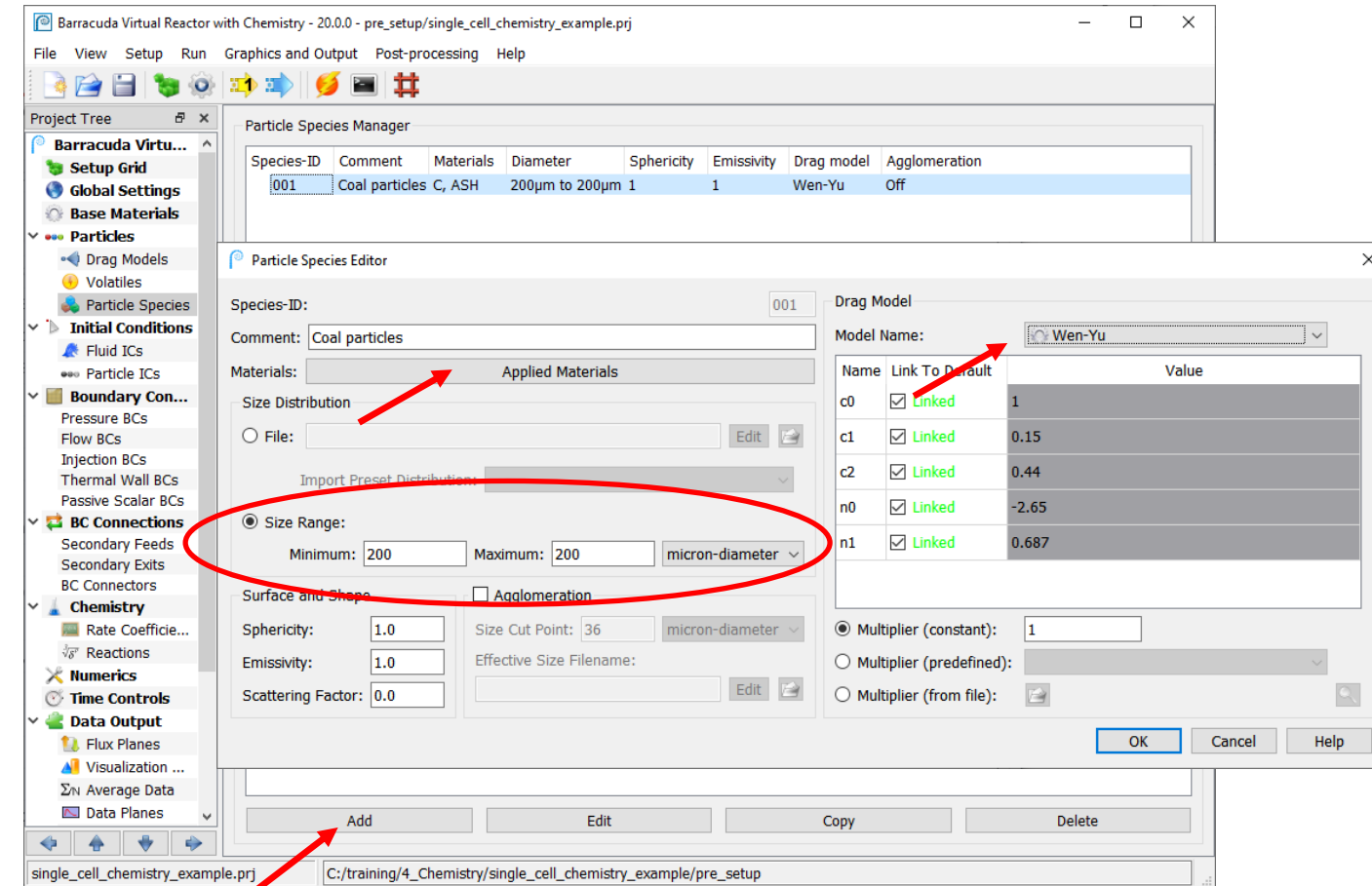
Particle Species

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.

Use Wen-Yu drag model

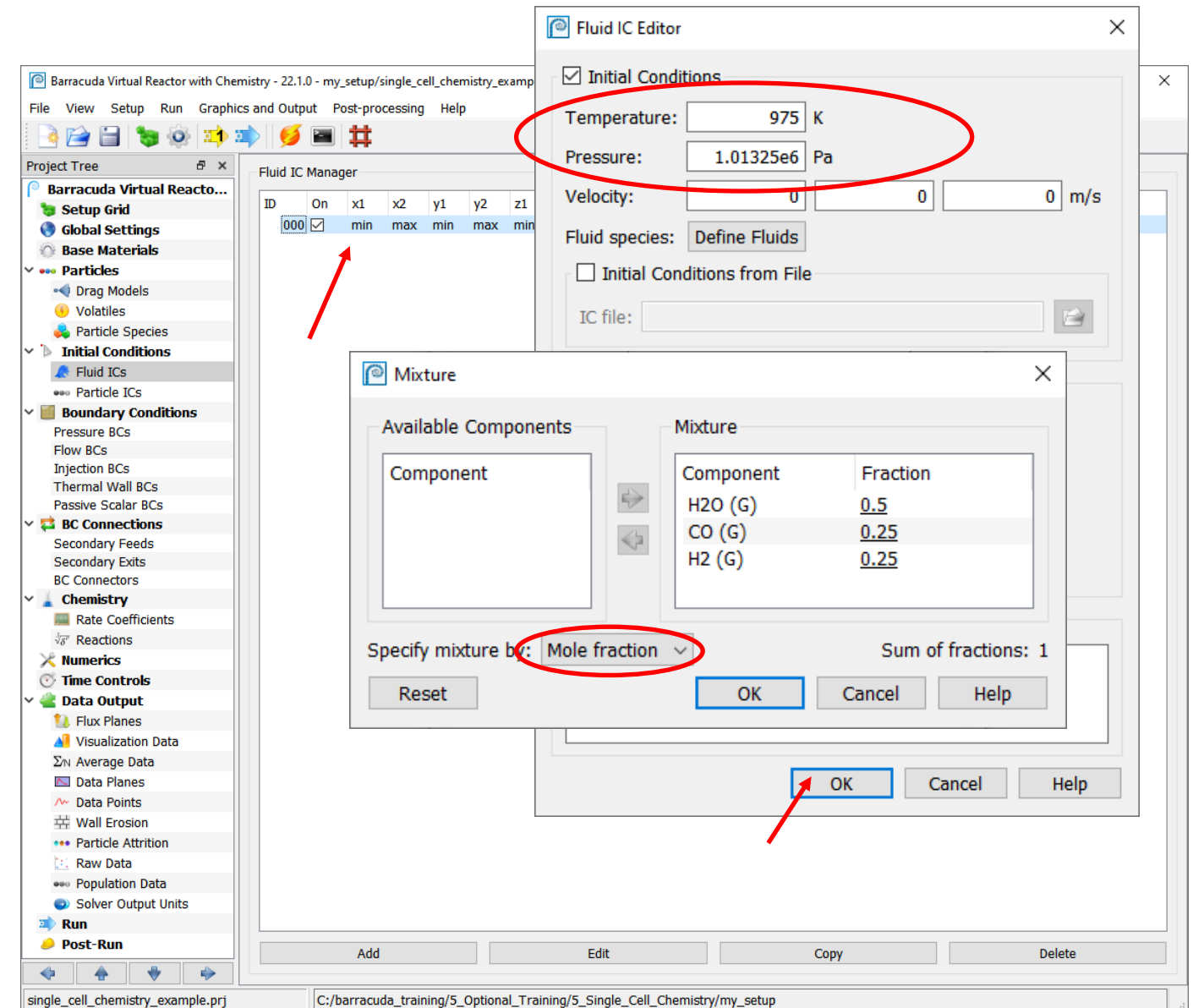


Fluid Initial Conditions

For the fluid initial condition:

