Chemistry Training Example 1: Volume-Average

February 2018

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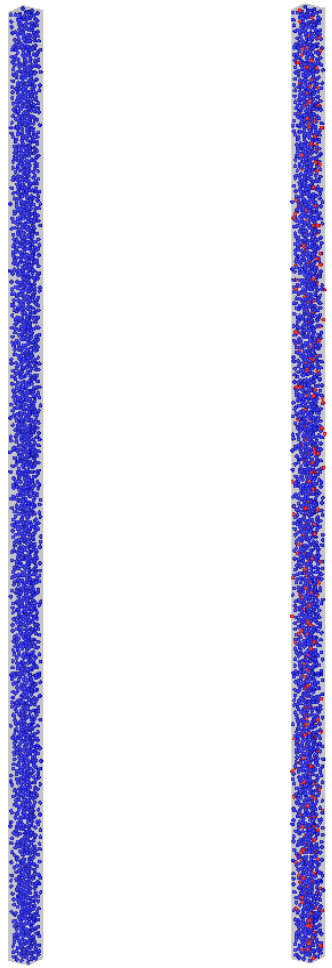
Training Plan

- Chemistry training will be provided in three parts
  - Lecture: Introduction to the Chemistry module
    - Volume Average Chemistry
    - Discrete Particle Chemistry
  - Example 1: Set up of training problem using Volume Average Chemistry
  - Example 2: Set up of training problem using Discrete Particle Chemistry

Steam Gasification Tube Setup

- The steam gasification system consists of
  - A narrow square tube (1 cm x 1 cm x 40 cm)
  - Tube is filled with 200 µm diameter coal particles.
  - Coal particle locations are fixed in space with a volume fraction of 0.4 and initial temperature of 975 K
  - Top of tube is pressurized to 10 atm.
  - Coal is assumed to be 90% carbon and 10% ash (SiO2)
- Two cases will be modeled in this system:
  - **Case #1**: Pure steam enters bottom of tube at 1 cm/s and 800 K.
  - **Case #2**: Steam containing 10% by volume fine coal particles (20 µm) enters the bottom of tube a 1 cm/s and 800 K. Fine coal particles pass through the interstitial spaces in the fixed coal bed.
- A model for Case #1 will be set up with volume average chemistry



Case #1 **Case #2**

Steam Gasification Reaction

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

$$\mathrm{C} + \mathrm{H_2O} \longleftrightarrow \mathrm{CO} + \mathrm{H_2}$$

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

Forward Reaction

$$\mathrm{C} + \mathrm{H_2O} \longrightarrow \mathrm{CO} + \mathrm{H_2}$$

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

Reverse Reaction

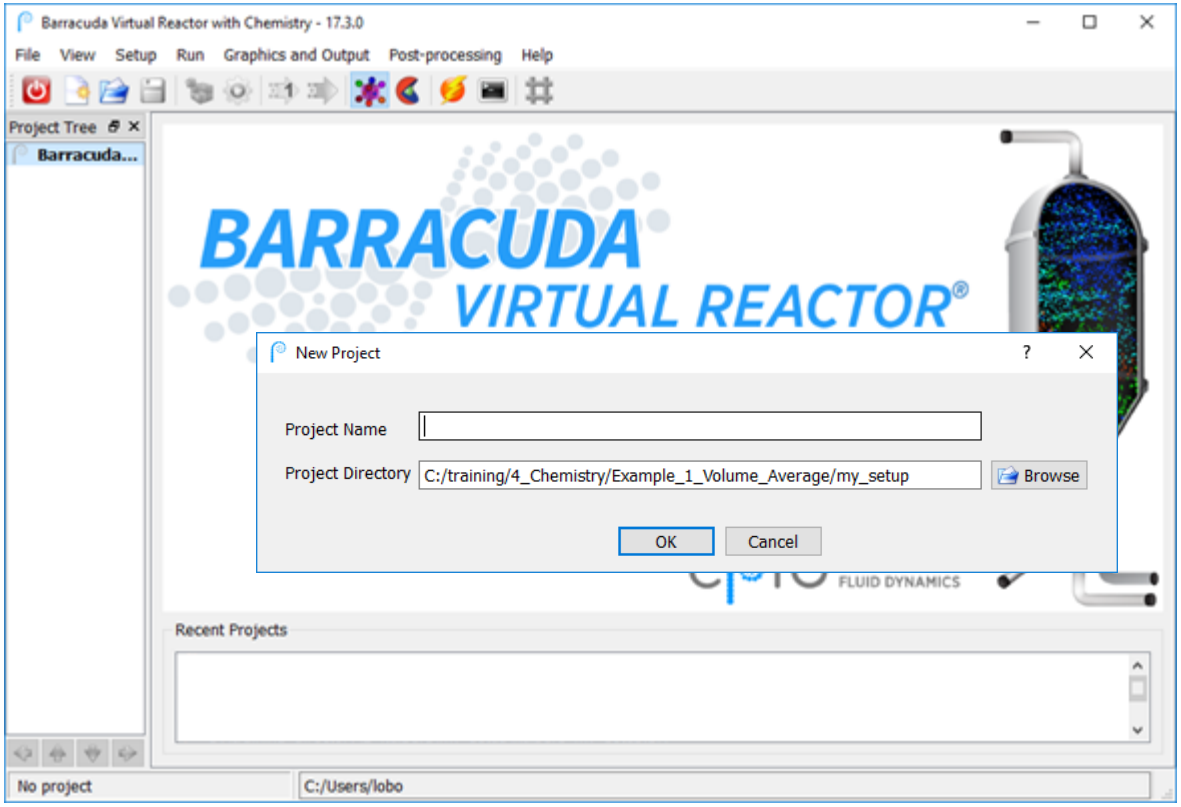
$$\mathrm{CO} + \mathrm{H_2} \longrightarrow \mathrm{C} + \mathrm{H_2O}$$

$$\frac{d[\mathrm{H_2O}]}{dt} = \left(15.7\ \frac{\mathrm{m}^6}{\mathrm{kg\,mol\,K^2\,s}}\right) T^2 \exp\left(\frac{-33190\,\mathrm{K}}{T}\right) \rho_{\mathrm{C}}\,[\mathrm{H_2}]\,[\mathrm{CO}]$$

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

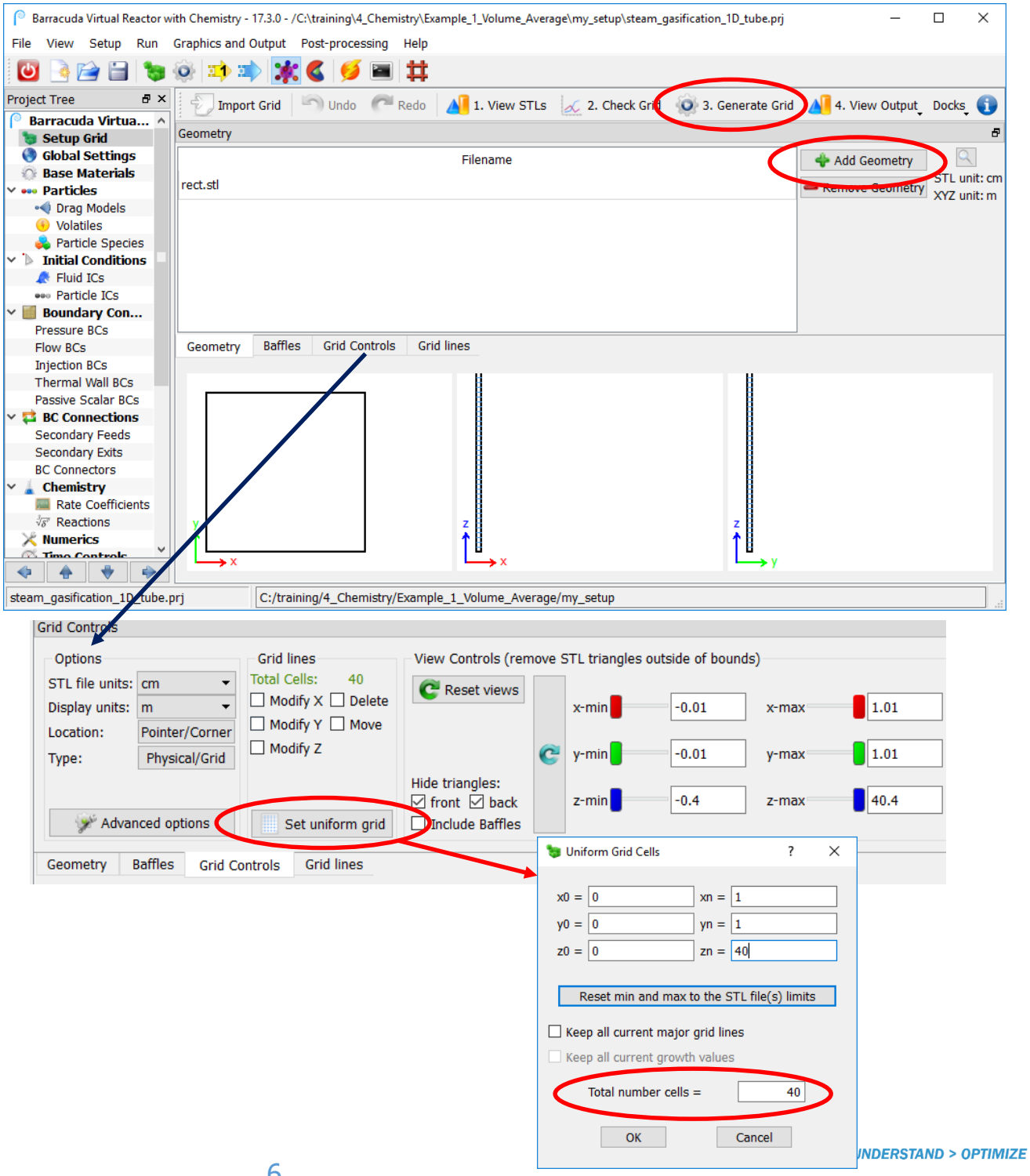
Volume Average Project File

- Create a new project file under the directory:
  - Linux: /home/training/barracuda_training/4_Chemistry/Example_1_Volume_Average/my_setup
  - Windows: C:\training\4_Chemistry\Example_1_Volume_Average\my_setup
- Enter an appropriate project name

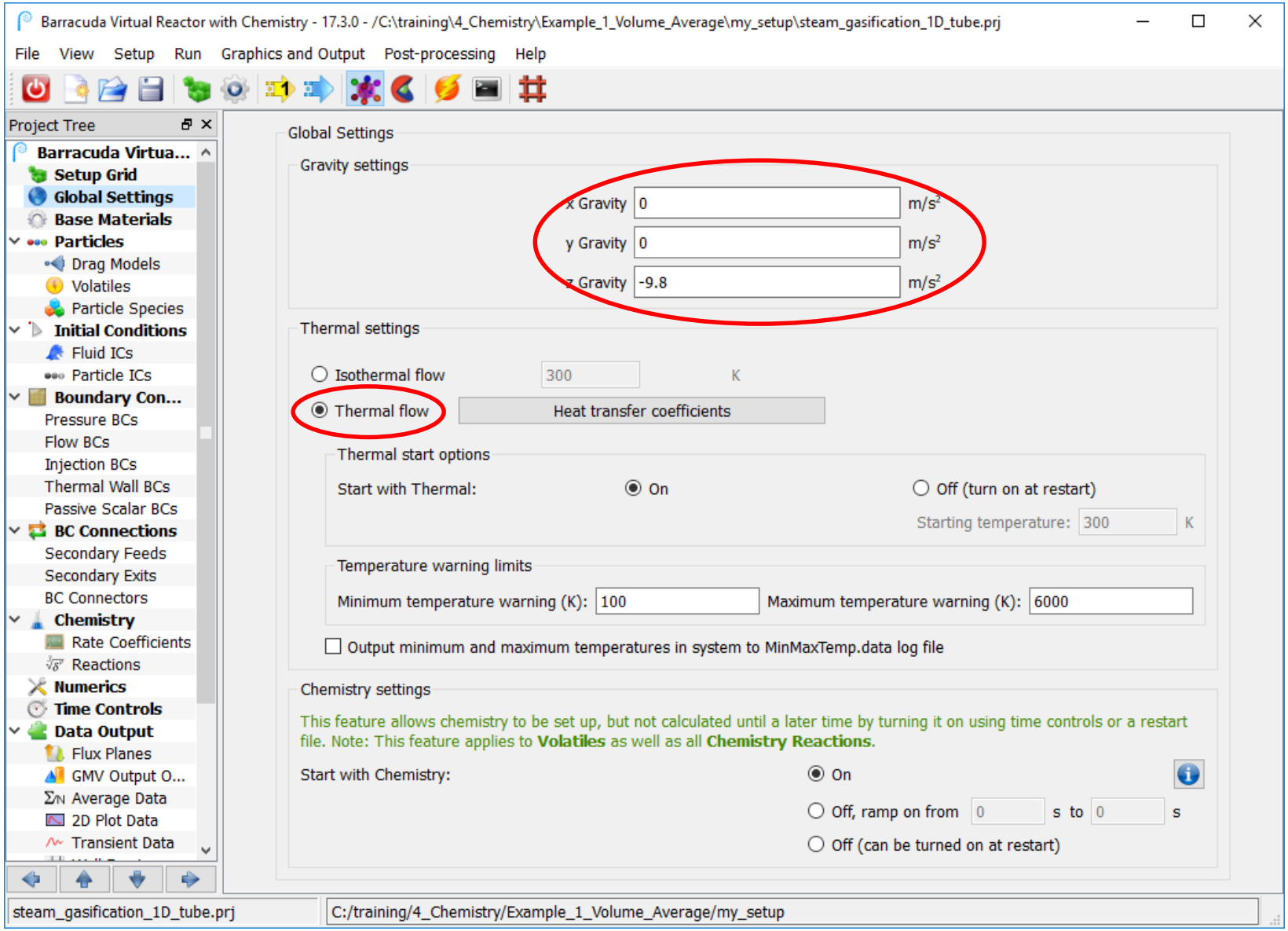


Generate the Grid

- In the **Geometry** tab, click **Add Geometry**
- An STL file is included in your project directory, named **rect.stl**
  - x-width = 1 cm
  - y-width = 1 cm
  - z-width = 40 cm
- In the **Grid Controls** tab:
  - Set STL units to “cm”
  - Click **Set uniform grid**
  - Set **Total number of cells** to “40”
- Make sure to click on **Generate Grid** when finished with the previous steps
- This type of 1-dimensional tube is useful when first exploring a set of chemical reactions

