Chemistry Training Example 2: Discrete Particle

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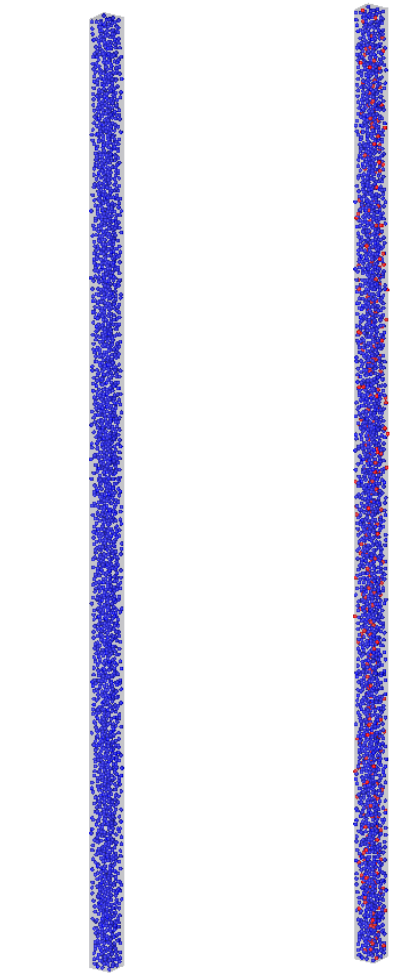
CPFD Software LLC
10899 Montgomery Blvd. NE, Suite A
Albuquerque, NM 87111
+1.505.275.3849
www.cpfd-software.com

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 void fraction is 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 #2 will be set up with discrete particle 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 become **mol/m³/s**.

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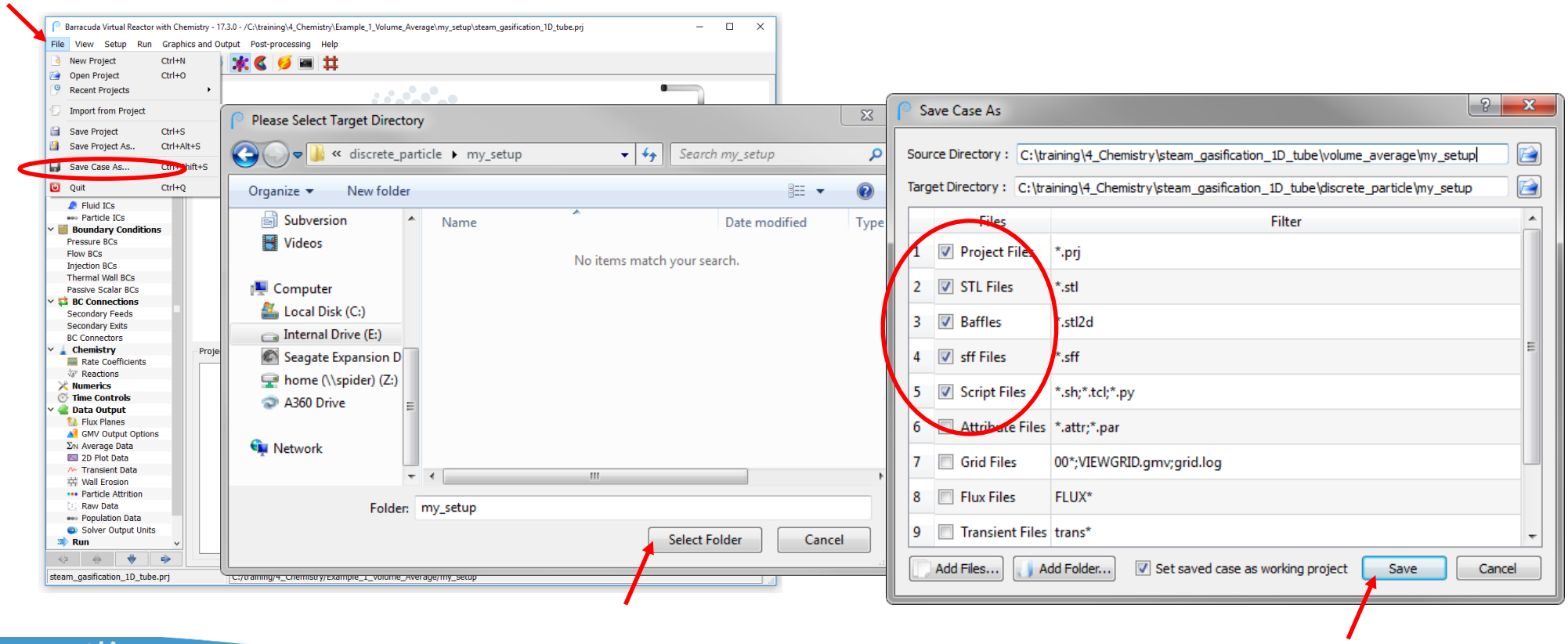
Modifications to Project Setup

- Discrete chemistry example will be set up by modifying the volume average chemistry example
- The following modifications will be made:
  - Save existing project as a new project file in a new directory
  - Add a new particle species
  - Adjust boundary conditions
  - Replace volume average reactions with discrete particle reactions

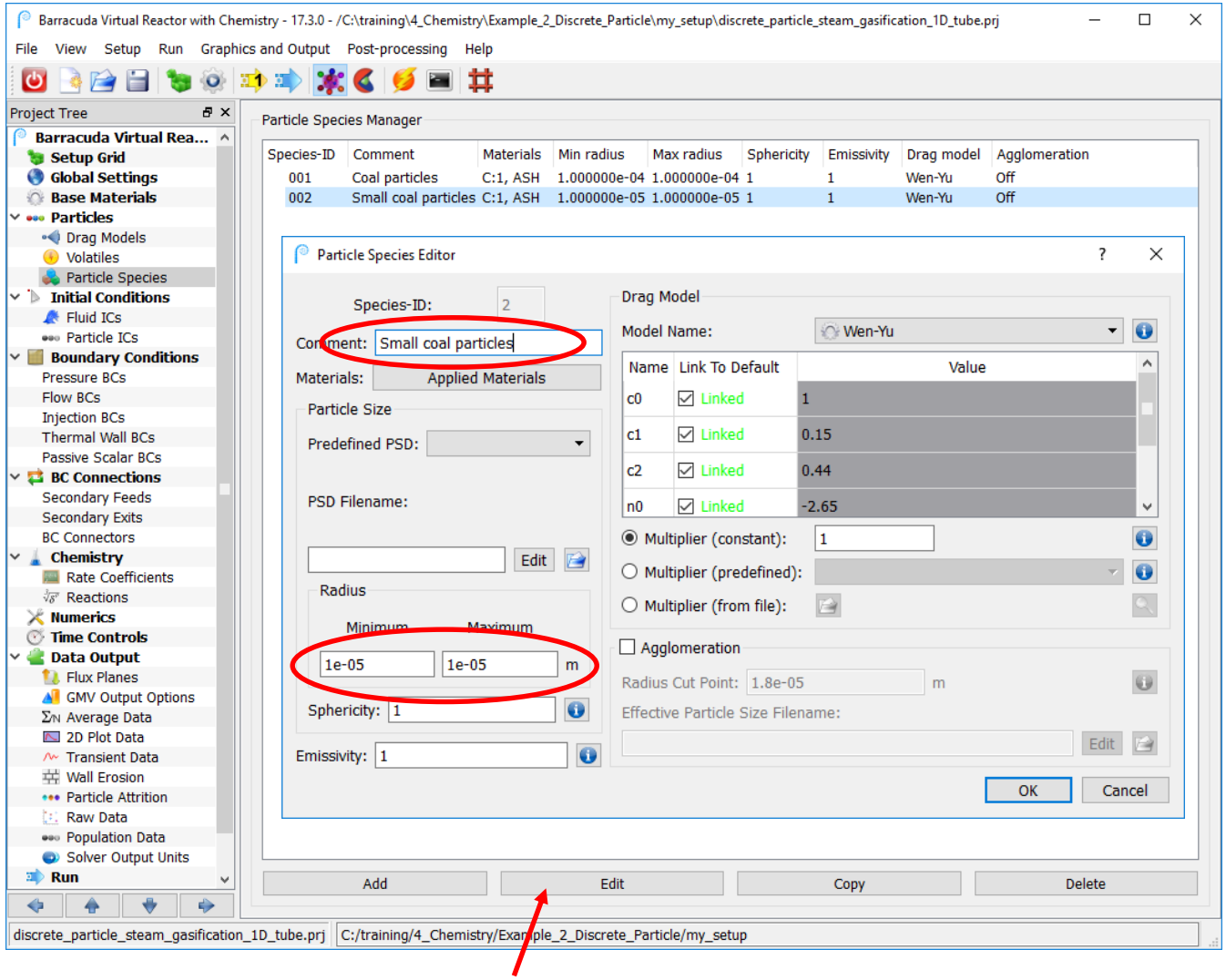
Saving a New Project File

- The existing project file will be used as the starting point for part II of this example
- Use the Save Case As command to save a copy of the project file in the directory shown below:
  - Linux: /home/training/barracuda_training/4_Chemistry/steam_gasification_1D_tube/discrete_particle/my_setup
  - Windows: C:\training\4_Chemistry\steam_gasification_1D_tube\discrete_particle\my_setup
- Select the files shown in the Save Case As dialog box and click **Save**



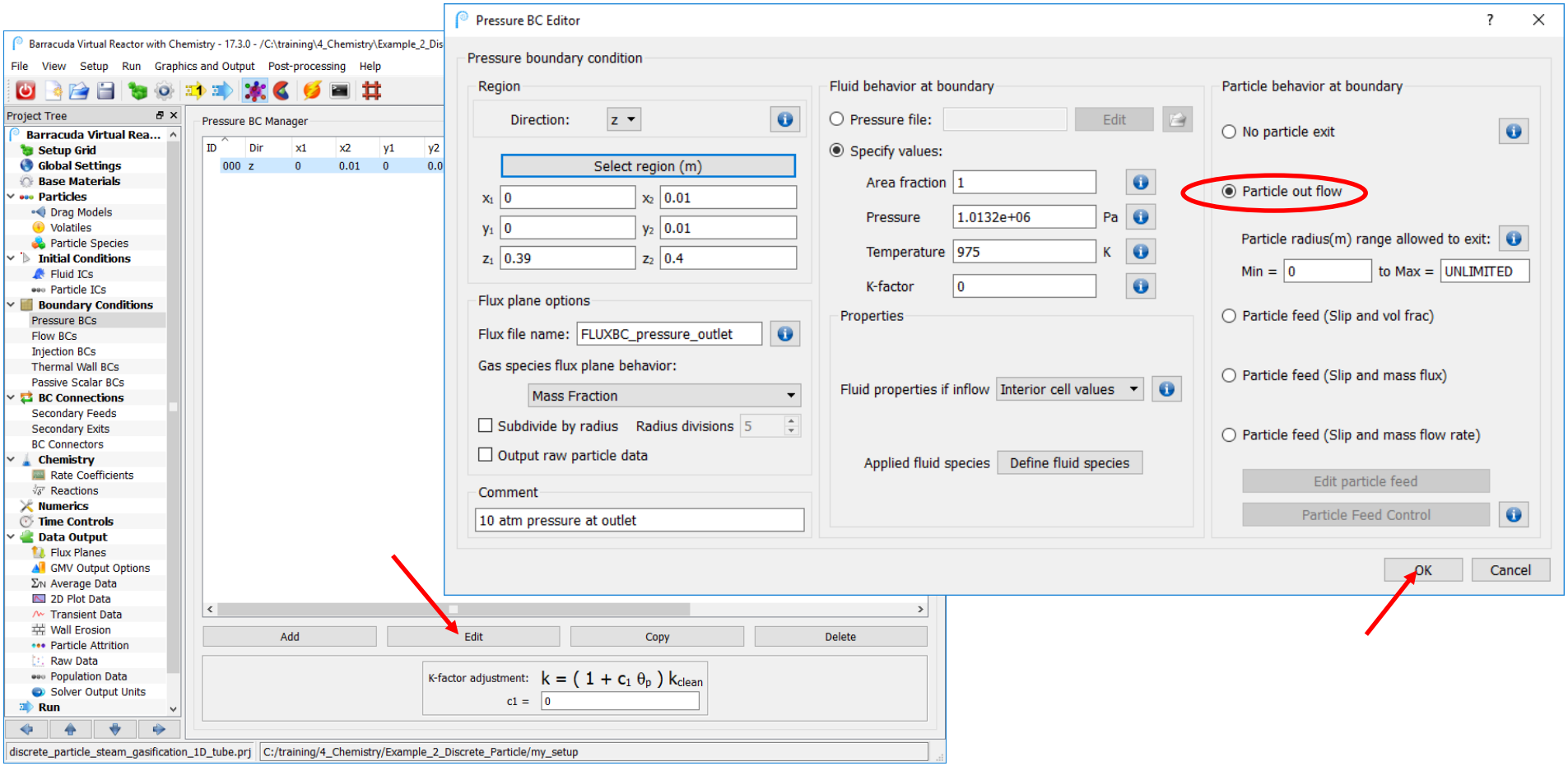
Adding a Particle Species

- Small coal particles need to be added as a new species for the reactor feed
- **Copy** particle species 001 to create a new particle species (002)
- **Edit** species 002, changing the **Radius** to “10 μm” (1e-5 m, 1e-5 m) and the **Comment** to “Small coal particles”
- Click **OK**



