

Chemistry Training Example 2: Discrete Particle

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Training Plan

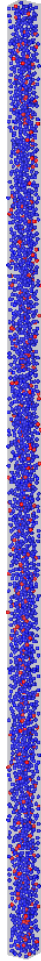
- Chemistry training will be provided in three parts
 - Lecture: Introduction to the Chemistry module
 - Volume Average Chemistry
 - Discrete Particle Chemistry
 - Example 1: Set up of training problem using Volume Average Chemistry
 - Example 2: Set up of training problem using Discrete Particle Chemistry

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 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 (SiO_2)
- 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



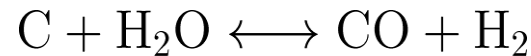
Case #1



Case #2

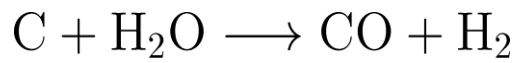
Steam Gasification Reaction

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



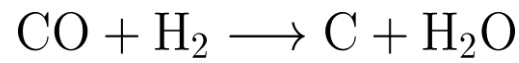
- Reaction is reversible, meaning that full reaction consists of a forward reaction and a reverse reaction.

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/m³**, the reaction rate units will become **mol/m³/s**.

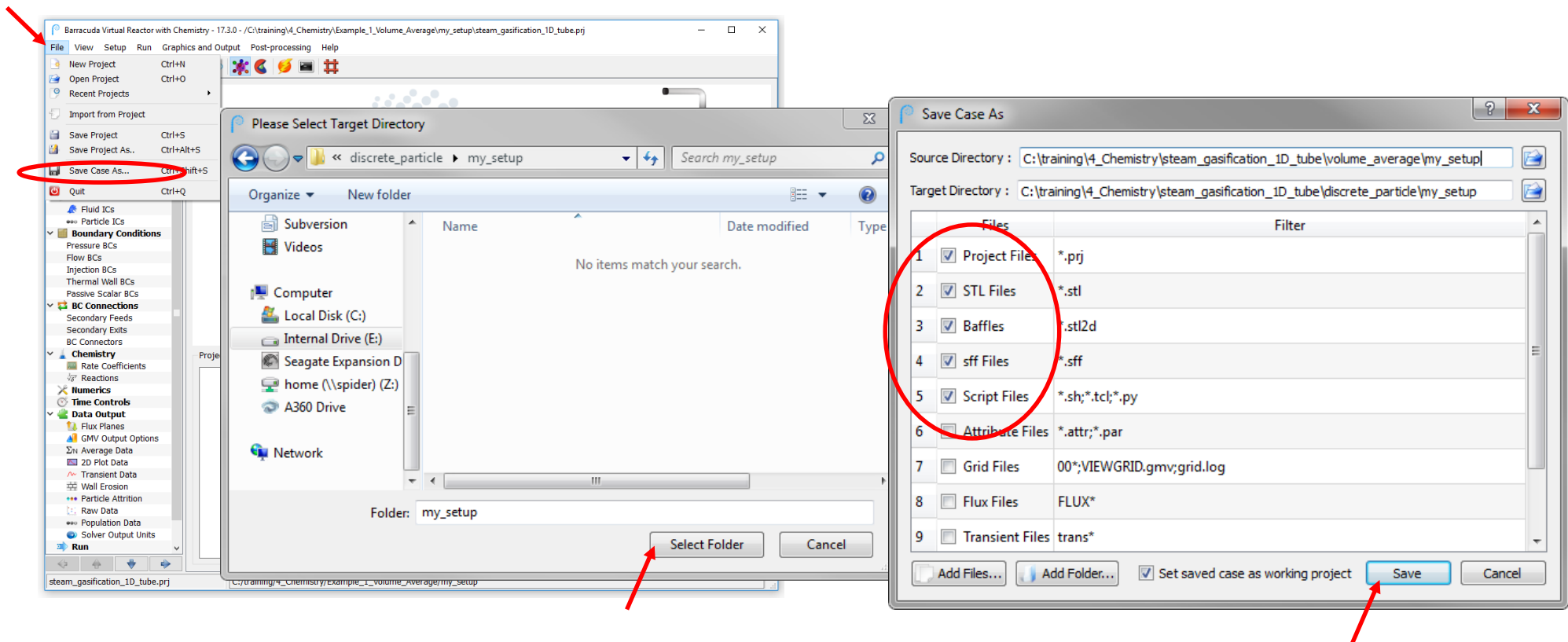
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Modifications to Project Setup

- 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

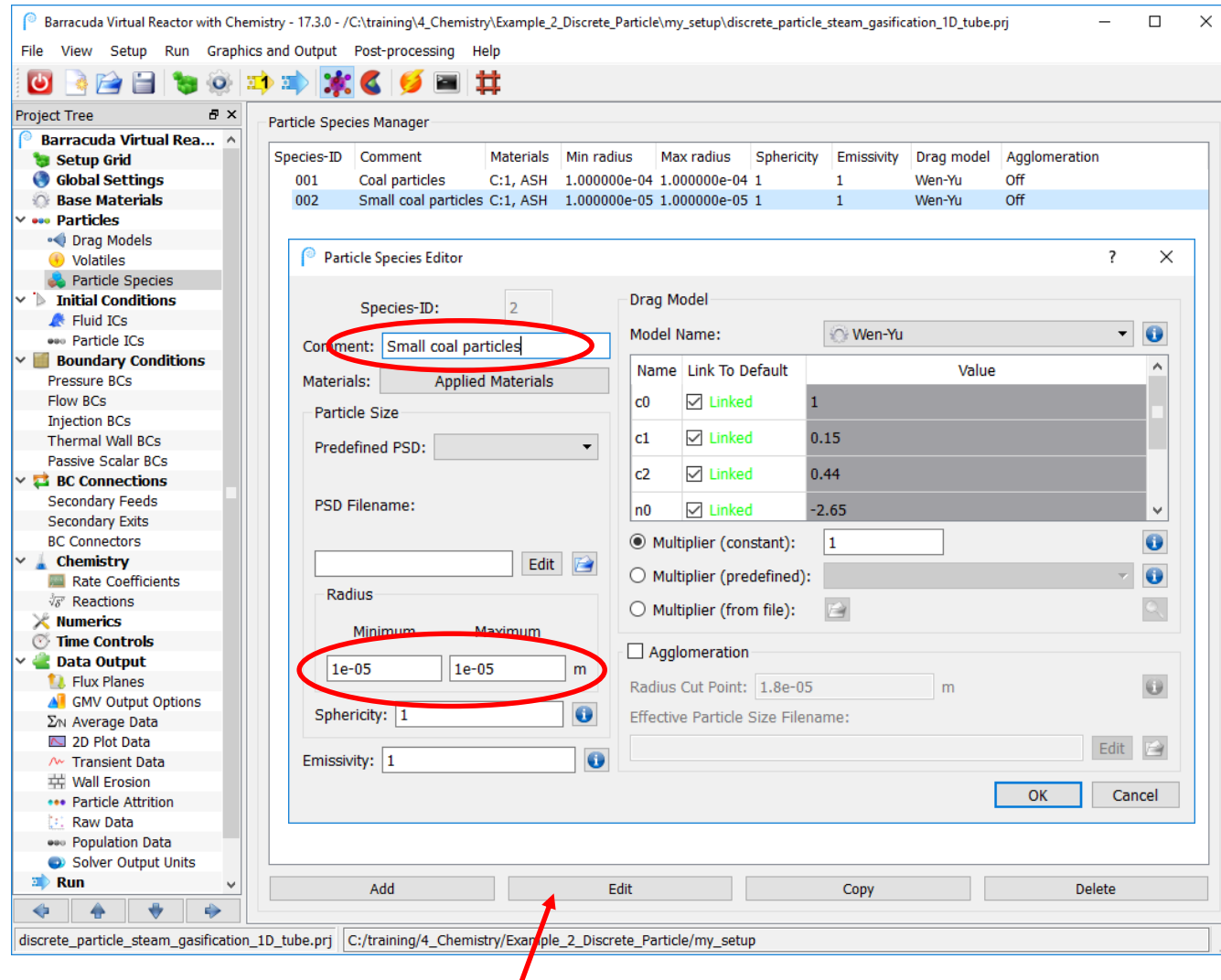
Saving a New Project File

- 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**

Pressure BC Editor

Pressure boundary condition

Region

Direction: **z**

Select region (m)

x₁ 0 x₂ 0.01
y₁ 0 y₂ 0.01
z₁ 0.39 z₂ 0.4

Flux plane options

Flux file name: **FLUXBC_pressure_outlet**

Gas species flux plane behavior:

Mass Fraction

☐ Subdivide by radius Radius divisions 5

☐ Output raw particle data

Comment

10 atm pressure at outlet

Fluid behavior at boundary

☐ Pressure file: **Edit**

☒ Specify values:

Area fraction 1

Pressure 1.0132e+06 Pa

Temperature 975 K

K-factor 0

Properties

Fluid properties if inflow Interior cell values

Applied fluid species Define fluid species

Particle behavior at boundary

☐ No particle exit

☒ Particle out flow

Particle radius(m) range allowed to exit:

Min = 0 to Max = UNLIMITED

☐ Particle feed (Slip and vol frac)

☐ Particle feed (Slip and mass flux)

☐ Particle feed (Slip and mass flow rate)

Edit particle feed

Particle Feed Control

OK **Cancel**

Pressure BC Manager

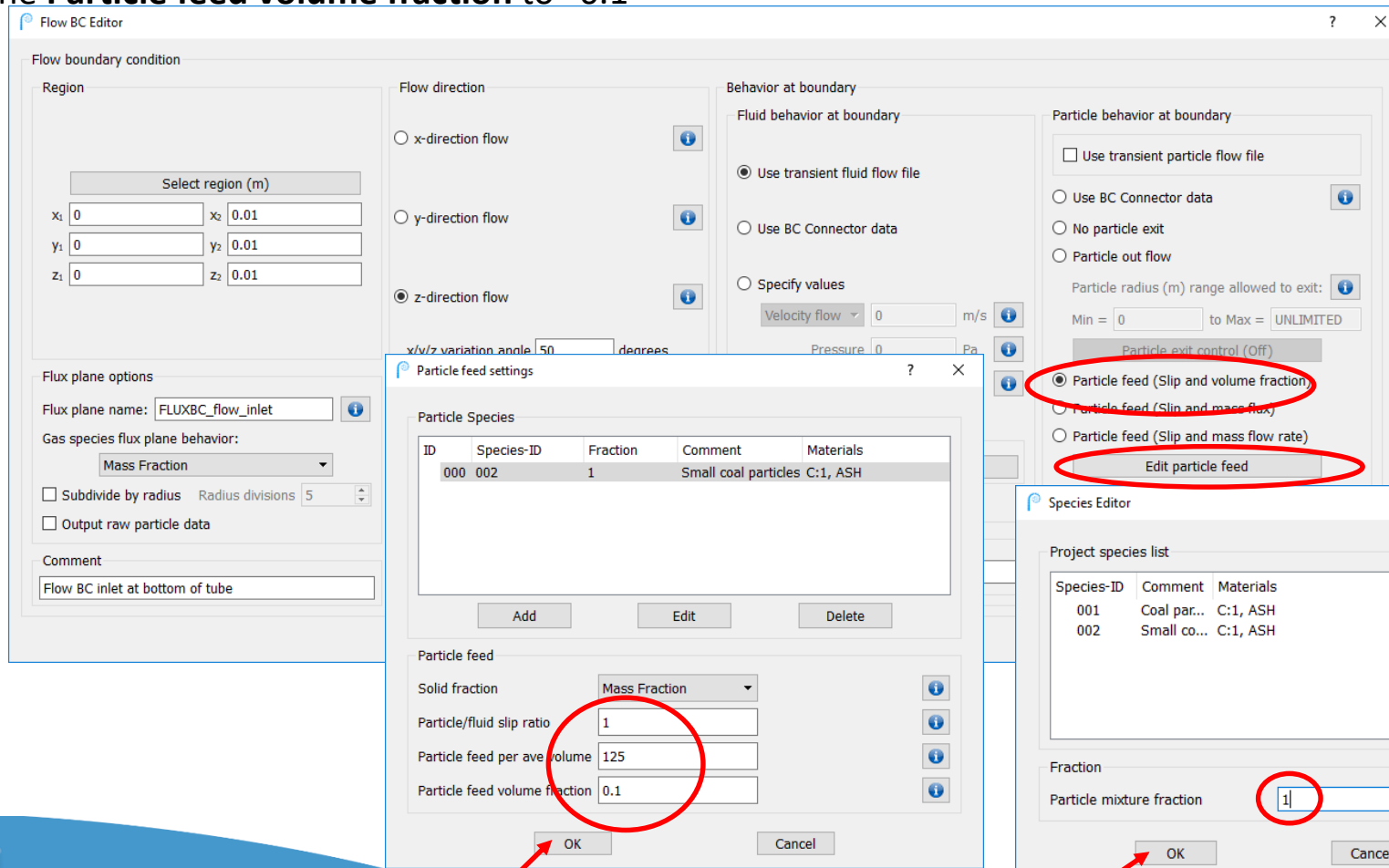
ID	Dir	x1	x2	y1	y2
000	z	0	0.01	0	0.0

Add Edit Copy Delete

K-factor adjustment: $k = (1 + c_1 \theta_p) k_{\text{clean}}$
c1 = 0

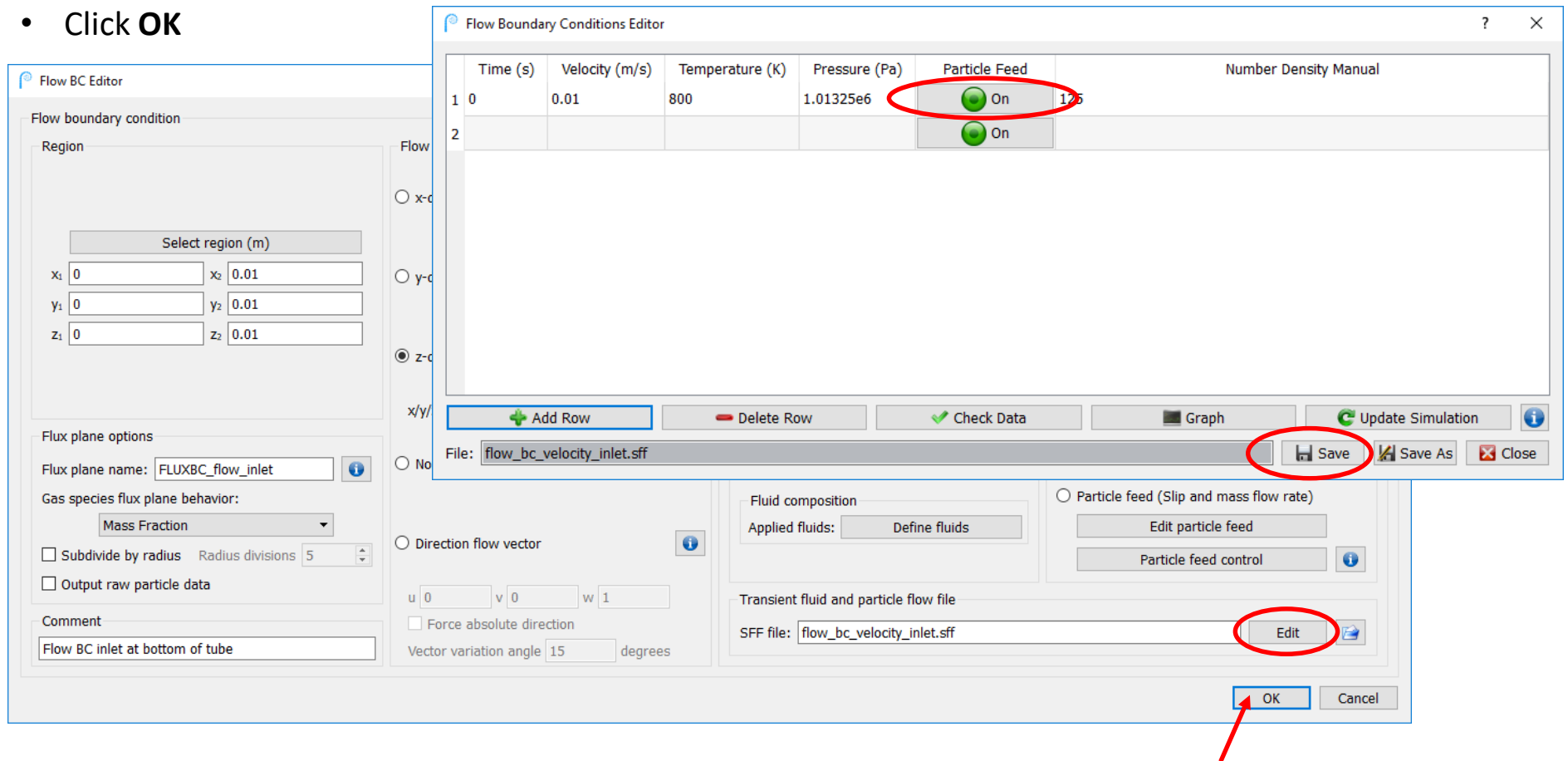
Flow Boundary Conditions

- 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”