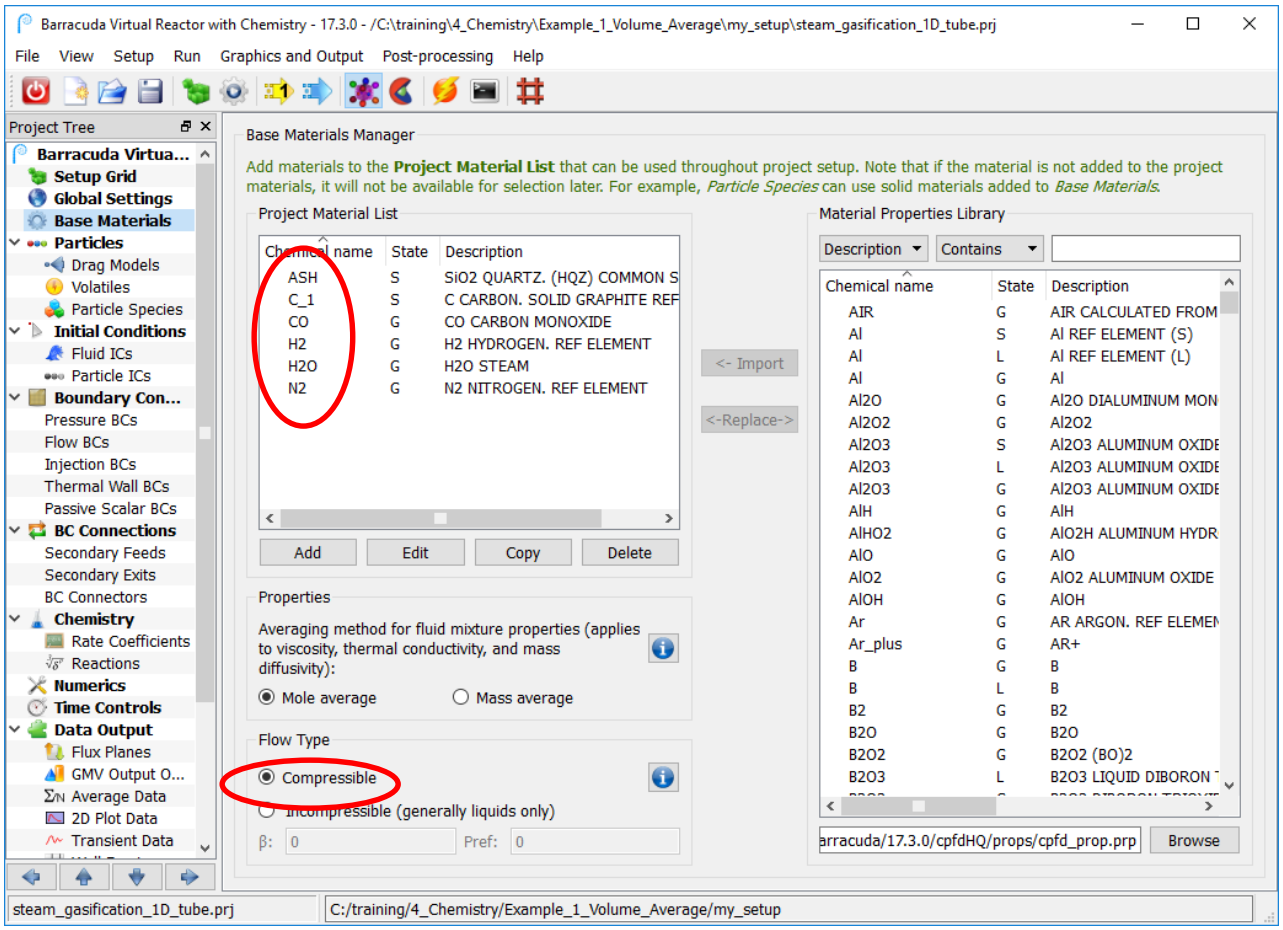


Global Settings



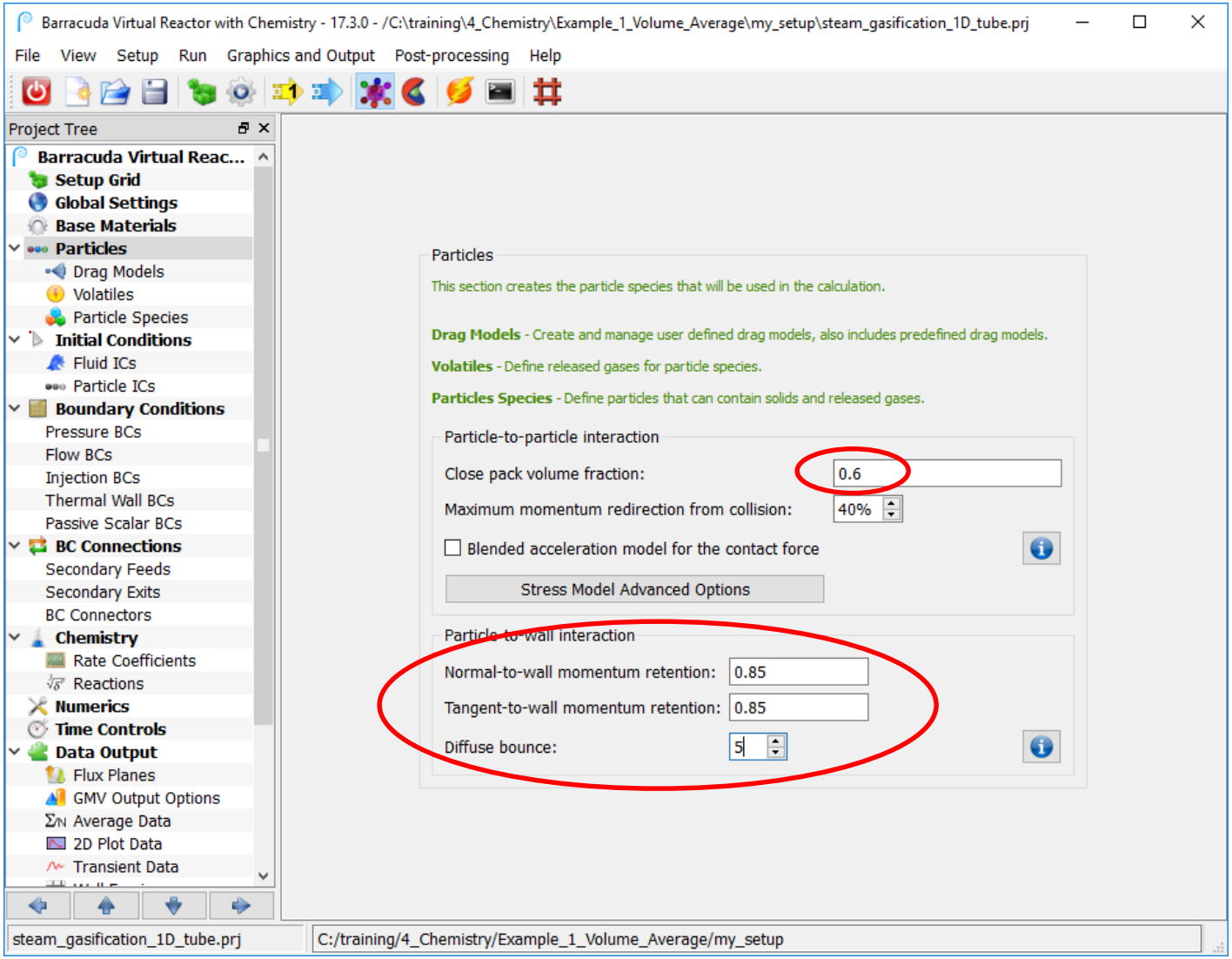
Base Materials

- 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"
- Choose **Compressible Flow** to add multiple fluids



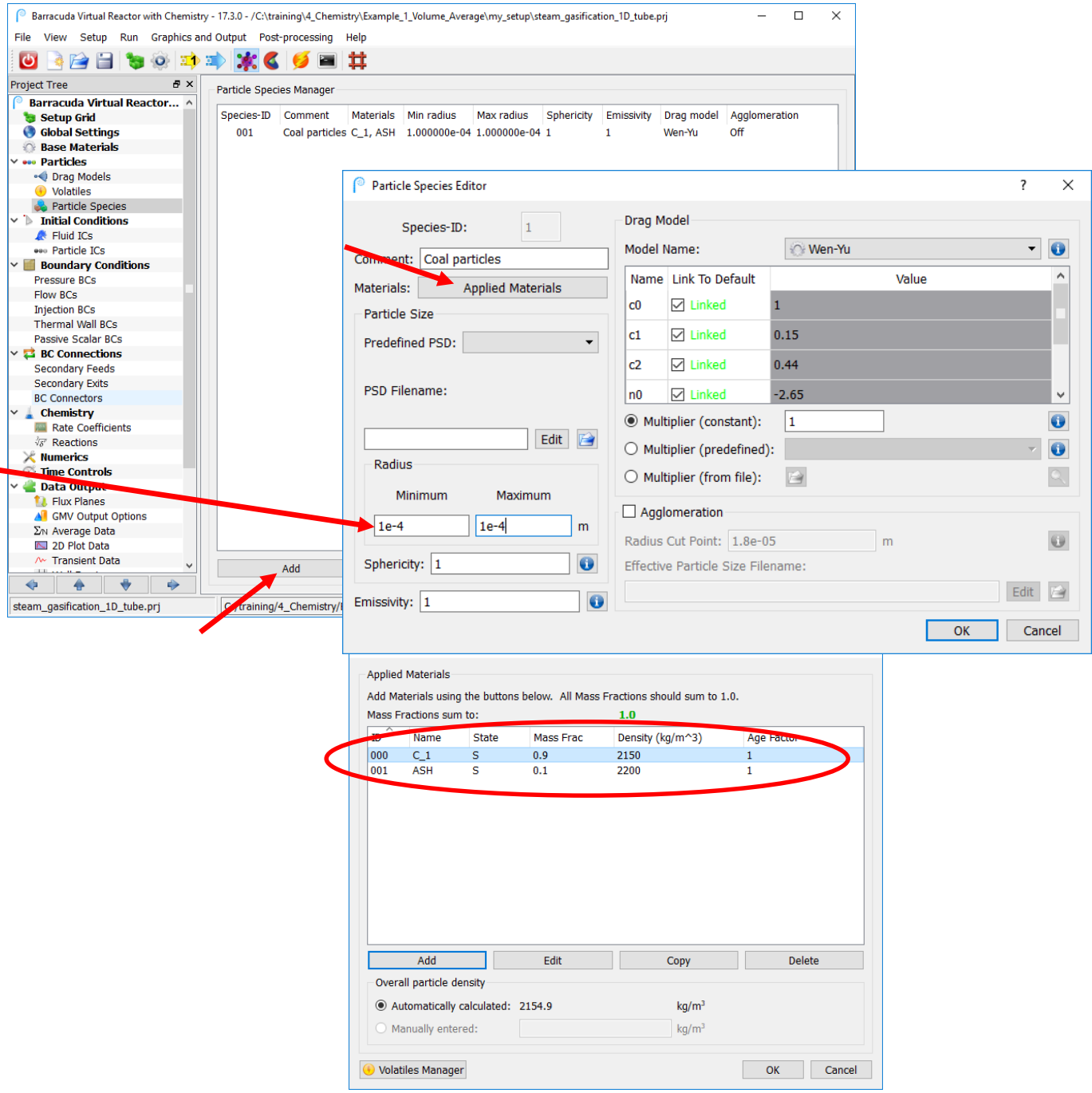
Particles

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



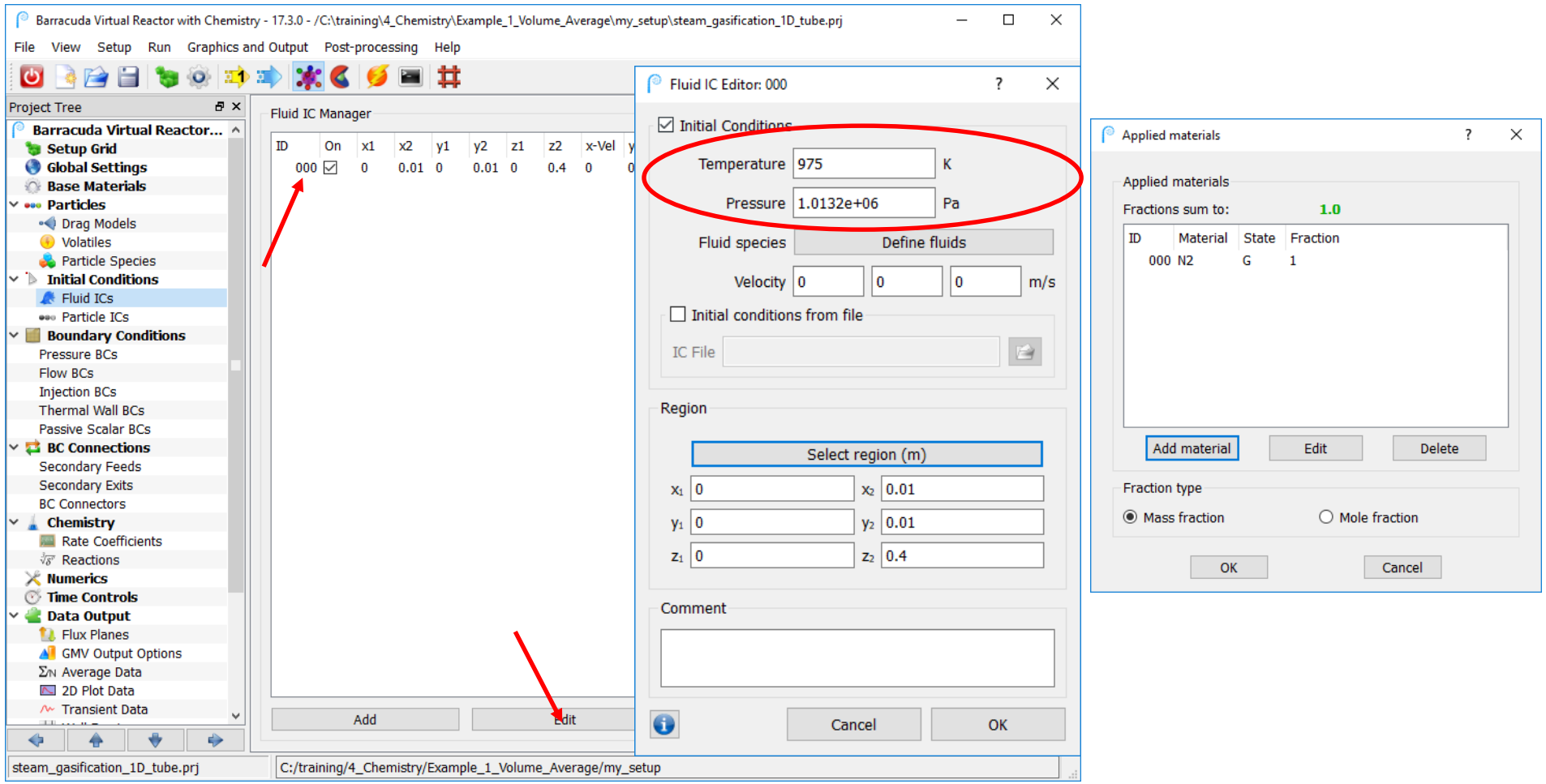
Particle Species

- Click on the Particle Species tab
- Click **Add** and then click **Applied Materials** to create a particle species consisting of 90% carbon and 10% ASH by mass
- A mono-sized particle will be used with a diameter of 200 microns. Remember that particle size is entered by radius in Barracuda
- In the Comment field, enter “Coal particles”



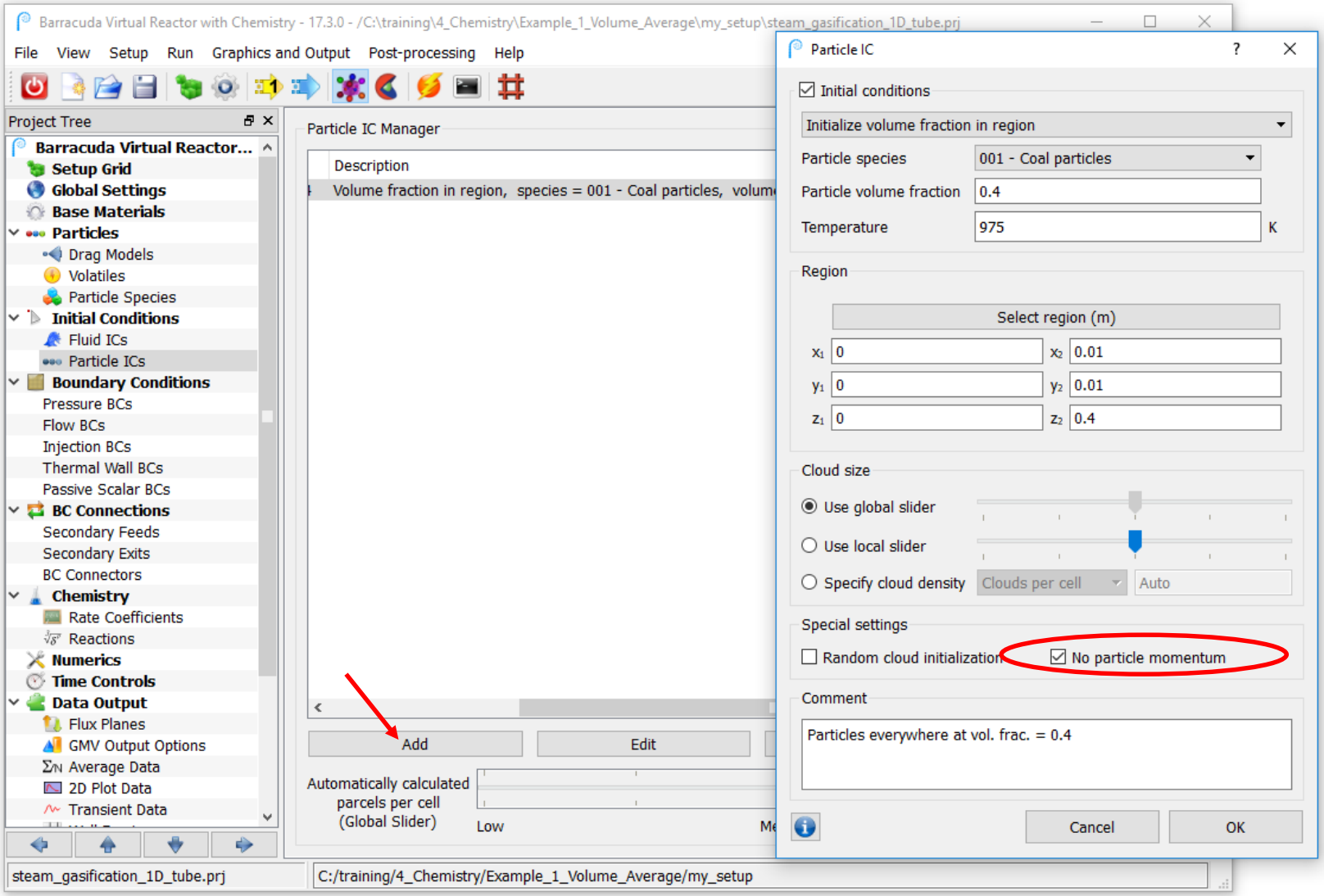
Fluid Initial Conditions

- For the fluid initial condition, fill the tube with 100% N_2, at a pressure of 10 atm and a temperature of 975 K