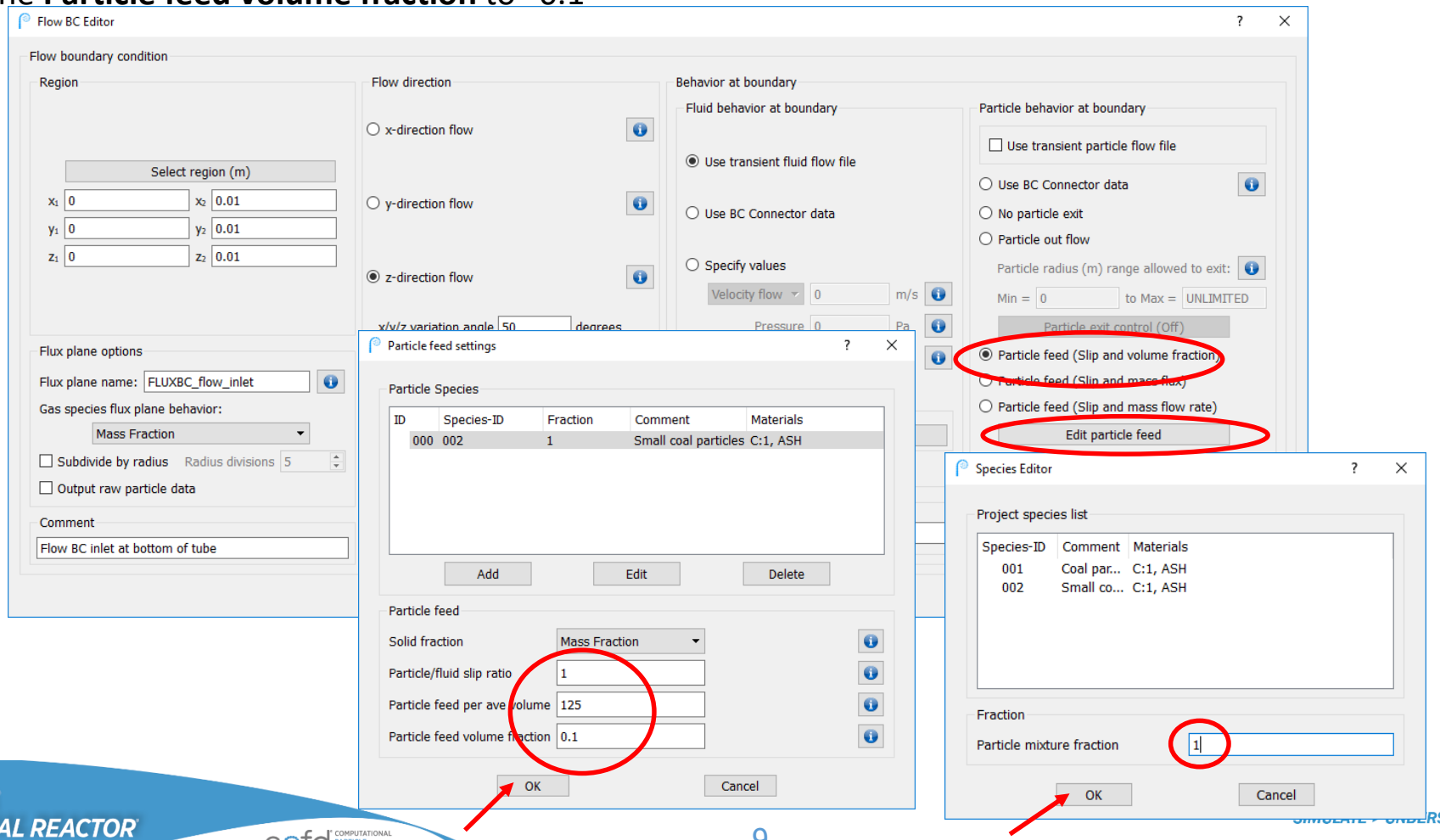
Pressure Boundary Conditions

- The small coal particles being added to the reactor will be allowed to leave at the reactor outlet
- Edit the **Particle behavior at boundary** from **No particle exit** to **Particle out flow**
- Click **OK**



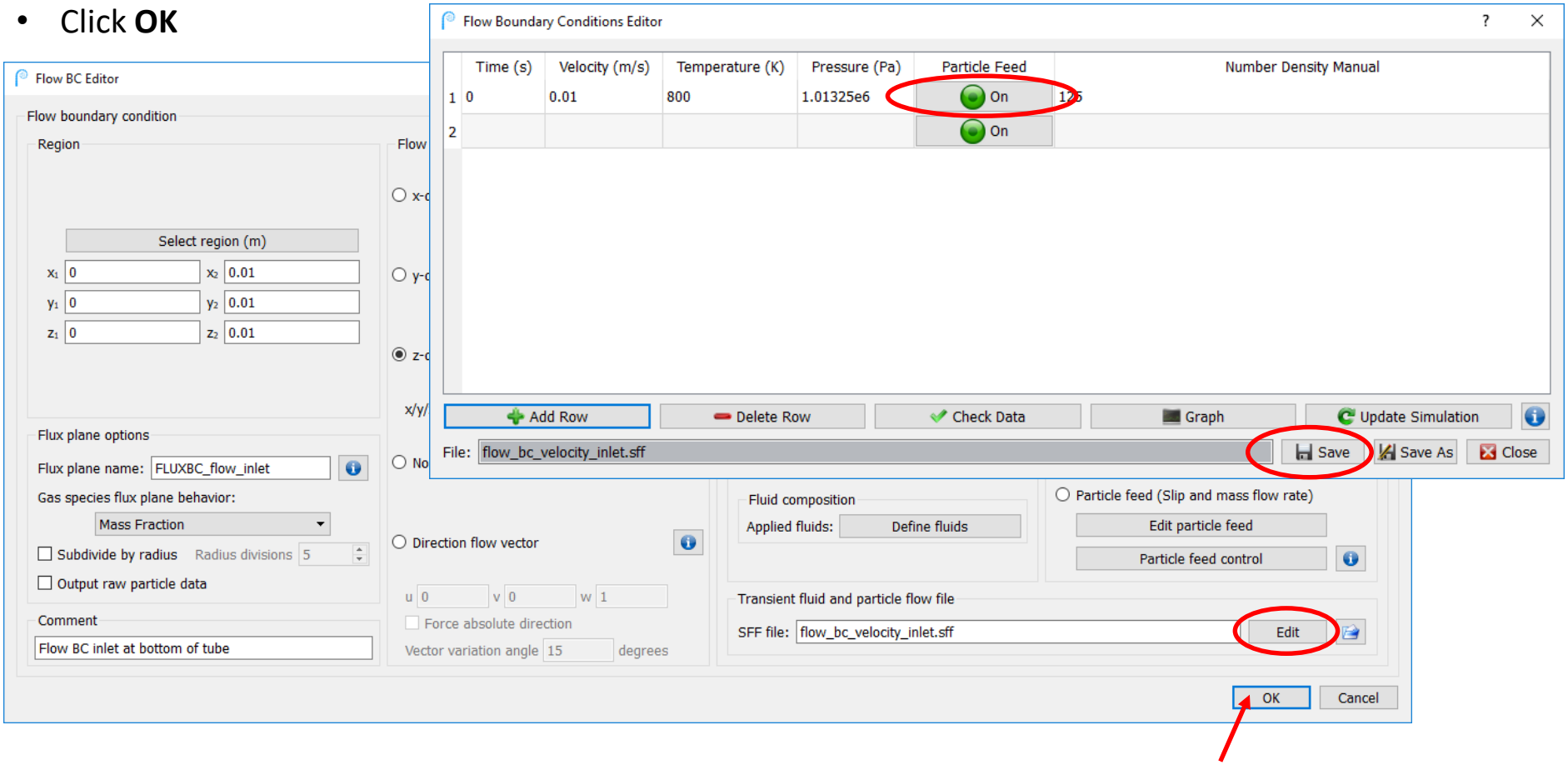
Flow Boundary Conditions

- Select **Particle feed (Slip and volume fraction)**
- Click on **Edit particle feed**
- Click on **Add** and select species 002- Small coal particles with a **Particle mixture fraction** of “1”
- In the **Particle feed settings** window, change the value for **Particle/fluid slip ratio** to “1”, and change the **Particle feed volume fraction** to “0.1”



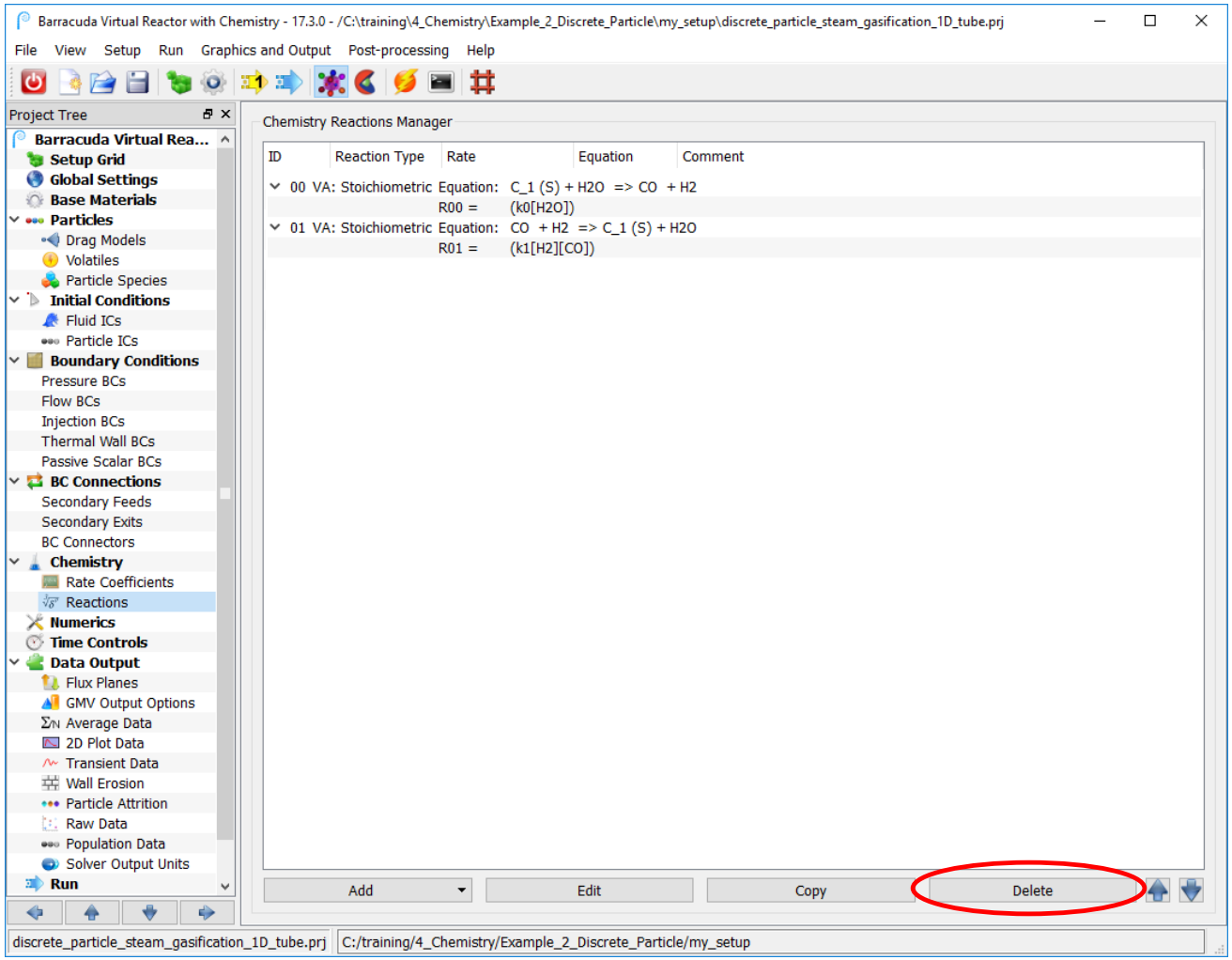
Flow Boundary Conditions

- **Edit** the velocity file changing the **Particle Feed** to “On”
- Remember to save the velocity file, before closing the file window
- Click **OK**



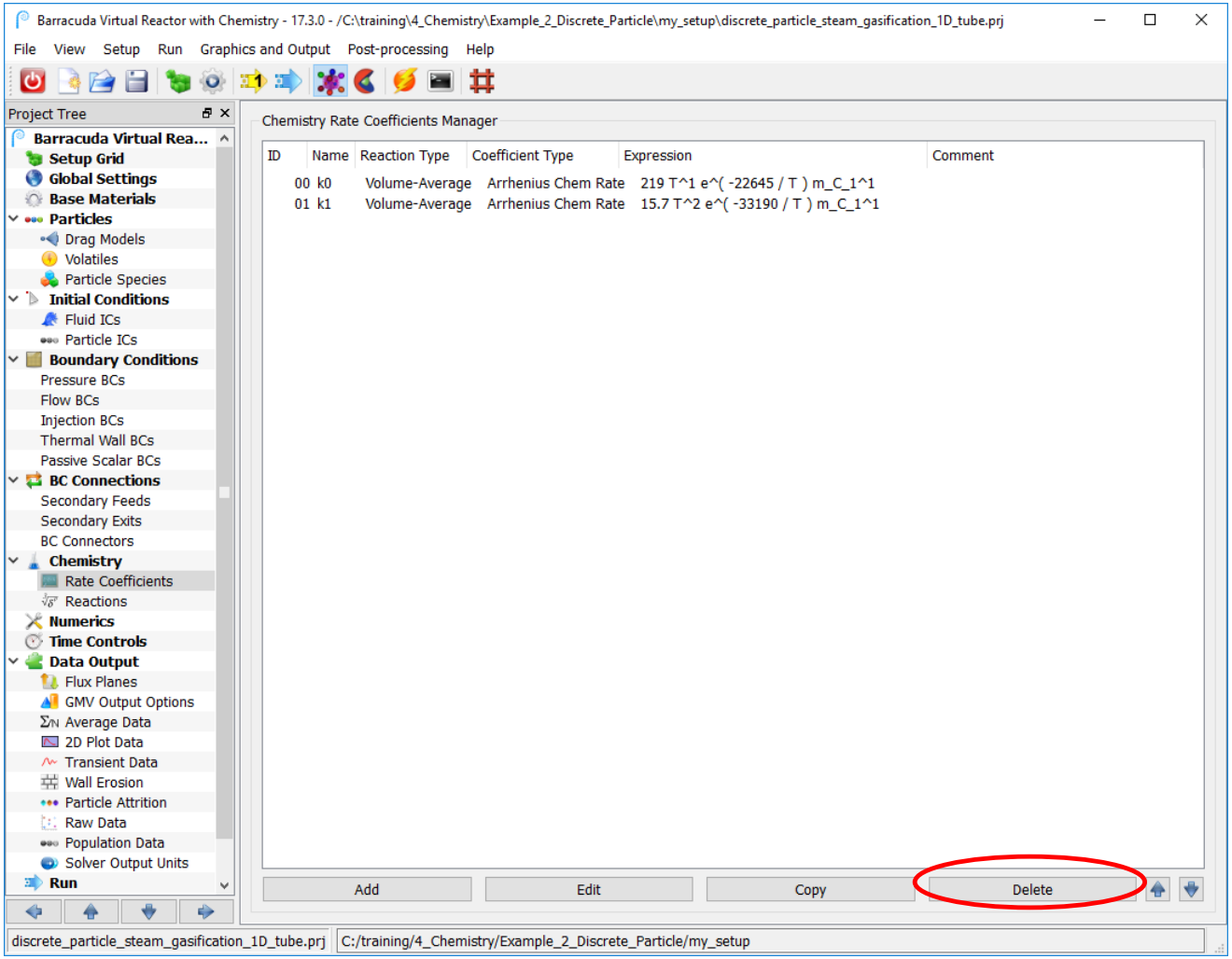
Deleting Existing Reactions

- Different reaction equations will be used since this example uses discrete particle chemistry
- Delete the existing reactions by selecting each and clicking **Delete**