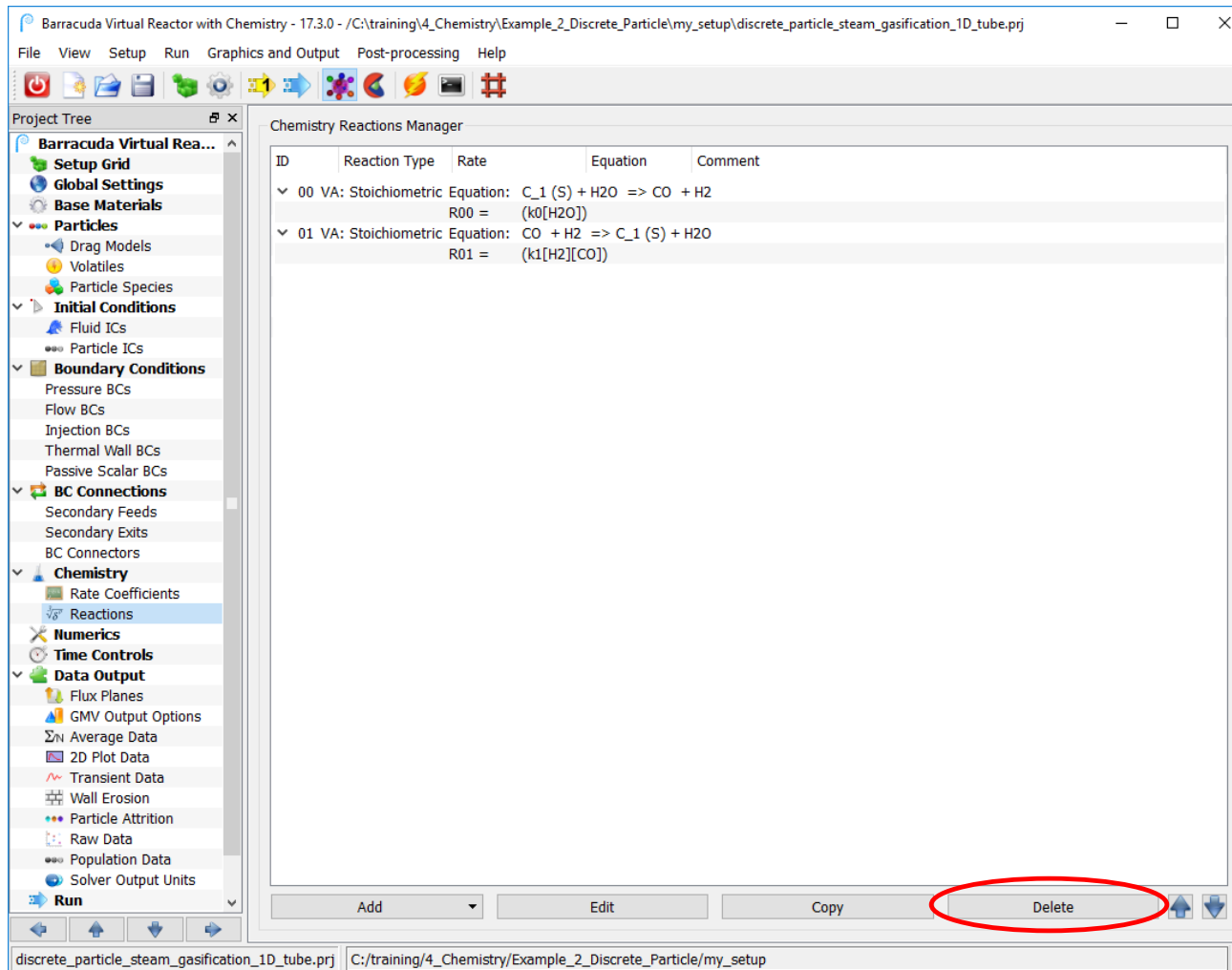
Flow Boundary Conditions

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



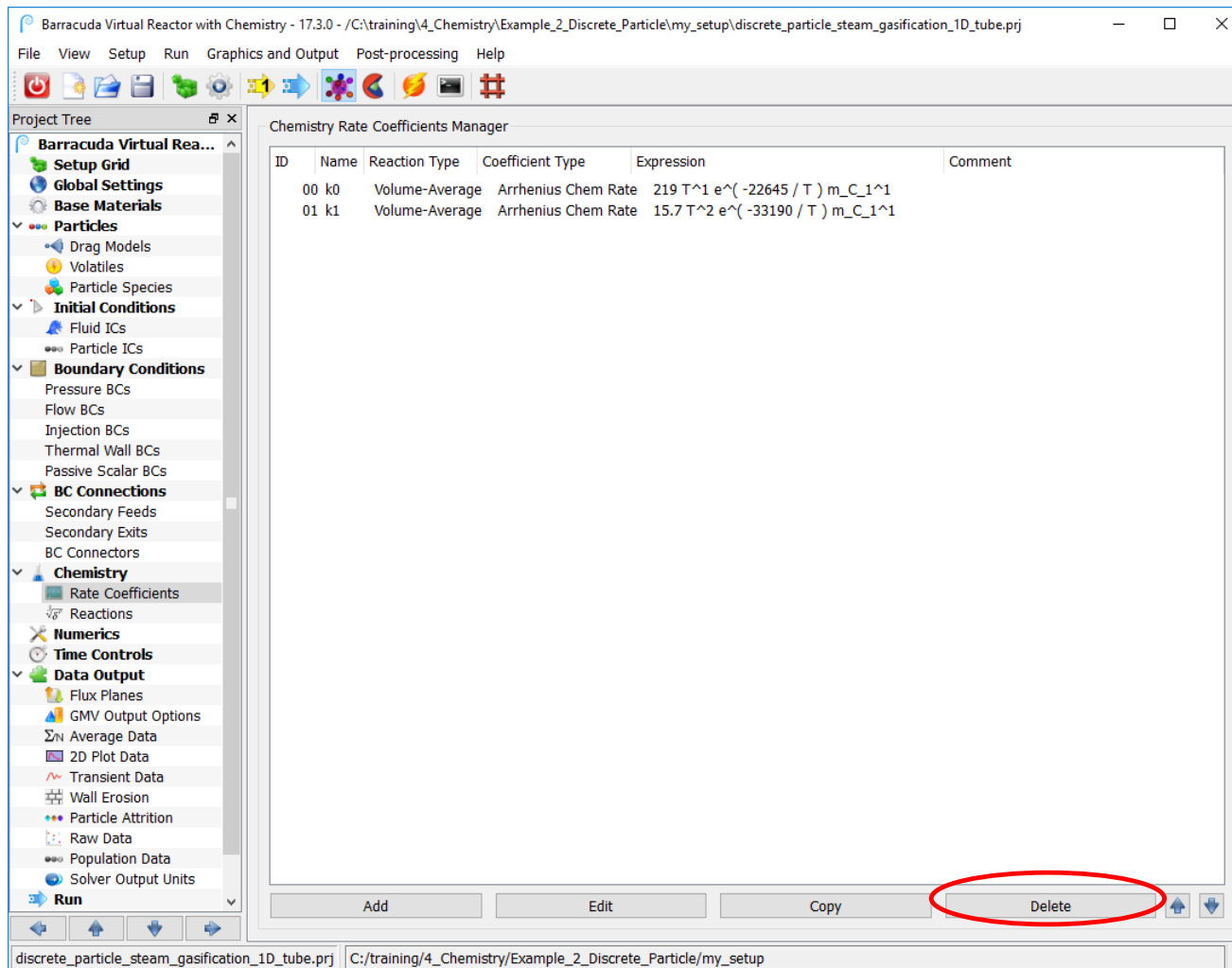
Deleting Existing Reactions

- 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

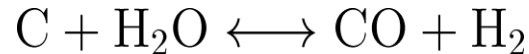


Adding Discrete Particle Chemistry

- 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)