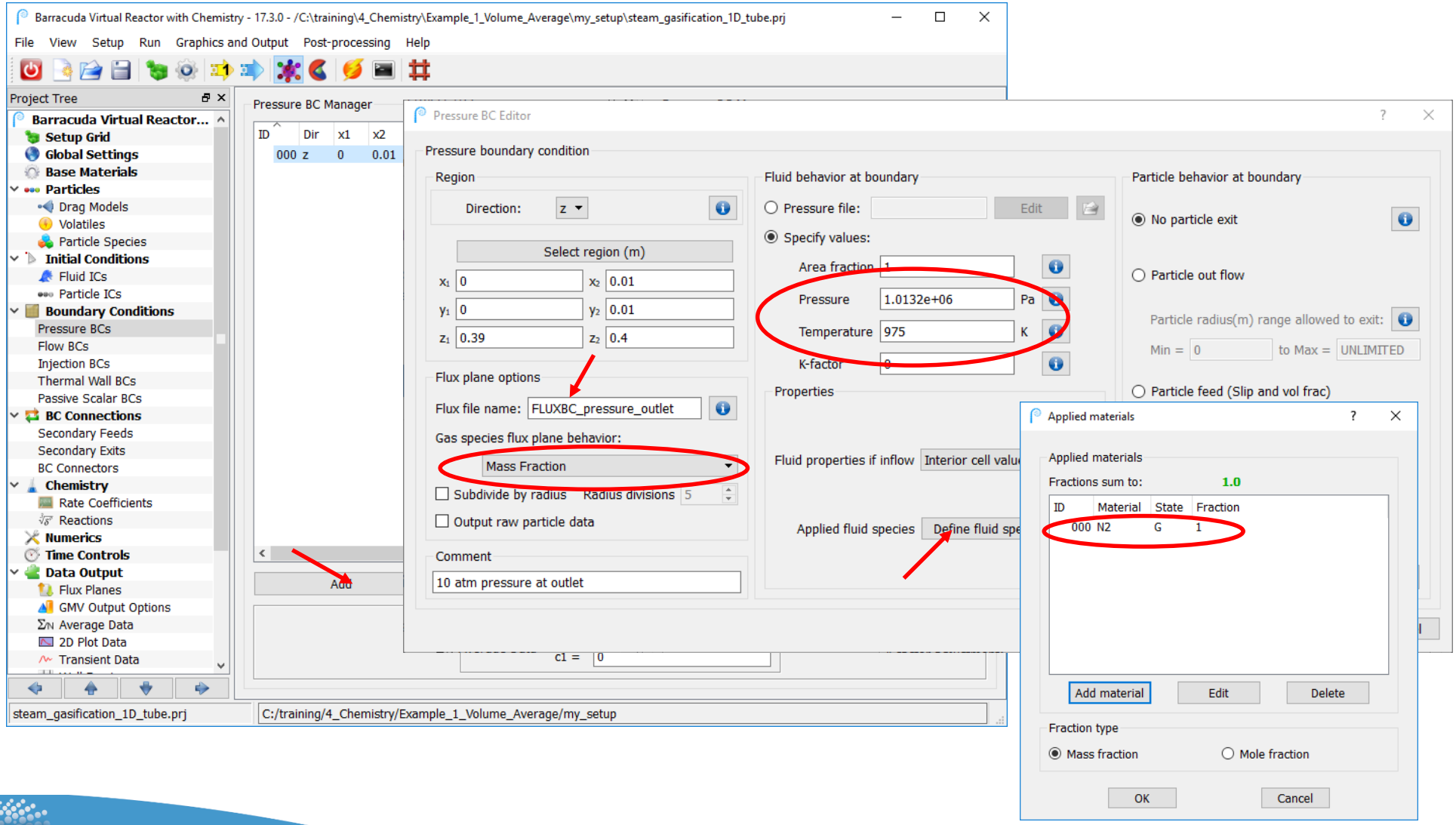
Particle Initial Conditions

- Click **Add** to specify the initial volume fraction of the coal particles at “0.4”



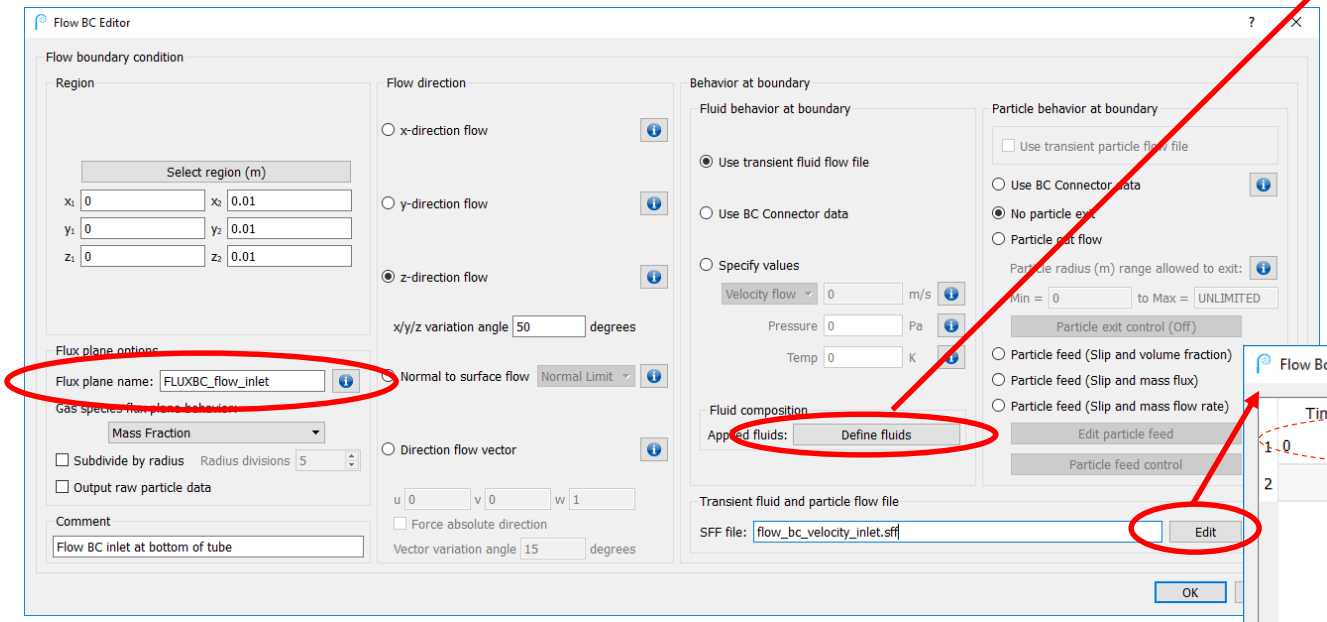
Pressure Boundary Conditions

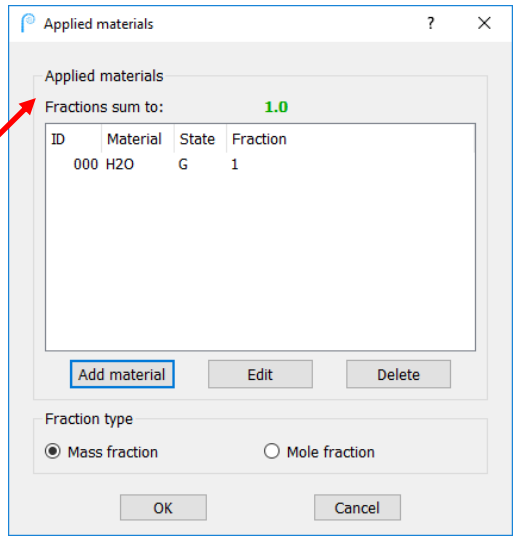
- Define the fluid species for the Pressure BC as 100% N_2
- Be sure to enter the **Flux plane name** as “FLUXBC_pressure_outlet”

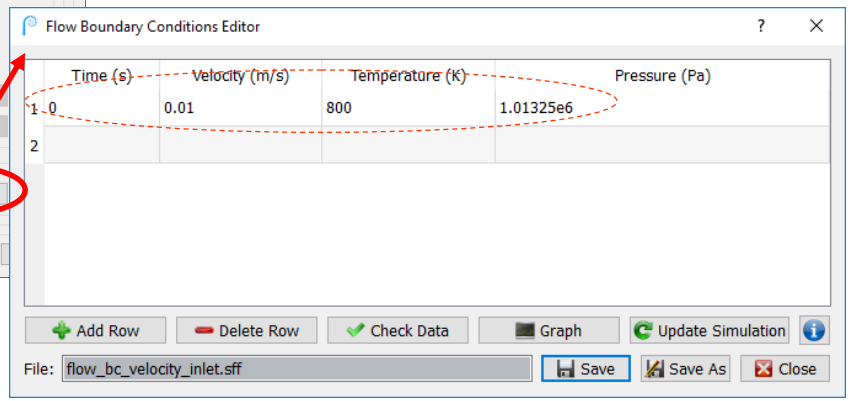


Flow Boundary Conditions

- For the **Flow BC**, use a velocity file to specify the flow of fluid into the bottom of the tube. Feed 0.01 m/s H_2O, at T = 800 K and P = 10 atm
- Remember to save the velocity file before closing the file window
- In the **Applied materials** window, select 100% H_2O
- Be sure to enter the **Flux plane name** as “FLUXBC_flow_inlet”





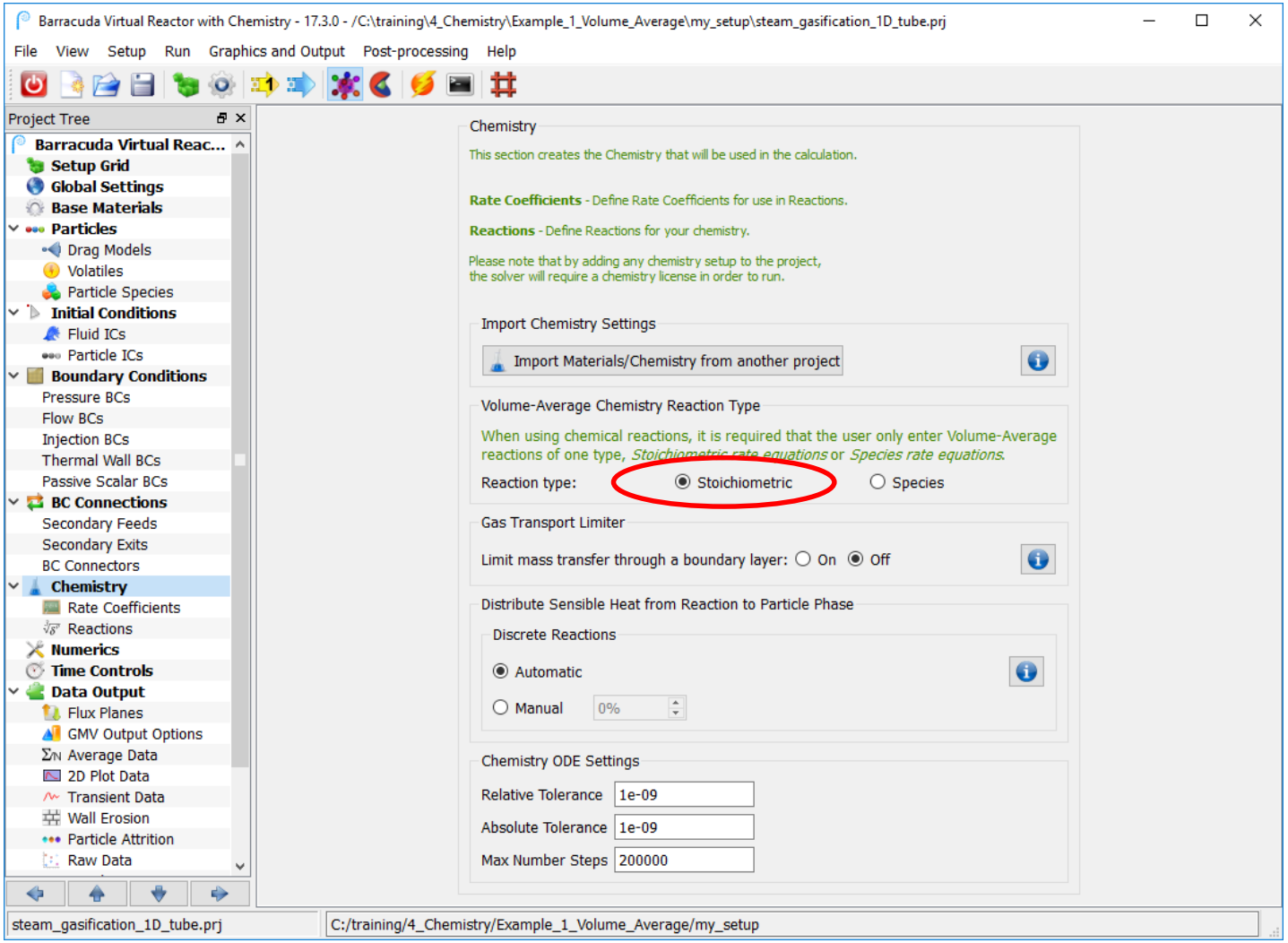


Adding Chemical Reactions

- Materials, particles, and boundaries for the example problem have now been set up.
- Chemistry will be added for the forward and reverse reactions
  - Rate coefficients
  - Stoichiometric reaction rates

Chemistry

- For volume average chemistry, the Stoichiometric and Species forms cannot be mixed.
- In this example, reactions will be entered in the Stoichiometric form



Chemistry

- Recall that the chemical reaction being modeled is:

$$\mathrm{C} + \mathrm{H_2O} \longleftrightarrow \mathrm{CO} + \mathrm{H_2}$$

- In Barracuda, a reversible reaction is defined by splitting it into the forward and reverse reactions, defining a reaction rate for both the forward and reverse directions

Forward Reaction

$$\mathrm{C} + \mathrm{H_2O} \longrightarrow \mathrm{CO} + \mathrm{H_2}$$

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

Reverse Reaction

$$\mathrm{CO} + \mathrm{H_2} \longrightarrow \mathrm{C} + \mathrm{H_2O}$$

$$\frac{d[\mathrm{H_2O}]}{dt} = \left(15.7\ \frac{\mathrm{m}^6}{\mathrm{kg\,mol\,K^2\,s}}\right) T^2 \exp\left(\frac{-33190\,\mathrm{K}}{T}\right) \rho_{\mathrm{C}}\,[\mathrm{H_2}]\,[\mathrm{CO}]$$

The chemical kinetics shown are for demonstration or education purpose only and have not been validated, nor are they recommended for any application. Development, validation, and use of chemical kinetics is the User's responsibility, and CPFD Software, LLC, does not warrant or endorse these chemical kinetics for any purpose.