Deleting Existing Rate Coefficients

- Slightly different rate coefficients also will be used
- Delete the existing rate coefficients by selecting each and clicking Delete



Adding Discrete Particle Chemistry

- The project file is now ready for the discrete particle chemistry
- Both the forward and reverse reactions will be added
  - Rate coefficients
  - Reaction rate expressions (species form)

Steam Gasification 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

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

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

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Converting the Forward Reaction Rate to Discrete Particle Chemistry

- As shown previously, the reaction rate needs to be converted to the discrete form

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

- Substituting the reaction rate and solid mass definition terms,

$$\rho_C = m_C / v_{cp} = m_C / \left(V_{cell}/N_p\right)$$

$$\frac{d\,[\mathrm{C}(s)]}{dt} = r\theta_f \left(V_{cell}/N_p\right) = -\left(219\ \frac{\mathrm{m}^3}{\mathrm{kg\,K\,s}}\right) T\theta_f \exp\left(\frac{-22645\mathrm{K}}{T}\right) m_{\mathrm{C}}\,[\mathrm{H_2O}]$$

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Forward Reaction in Discrete Particle Form

- Discrete Particle Reaction Rate

$$\frac{d\left[\mathrm{C}(s)\right]}{dt} = -\underbrace{\left(219\ \frac{\mathrm{m}^3}{\mathrm{kg\,K\,s}}\right) T\theta_f \exp\left(\frac{-22645\mathrm{K}}{T}\right) m_{\mathrm{C}}}_{\text{Rate Coefficient}}\left[\mathrm{H_2O}\right]$$

- Additional reactants and products

$$\frac{d[\mathrm{H_2O}]}{dt} = 1\ \frac{d[\mathrm{C}(s)]}{dt}$$
$$\frac{d[\mathrm{CO}]}{dt} = -1\ \frac{d[\mathrm{C}(s)]}{dt}$$
$$\frac{d[\mathrm{H_2}]}{dt} = -1\ \frac{d[\mathrm{C}(s)]}{dt}$$

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Rate Coefficient: Forward Reaction

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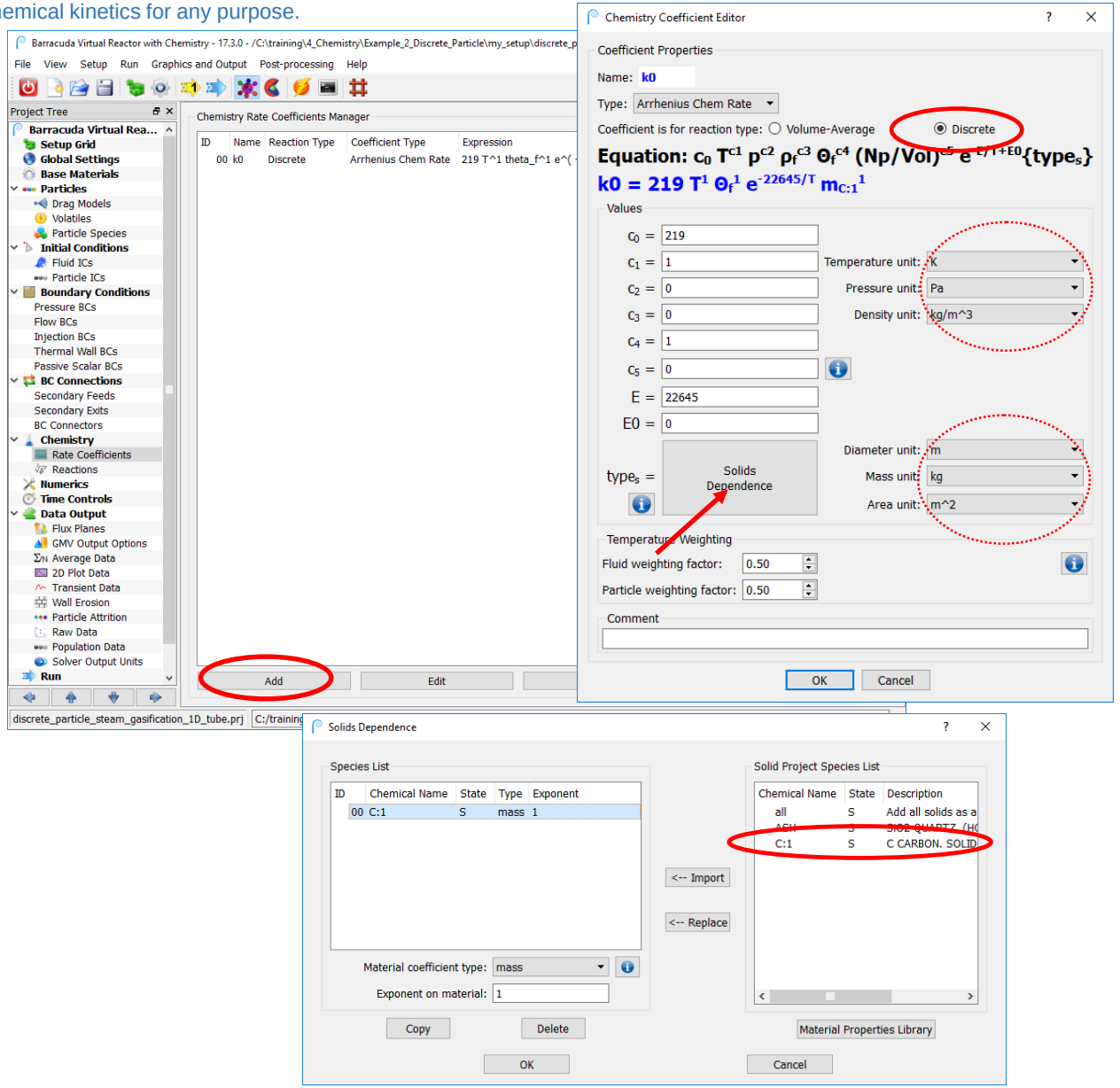
- Enter a new rate coefficient
- Click on **Add**
- Enter the equation for k0 as follows:

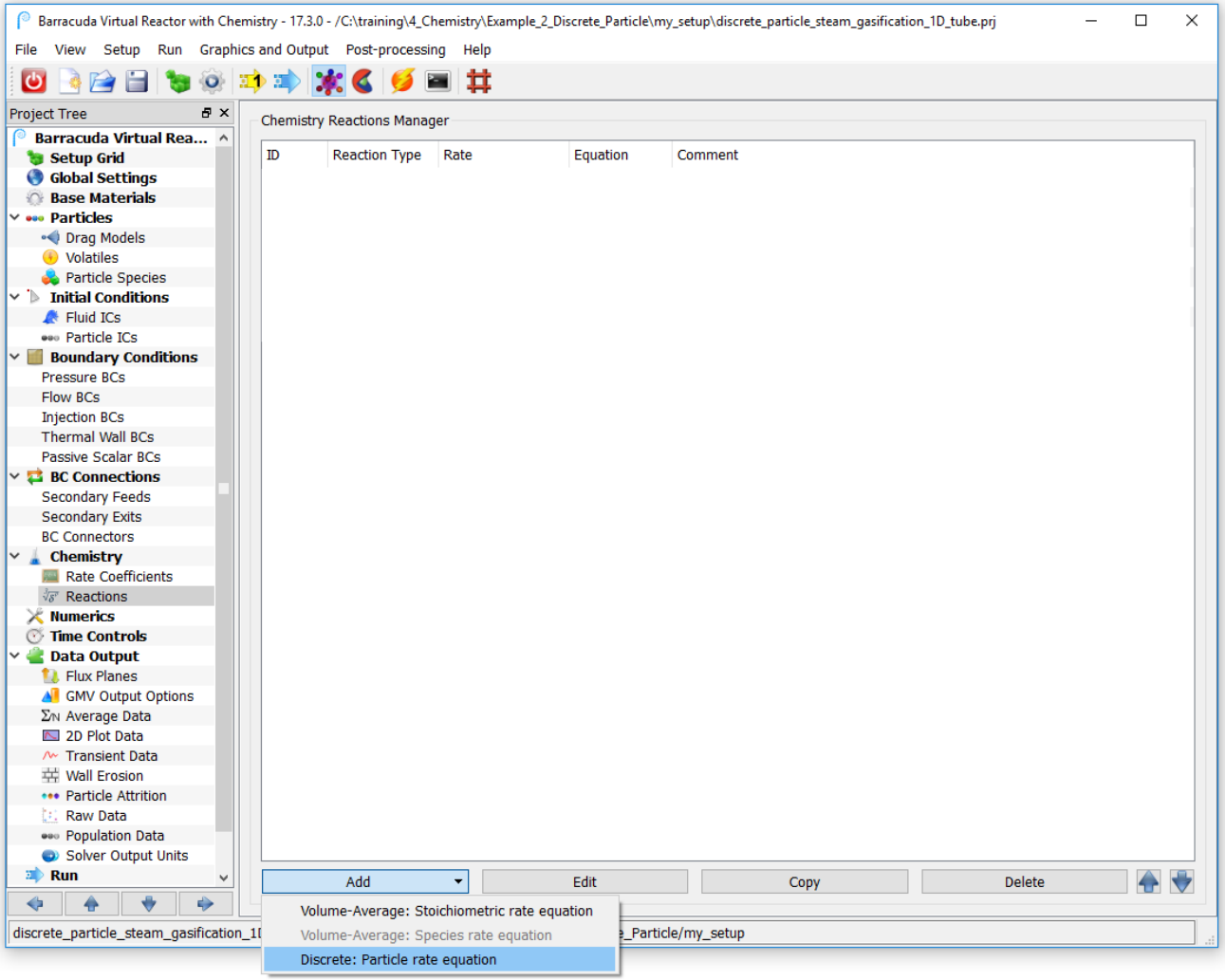
c_0 c_1 c_4 E solids dependence

- $k0 = 219\ T^1\ \Theta_f^1 \exp(-22645/T) m_{C:1}$
- Check that **Discrete** is selected
- Remember to click on **Solids Dependence** and select **C:1**
- Click **OK**