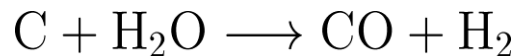
Steam Gasification Chemistry

- Recall that the chemical reaction being modeled is:



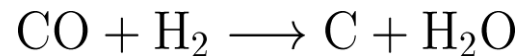
- In Barracuda, a reversible reaction is defined by splitting it into the forward and reverse reactions, defining a reaction rate for both the forward and reverse directions

Forward Reaction



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

Reverse Reaction



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

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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

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

- Substituting the reaction rate and solid mass definition terms,

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

$$\frac{d[C(s)]}{dt} = r \theta_f (V_{cell} / N_p) = - \left(219 \frac{\text{m}^3}{\text{kg K s}} \right) T \theta_f \exp \left(\frac{-22645\text{K}}{T} \right) m_C [\text{H}_2\text{O}]$$

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Forward Reaction in Discrete Particle Form

- Discrete Particle Reaction Rate

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

- Additional reactants and products

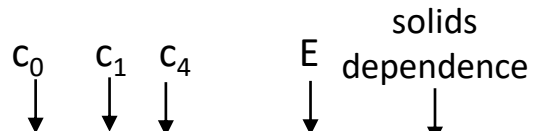
$$\begin{aligned}\frac{d[H_2O]}{dt} &= 1 \frac{d[C(s)]}{dt} \\ \frac{d[CO]}{dt} &= -1 \frac{d[C(s)]}{dt} \\ \frac{d[H_2]}{dt} &= -1 \frac{d[C(s)]}{dt}\end{aligned}$$

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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:



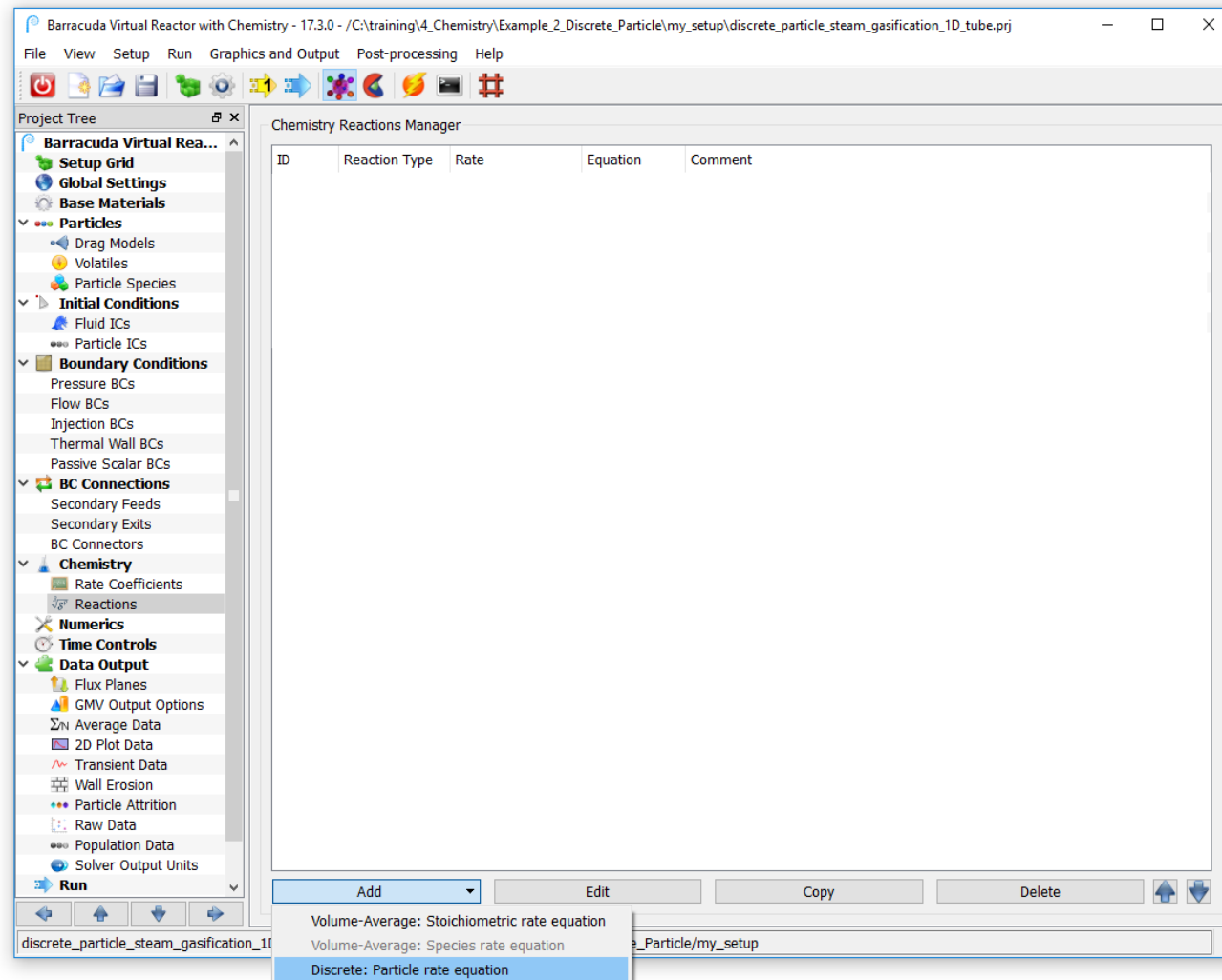
- $k_0 = 219 T^1 \Theta_f^1 \exp(-22645/T) m_{C:1}$
- Check that **Discrete** is selected
- Remember to click on **Solids Dependence** and select **C:1**
- Click **OK**

The image displays three screenshots from the Barracuda Virtual Reactor software interface:

- Top Left:** The main project tree with the 'Chemistry' section expanded, showing 'Rate Coefficients' and 'Reactions'.
- Top Right:** The 'Chemistry Coefficient Editor' dialog box. The 'Name' is 'k0', 'Type' is 'Arrhenius Chem Rate', and 'Coefficient is for reaction type' is 'Discrete' (circled in red). The 'Equation' is $k_0 = 219 T^1 \Theta_f^1 e^{-22645/T} m_{C:1}$. The 'Values' section shows $C_0 = 219$, $C_1 = 1$, $C_2 = 0$, $C_3 = 0$, $C_4 = 1$, $C_5 = 0$, $E = 22645$, and $E_0 = 0$. The 'type_s' dropdown is set to 'Solids Dependence' (indicated by a red arrow). The 'Temperature unit' is 'K', 'Pressure unit' is 'Pa', 'Density unit' is 'kg/m^3', 'Diameter unit' is 'm', 'Mass unit' is 'kg', and 'Area unit' is 'm^2'. The 'Fluid weighting factor' and 'Particle weighting factor' are both 0.50.
- Bottom:** The 'Solids Dependence' dialog box. The 'Species List' table shows 'C:1' with state 'S' and type 'mass'. The 'Material coefficient type' is 'mass' and the 'Exponent on material' is '1'. The 'Solid Project Species List' table shows 'C:1' with state 'S' and description 'C CARBON, SOLID' (circled in red).