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

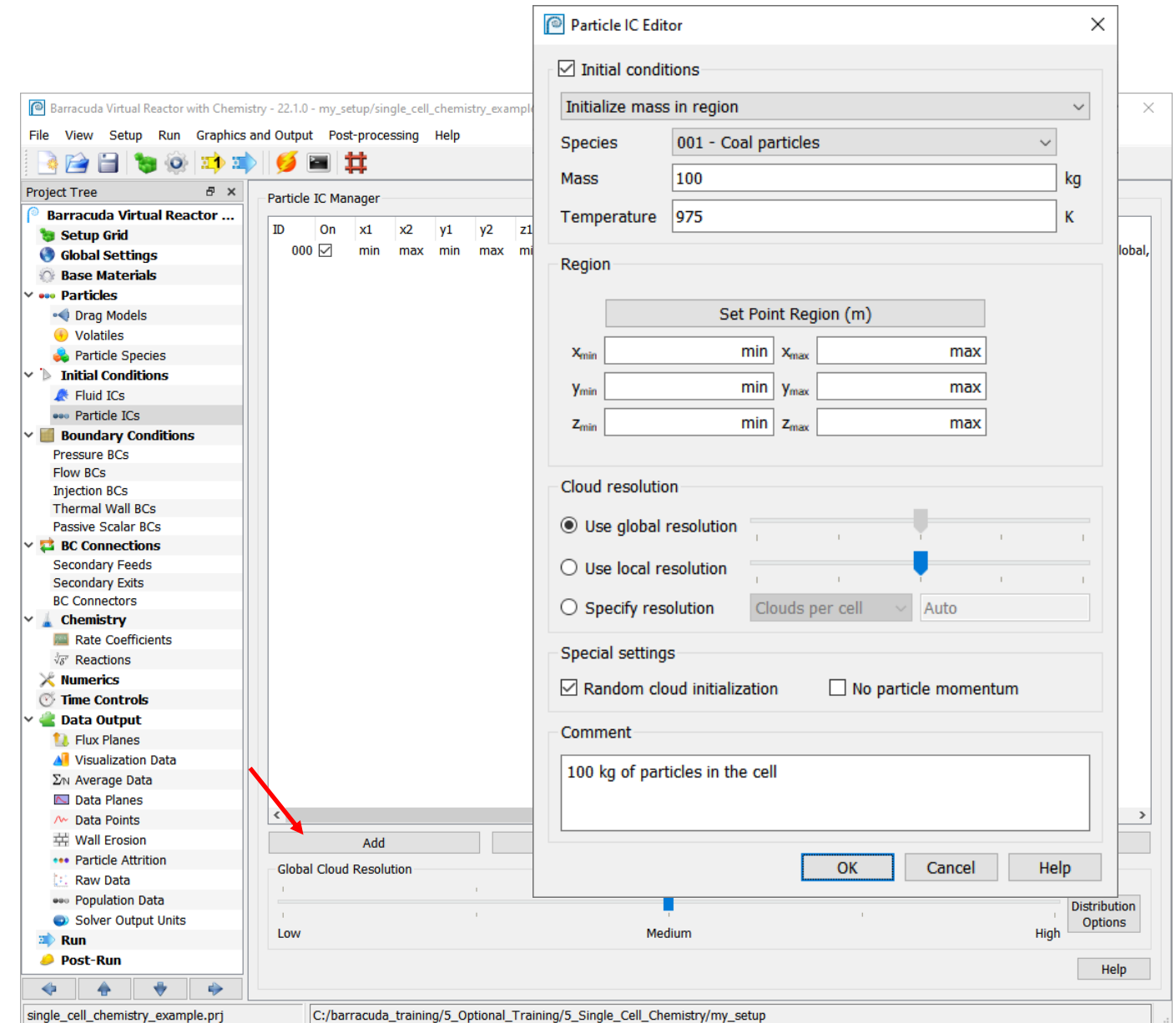
The mixture should be specified by Mole fraction



Particle Initial Conditions

Click Add

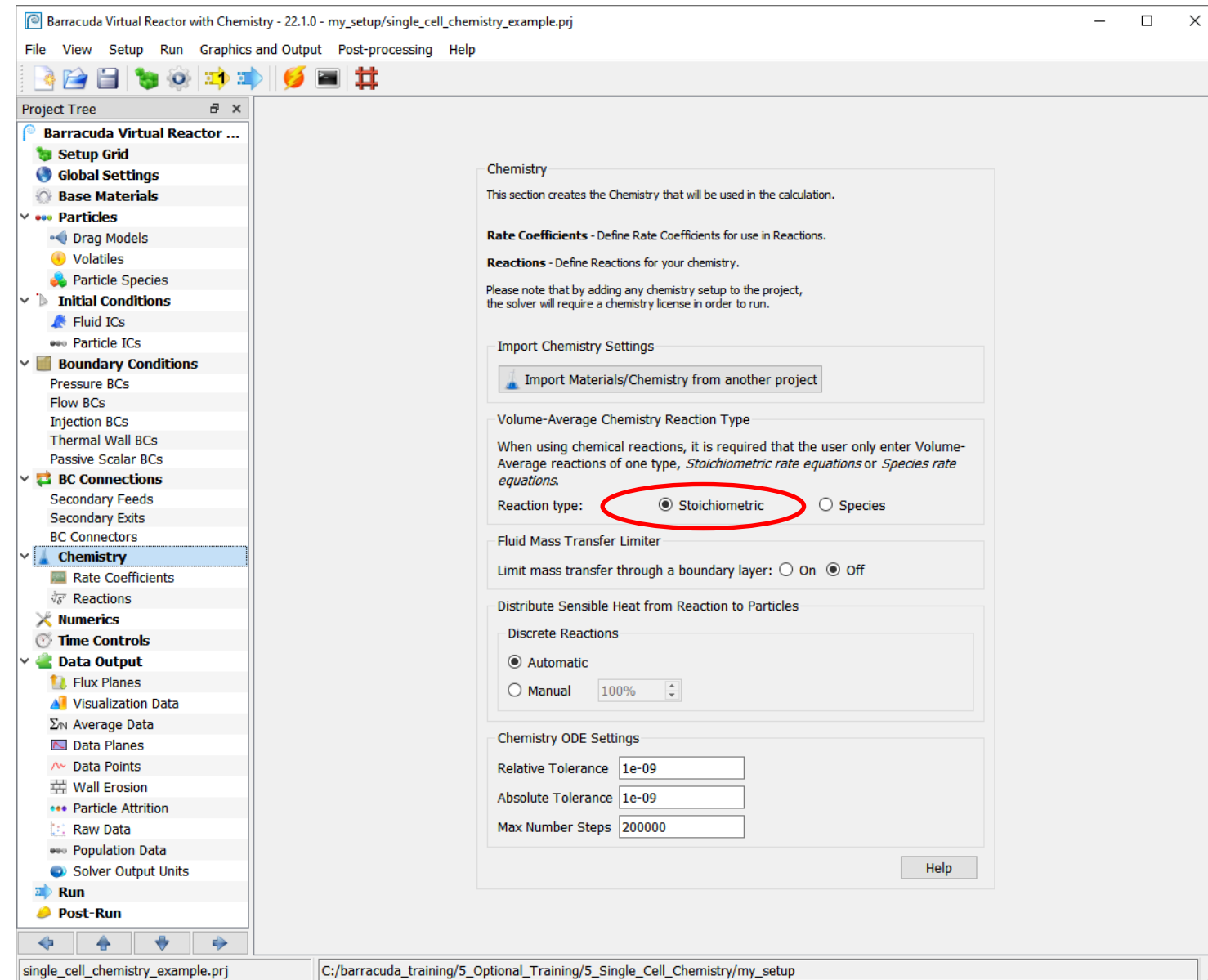
- Initialize mass in region
- Initial mass of 100 kg of coal particles
- $T = 975\text{ K}$



Chemistry

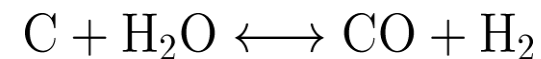
For volume average chemistry, the Stoichiometric and Species forms cannot be mixed.

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



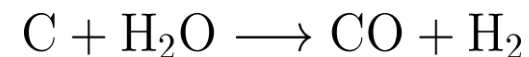
Steam Gasification Reaction

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



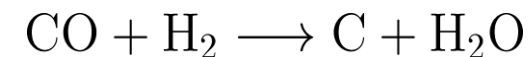
Reaction is reversible, meaning that full reaction consists of a forward reaction and a reverse reaction.