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:

$$\mathrm{C} + \mathrm{H_2O} \longrightarrow \mathrm{CO} + \mathrm{H_2}$$

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

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

- In Barracuda:

Reaction rate expression: $r_{\text{forward}} = k_0\,[\mathrm{H_2O}]$

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

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

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

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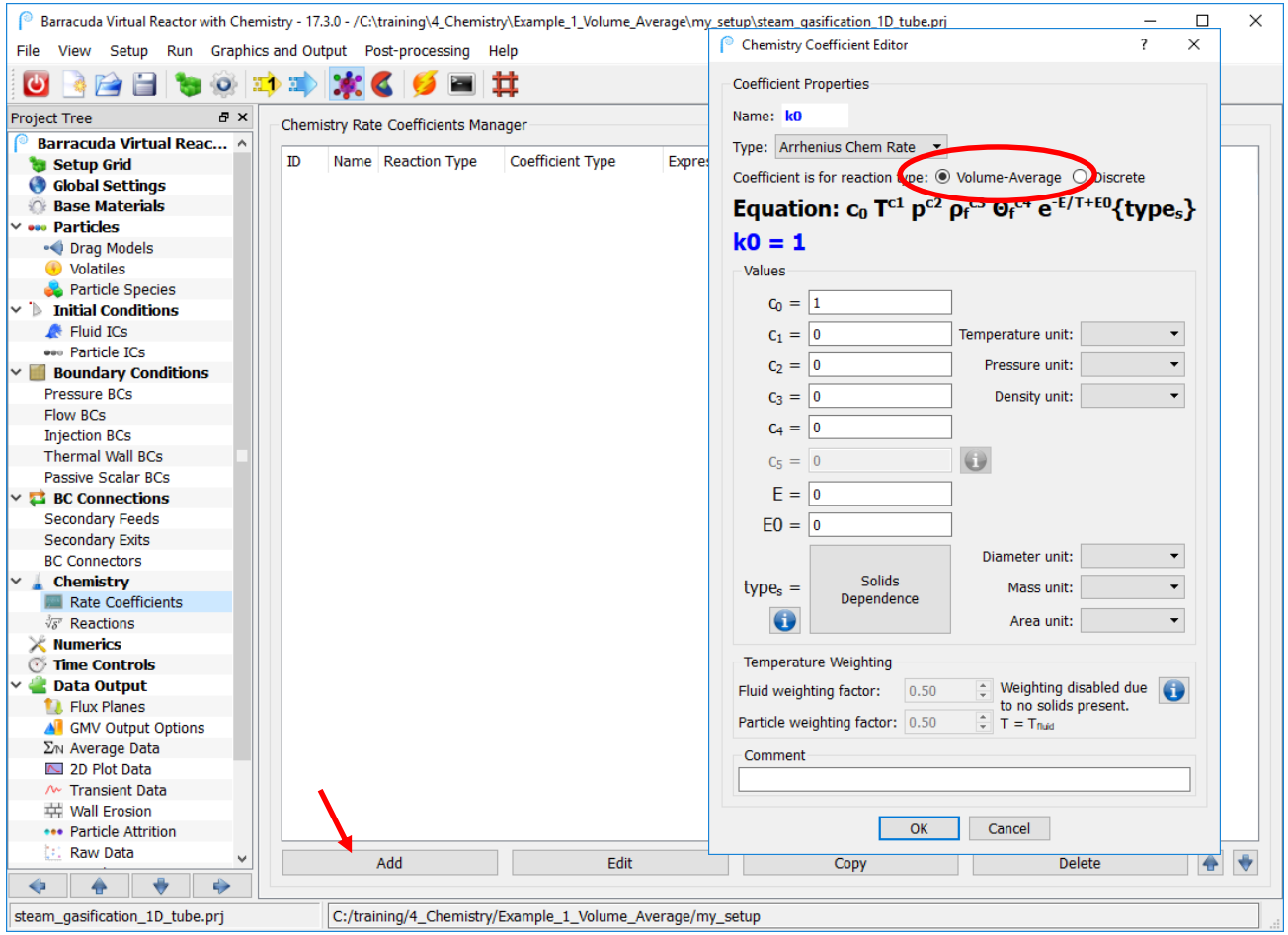
Creating the Forward Rate Coefficient

- To create the rate coefficient for the forward reaction, go to the **Rate Coefficients** section of the tree
- Click **Add**
- The Chemistry Coefficient Editor window will pop up
- Check that **Volume-Average** is selected

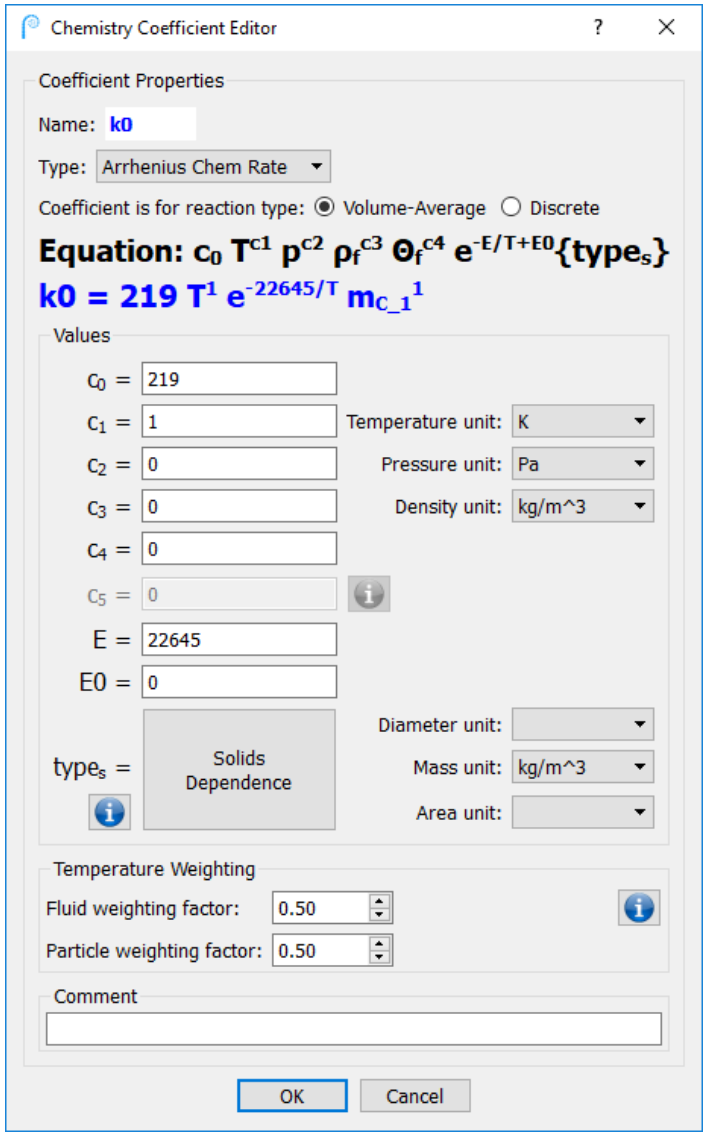


Forward Rate Coefficients

- Enter the equation for k0 as follows:

c_0 c_1 E solids dependence

- $k0 = 219\ T^1 \exp(-22645/T) m_{C\_1}$
- 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



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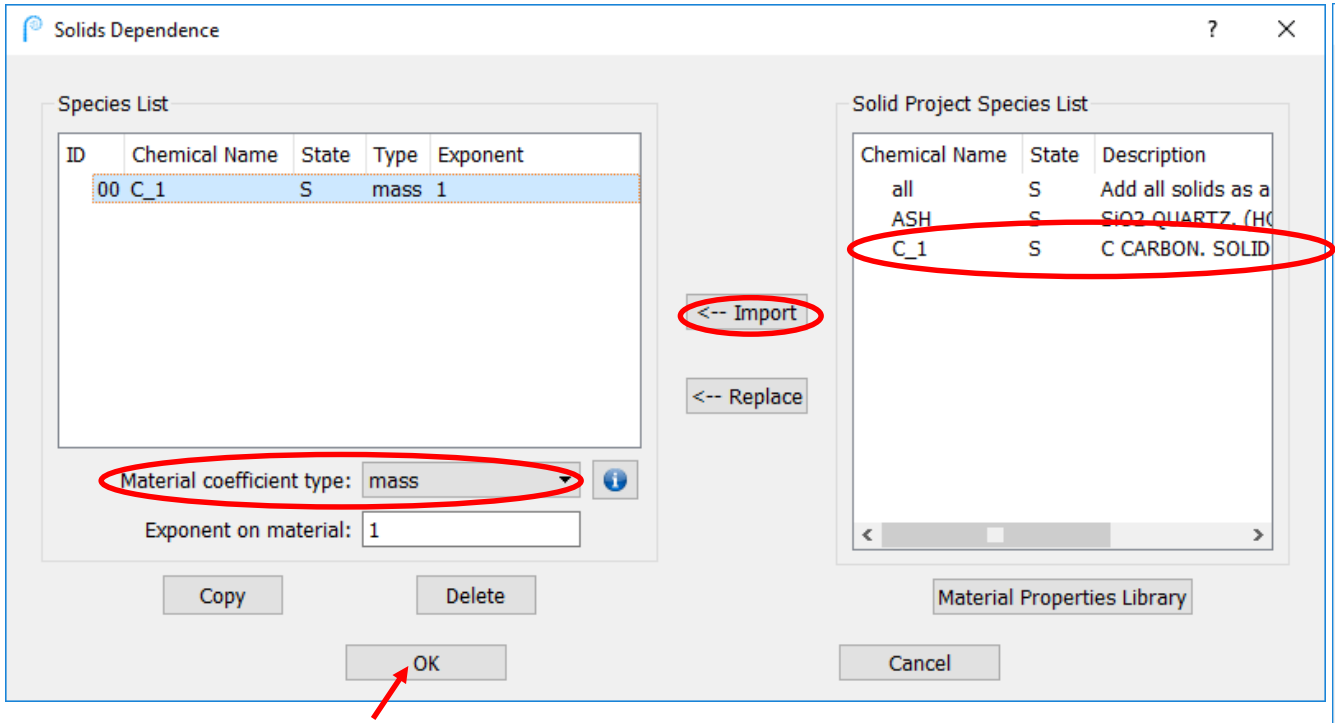
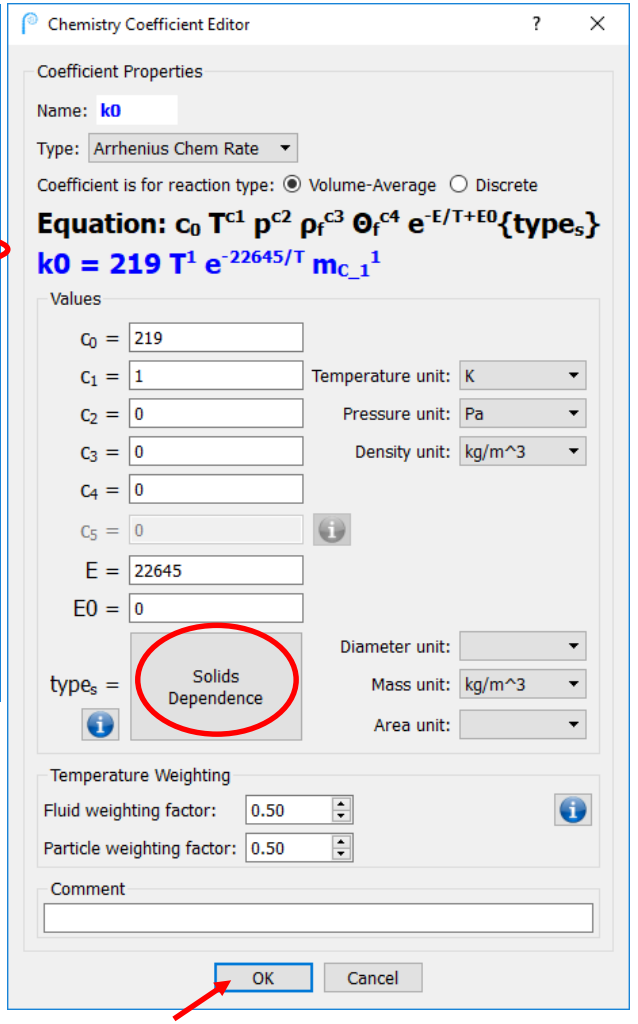
Rate Coefficients: Solids Term

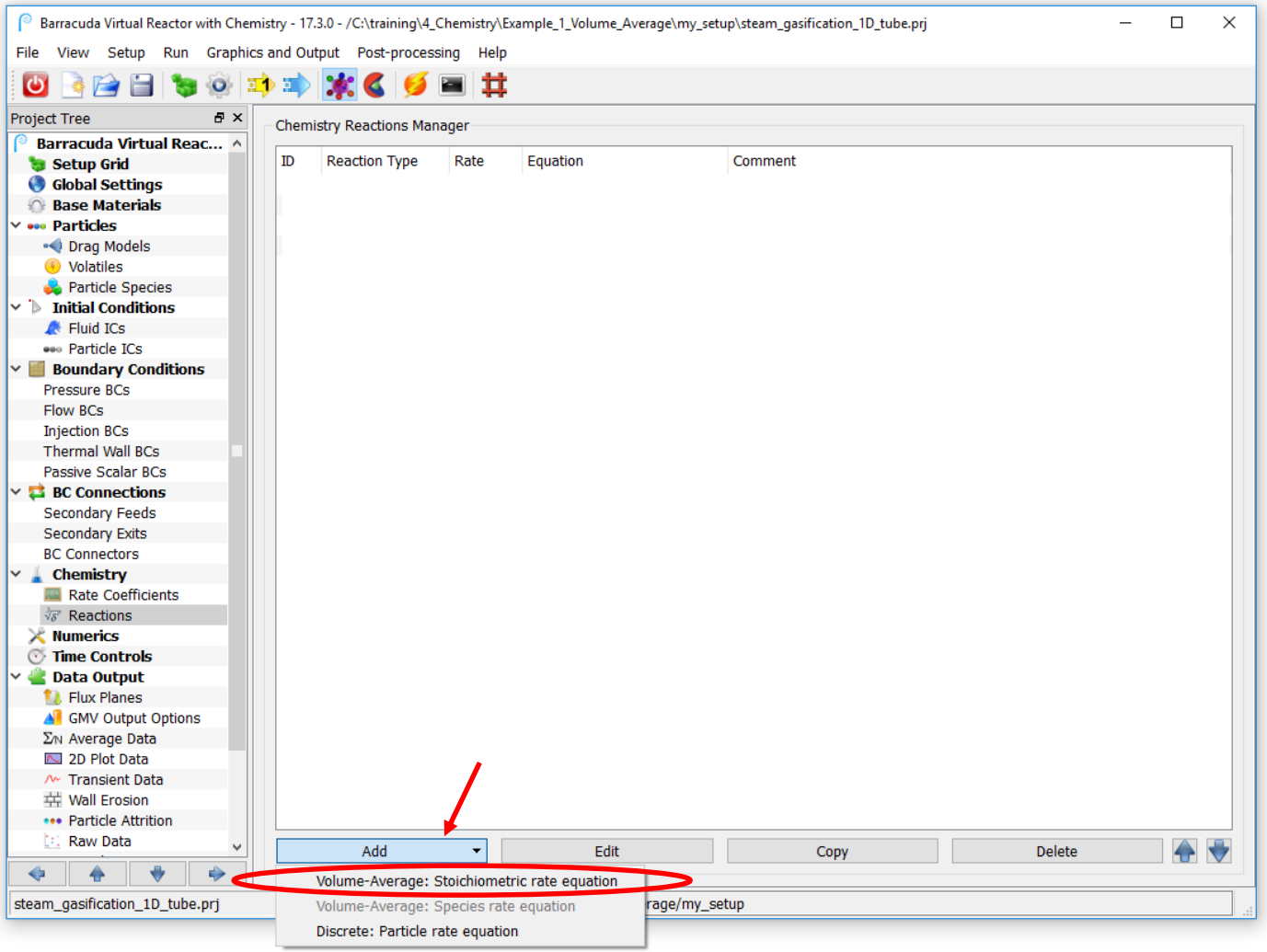
- Click on **Solids Dependence** in the **Chemistry Coefficient Editor** window
- Select C_1 then click **Import**, make sure that **Material coefficient type** is set to **mass**, click **OK**
- Click **OK** in the **Chemistry Coefficient Editor** window