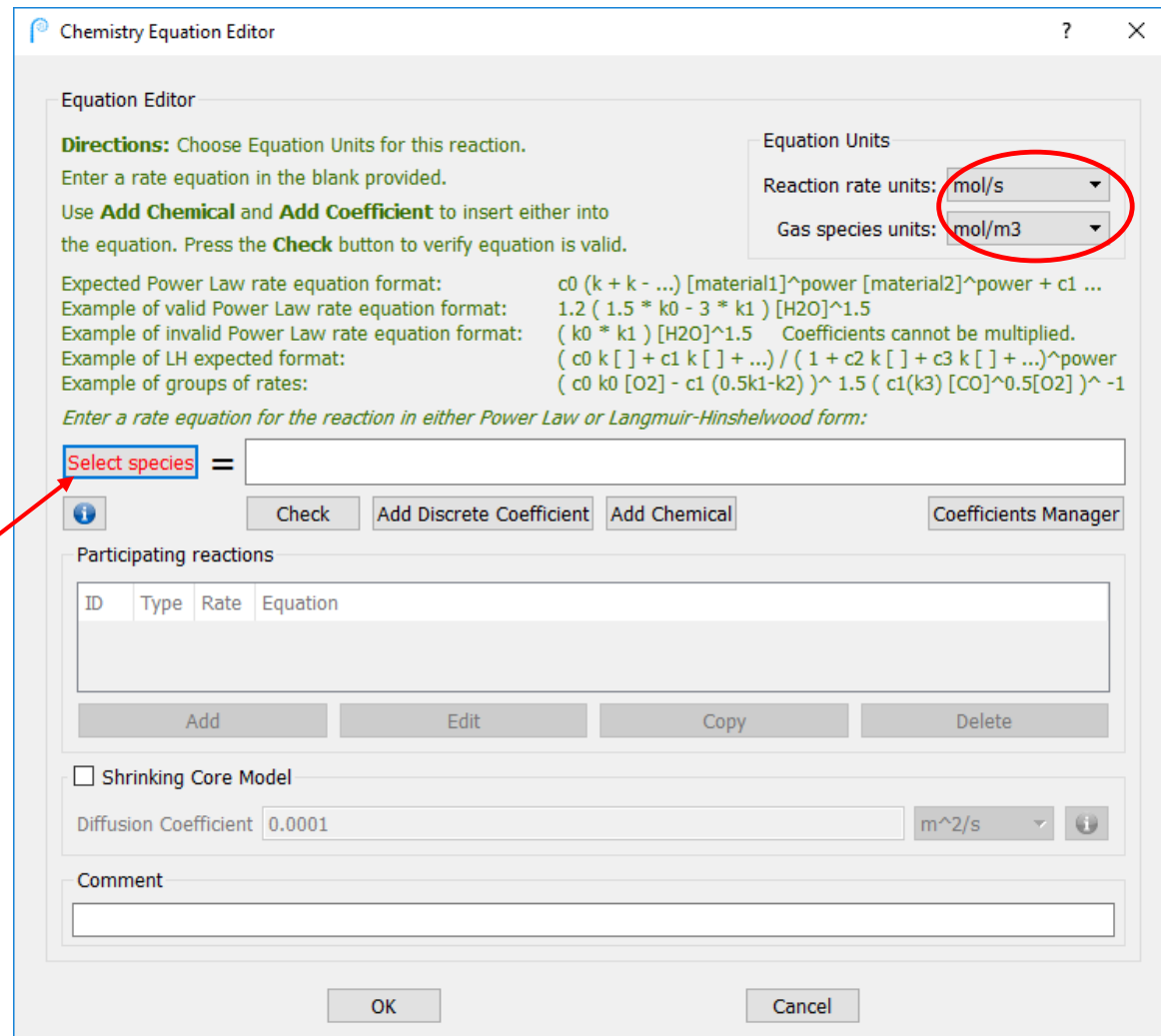
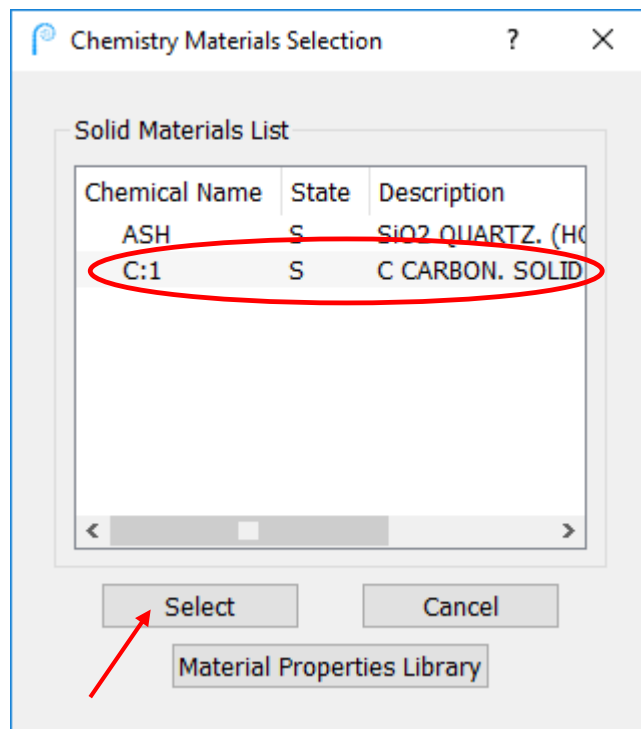
Creating the Forward Reaction

- 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

The screenshot shows the **Chemistry Equation Editor** window with the equation $d[C:1(S)]/dt = (-1k_0[H_2O])$ entered. The **Add Discrete Coefficient** and **Add Chemical** buttons are circled in red. Below the editor, two windows are shown: **Chemistry Coefficient Selection** and **Chemistry Materials Selection**.

Chemistry Coefficient Selection window:

ID	Name	Reaction Type	Coefficient Type	Expression
00	k0	Discrete	Arrhenius Chem Rate	219 T ⁻¹ theta_f ⁻¹

Chemistry Materials Selection window:

Chemical Name	State	Description
CO	G	CO CARBON MONO
H2	G	H2 HYDROGEN. RE
H2O	G	H2O STEAM
N2	G	N2 NITROGEN. RE

Specifying Participating Reactions

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

$$\frac{d[\text{H}_2\text{O}]}{dt} = 1 \frac{d[\text{C}(s)]}{dt}$$

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

Chemistry Equation Editor

Equation Editor

Directions: Choose Equation Units for this reaction. Enter a rate equation in the blank provided. Use **Add Chemical** and **Add Coefficient** to add species and coefficients to the equation. Press the **Check** button to verify the equation.

Expected Power Law rate equation form: $\frac{d[\text{C}]}{dt} = k[\text{H}_2\text{O}]^n$
 Example of valid Power Law rate equation: $\frac{d[\text{C}]}{dt} = k[\text{H}_2\text{O}]^n$
 Example of invalid Power Law rate equation: $\frac{d[\text{C}]}{dt} = k[\text{H}_2\text{O}]^n + k[\text{H}_2\text{O}]^m$
 Example of LH expected format: $\frac{d[\text{C}]}{dt} = k[\text{H}_2\text{O}]^n$
 Example of groups of rates: $\frac{d[\text{C}]}{dt} = k[\text{H}_2\text{O}]^n$
 Enter a rate equation for the reaction in the blank provided.

Equation Units: Reaction rate units:

Chemistry Product Editor

Directions: Click on the buttons to select a chemical species and coefficient. Enter a constant in the text box if needed.

= d[C:1(S)]/dt

OK Cancel

Chemistry Materials Selection

Materials List

Chemical Name	State	Description
ASH	S	SiO2 QUARTZ. (H2O)
C:1	S	C CARBON. SOLID
CO	G	CO CARBON MONOXIDE
H2	G	H2 HYDROGEN. REACTANT
H2O	G	H2O STEAM
N2	G	N2 NITROGEN. REACTANT

Select Cancel

Material Properties Library

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Specifying Participating Reactions

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

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

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

Chemistry Equation Editor

Equation Editor

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

Expected Power Law rate equation format:
Example of valid Power Law rate equation:
Example of invalid Power Law rate equation:
Example of LH expected format:
Example of groups of rates:
Enter a rate equation for the reaction in e

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

d[C:1(S)]/dt = (-1k0[H2O])

Check Add Dis

Participating reactions

ID	Type	Rate	Equation
00	Discrete	d[H2O(G)]/dt =	1 d[C:1(S)]/dt

Add Edit

☐ Shrinking Core Model

Diffusion Coefficient 0.0001

Comment

OK

Chemistry Product Editor

Directions: Click on the buttons to select a chemical species and coefficient.
Enter a constant in the text box if needed.