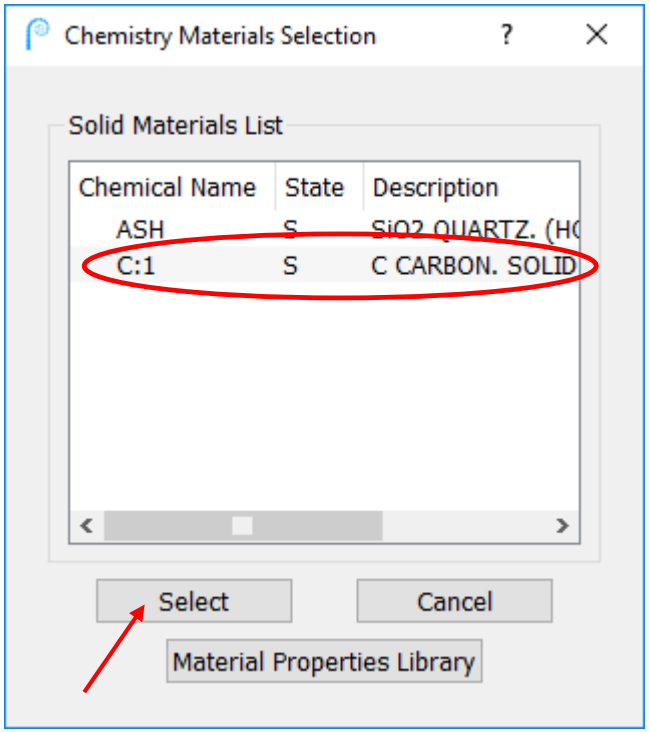
Creating the Forward Reaction

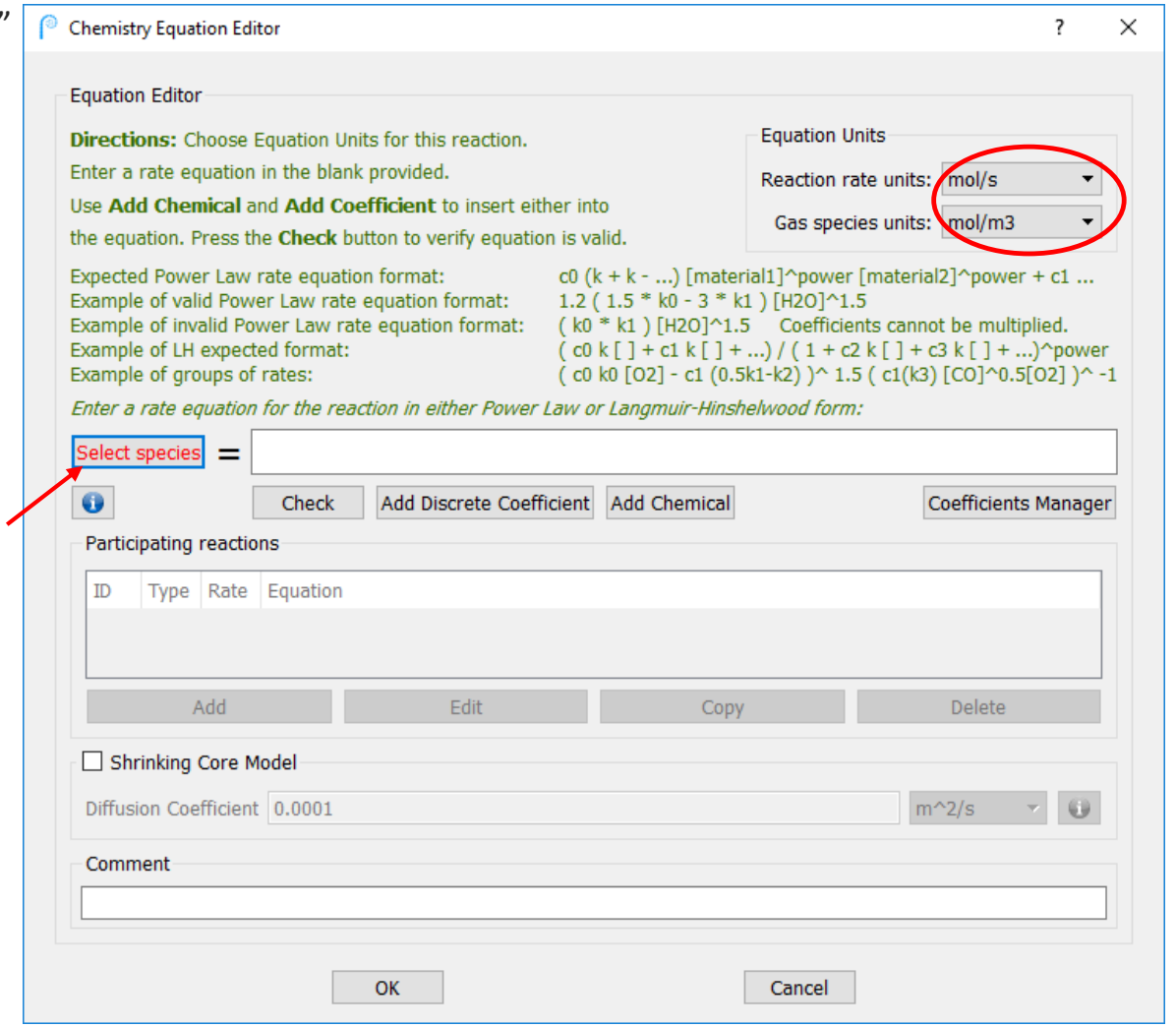
- Now enter the chemical equation for the forward reaction
- Under Reactions click on **Add → Discrete Particle rate equation** to define the chemical reaction and its reaction rate



Specifying the Forward Reaction Stoichiometry

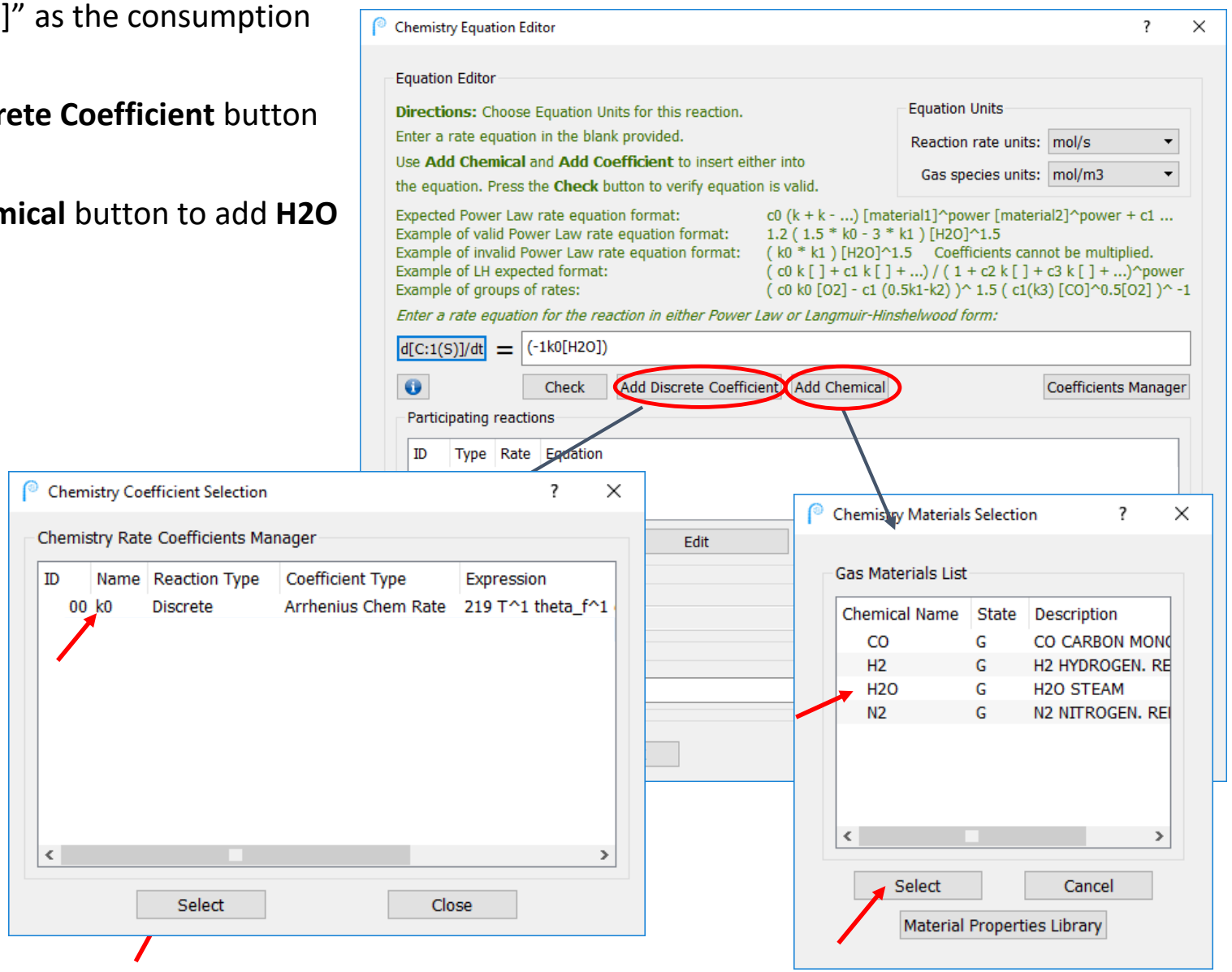
- In the **Chemistry Equation Editor** window:
  - Set the Reaction rate units to “mol/s”
  - Set the Gas species units to “mol/m3”
  - Click on **Select species**
  - Select **C:1** and click **Select**





Specifying the Forward Reaction Stoichiometry

- Enter “-1 k0 [H2O]” as the consumption rate of carbon
- Use the **Add Discrete Coefficient** button to add **k0**
- Use the **Add Chemical** button to add **H2O**

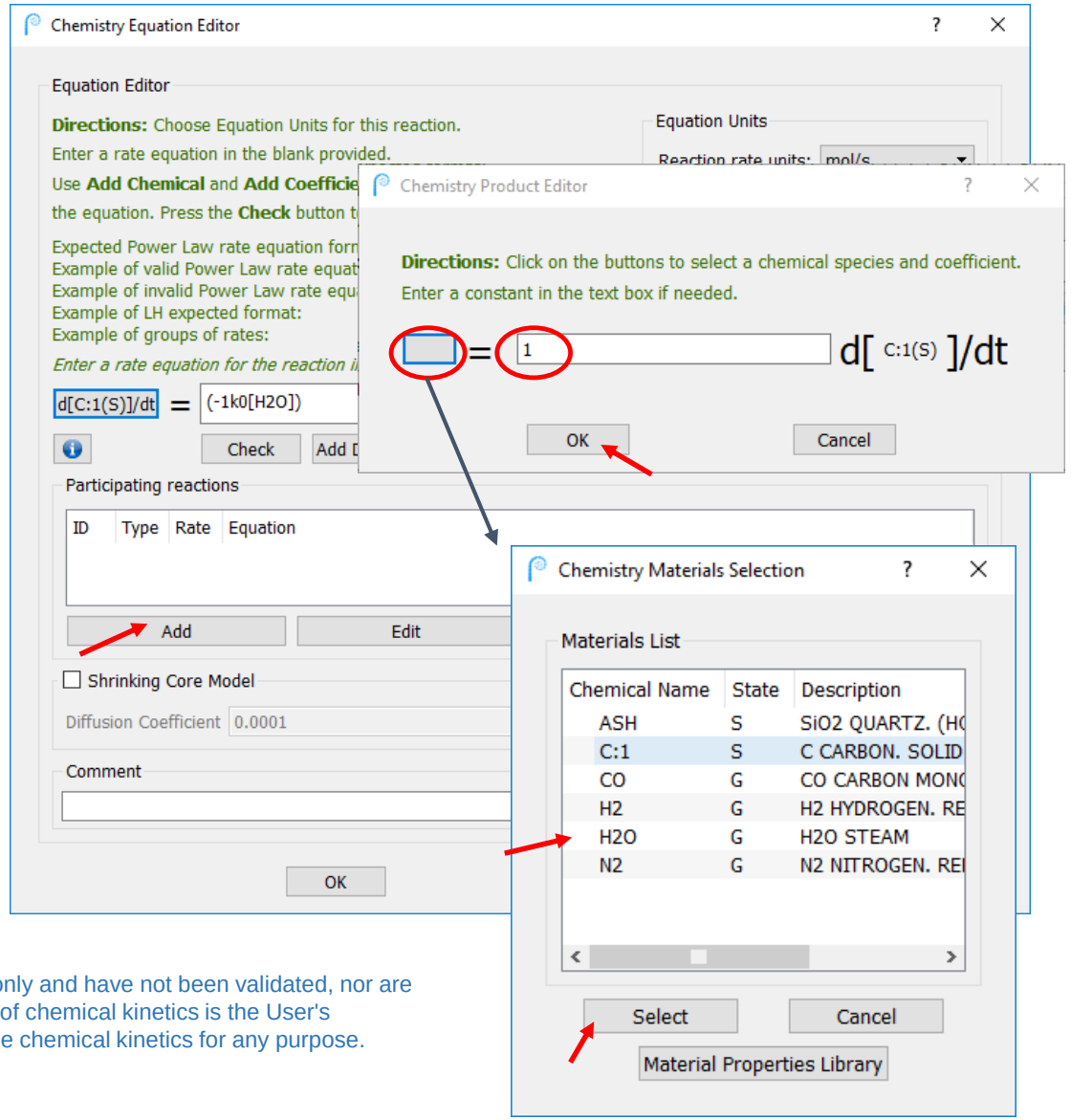


Specifying Participating Reactions

- Under **Participating reactions** click **Add** to enter the rate equation for the consumption of H2O

$$\frac{d[\mathrm{H_2O}]}{dt} = 1\ \frac{d[\mathrm{C}(s)]}{dt}$$

- In the **Chemistry Product Editor** window select a chemical species (H2O) and a coefficient of “1”
- Click **OK**



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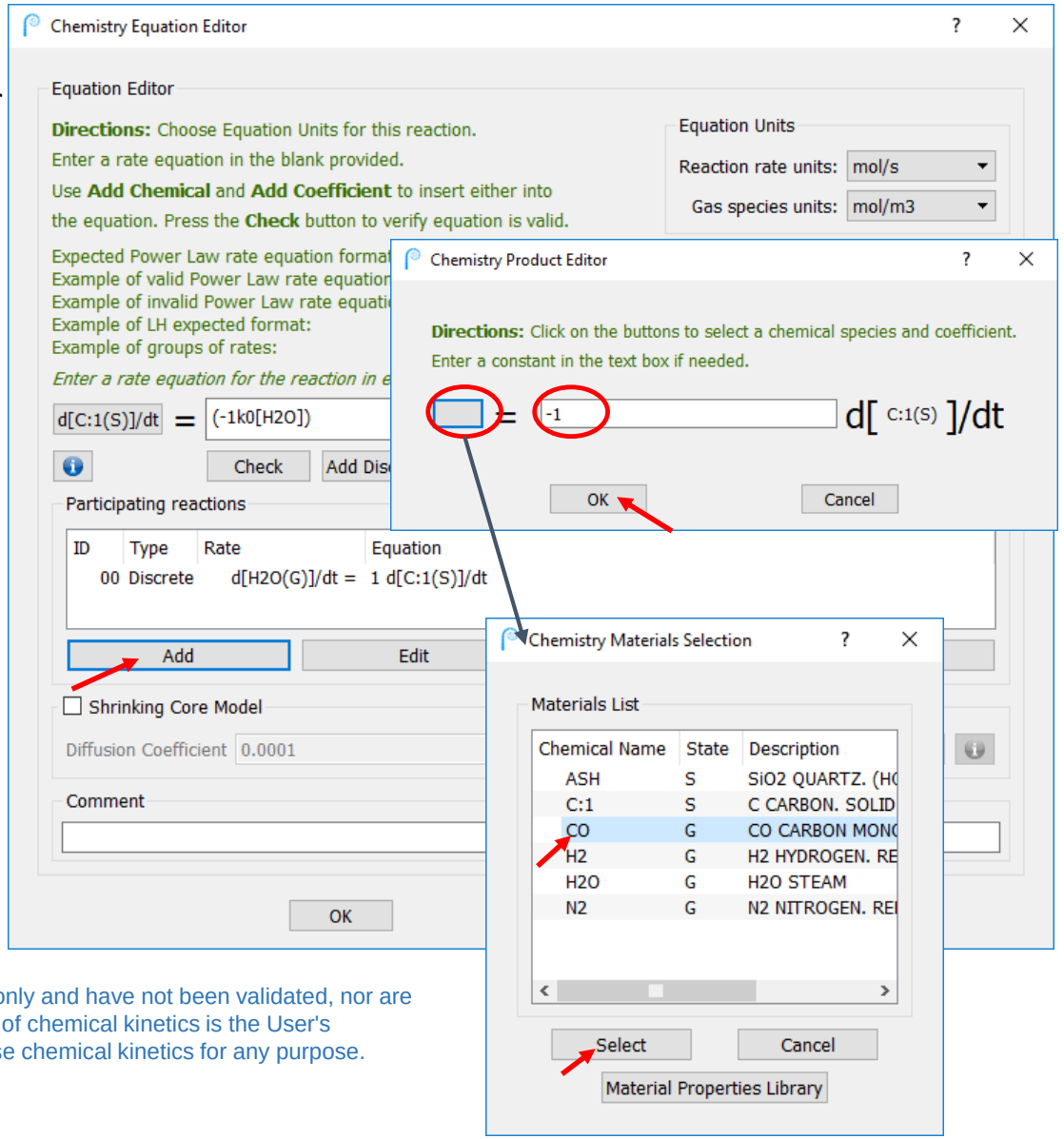
Specifying Participating Reactions