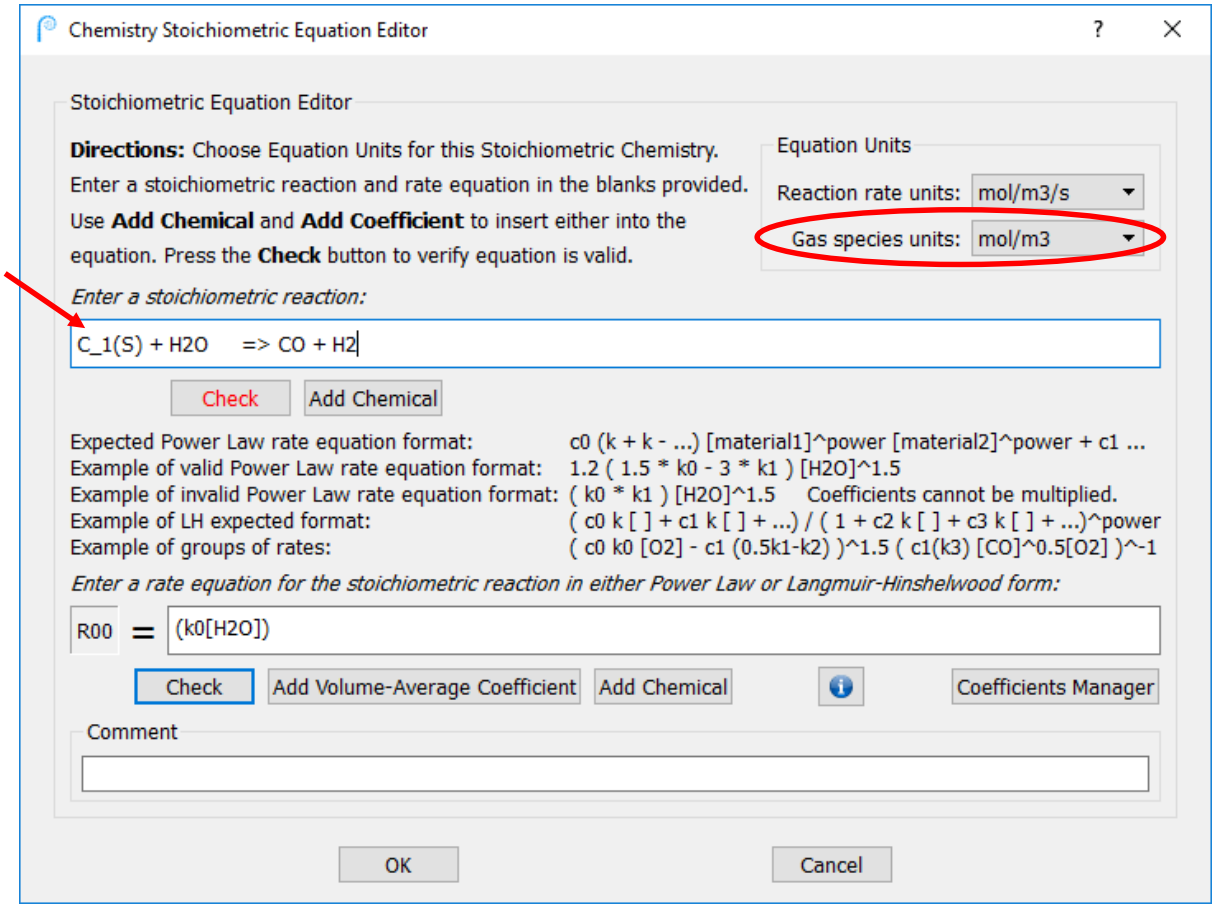
Creating the Forward Reaction

- 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



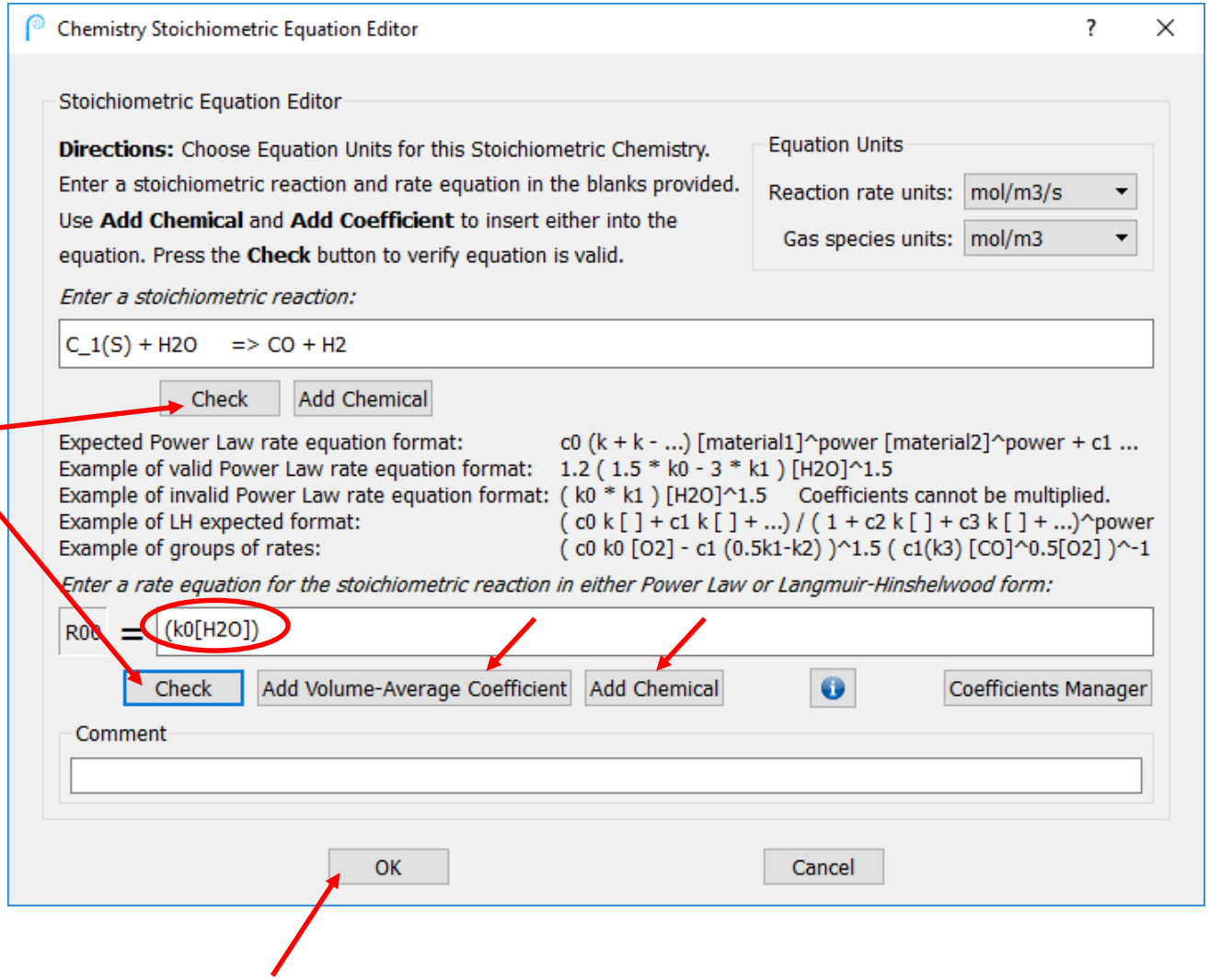
Specifying the Forward Reaction Stoichiometry

- 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, i.e. carbon needs to be entered as “C_1”
  - 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**



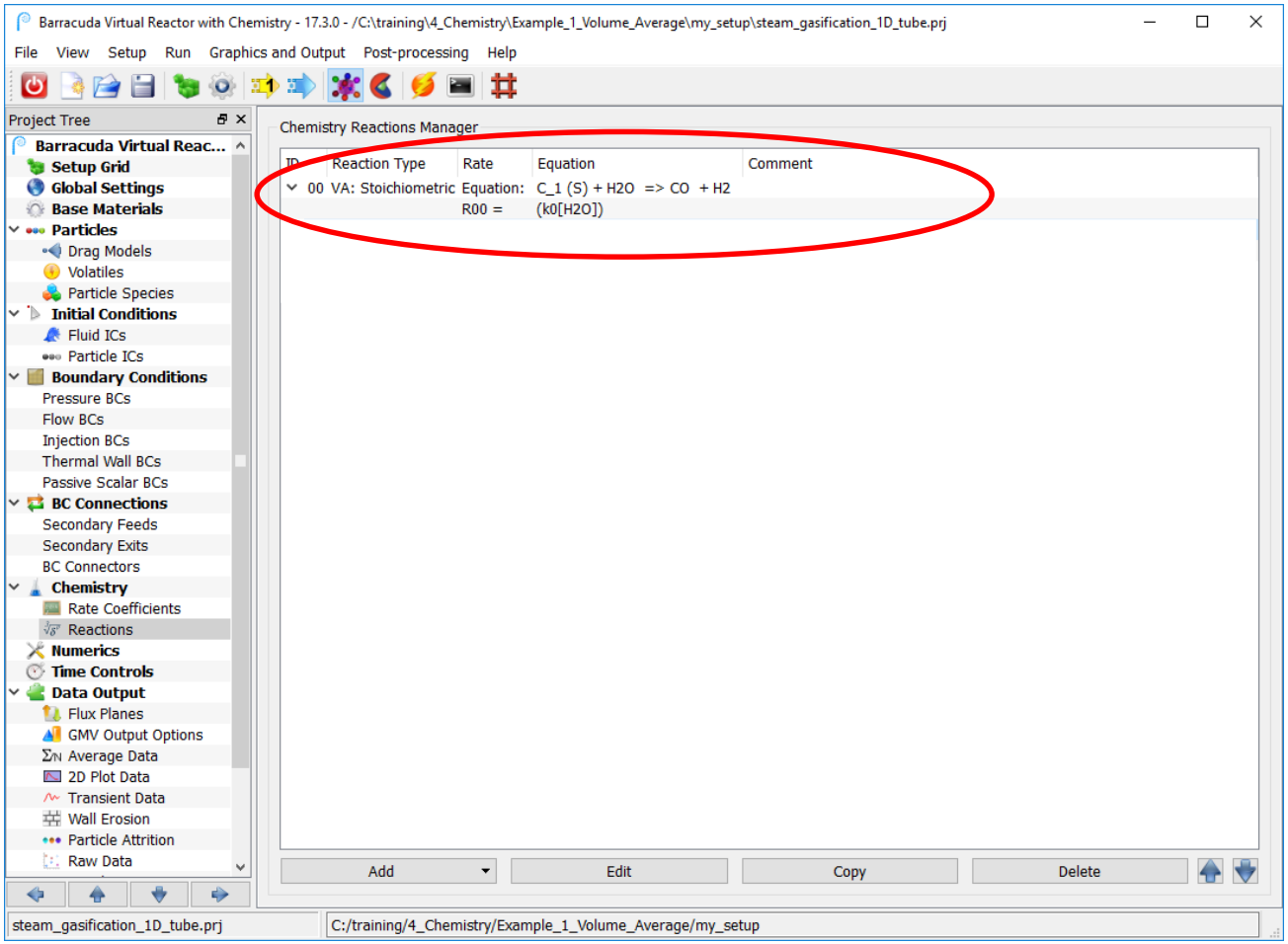
Specifying the Forward Reaction Rate

- To enter the rate equation for the reaction, click **Add Volume-Average Coefficient** and select $\mathbf{k_0}$, then 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**



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 be able to specify the reverse reaction by the stoichiometric equation.

$$\mathrm{CO} + \mathrm{H_2} \longrightarrow \mathrm{C} + \mathrm{H_2O}$$

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

- In Barracuda,

$$\frac{d[\mathrm{H_2O}]}{dt} = \left(15.7 \, \frac{\mathrm{m^6}}{\mathrm{kg\,mol\,K^2\,s}}\right) T^2 \exp\left(\frac{-33190\,\mathrm{K}}{T}\right) \rho_{\mathrm{C}} \, [\mathrm{H_2}] \, [\mathrm{CO}]$$

Reaction rate expression: $r_{\mathrm{reverse}} = k_1 \, [\mathrm{H_2}] \, [\mathrm{CO}]$

Reaction rate units: mol/m^3/s **Gas concentration units:** mol/m^3

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

Temperature units: K **Solid Mass units:** kg/m^3

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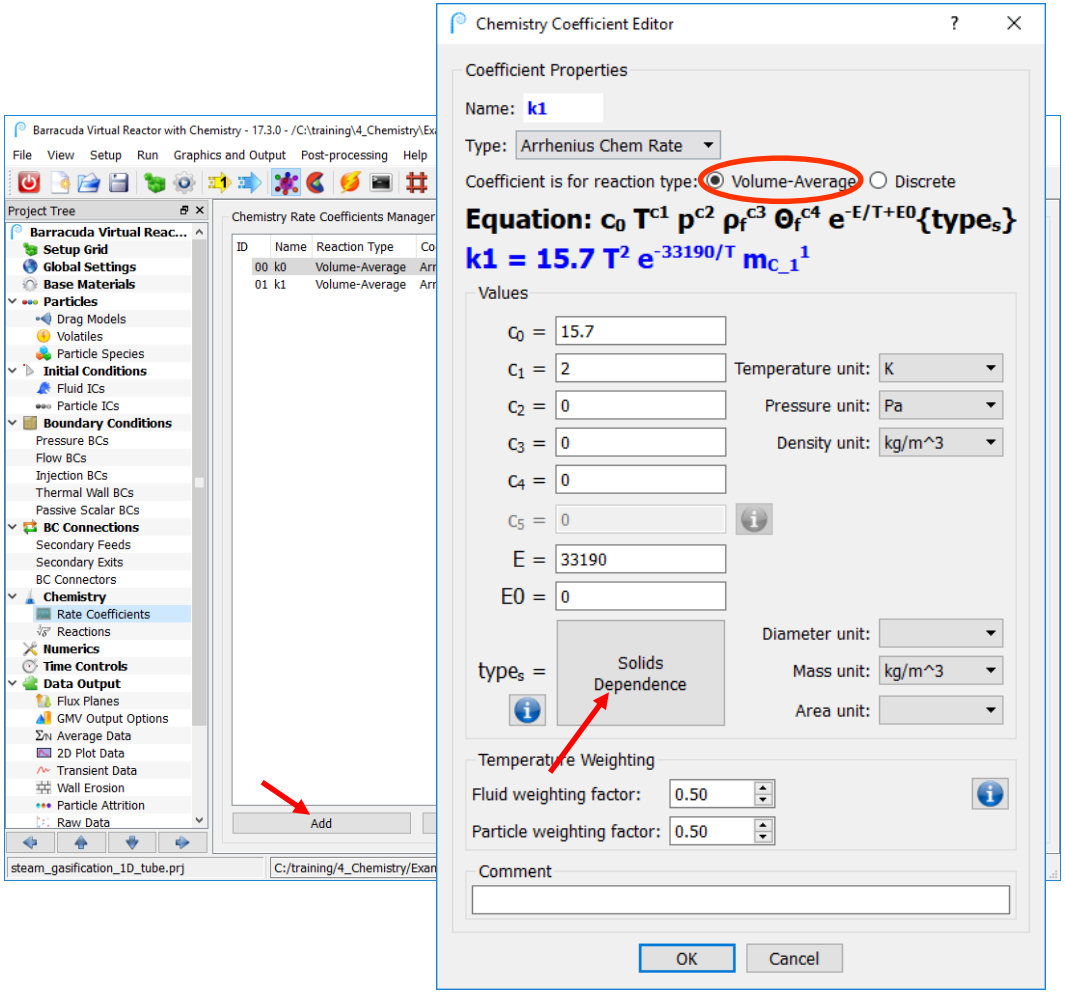
Rate Coefficient: Reverse Reaction

- 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

- $k1 = 15.7\ T^2 \exp(-33190/T) m_{C:1}$
- 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_1** and set **Material coefficient type** to **mass**



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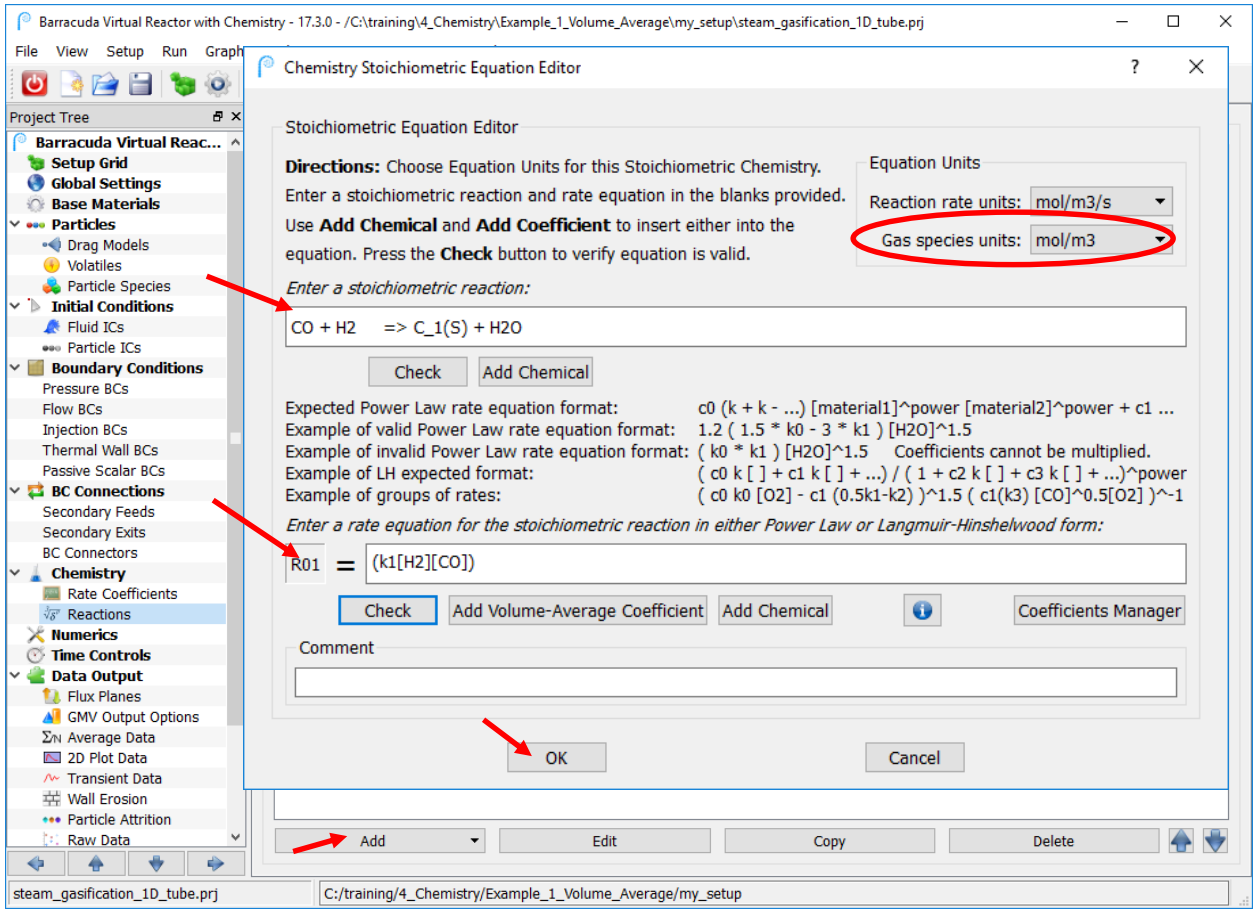
Chemical Equations: Reverse Reaction