= -1 d[C:1(S)]/dt

OK Cancel

Chemistry Materials Selection

Materials List

Chemical Name	State	Description
ASH	S	SiO2 QUARTZ. (H)
C:1	S	C CARBON. SOLID
CO	G	CO CARBON MONO
H2	G	H2 HYDROGEN. RE
H2O	G	H2O STEAM
N2	G	N2 NITROGEN. RE

Select Cancel

Material Properties Library

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Specifying Participating Reactions

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

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

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

Chemistry Equation Editor

Equation Editor

Directions: Choose Equation Units for this reaction.
Enter a rate equation in the blank 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/s
Gas species units: mol/m3

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

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

$d[C:1(S)]/dt = (-1k0[H2O])$

Check **Add Discrete Coefficient** **Add Chemical** **Coefficients Manager**

Participating reactions

ID	Type	Rate	Equation
00	Discrete	$d[H2O(G)]/dt =$	$1 d[C:1(S)]/dt$
01	Discrete	$d[CO(G)]/dt =$	$-1 d[C:1(S)]/dt$
02	Discrete	$d[H2(G)]/dt =$	$-1 d[C:1(S)]/dt$

Add **Edit** **Copy** **Delete**

☐ **Shrinking Core Model**

Diffusion Coefficient: 0.0001 m^2/s

Comment

OK **Cancel**

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Forward Reaction Rate

- The forward reaction rate equation is now complete

Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/4_Chemistry/Example_2_Discrete_Particle/my_setup/discrete_particle_steam_gasification_1D_tube.prj

File View Setup Run Graphics and Output Post-processing Help

Project Tree

- Barracuda Virtual Rea...
- Setup Grid
- Global Settings
- Base Materials
- Particles
 - Drag Models
 - Volatiles
 - Particle Species
- Initial Conditions
 - Fluid ICs
 - Particle ICs
- Boundary Conditions
 - Pressure BCs
 - Flow BCs
 - Injection BCs
 - Thermal Wall BCs
 - Passive Scalar BCs
- BC Connections
 - Secondary Feeds
 - Secondary Exits
 - BC Connectors
- Chemistry
 - Rate Coefficients
 - Reactions
- Numerics
- Time Controls
- Data Output
 - Flux Planes
 - GMV Output Options
 - Average Data
 - 2D Plot Data
 - Transient Data
 - Wall Erosion
 - Particle Attrition
 - Raw Data
 - Population Data
 - Solver Output Units
- Run

Chemistry Reactions Manager

ID	Reaction Type	Rate	Equation	Comment
00	Discrete	$d[C:1(S)]/dt =$	$(-1k_0[H_2O])$	
00		$d[H_2O(G)]/dt =$	$1 d[C:1(S)]/dt$	
01		$d[CO(G)]/dt =$	$-1 d[C:1(S)]/dt$	
02		$d[H_2(G)]/dt =$	$-1 d[C:1(S)]/dt$	

discrete_particle_steam_gasification_1D_tube.prj C:/training/4_Chemistry/Example_2_Discrete_Particle/my_setup

Converting the Reverse Reaction Rate to Discrete Particle Chemistry

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

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

- Substituting the reaction rate and solid mass definition terms

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

$$\frac{d[C(s)]}{dt} = r \theta_f (V_{cell} / N_p) = \left(15.7 \frac{\text{m}^6}{\text{kg mol K}^2 \text{s}} \right) T^2 \theta_f \exp \left(\frac{-33190 \text{ K}}{T} \right) m_C [\text{H}_2] [\text{CO}]$$

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Reverse Reaction in Discrete Particle Form

- Discrete Particle Reaction Rate

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

- Additional reactants and products

$$\begin{aligned} \frac{d[H_2O]}{dt} &= 1 \frac{d[C(s)]}{dt} \\ \frac{d[CO]}{dt} &= -1 \frac{d[C(s)]}{dt} \\ \frac{d[H_2]}{dt} &= -1 \frac{d[C(s)]}{dt} \end{aligned}$$

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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
 \downarrow \downarrow \downarrow \downarrow \downarrow
 $k_1 = 15.7 T^2 \Theta_f^1 \exp(-33190/T) m_{C:1}$
- 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**

The screenshot shows the Barracuda Virtual Reactor software interface. The Project Tree on the left highlights the 'Chemistry' section, specifically 'Rate Coefficients'. The 'Add' button is highlighted with a red arrow. The 'Chemistry Rate Coefficients Manager' window shows a table with columns: ID, Name, Reaction Type, and Coefficient. The first entry is '00 k0 Discrete Arrhenius'. The 'Chemistry Coefficient Editor' window is open for 'k1'. It shows the 'Coefficient Properties' tab with the following settings:

- Name: k1
- Type: Arrhenius Chem Rate
- Coefficient is for reaction type: ☒ Discrete
- Equation: $c_0 T^{c_1} p^{c_2} \rho_f^{c_3} \Theta_f^{c_4} (Np/Vol)^{c_5} e^{-E/T+E0} \{type_s\}$
- Equation for k1: $k_1 = 15.7 T^2 \Theta_f^1 e^{-33190/T} m_{C:1}$
- Values:
 - $c_0 = 15.7$
 - $c_1 = 2$
 - $c_2 = 0$
 - $c_3 = 0$
 - $c_4 = 1$
 - $c_5 = 0$
 - $E = 33190$
 - $E0 = 0$
- Units:
 - Temperature unit: K
 - Pressure unit: Pa
 - Density unit: kg/m³
 - Diameter unit: m
 - Mass unit: kg
 - Area unit: m²
- type_s = Solids Dependence (highlighted with a red arrow)
- Temperature Weighting:
 - Fluid weighting factor: 0.50
 - Particle weighting factor: 0.50
- Comment: (empty field)

The 'OK' and 'Cancel' buttons are at the bottom right of the editor window.

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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

The screenshot displays the Barracuda Virtual Reactor software interface. On the left is the **Project Tree** with a hierarchical list of settings including Setup Grid, Global Settings, Base Materials, Particles, Initial Conditions, Boundary Conditions, BC Connections, Chemistry, Numerics, Time Controls, and Data Output. The **Chemistry** section is expanded, showing **Reactions**. A red arrow points to the **Add** button at the bottom of the Project Tree.

The main window is the **Chemistry Equation Editor**. It contains the following elements:

- Equation Editor** section:
 - Directions:** Choose Equation Units for this reaction. Enter a rate equation in the blank 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/s** (circled in red)
 - Gas species units: **mol/m3** (circled in red)
 - 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: $(c_0 k_0 [\text{O}_2] - c_1 (0.5k_1 - k_2))^{\wedge} 1.5 (c_1(k_3) [\text{CO}]^{\wedge} 0.5 [\text{O}_2])^{\wedge} -1$
 - Instruction: Enter a rate equation for the reaction in either Power Law or Langmuir-Hinshelwood form:
 - Equation input field: $d[\text{C:1(S)}]/dt = (k_1[\text{H}_2][\text{CO}])$ (The entire equation is circled in red).
 - Buttons: **Check**, **Add Discrete Coefficient**, **Add Chemical**, **Coefficients Manager**.
- Participating reactions** section:

ID	Type	Rate	Equation

 Buttons: **Add**, **Edit**, **Copy**, **Delete**.
- Shrinking Core Model** checkbox (unchecked).
- Diffusion Coefficient** input: 0.0001, units: **m^2/s**.
- Comment** text area.
- OK** and **Cancel** buttons.

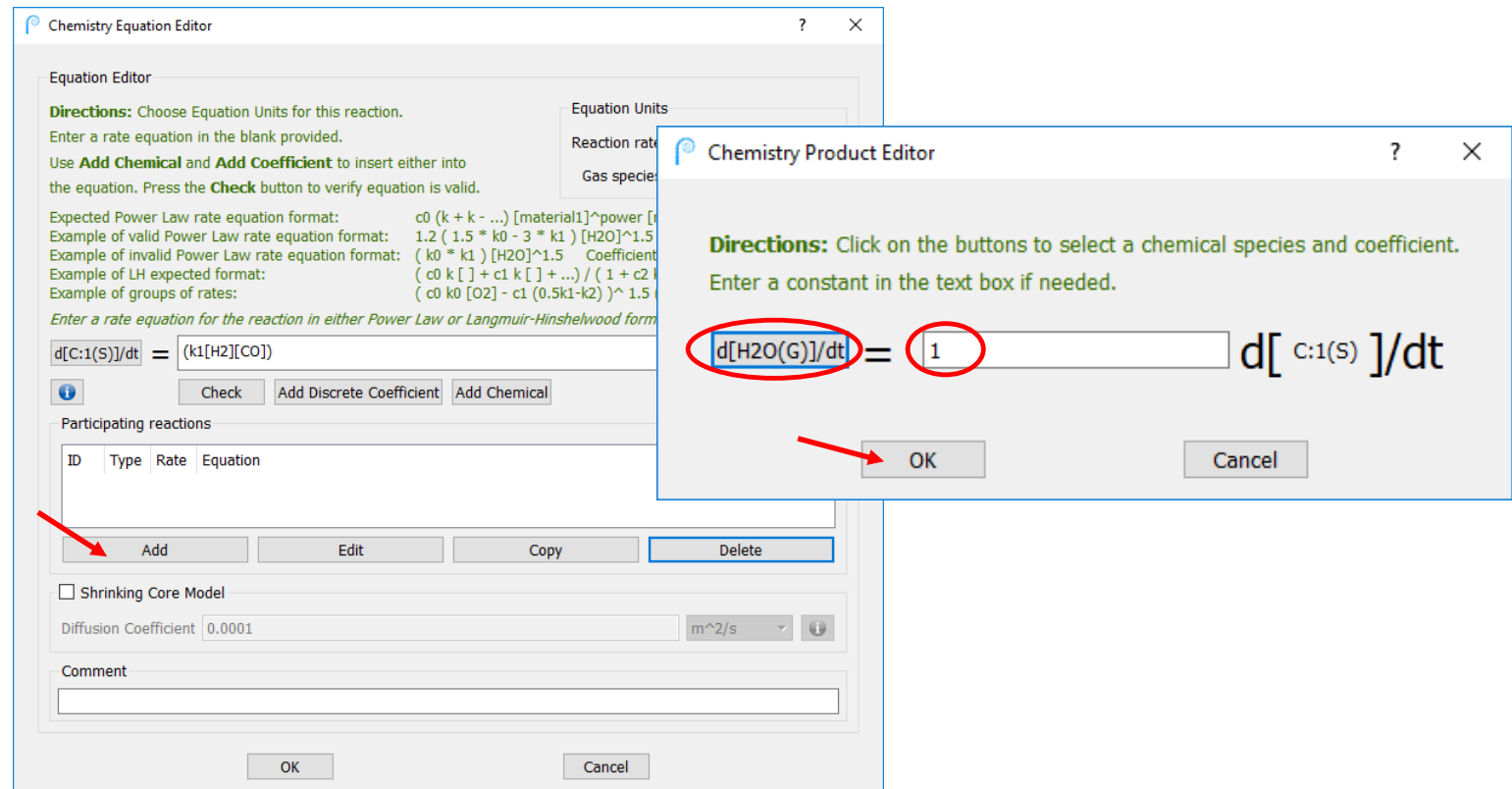
At the bottom of the window, there is a status bar with file names: `discrete_particle_steam_gasification_1D_tube.prj` and `C:/training/4_Chemistry/Example_2_Discrete_Particle/my_setup`.