- Next, click **Add** to enter the rate equation for the production of CO

$$\frac{d[\mathrm{CO}]}{dt} = -1\,\frac{d[\mathrm{C}(s)]}{dt}$$

- In the **Chemistry Product Editor** window select a chemical species (CO) and a coefficient of "-1"
- Click **OK**



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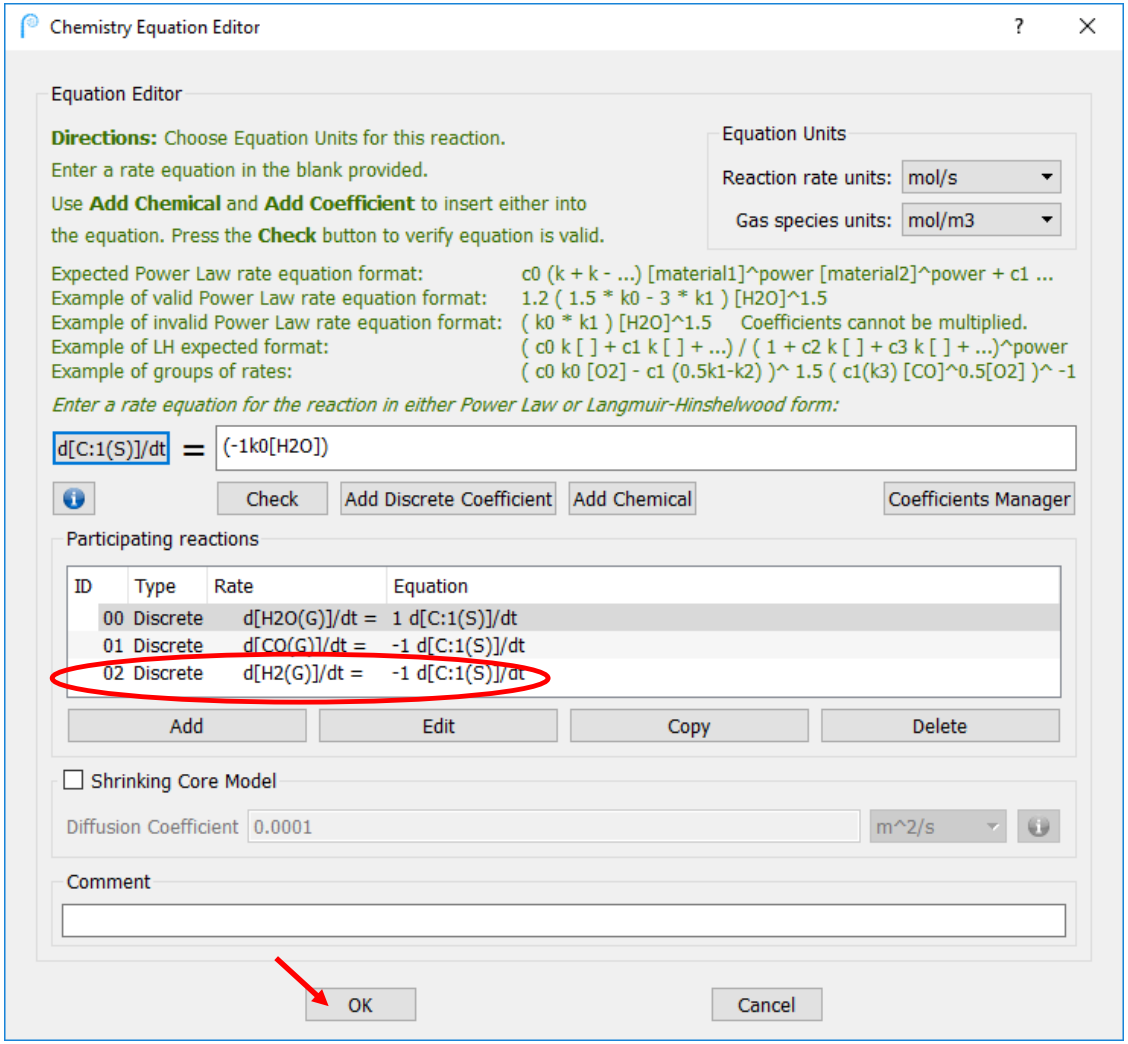
Specifying Participating Reactions

- In a similar manner, enter the rate equation for the production of H2

$$\frac{d[\mathrm{H_2}]}{dt} = -1\,\frac{d[\mathrm{C}(s)]}{dt}$$

- When finished, click **OK** in the **Chemistry Equation Editor** window



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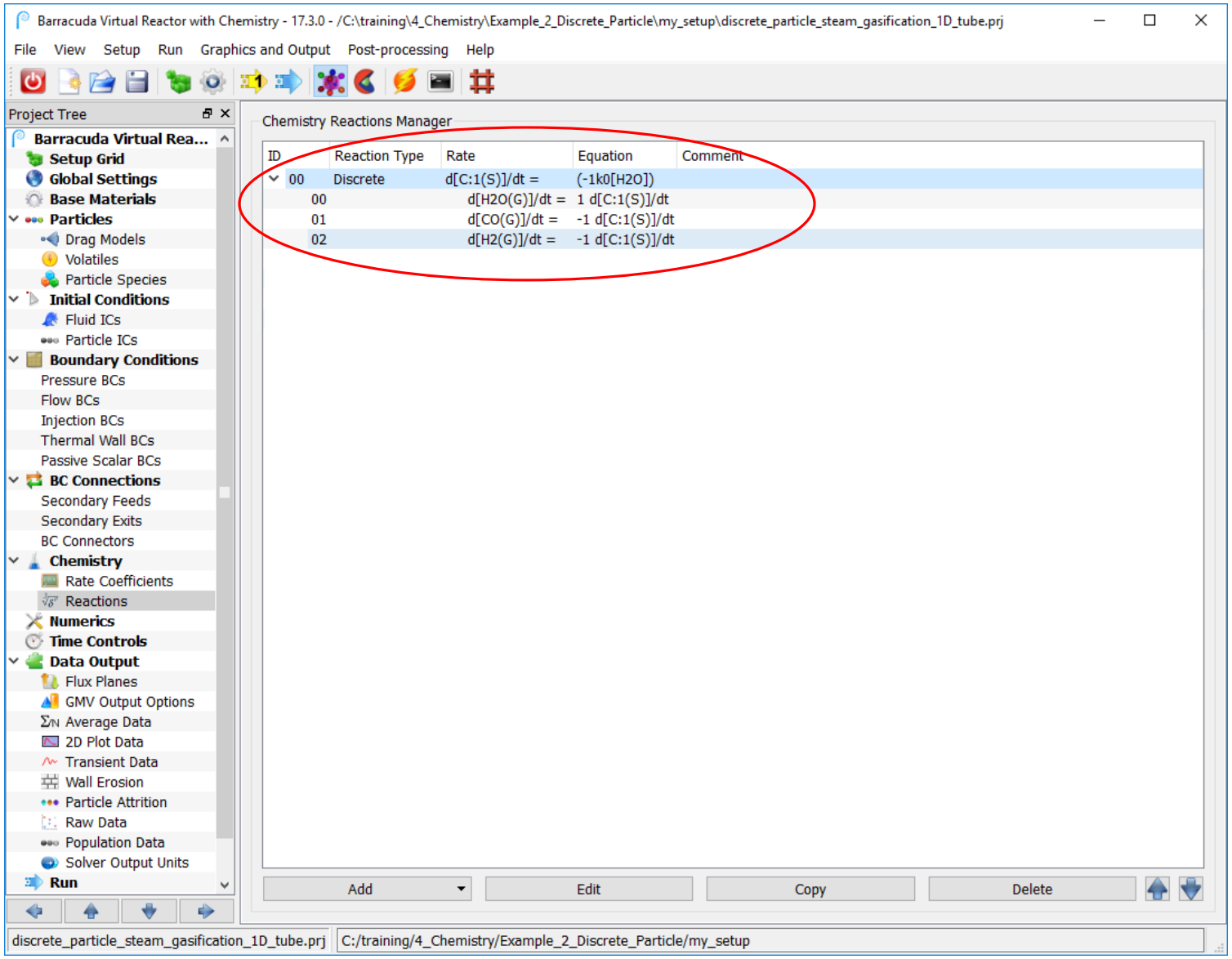
Forward Reaction Rate

- The forward reaction rate equation is now complete



Converting the Reverse Reaction Rate to Discrete Particle Chemistry

- The reverse reaction rate needs to be converted to the discrete form

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

- Substituting the reaction rate and solid mass definition terms

$$\rho_C = m_C / v_{cp} = m_C / \left(V_{cell}/N_p\right)$$

$$\frac{d\,[\mathrm{C}(s)]}{dt} = r\theta_f \left(V_{cell}/N_p\right) = \left(15.7\ \frac{\mathrm{m}^6}{\mathrm{kg\,mol\,K^2\,s}}\right) T^2\theta_f \exp\left(\frac{-33190\ \mathrm{K}}{T}\right) m_{\mathrm{C}}\,[\mathrm{H_2}]\,[\mathrm{CO}]$$

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Reverse Reaction in Discrete Particle Form

- Discrete Particle Reaction Rate

$$\frac{d\left[\mathrm{C}(s)\right]}{dt} = \underbrace{\left(15.7\ \frac{\mathrm{m}^6}{\mathrm{kg\,mol\,K^2\,s}}\right) T^2 \theta_f \exp\left(\frac{-33190\ \mathrm{K}}{T}\right) m_{\mathrm{C}}}_{\text{Rate Coefficient}} \left[\mathrm{H_2}\right]\left[\mathrm{CO}\right]$$

- Additional reactants and products

$$\frac{d[\mathrm{H_2O}]}{dt} = 1\ \frac{d[\mathrm{C}(s)]}{dt}$$
$$\frac{d[\mathrm{CO}]}{dt} = -1\ \frac{d[\mathrm{C}(s)]}{dt}$$
$$\frac{d[\mathrm{H_2}]}{dt} = -1\ \frac{d[\mathrm{C}(s)]}{dt}$$

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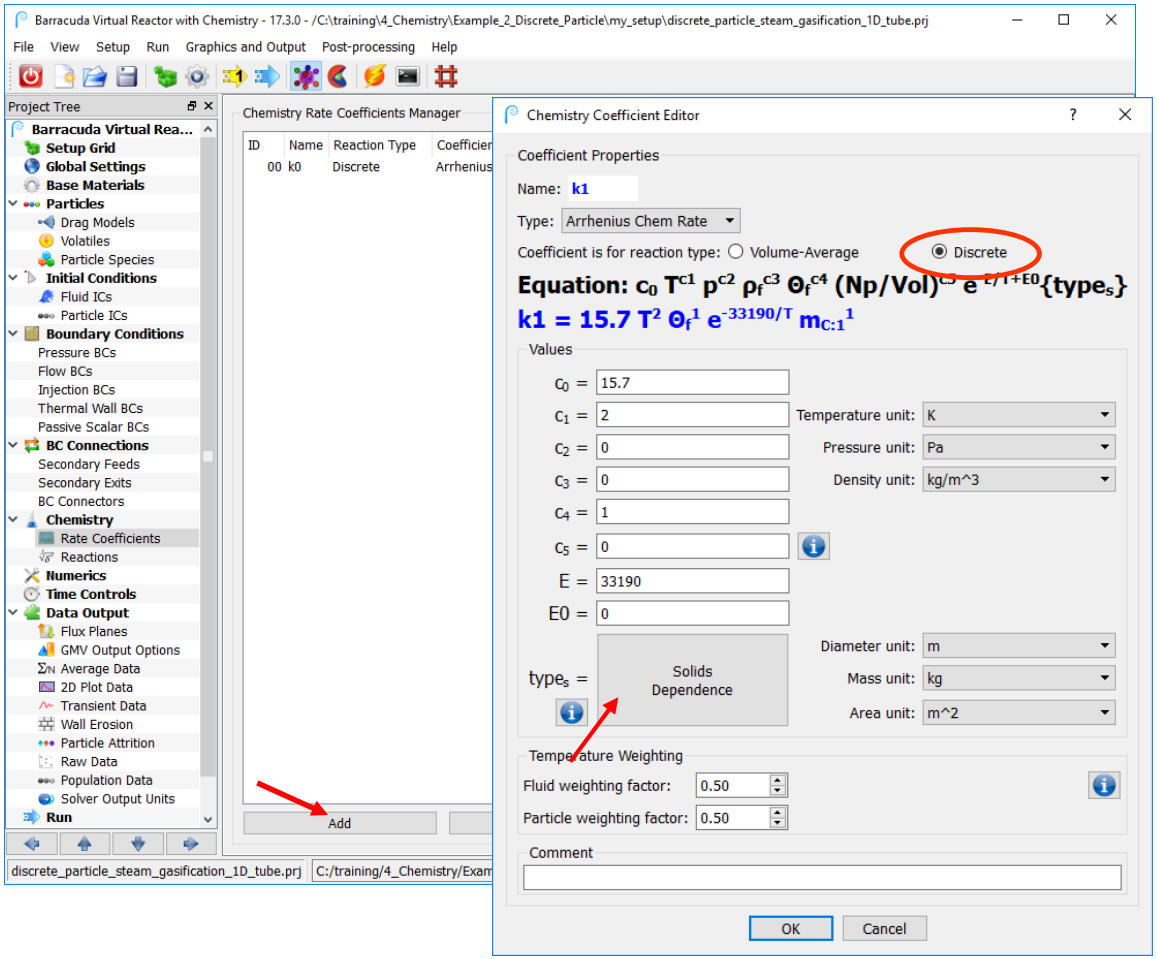
Rate Coefficient: Reverse Reaction

- 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 c_4 E solids dependence

- $k_1 = 15.7\ T^2\ \Theta_f^1 \exp(-33190/T) m_{C:1}$
- Check that Discrete is selected and that units are selected for temperature, pressure, density, mass, etc.
- Remember to click on **Solids Dependence** and select **C:1**