- Define the stoichiometric equation for the reverse reaction:
  CO + H2 → C + H2O
- Enter the rate equation for the reverse reaction as follows:
  R01 = $k_1[H_2][CO]$
- 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** when finished



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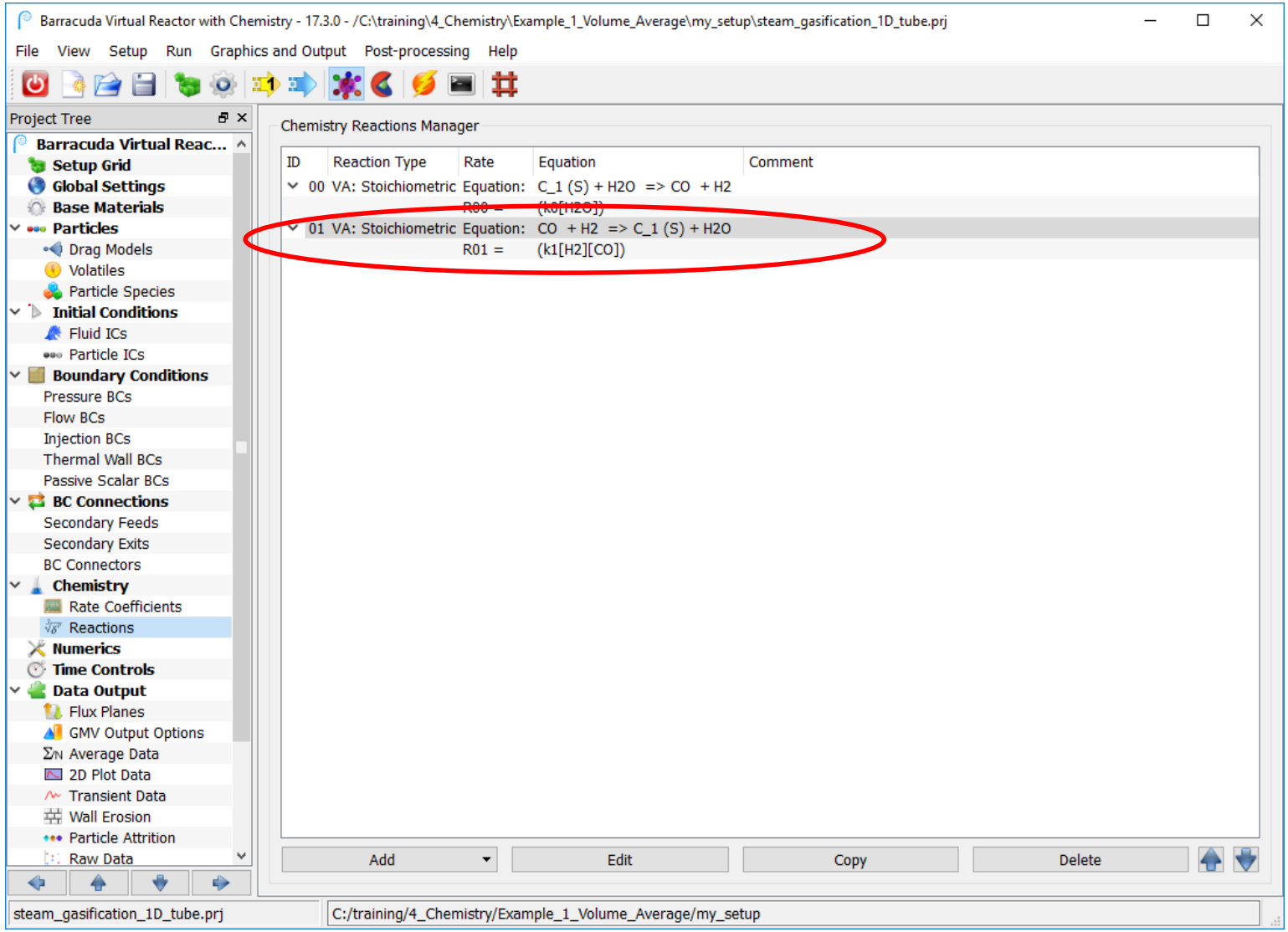
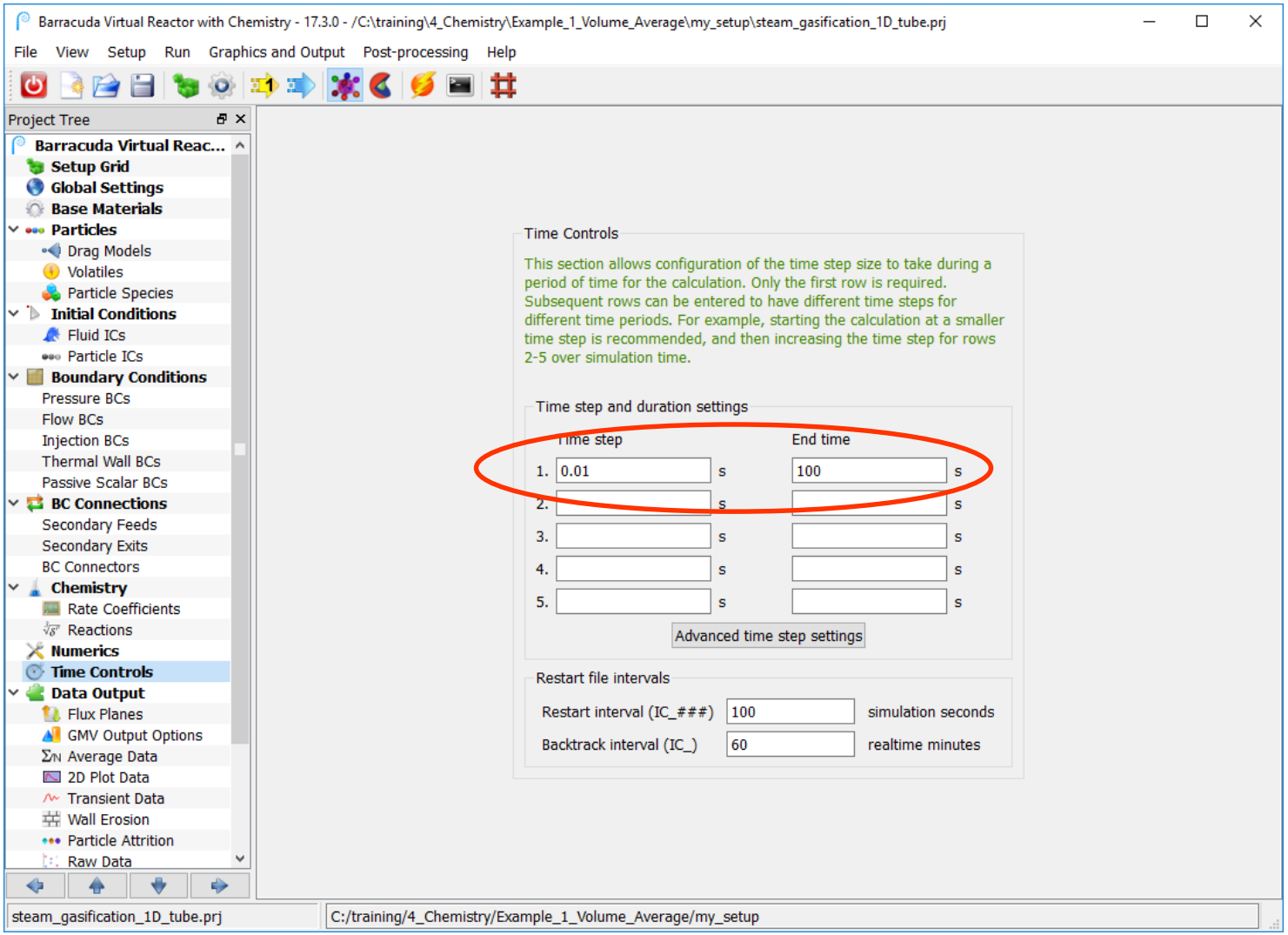
Reverse Reaction

- The reverse reaction is now complete



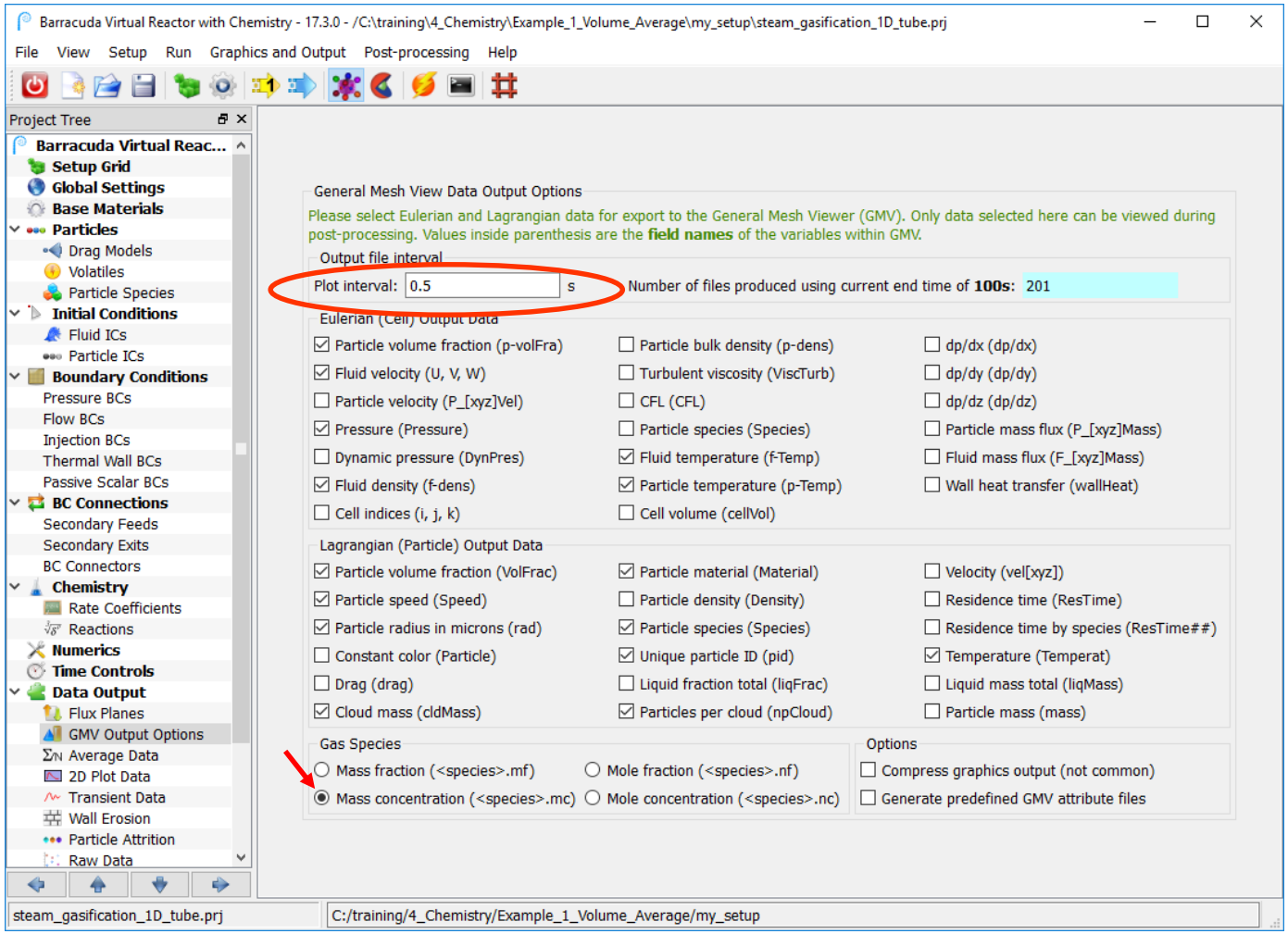
Time Controls

- Enter **Time step** and **End time** as shown below:

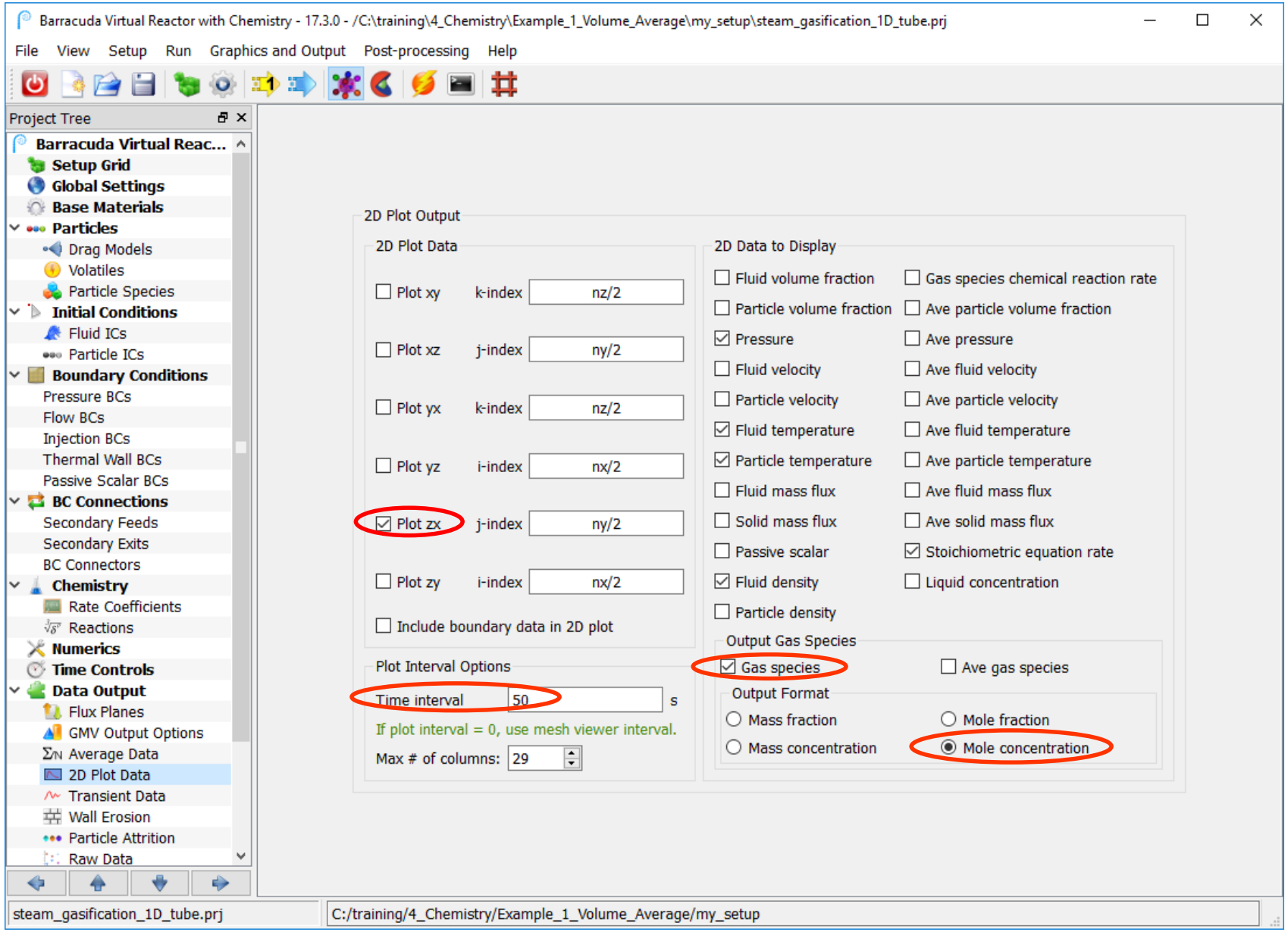


GMV Output Options

- Enter a **Plot interval** of “0.5” s
- Choose the GMV output variables shown on the right
- Note that only one Gas Species option can be chosen, in this case use **Mass concentration**