Specifying Participating Reactions

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

$$\frac{d[\text{H}_2\text{O}]}{dt} = 1 \frac{d[\text{C}(s)]}{dt}$$

- Click **OK**



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Specifying Participating Reactions

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

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

$$\frac{d[\text{H}_2]}{dt} = -1 \frac{d[\text{C}(s)]}{dt}$$

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

Chemistry Equation Editor

Equation Editor

Directions: Choose Equation Units for this reaction.
Enter a rate equation in the blank 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/s
Gas species units: mol/m3

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

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

$d[\text{C:1(S)}]/dt = (k_1[\text{H}_2][\text{CO}])$

Check Add Discrete Coefficient Add Chemical Coefficients Manager

Participating reactions

ID	Type	Rate	Equation
00	Discrete	$d[\text{H}_2\text{O}(\text{G})]/dt =$	$1 d[\text{C:1(S)}]/dt$
01	Discrete	$d[\text{CO}(\text{G})]/dt =$	$-1 d[\text{C:1(S)}]/dt$
02	Discrete	$d[\text{H}_2(\text{G})]/dt =$	$-1 d[\text{C:1(S)}]/dt$

Add Edit Copy Delete

☐ Shrinking Core Model

Diffusion Coefficient 0.0001 m²/s

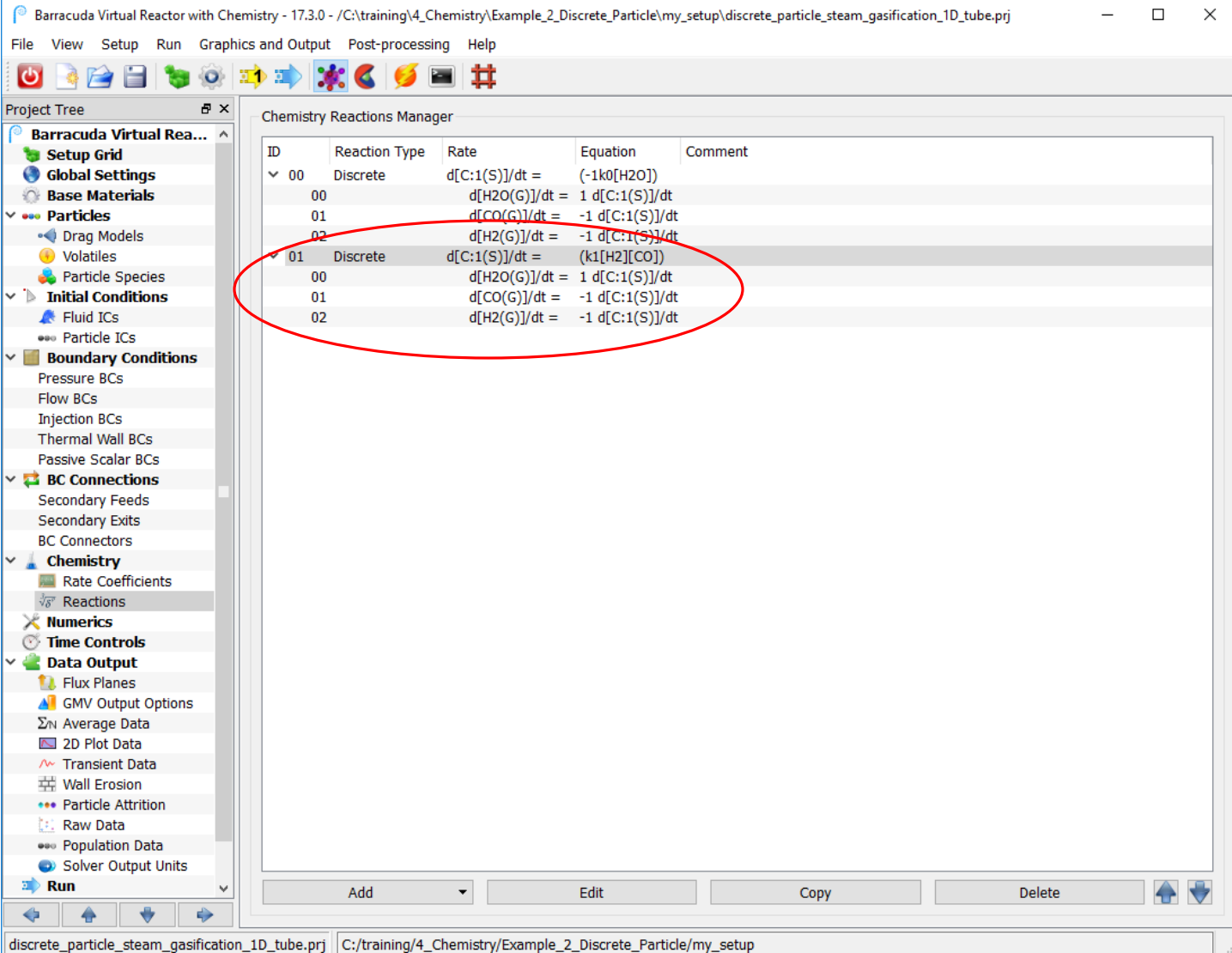
Comment

OK Cancel

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Reverse Reaction Rate

- The reverse reaction rate equation is now complete



Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/4_Chemistry/Example_2_Discrete_Particle/my_setup/discrete_particle_steam_gasification_1D_tube.prj

File View Setup Run Graphics and Output Post-processing Help

Project Tree

- Barracuda Virtual Rea...
- Setup Grid
- Global Settings
- Base Materials
- Particles
 - Drag Models
 - Volatiles
 - Particle Species
- Initial Conditions
 - Fluid ICs
 - Particle ICs
- Boundary Conditions
 - Pressure BCs
 - Flow BCs
 - Injection BCs
 - Thermal Wall BCs
 - Passive Scalar BCs
- BC Connections
 - Secondary Feeds
 - Secondary Exits
 - BC Connectors
- Chemistry
 - Rate Coefficients
 - Reactions
- Numerics
- Time Controls
- Data Output
 - Flux Planes
 - GMV Output Options
 - Average Data
 - 2D Plot Data
 - Transient Data
 - Wall Erosion
 - Particle Attrition
 - Raw Data
 - Population Data
 - Solver Output Units
- Run