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

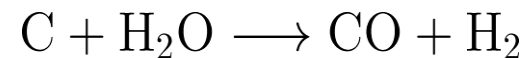


$$\frac{d[\text{H}_2\text{O}]}{dt} = \left(15.7 \frac{\text{m}^6}{\text{kg mol K}^2 \text{s}} \right) T^2 \exp \left(\frac{-33190 \text{K}}{T} \right) \rho_{\text{C}} [\text{H}_2] [\text{CO}]$$

Note: If fluid 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:



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/m³/s **Fluid concentration units:** mol/m³

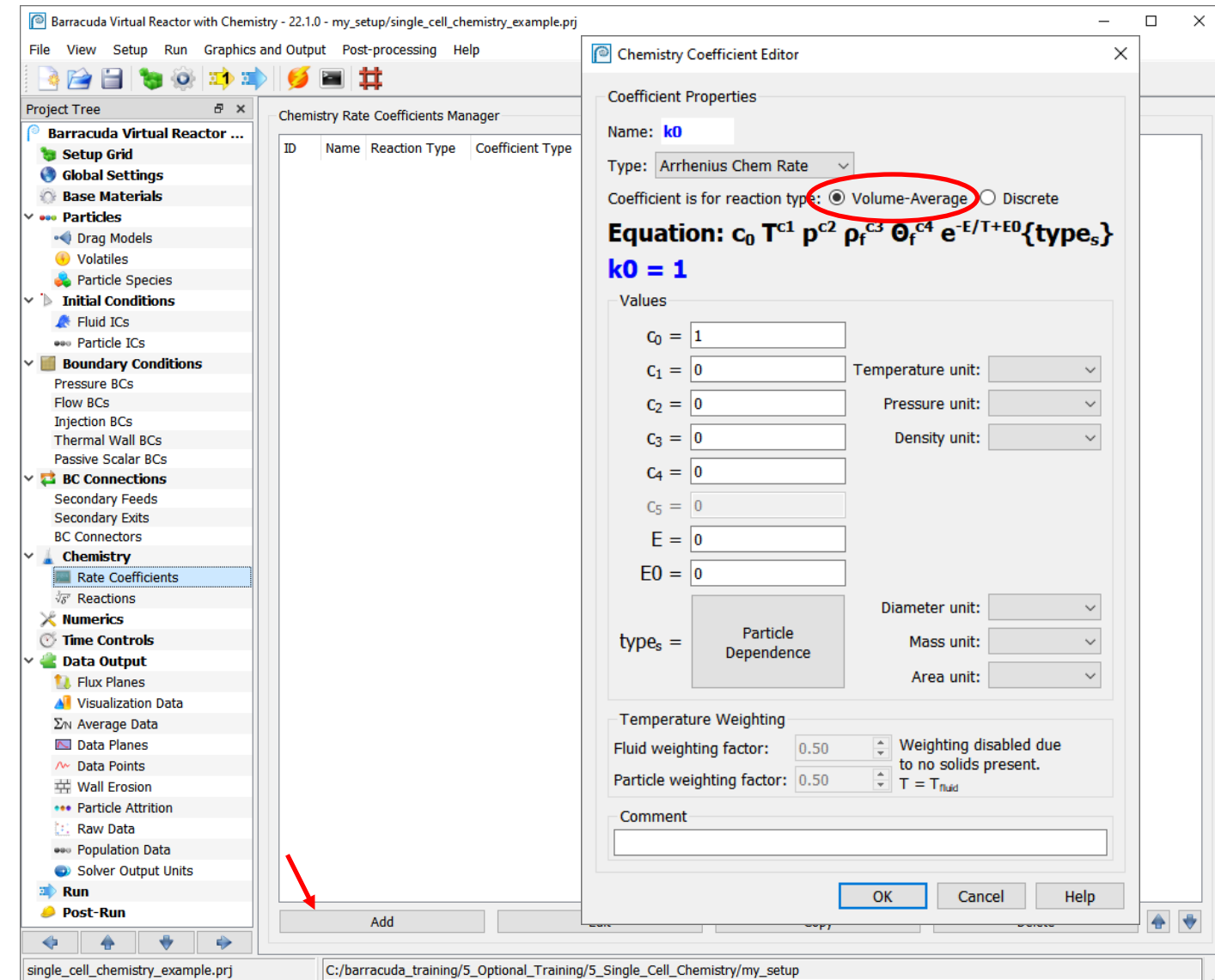
Rate coefficient: $k_0 = 219T \exp\left(\frac{-22645}{T}\right) \rho_{\text{C}}$

Temperature units: K **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:

$$k_0 = 219 T^1 \exp(-22645/T) m_c$$

c_0 c_1 E particle dependence
 \downarrow \downarrow \downarrow \downarrow

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 ☐ 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 input: **k0 = 219 T¹ e^{-22645/T} m_c¹**

The 'Values' section contains input fields for:

- C₀ = 219
- C₁ = 1
- C₂ = 0
- C₃ = 0
- C₄ = 0
- C₅ = 0
- E = 22645
- E0 = 0
- Temperature unit: K
- Pressure unit: (empty)
- Density unit: (empty)
- type_s = Particle Dependence
- Diameter unit: (empty)
- Mass unit: kg/m³
- Area unit: (empty)

The 'Temperature Weighting' section has:

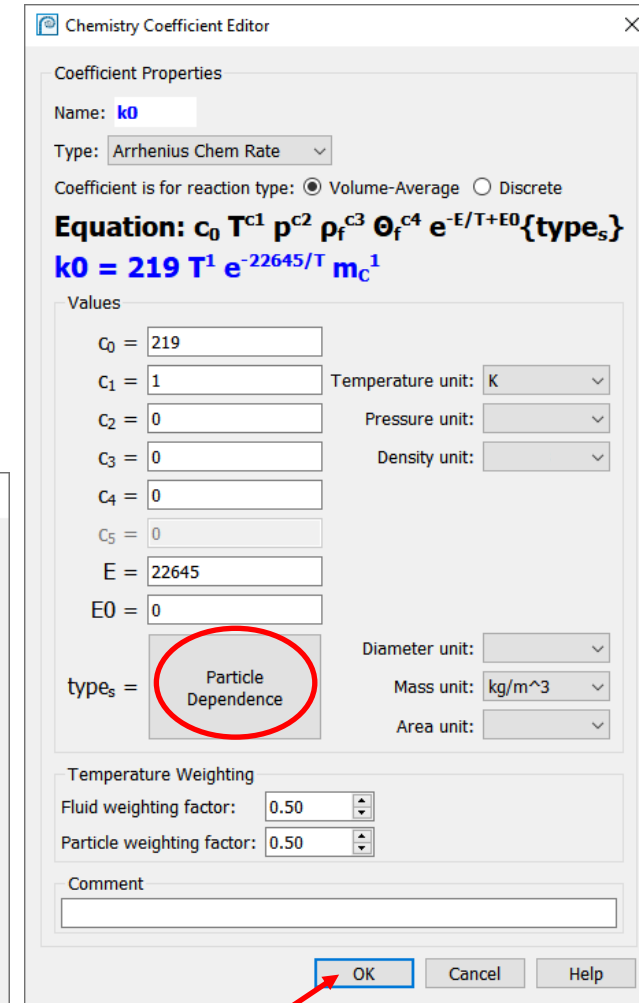
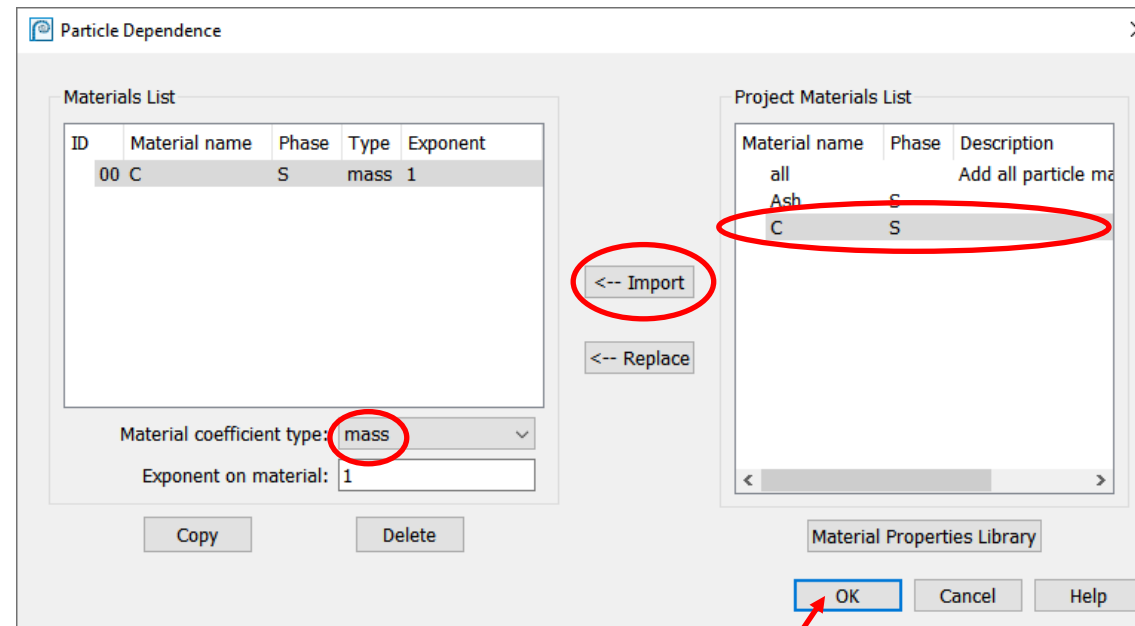
- Fluid weighting factor: 0.50
- Particle weighting factor: 0.50

At the bottom, there is a 'Comment' text area and buttons for 'OK', 'Cancel', and 'Help'.