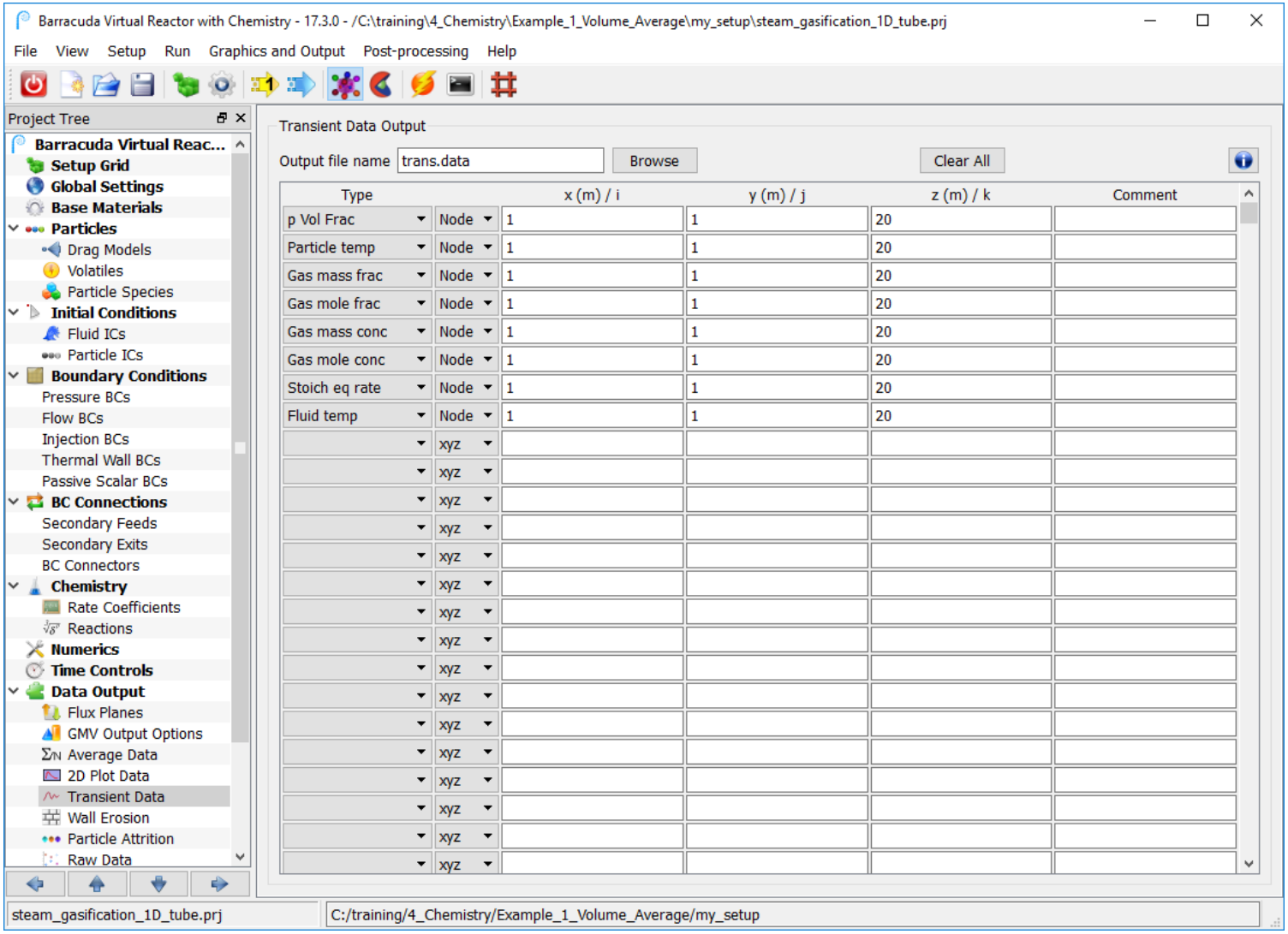


Select 2D Data



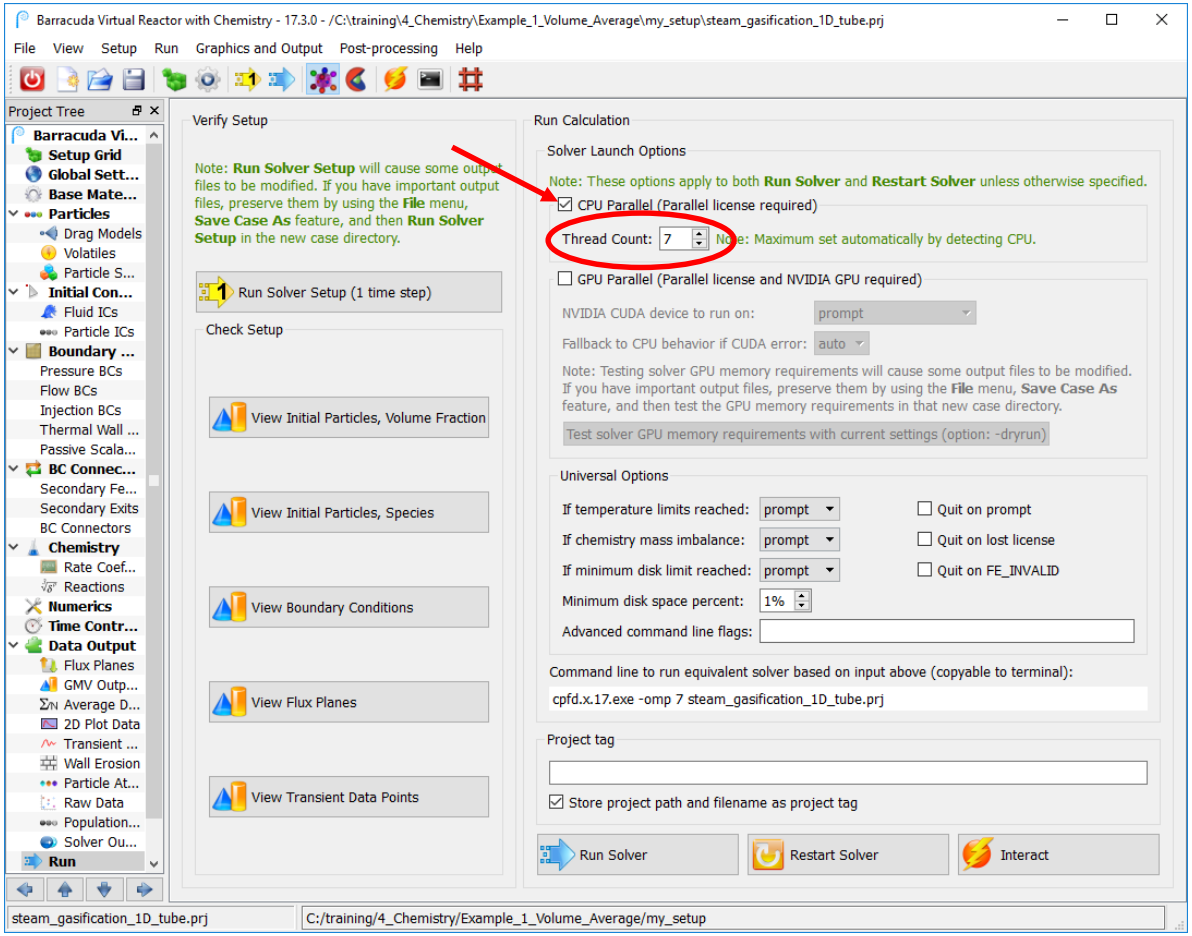
Transient Data Output

- For transient data, choose the options shown below



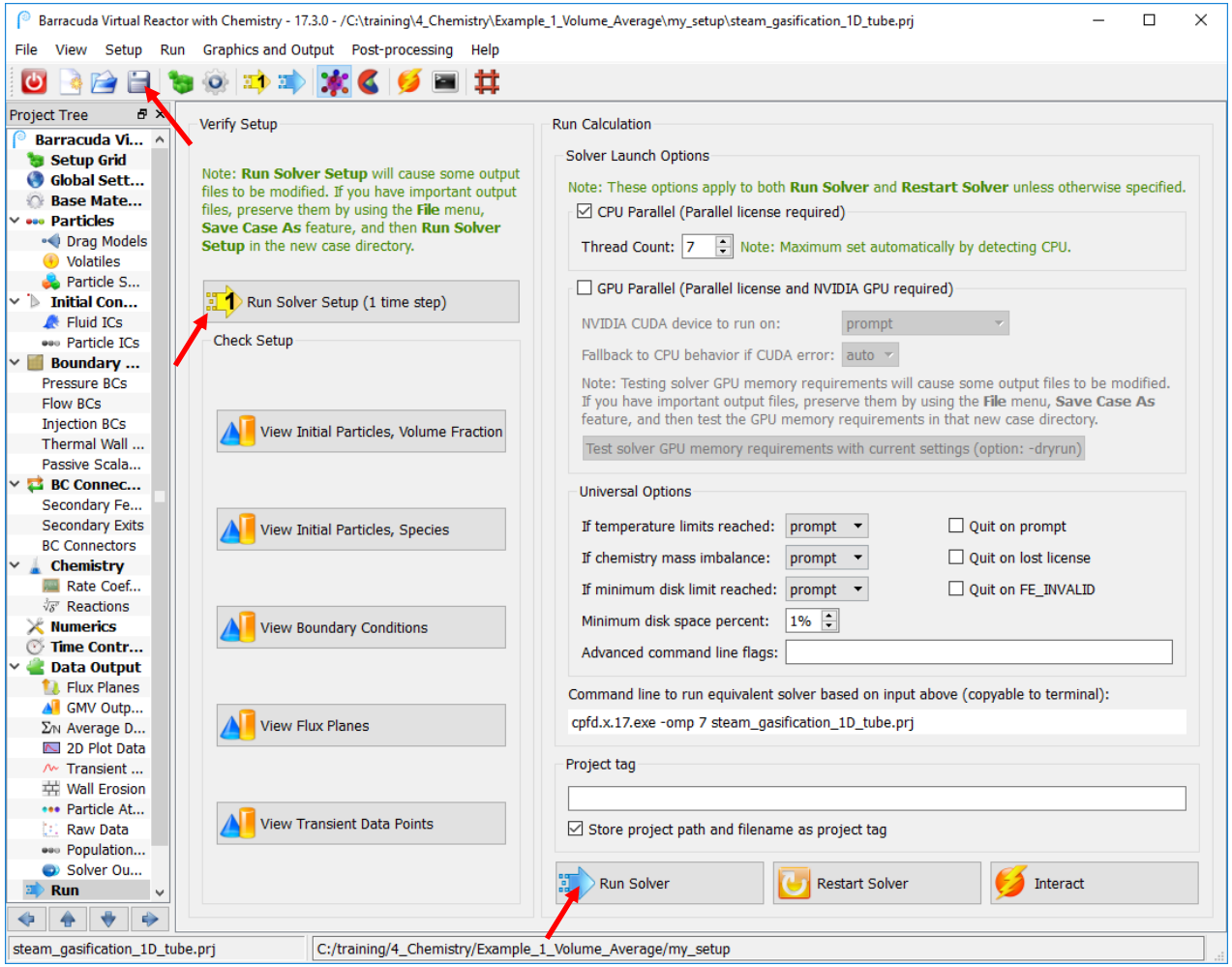
Set CPU Parallel

- Set CPU Parallel to one less than system virtual (logical) cores
  - Virtual (logical) cores are the physical cores multiplied by the hyper-threading count
  - Barracuda Virtual Reactor GUI will automatically detect this number
  - When running multiple simulations keep at least 1 CPU for running operating system
- CPU Parallel is only applied to volume averaged chemistry calculations



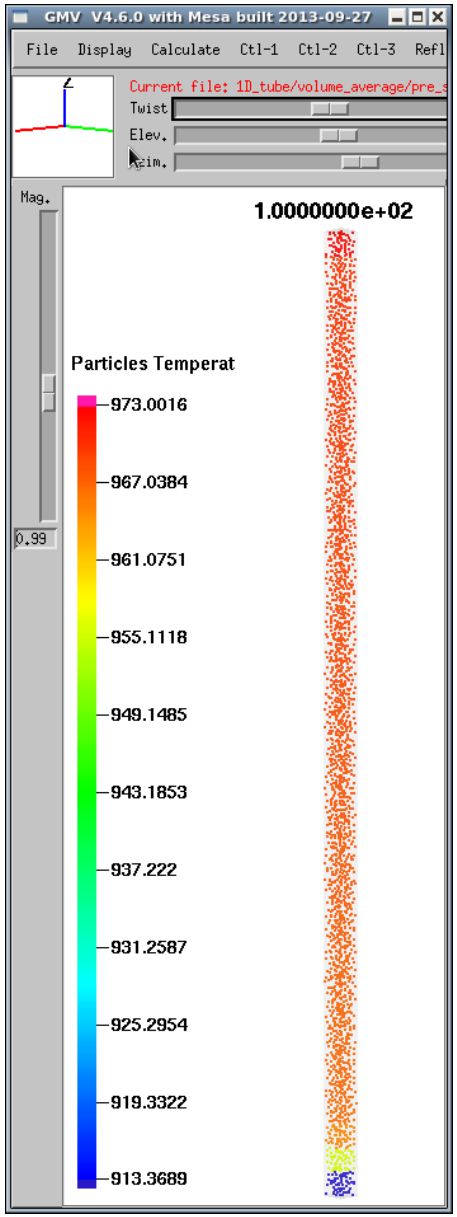
Start the Barracuda Solver

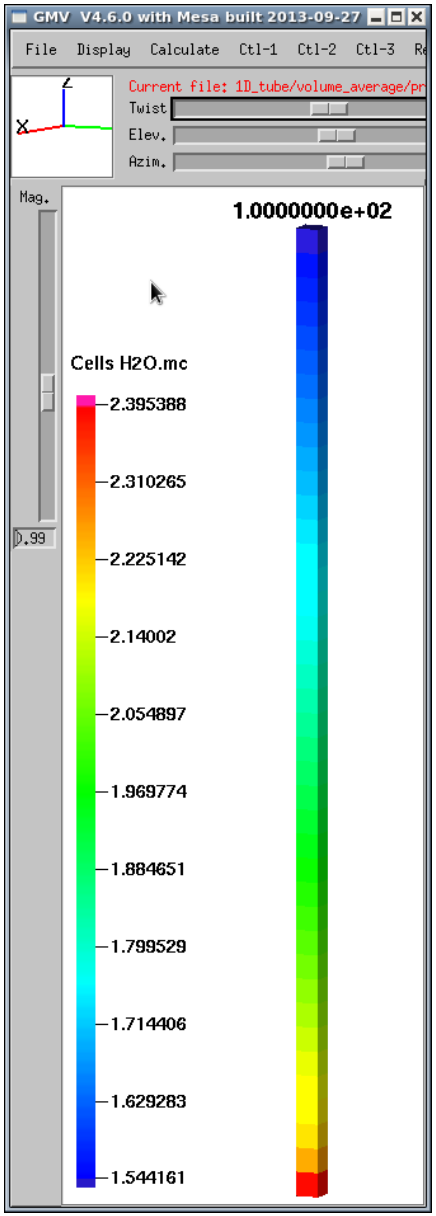
- Save the project file
- Verify your setup with **Run Solver Setup (1 time step)**
- Start the simulation



Post Processing

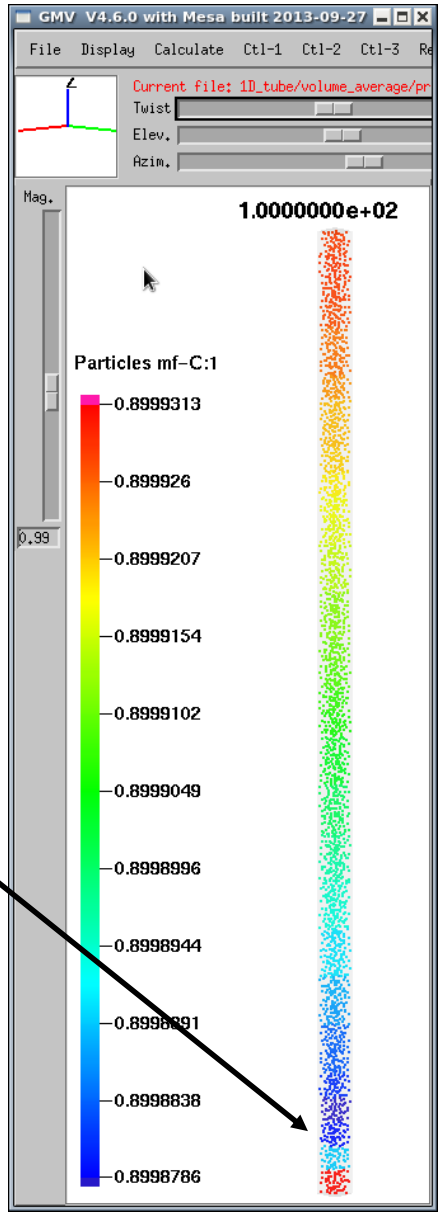
- Analyze the particle temperature and steam concentration in GMV
  - To view the particle temperature throughout the tube, use the **Particle Temperature** button
  - To view the mass concentration of steam throughout the tube, color cells by **Cell Field: H2O.mc**