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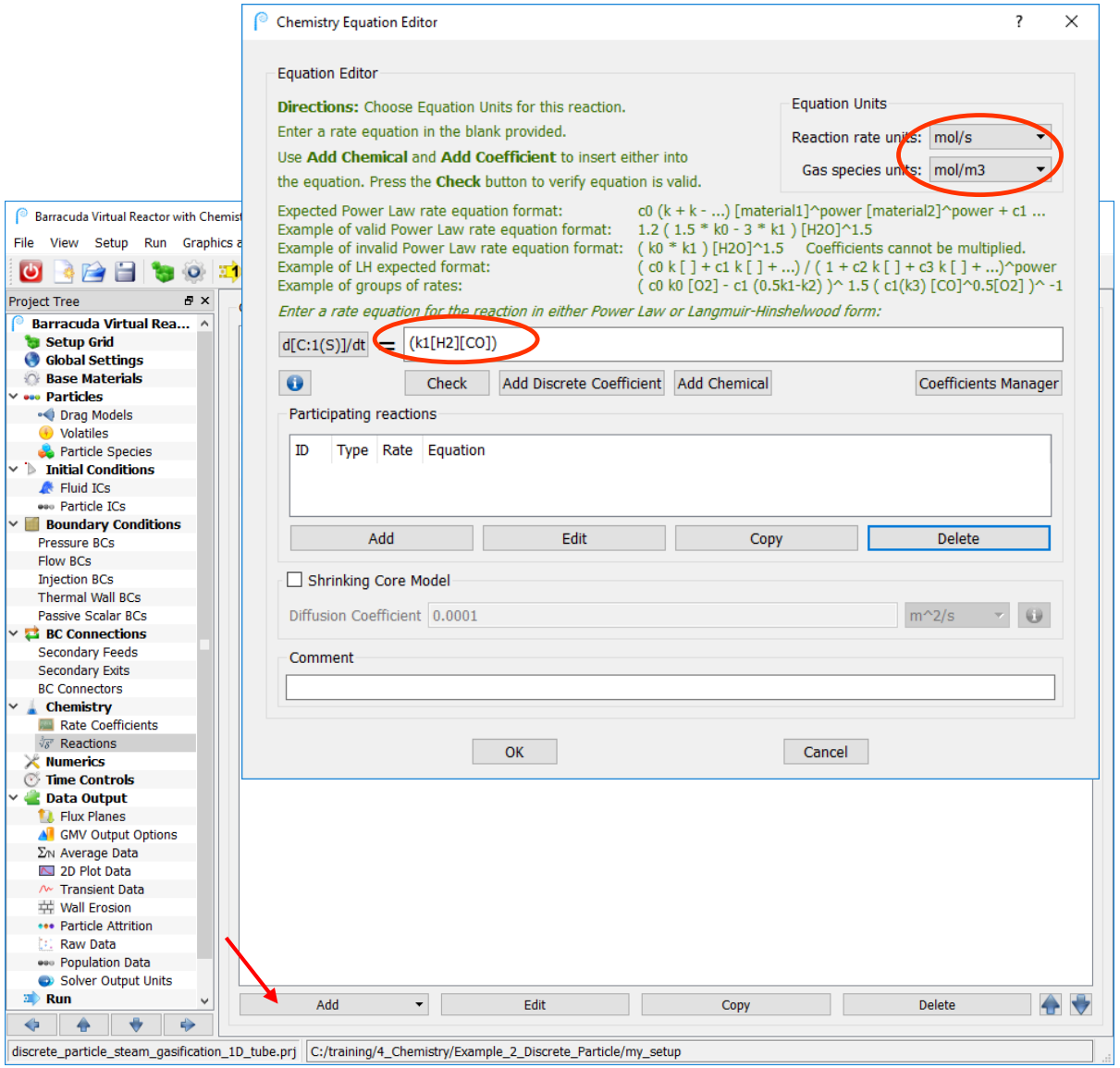
Creating the Reverse Reaction

- Next enter the chemical equation for the reverse reaction
- Under **Reactions** click on **Add** → **Discrete Particle rate equation** to raise the **Chemical Equation Editor** window
- Set the **Reaction rate units** to "mol/s" and the **Gas species units** to "mol/m3"
- Enter the rate equation for the production of C:1 as "k1 [H2] [CO]" using the **Add Discrete Coefficient** and the **Add Chemical** buttons

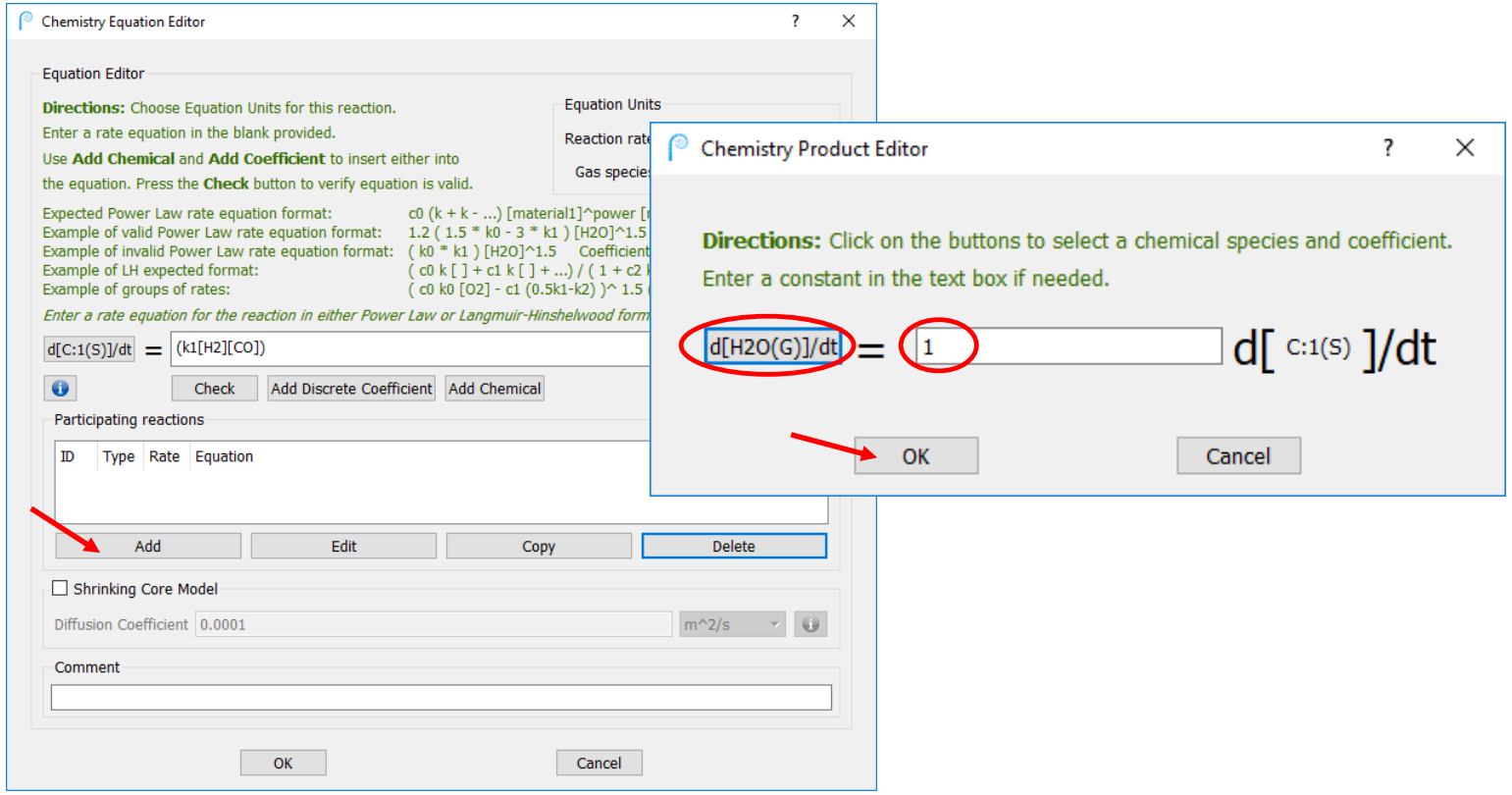


Specifying Participating Reactions

- Under **Participating reactions** click **Add** to enter the rate equation for the production of H2O

$$\frac{d[\mathrm{H_2O}]}{dt} = 1\ \frac{d[\mathrm{C}(s)]}{dt}$$

- Click **OK**



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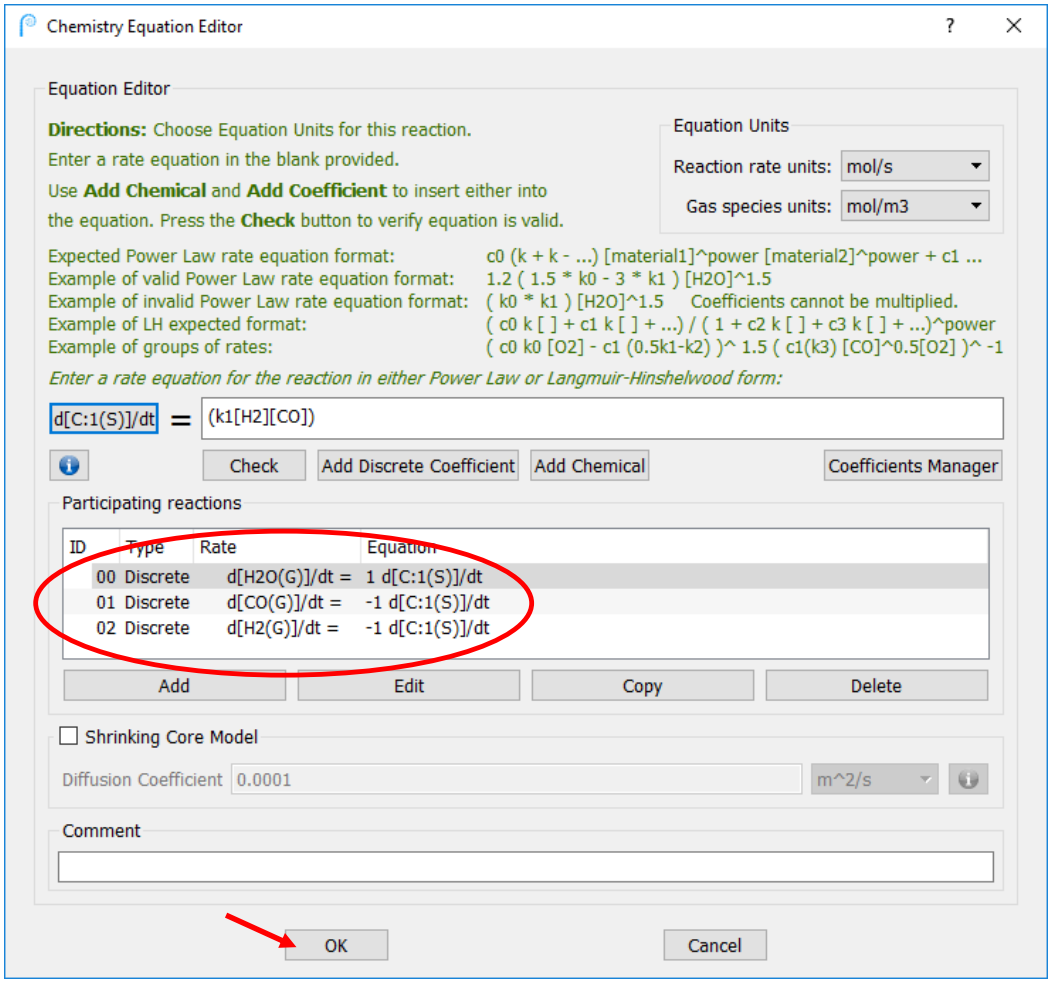
Specifying Participating Reactions