Rate Coefficients: Solids Term

Click on Particle 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

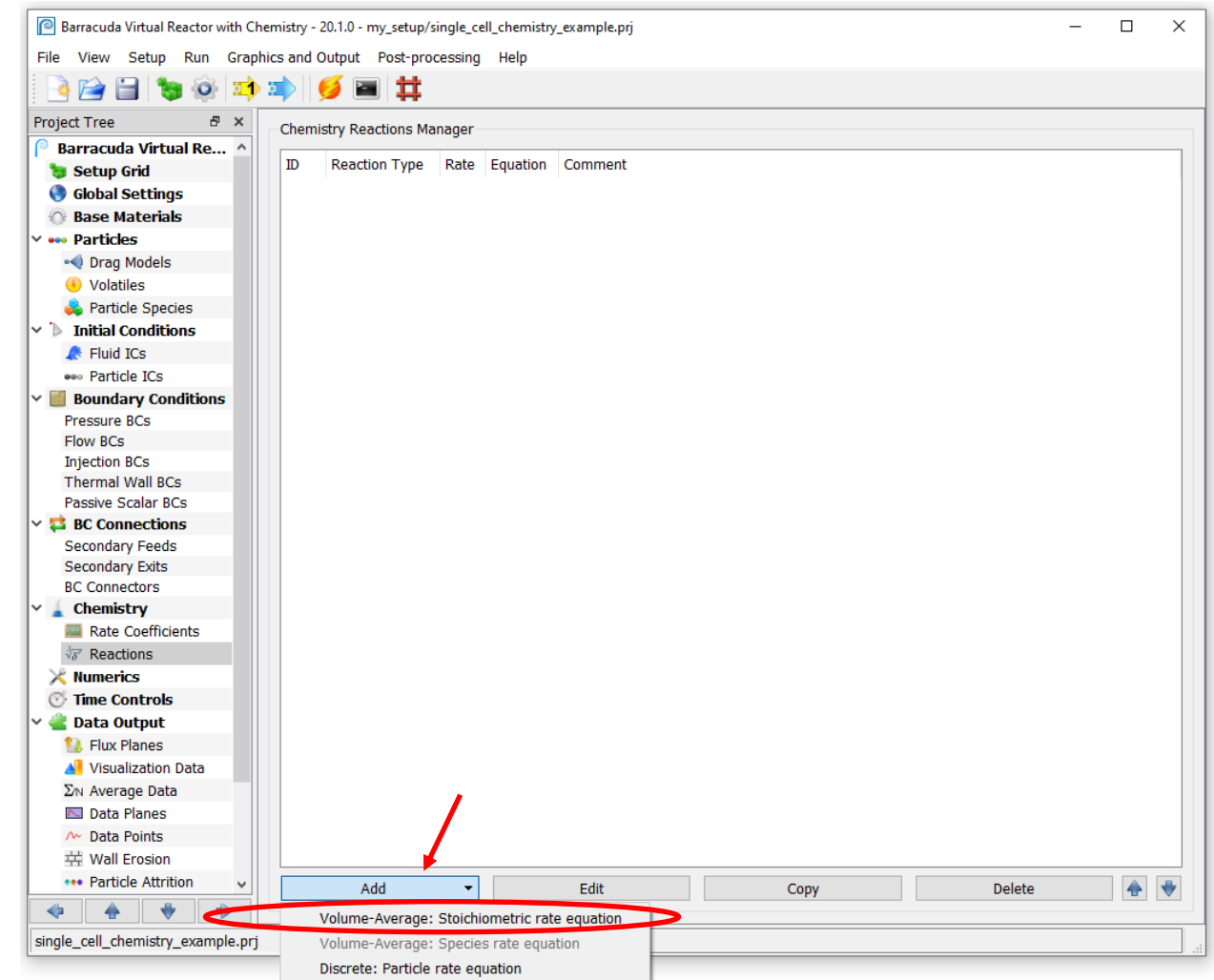


Creating the Forward Reaction

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 Fluid 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 Material** 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
Fluid species units: mol/m3

Enter a stoichiometric reaction:

C(S) + H2O => CO + H2

Check Add Material

Expected Power Law rate equation format: $c0 (k + k - \dots) [\text{material1}]^{\text{power}} [\text{material2}]^{\text{power}} + c1 \dots$
Example of valid Power Law rate equation format: $1.2 (1.5 * k0 - 3 * k1) [\text{H2O}]^{1.5}$
Example of invalid Power Law rate equation format: $(k0 * k1) [\text{H2O}]^{1.5}$ Coefficients cannot be multiplied.
Example of LH expected format: $(c0 k [] + c1 k [] + \dots) / (1 + c2 k [] + c3 k [] + \dots)^{\text{power}}$
Example of groups of rates: $(c0 k0 [\text{O2}] - c1 (0.5k1-k2))^{1.5} (c1(k3) [\text{CO}]^{0.5} [\text{O2}])^{-1}$

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 Material 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 H₂O

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 Material** 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
Fluid species units: mol/m³

Enter a stoichiometric reaction:

C(S) + H₂O => CO + H₂

Check Add Material

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: $(c_0 k_0 [\text{O}_2] - c_1 (0.5k_1 - k_2))^{\wedge 1.5} (c_1 (k_3) [\text{CO}]^{\wedge 0.5} [\text{O}_2])^{\wedge -1}$

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 Material Coefficients Manager

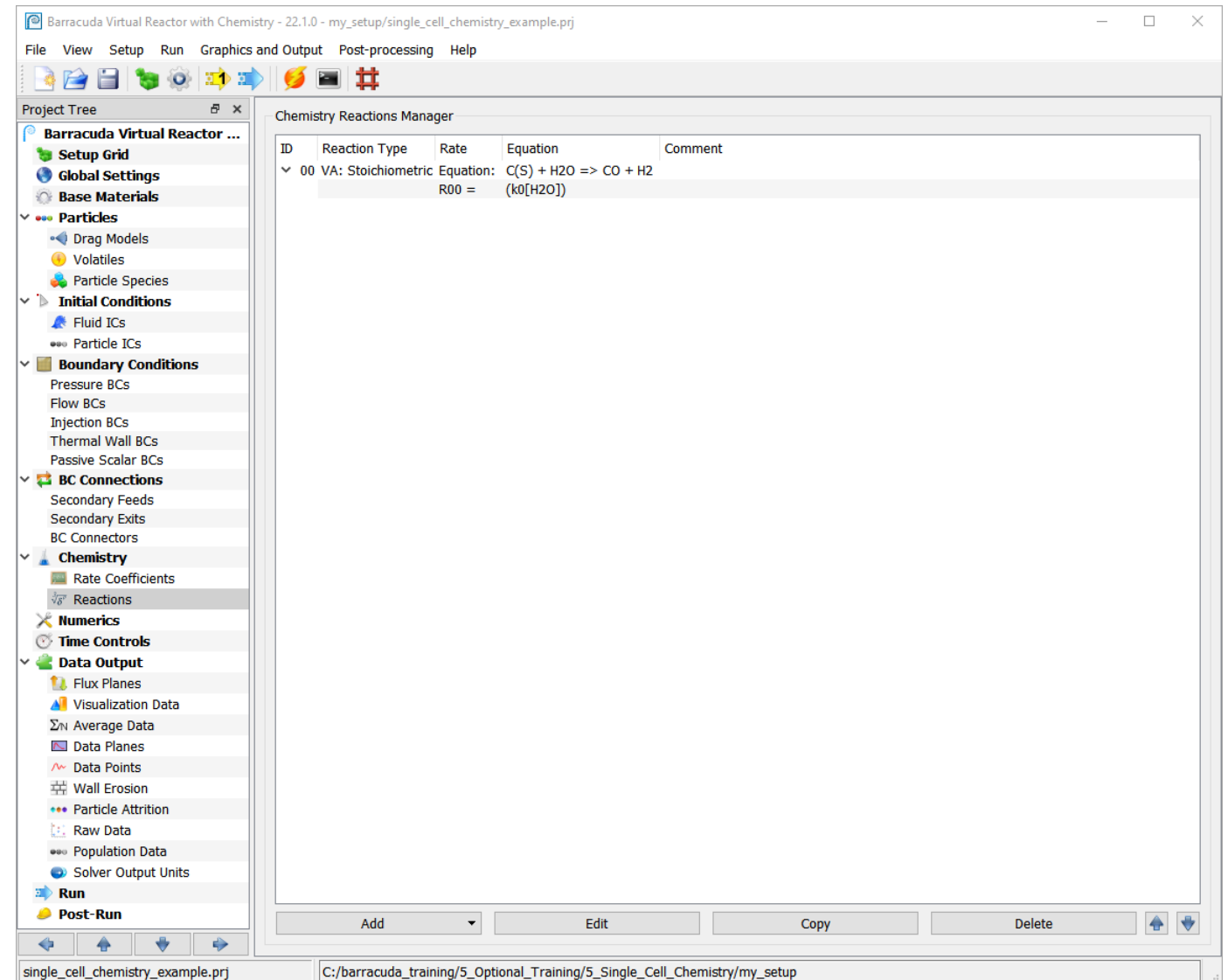
Comment

OK Cancel Help

Forward Reaction Rate

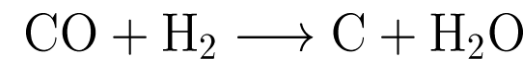
The forward reaction rate equation is now complete:

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



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.