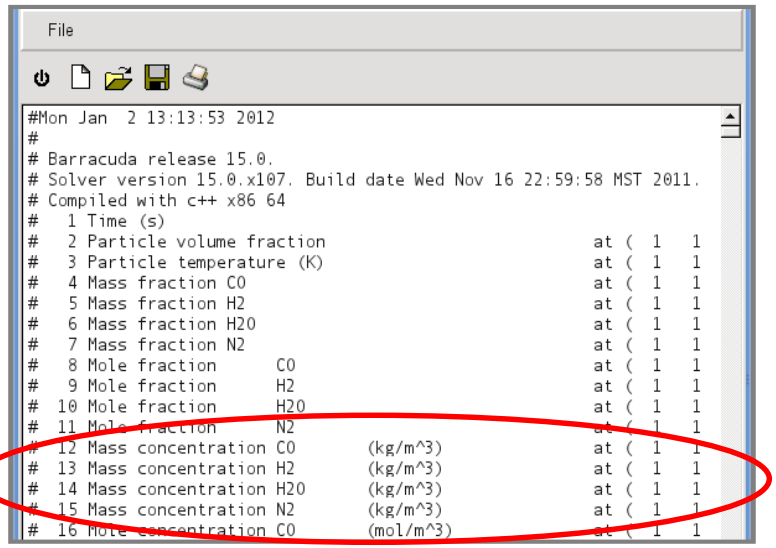
Post Processing

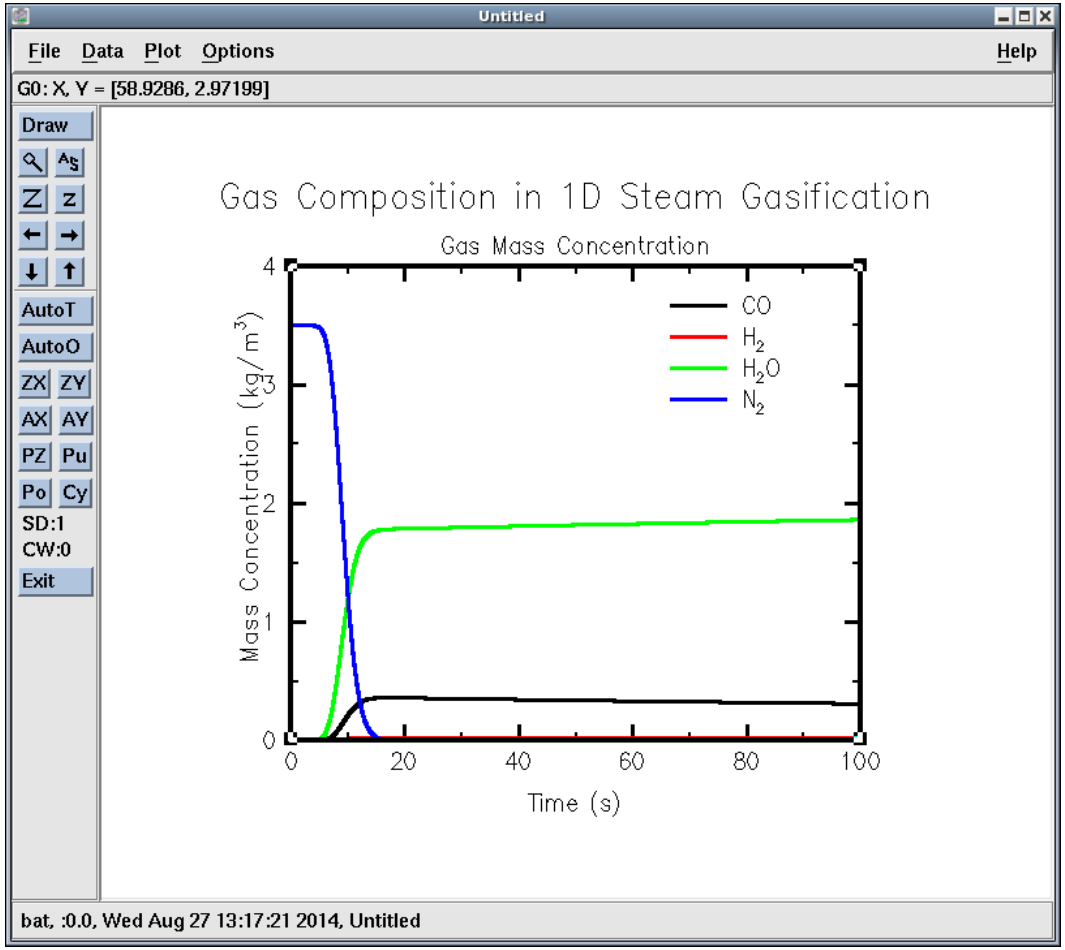
- Analyze the mass fraction of carbon in GMV
  - Hint: Display particles and color by **mf-C_1**
- How do the temperature and steam concentration help explain the mass fraction of carbon throughout the tube at 100 seconds?
- What is happening here?



Plotting Transient Data

- Make a plot of the mass concentration of all gas species versus time in Plot Manager
  - Hint: refer to the Kuipers post processing exercise in plotting
  - Data is in the **trans.data00** file
  - The plot shows the gas concentrations in the cell containing the transient data (z ~ 0.2 m)

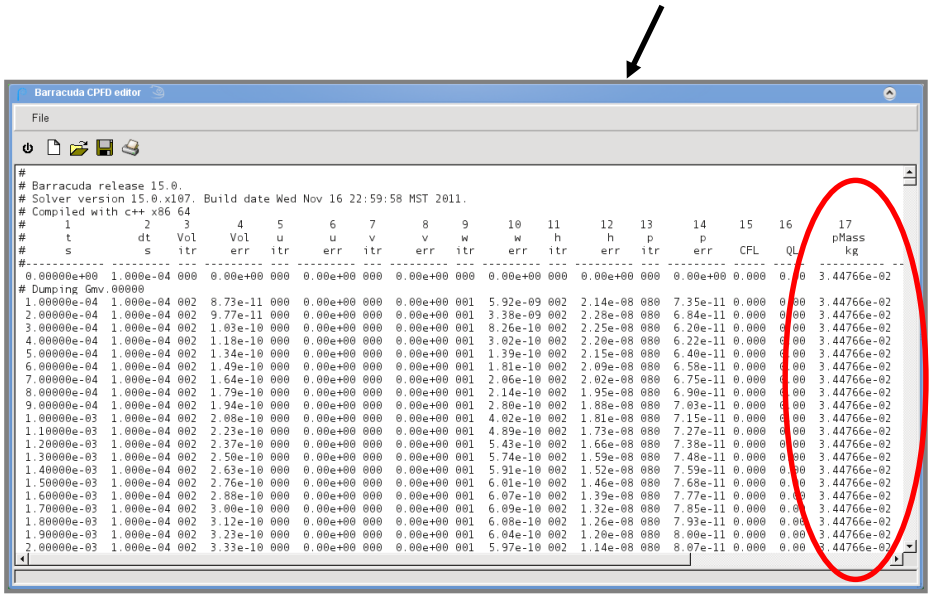


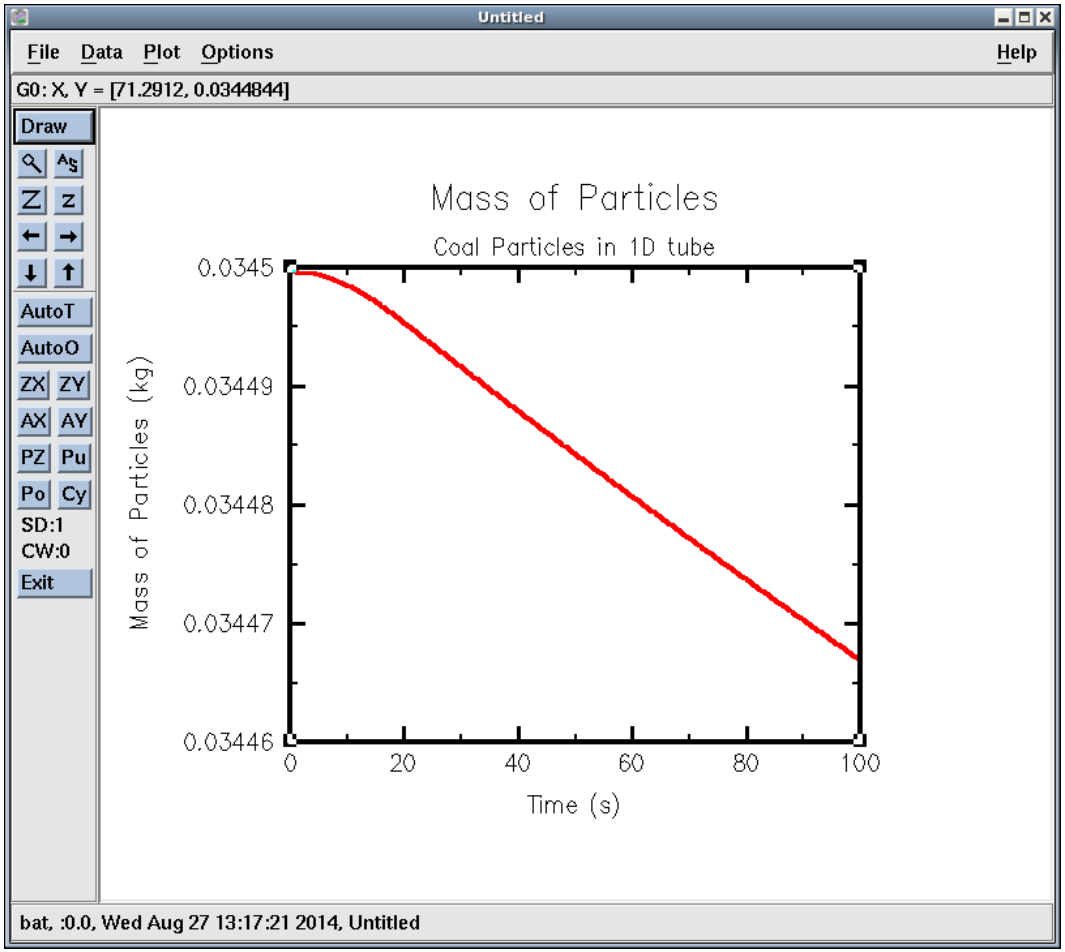


N_2 concentration goes to zero as H_2O is fed into the system and H_2 and CO are produced. All N_2 initially in tube is pushed out.

Plotting Transient Data

- Next, make a plot of the mass of coal particles versus time in Plot Manager
  - Hint: Data is in the **history.log** file



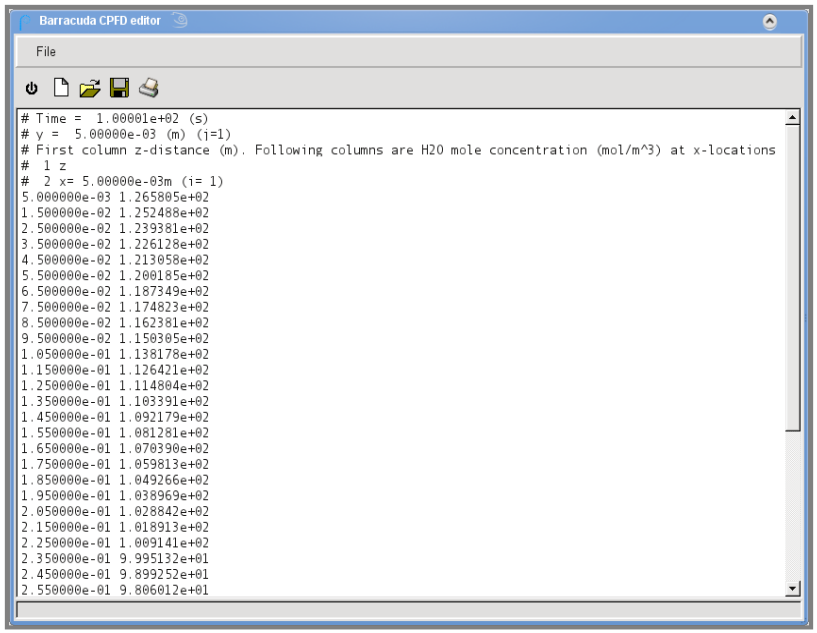


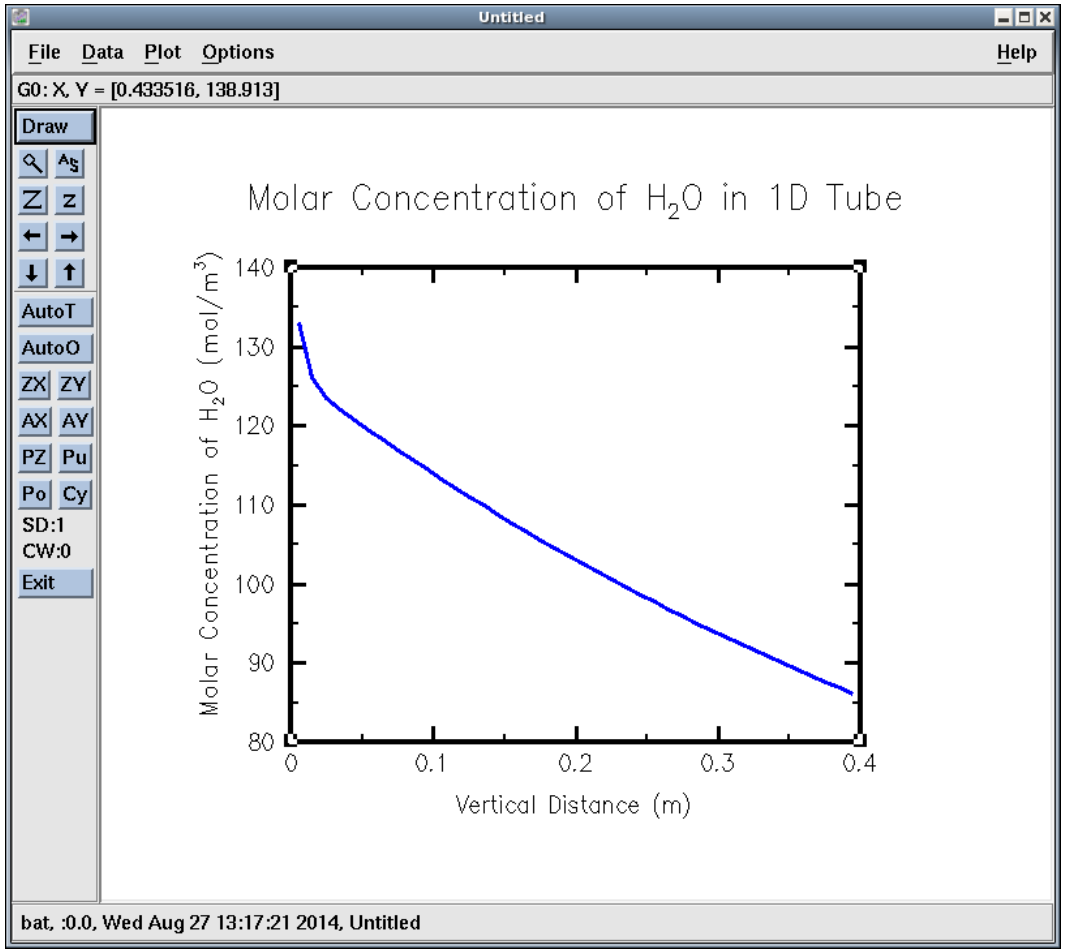
The solids mass in the system decreases as carbon is consumed in the reaction.

Plotting 2D Data

- Make a plot of the molar concentration of H_2O versus vertical distance in Plot Manager
  - Hint: Data is in the **H2O_zx_MoleConc_00100.003.dat** file

Note that this filename may be slightly different, due to the time-stamp. Choose the file closest to t = 100 s.





The concentration of H_2O is highest at the bottom of the tube.

Summary

- This example problem introduced several important components of a typical Barracuda simulation with chemistry:
  - Defining material properties
  - Defining stoichiometric chemical reactions
  - Defining a reversible chemical reaction by splitting the reaction into forward and reverse directions
  - Defining reaction rate equations for chemical reactions
- Additionally, some generally useful concepts were presented:
  - The “No particle momentum” option is useful for simulations in which you are first exploring the behavior of a set of chemical reactions. The simulation runs faster because the momentum equations are not solved for the particles, but they still participate fully in thermal and chemical calculations