- In a similar manner, enter the rate equation for the consumption of CO and H2

$$\frac{d[\mathrm{CO}]}{dt} = -1\ \frac{d[\mathrm{C}(s)]}{dt}$$

$$\frac{d[\mathrm{H_2}]}{dt} = -1\ \frac{d[\mathrm{C}(s)]}{dt}$$

- When finished, click **OK** in the **Chemistry Equation Editor** window



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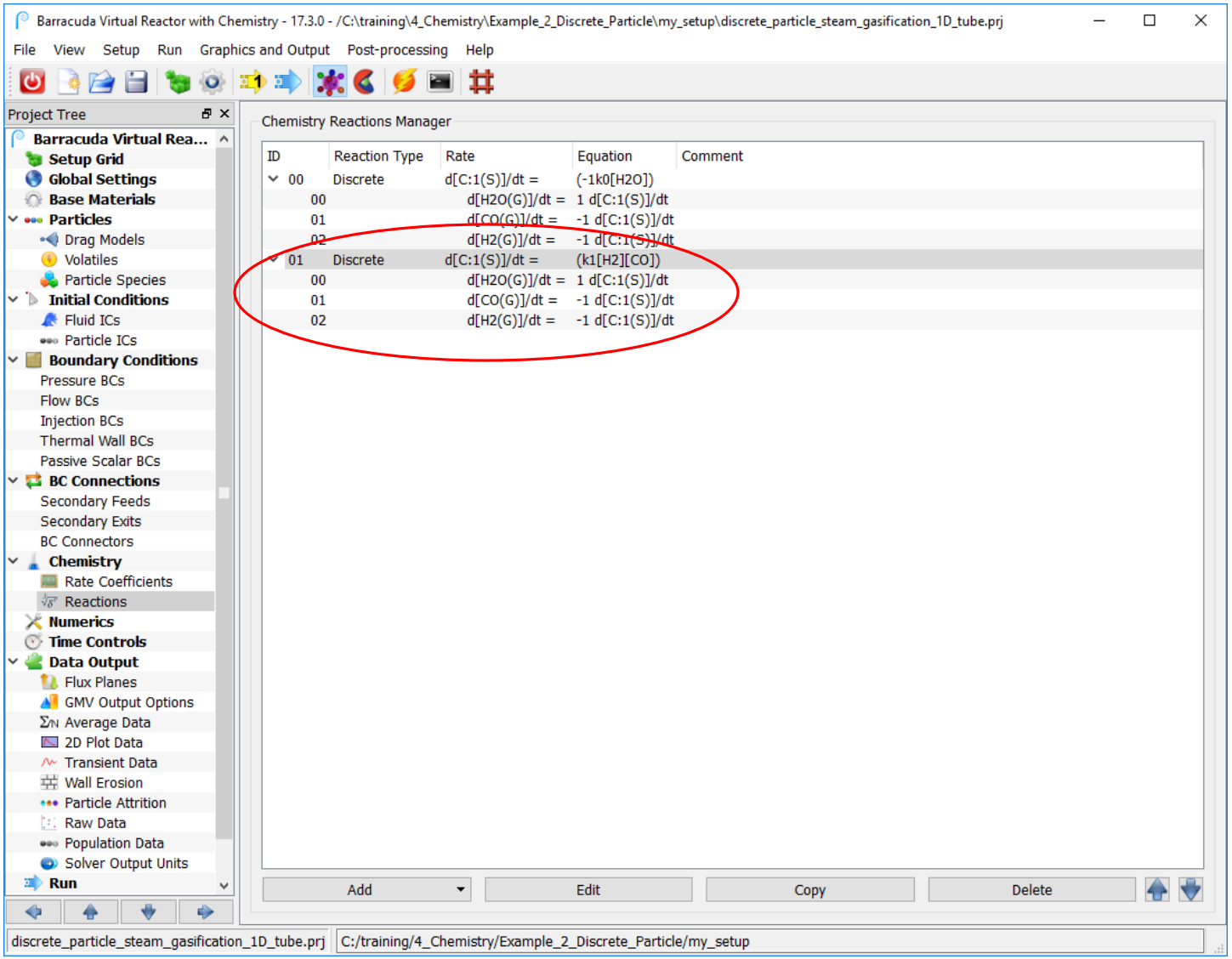
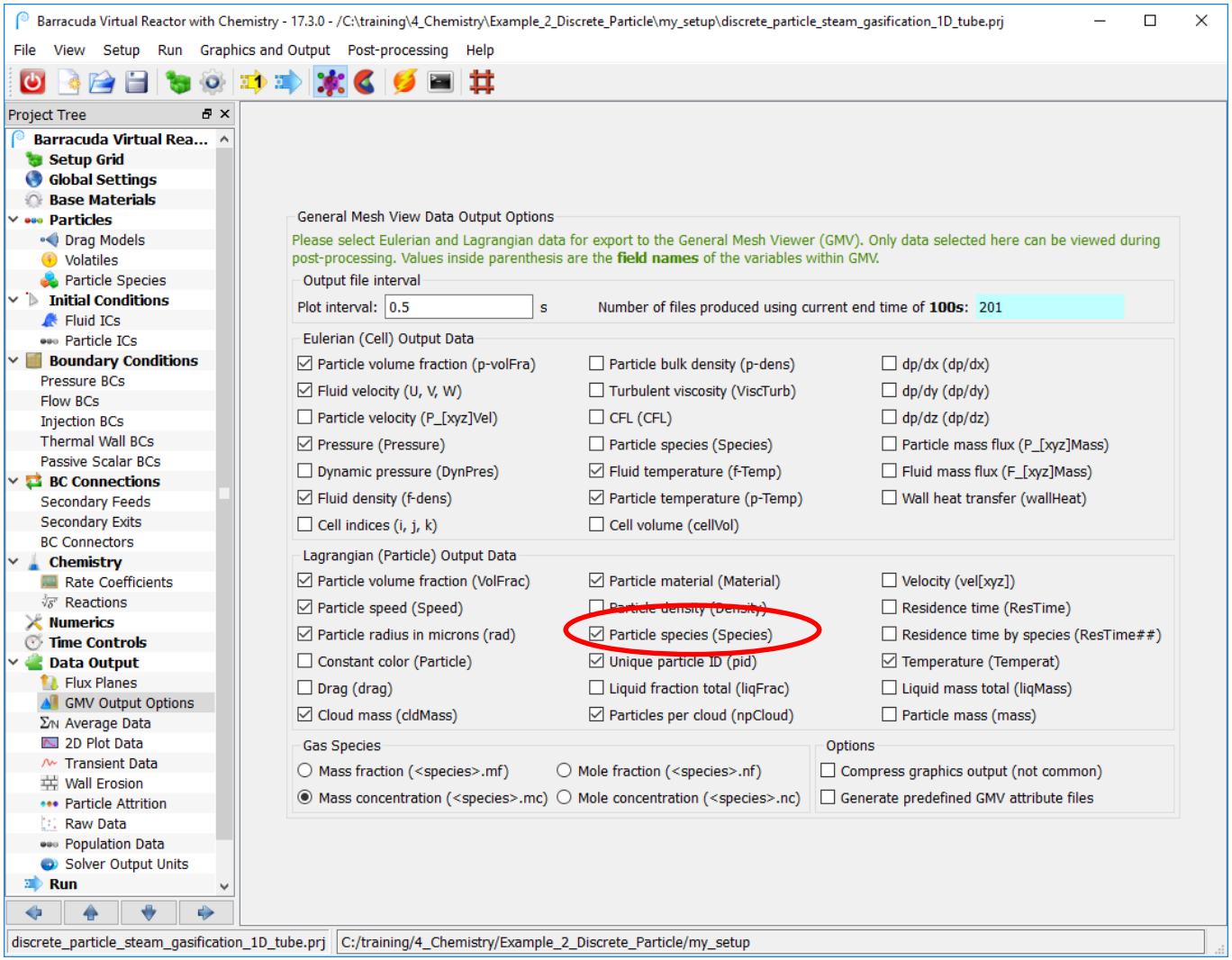
Reverse Reaction Rate

- The reverse reaction rate equation is now complete



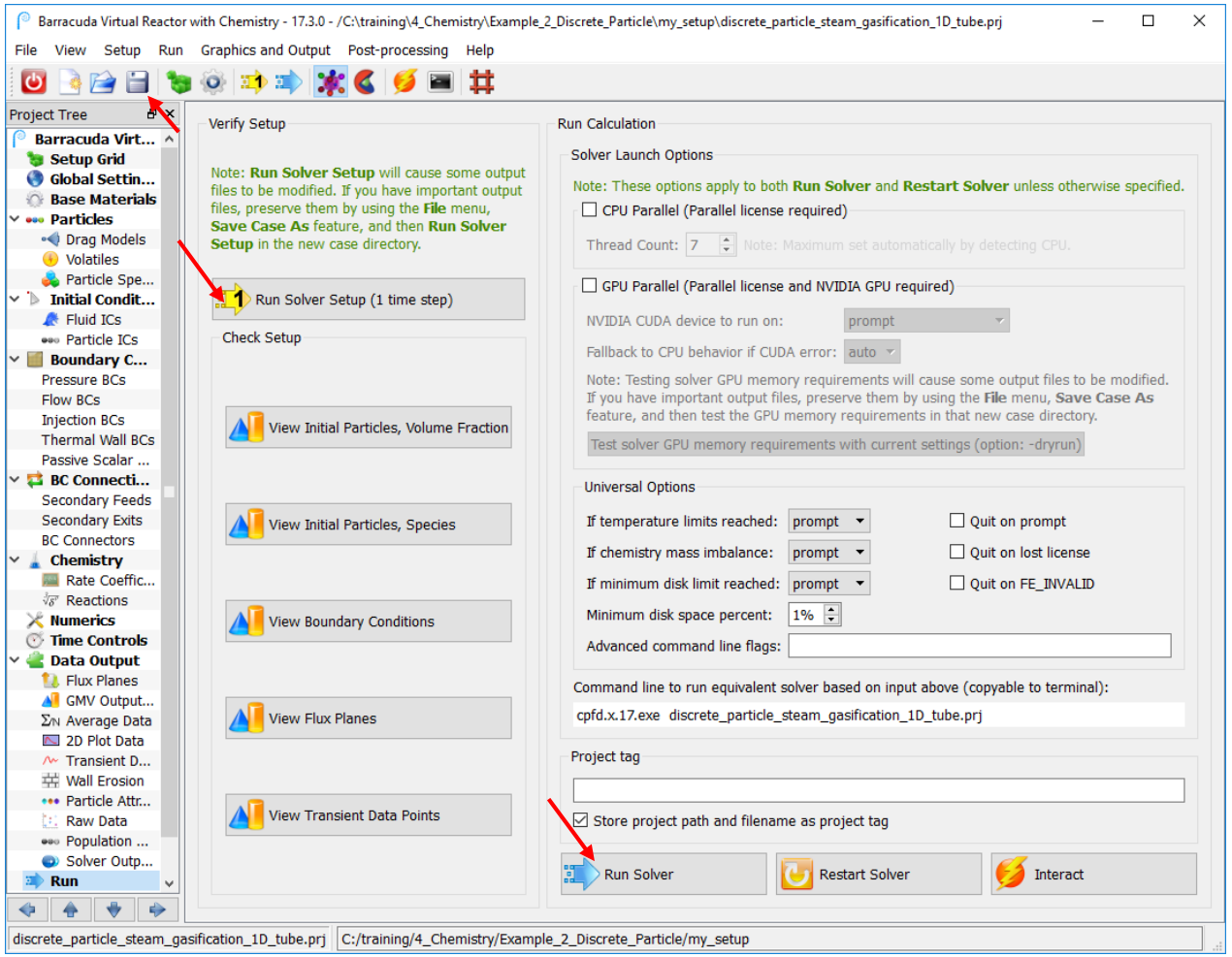
GMV Output Options

- Under **GMV Output Options** select **Particle species** in addition to the variables already selected
- All other parameters (Time Controls, 2D Plot Data, Transient Data, etc.) remain unchanged



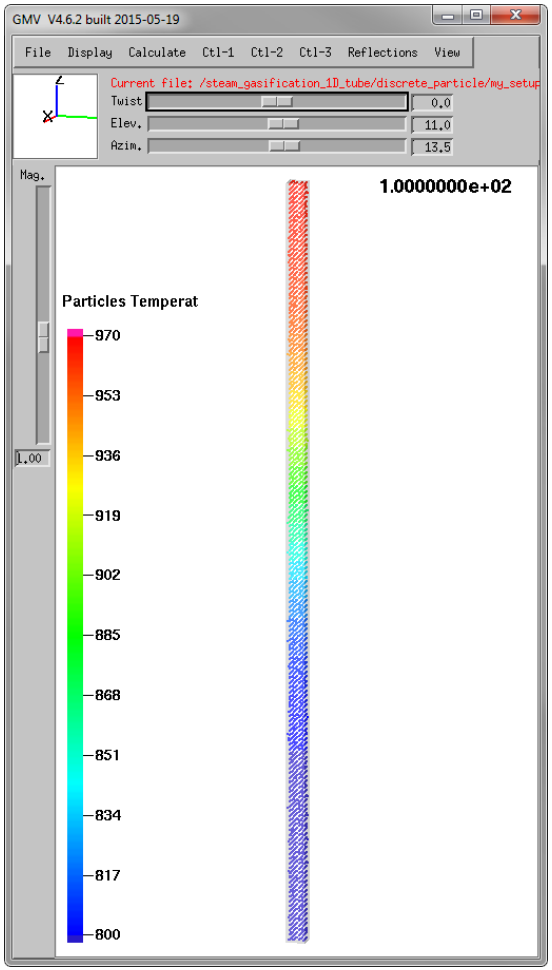
Start the Barracuda Solver

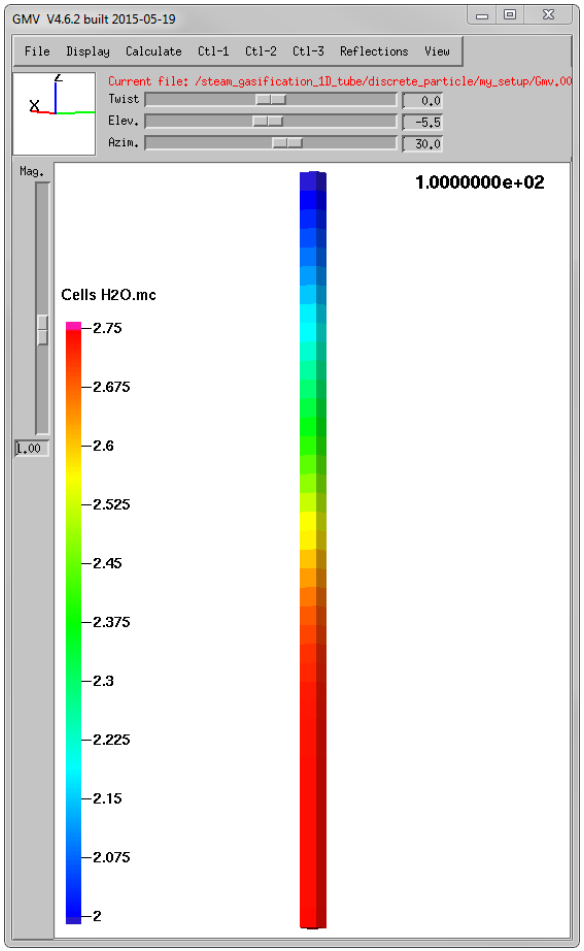
- **Remove** CPU Parallel
- **Save** the project file and **Run Solver Setup (1 time step)** to verify setup is correct
- **Run Solver**