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

In Barracuda:

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

Reaction rate units: mol/m³/s **Fluid concentration units:** mol/m³

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

Temperature units: K **Mass units:** kg/m³

Rate Coefficient: Reverse Reaction

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

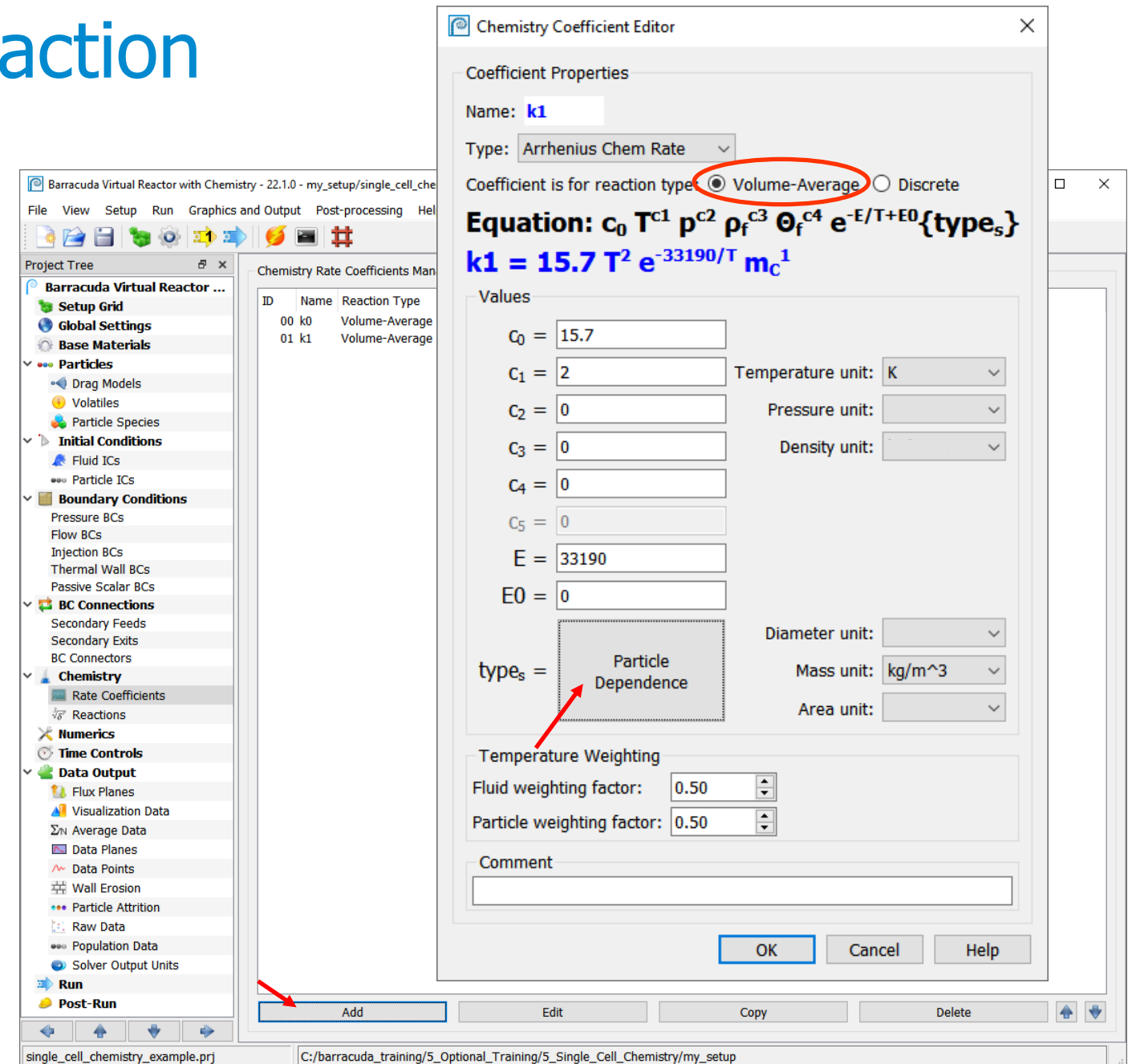
Under Rate Coefficients, click Add and enter the equation for k1 as follows:

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

c_0 c_1 E particle dependence
↓ ↓ ↓ ↓

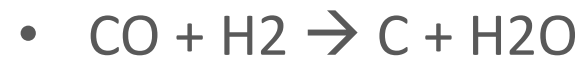
Check that Volume-Average is selected and that units are selected for temperature, pressure, density, mass, etc.

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



Chemical Equations: Reverse Reaction

Define the stoichiometric equation for the reverse reaction:



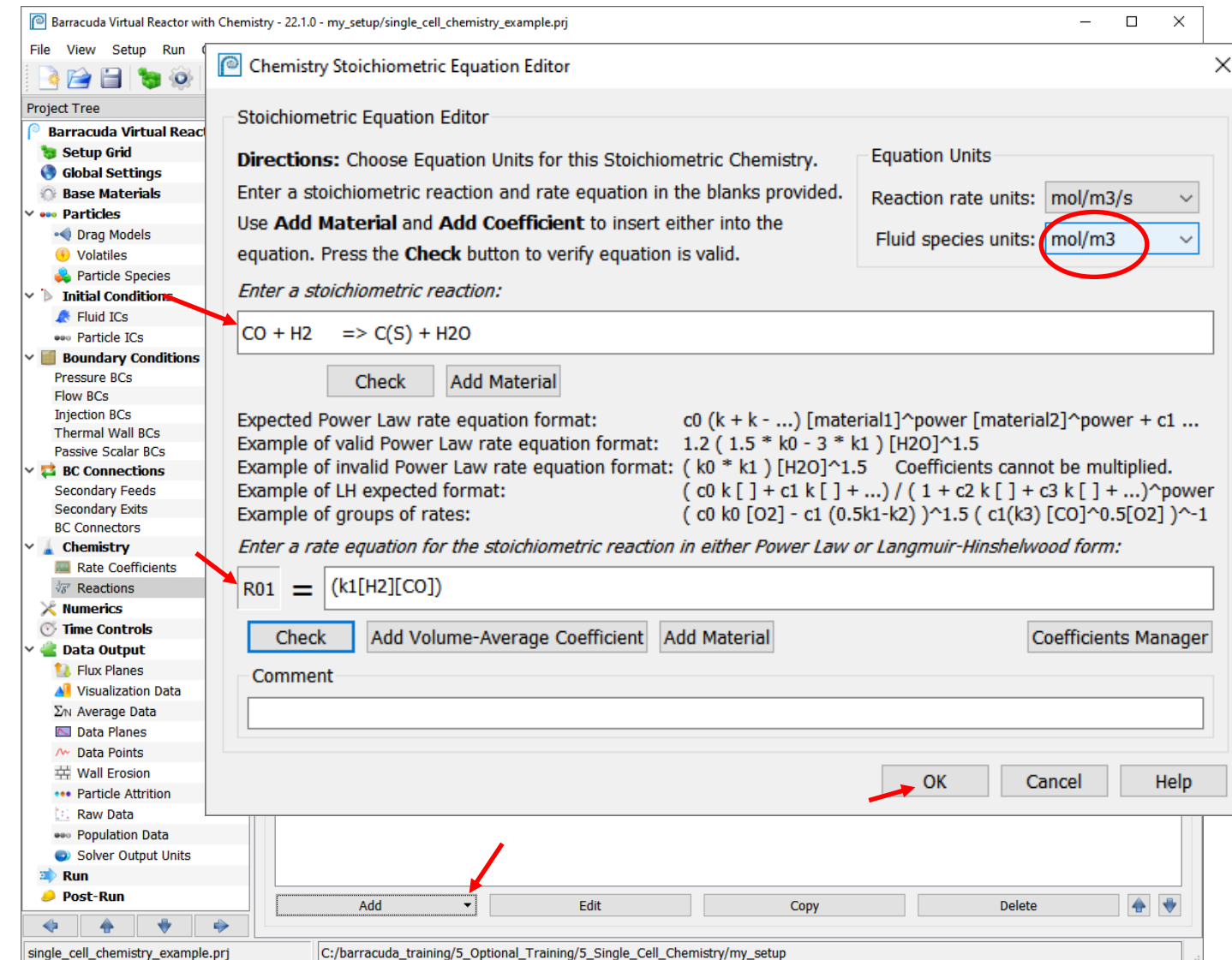
Enter the rate equation for the reverse reaction as follows:

- $R01 = k1[\text{H}_2][\text{CO}]$

Set Fluid 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



Reverse Reaction

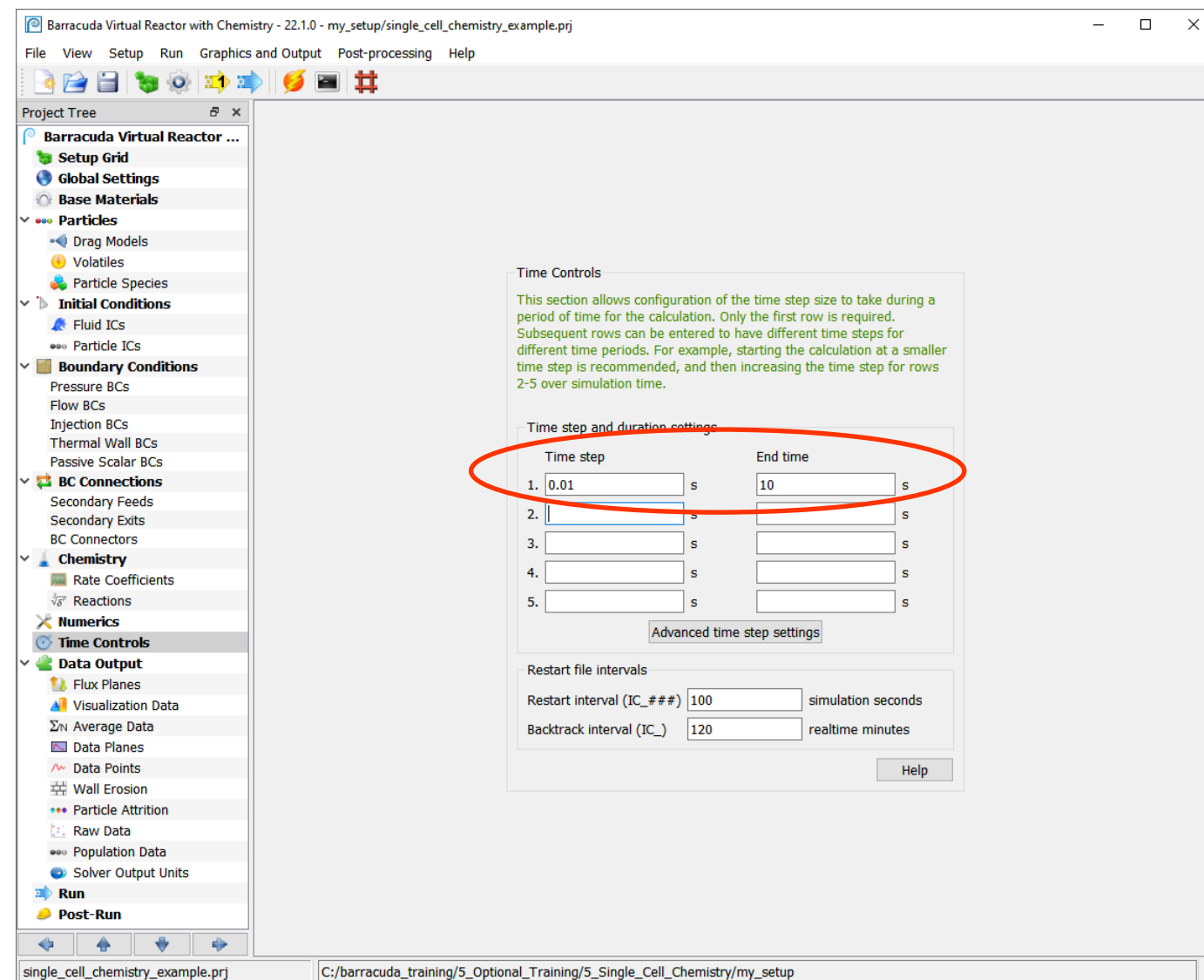
The reverse reaction is now complete

The screenshot shows the Barracuda Virtual Reactor software interface. The left sidebar contains a Project Tree with various settings categories. The main window displays the Chemistry Reactions Manager, which lists two reactions. The second reaction, ID 01, is highlighted with a red circle. It 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	$R00 = (k0[\text{H}_2\text{O}])$	$\text{C(S)} + \text{H}_2\text{O} \Rightarrow \text{CO} + \text{H}_2$	
01	VA: Stoichiometric	$R01 = (k1[\text{H}_2][\text{CO}])$	$\text{CO} + \text{H}_2 \Rightarrow \text{C(S)} + \text{H}_2\text{O}$	