Post Processing

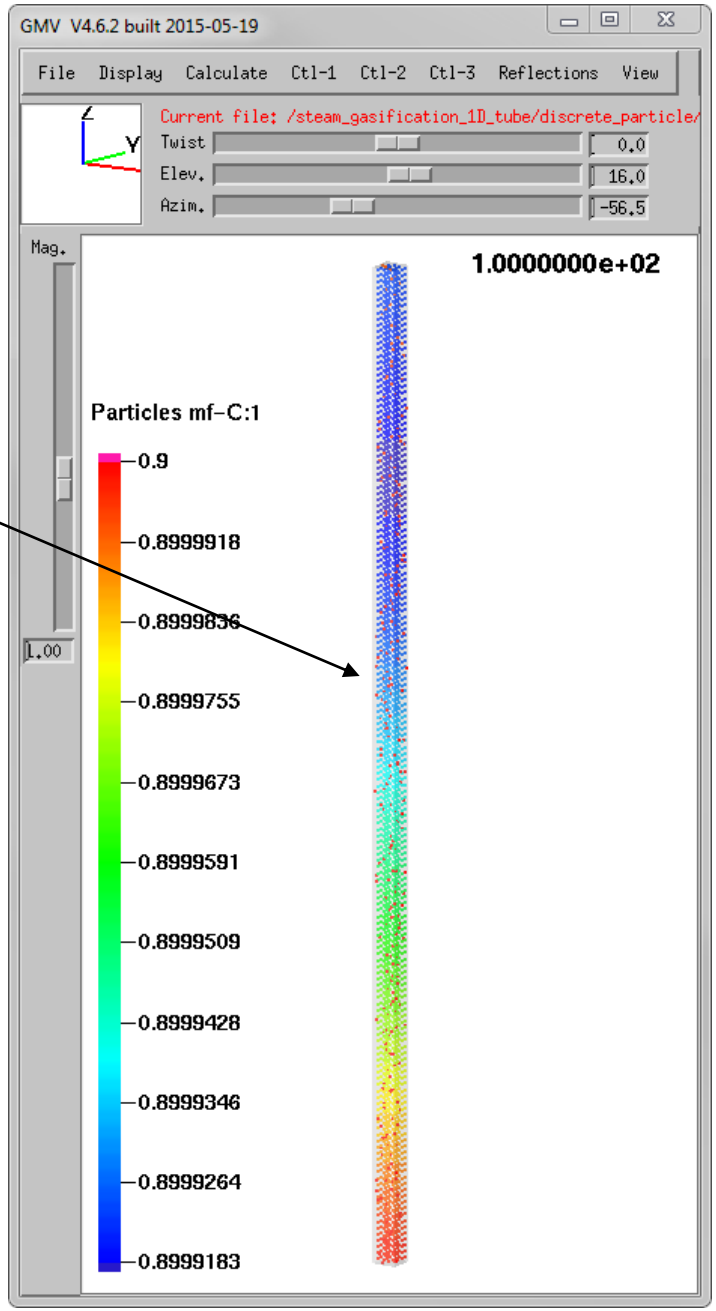
- Analyze the particle temperature and steam concentration in GMV
  - Use the **Particle Temperature** button
  - To view the mass concentration of steam throughout the tube, use the **Cell Volume Fraction** button and color cells by **Cell Field: H2O.mc**





Post Processing

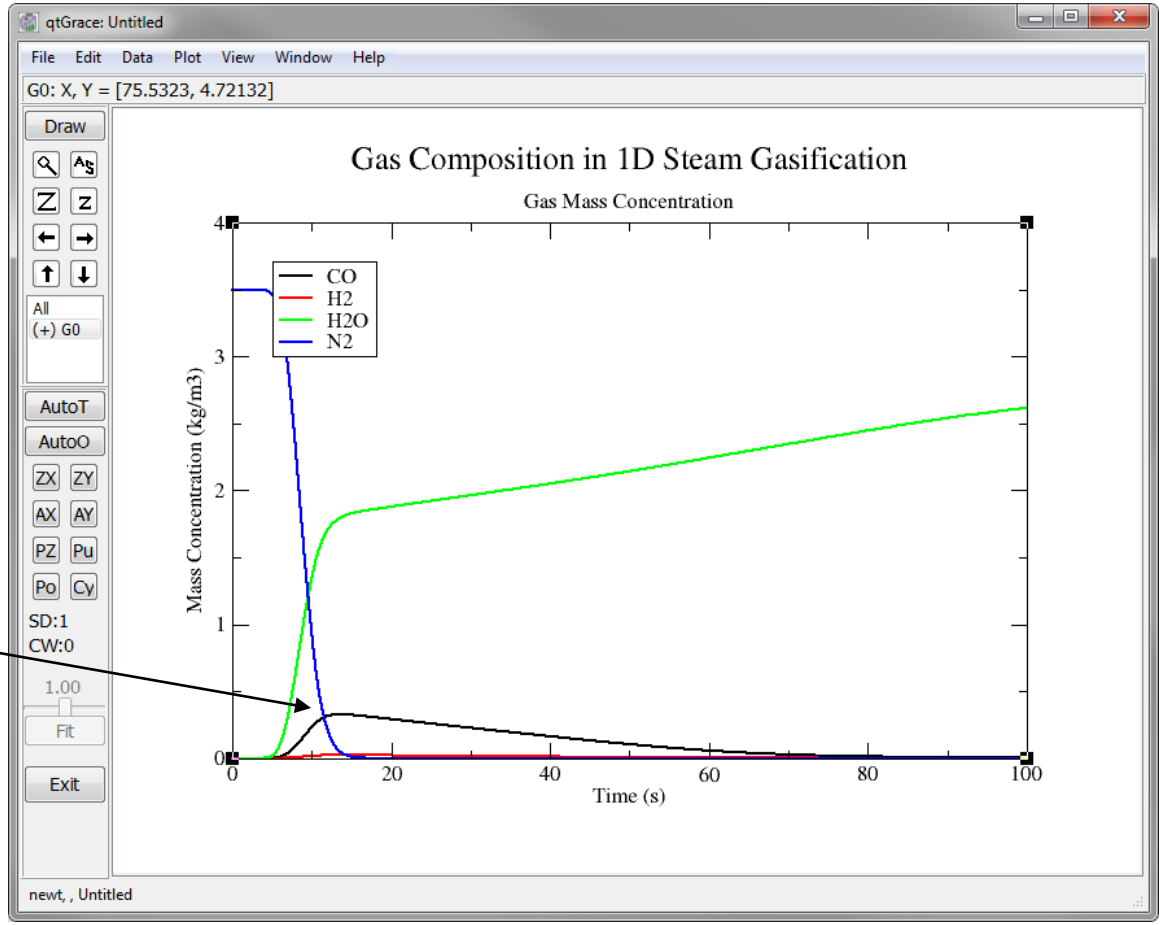
- Analyze the mass fraction of carbon in GMV
  - Hint: Display particles for **mf-C:1**
- Why do the moving particles have a higher mass fraction of carbon?
- How do the temperature and steam concentration help explain the mass fraction of carbon throughout the tube at 100 seconds?



Plotting Transient Data

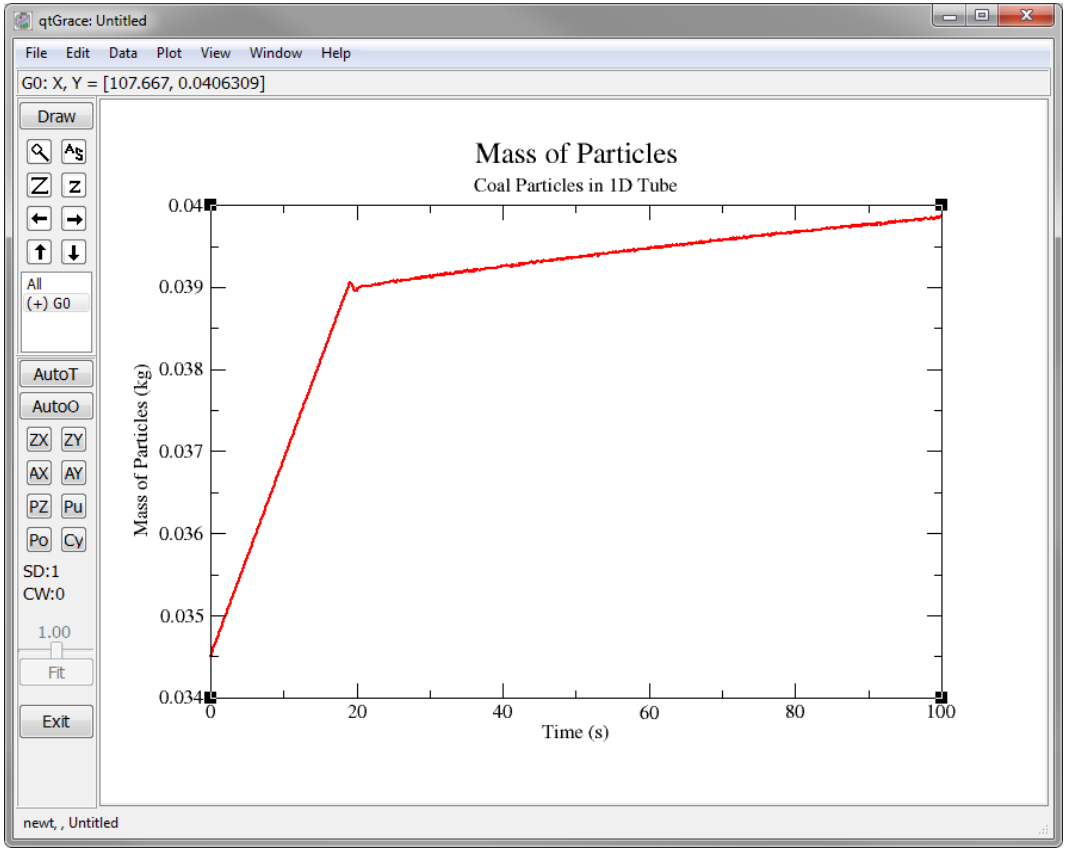
- Make a plot of the mass concentration of all gas species versus time in Plot Manager
  - Hint: refer to the Kuipers post processing exercise in plotting
  - Data is in the **trans.data00** file
  - The plot shows the gas concentrations in the cell containing the transient data (z ~ 0.2 m)

- Why is there a peak in CO concentration?
- 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.



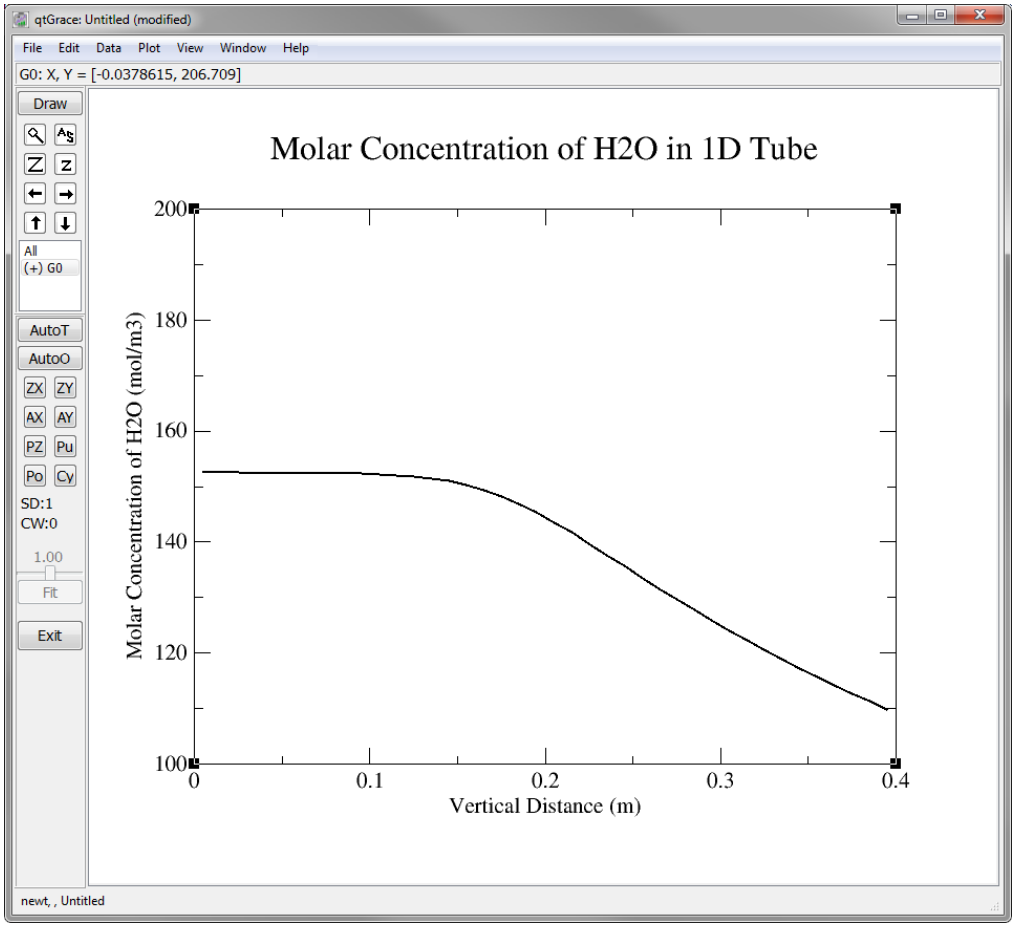
Plotting Transient Data

- Next, make a plot of the mass of coal particles versus time in Plot Manager
  - Hint: Data is in the **history.log** file
- Was 100 seconds long enough to reach “steady state” behavior in the reactor?
- The solids mass in the system increases even though carbon is consumed in the reaction because fine coal particles are fed into the reactor



Plotting 2D Data

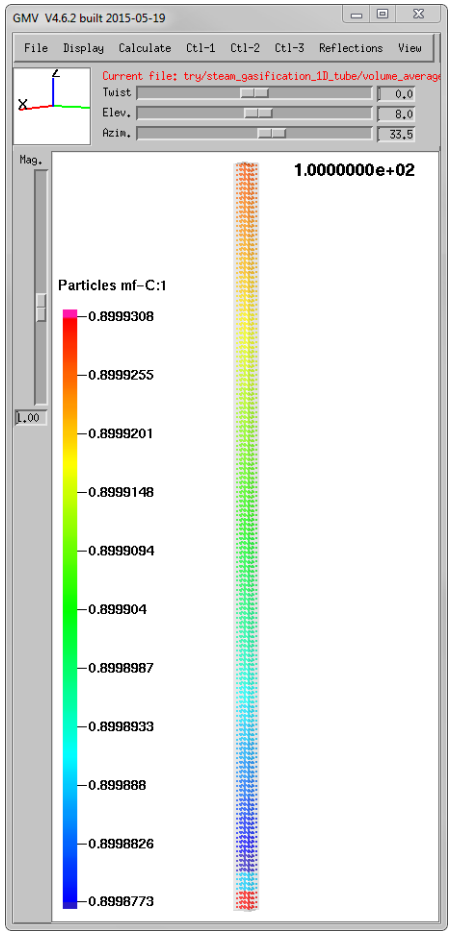
- Make a plot of the molar concentration of H_2O versus vertical distance in Plot Manager
  - Hint: Data is in the **H2O_zxMoleConc_00100.000.dat** file
- The concentration of H_2O is highest at the bottom of the tube.



1D Tube Comparisons

- Note close coupling of particle dynamics, reaction chemistry, and thermal dynamics in reactor
- Adding a feed of small coal particles dramatically changed the reactor dynamics

Case #1



Case #2