Time Controls

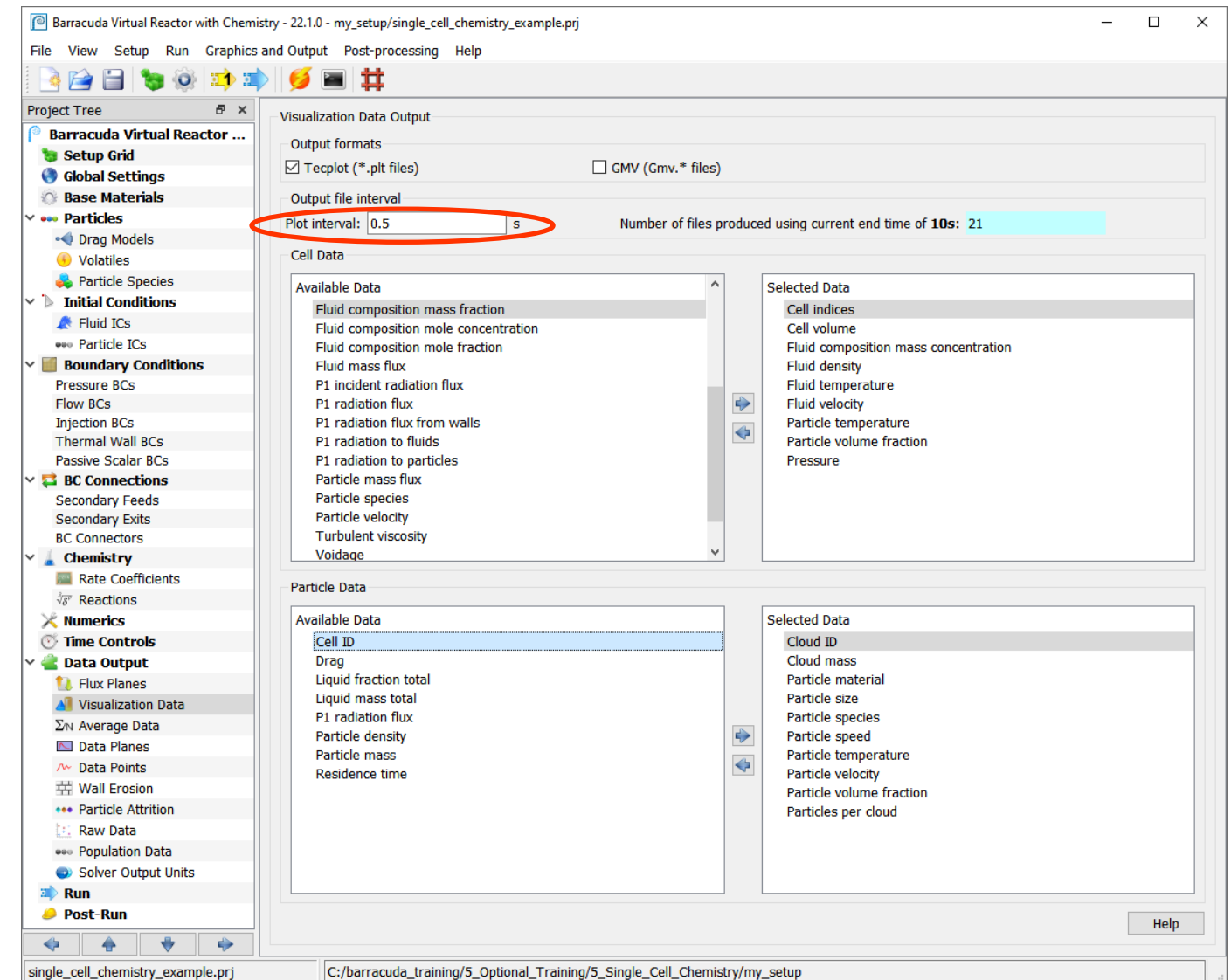
Enter Time step and End time as shown



Visualization Output Options

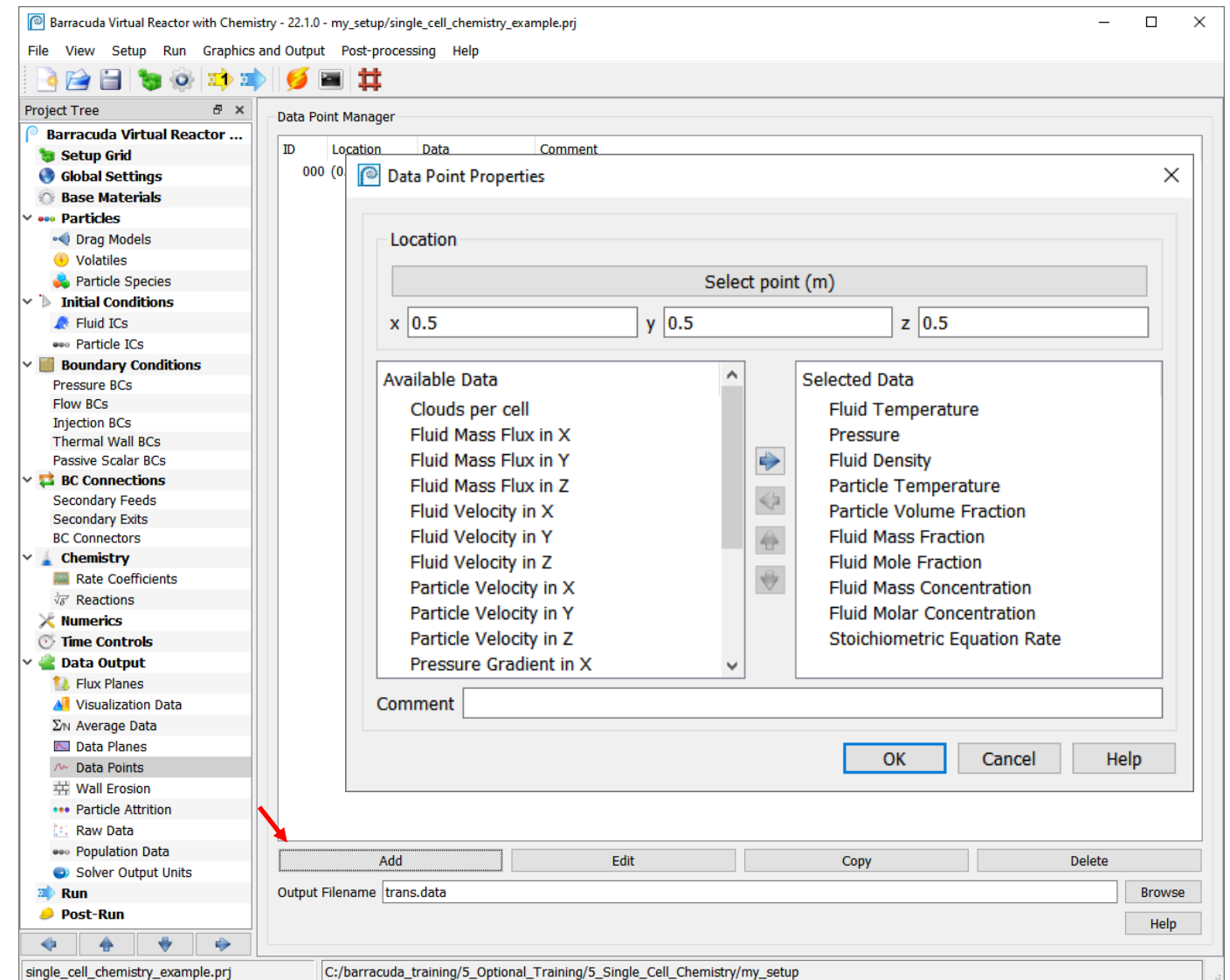
Enter a Plot interval of 0.5 s

Choose the output variables shown on the right



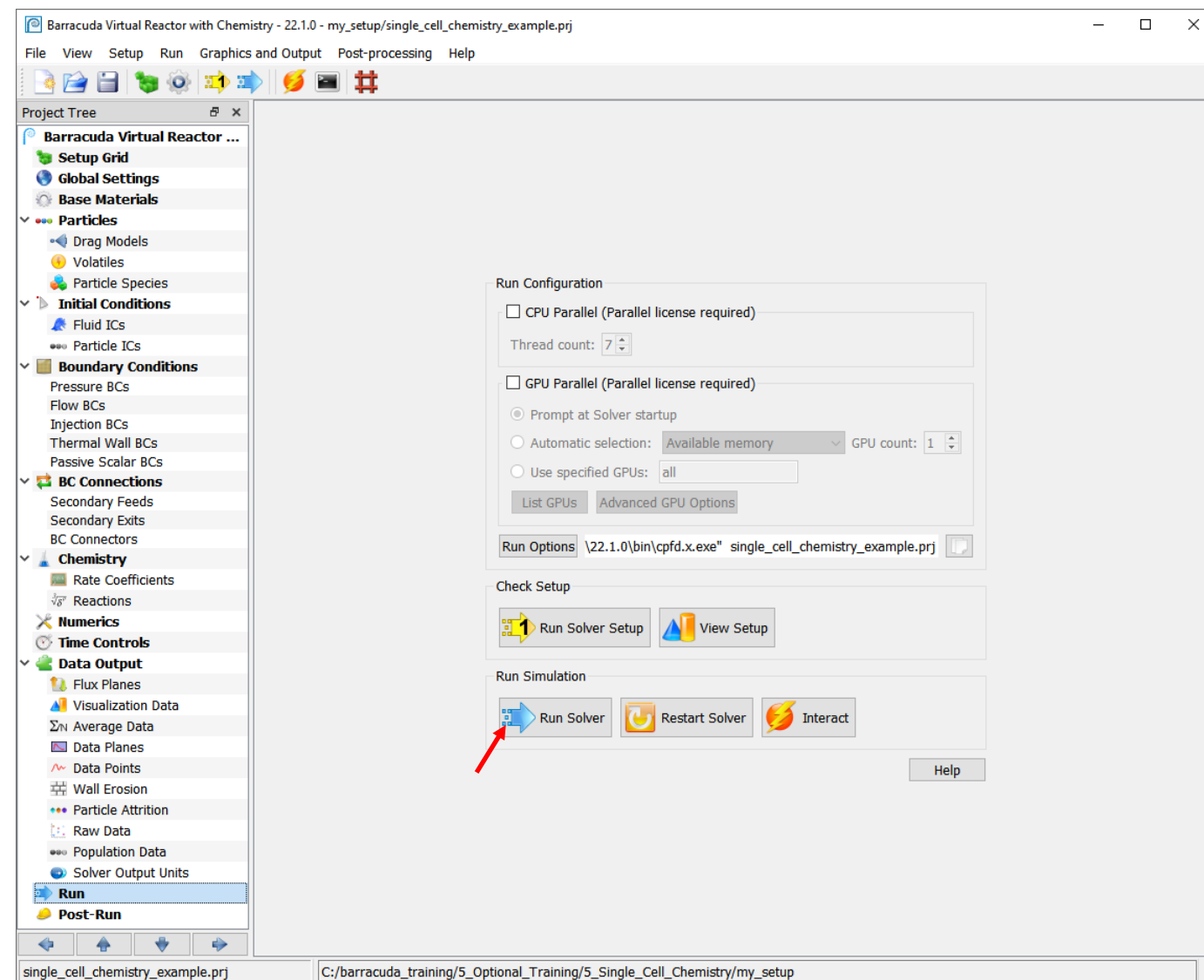
Data Points

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



Run the Simulation

Click on Run Solver



Plotting Data Point Information in Tecplot for Barracuda

Follow along with this [video](#) to create the grid of xy plots.

Open Tecplot for Barracuda using the Launch Tecplot 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)

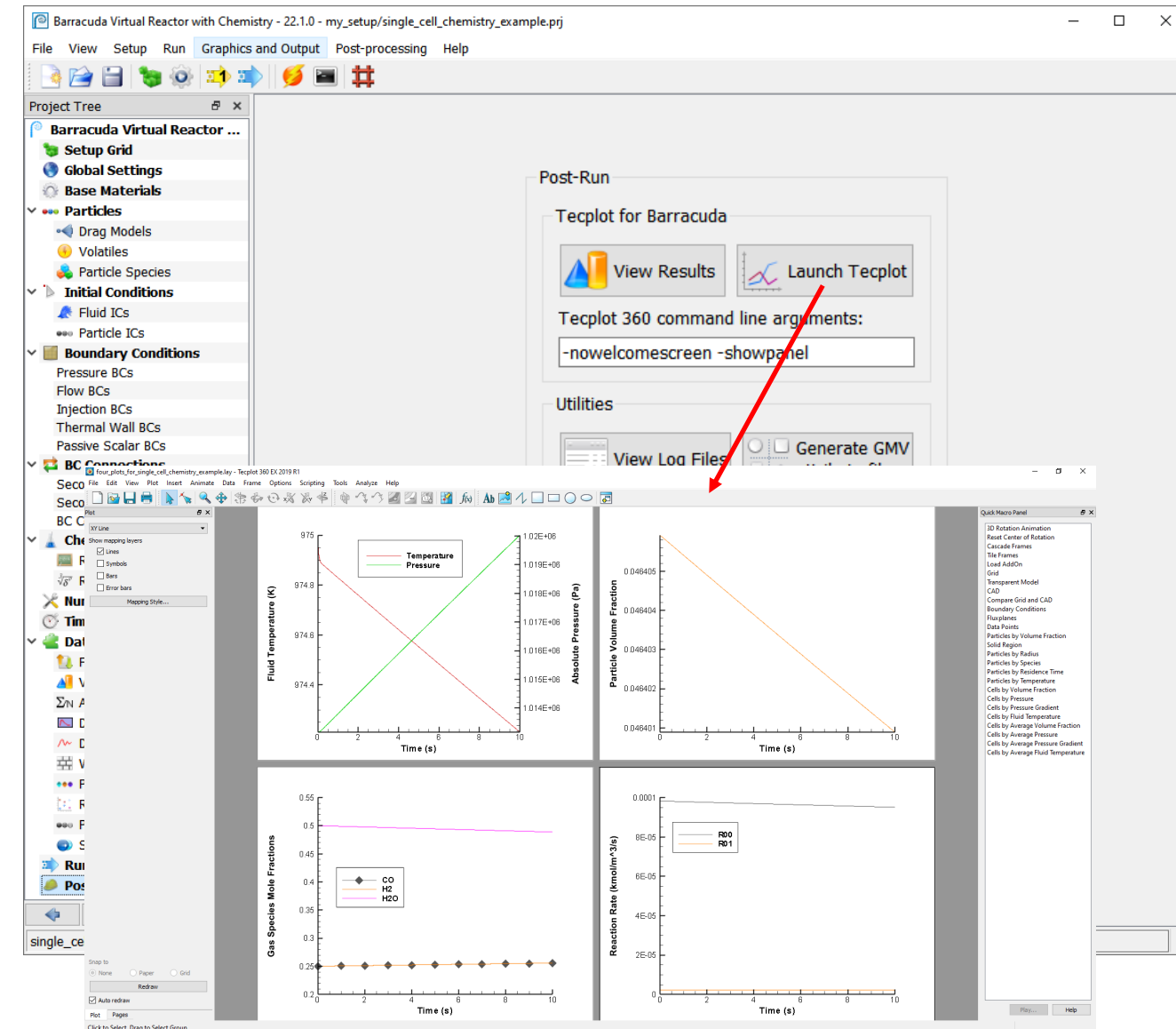
Create the following 4 plots (see next slide for larger version of final result):

- 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

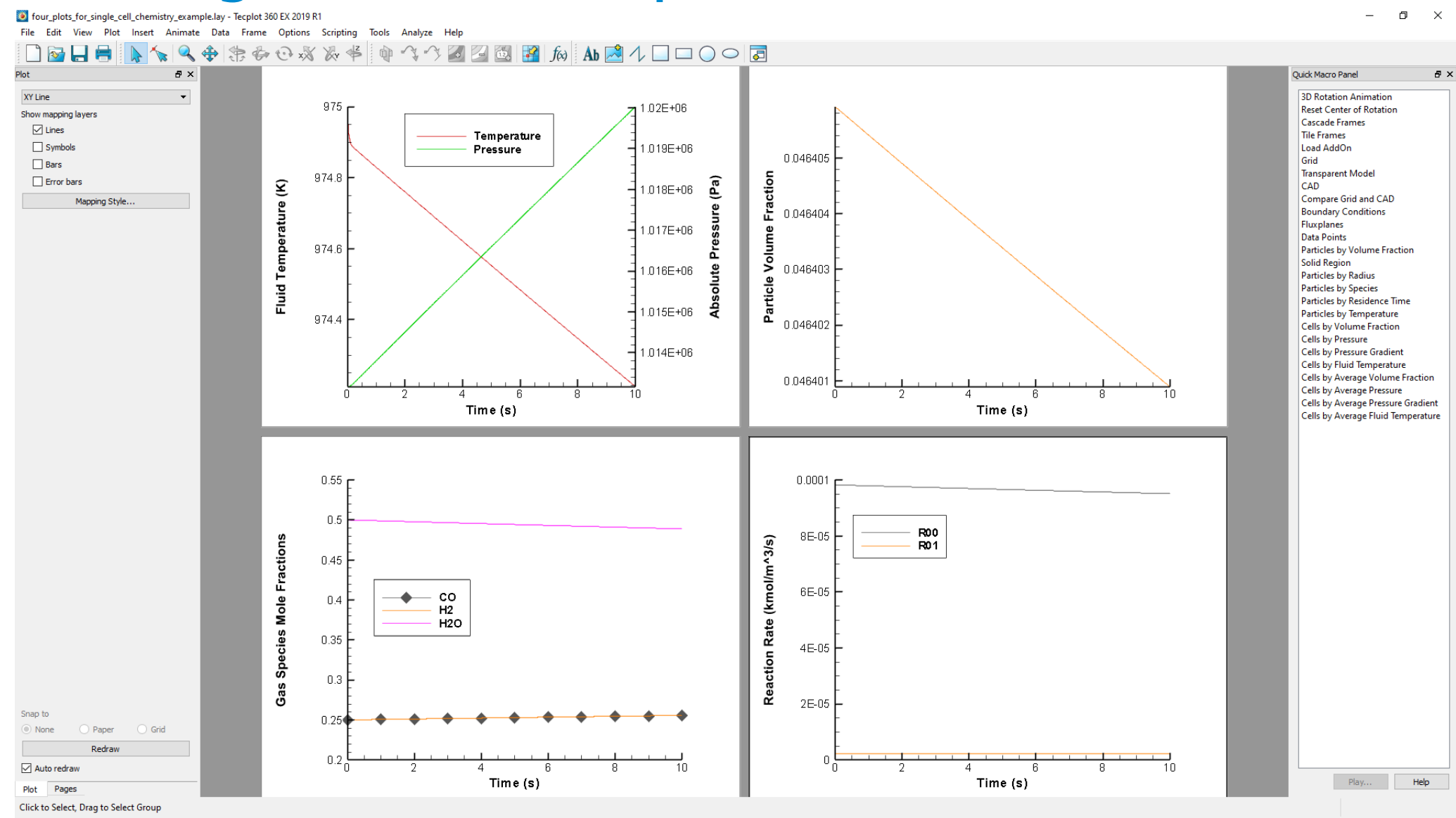
Hint: use Ctrl+F to rescale axes after selecting data or adjusting plot sizes

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	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 H ₂ O	0.50	
10	Mole fraction of H ₂	0.25	
11	Mole fraction of CO	0.25	
12	Molar concentration of H ₂ O	6.2492E+01	mol/m ³
13	Molar concentration of H ₂	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

trans.data00 (C:\training\4_Chemistry\single_cell_chemistry_example\pre_setup) - GVIM

File Edit Tools Syntax Buffers Window Help

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 9.750000000e+02 1.013200000e+06 2.062242989e+00 9.750000000e+02 4.6405919662e-02 4.242424242e-01 3.0303030303e-02 5.454545454e-01 0.000000000e+00

2.500000000e-01 2.500000000e-01 5.000000000e-01 0.000000000e+00 0.000000000e+00 0.000000000e+00 0.000000000e+00 0.000000000e+00 0.000000000e+00 0.000000000e+00

01 6.2492211603e+01 0.000000000e+00 9.8344346441e-05 2.1573151680e-06

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

Fluid Mass Transfer Limiter
Limit mass transfer through a boundary layer: ☐ On ☒ Off

Distribute Sensible Heat from Reaction to Particles

Discrete Reactions

☒ Automatic ☐ Manual 100%

Chemistry ODE Settings

Relative Tolerance 1e-09
Absolute Tolerance 1e-09
Max Number Steps 200000

Help