Chemistry Reactions Manager

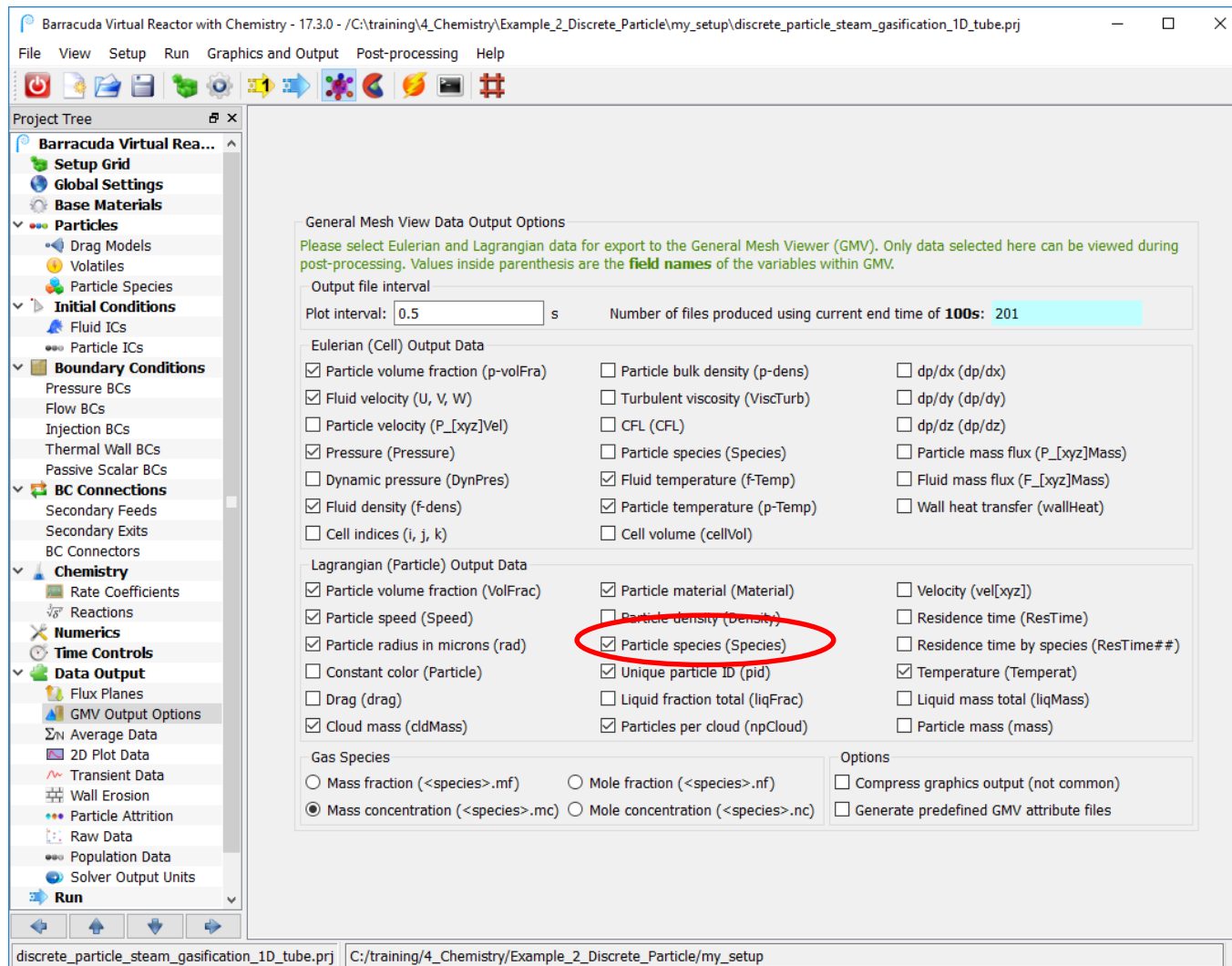
ID	Reaction Type	Rate	Equation	Comment
00	Discrete	$d[C:1(S)]/dt =$	$(-1k0[H2O])$	
01		$d[H2O(G)]/dt =$	$1 d[C:1(S)]/dt$	
02		$d[CO(G)]/dt =$	$-1 d[C:1(S)]/dt$	
03		$d[H2(G)]/dt =$	$-1 d[C:1(S)]/dt$	
01	Discrete	$d[C:1(S)]/dt =$	$(k1[H2][CO])$	
00		$d[H2O(G)]/dt =$	$1 d[C:1(S)]/dt$	
01		$d[CO(G)]/dt =$	$-1 d[C:1(S)]/dt$	
02		$d[H2(G)]/dt =$	$-1 d[C:1(S)]/dt$	

Add Edit Copy Delete

discrete_particle_steam_gasification_1D_tube.prj C:/training/4_Chemistry/Example_2_Discrete_Particle/my_setup

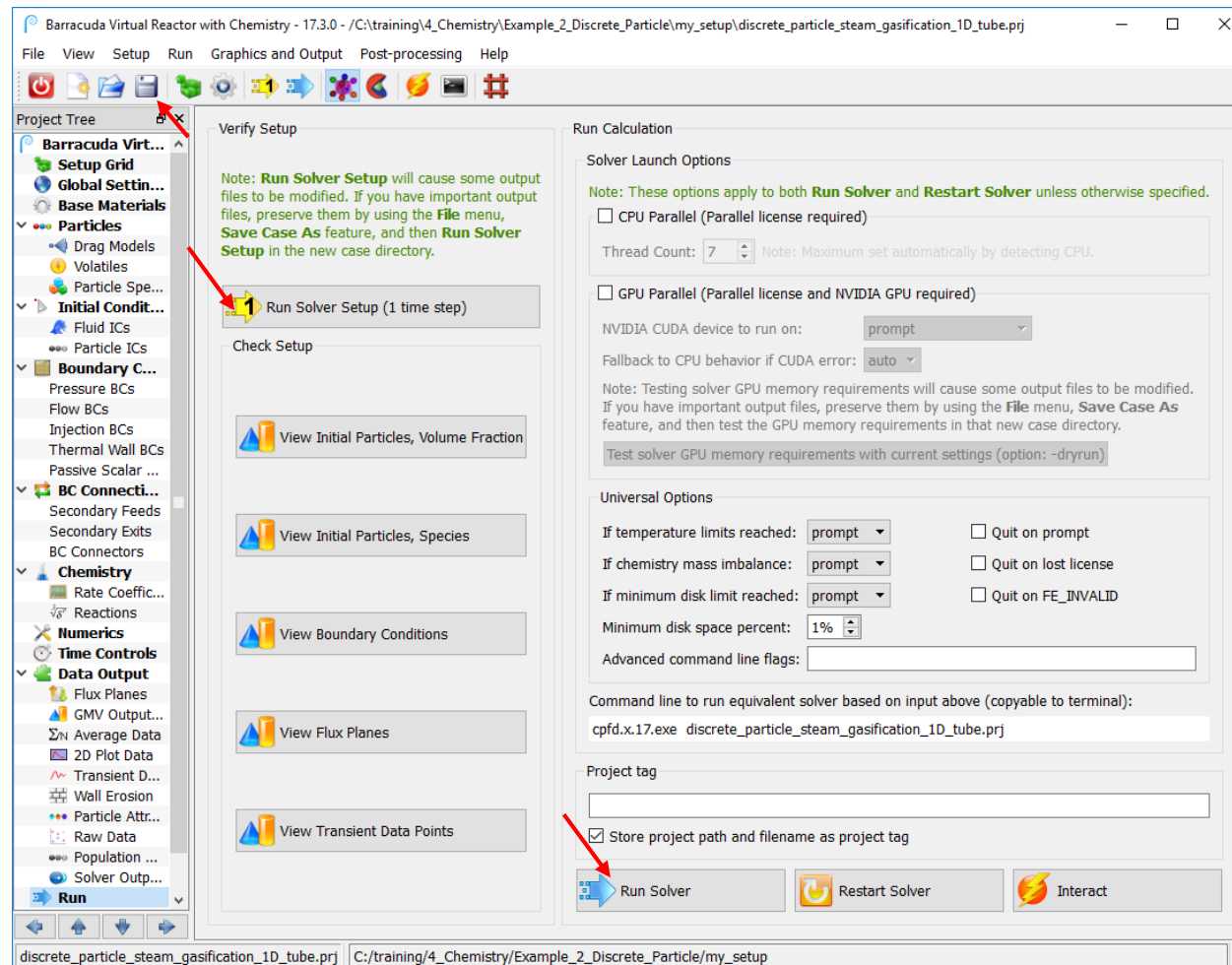
GMV Output Options

- 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



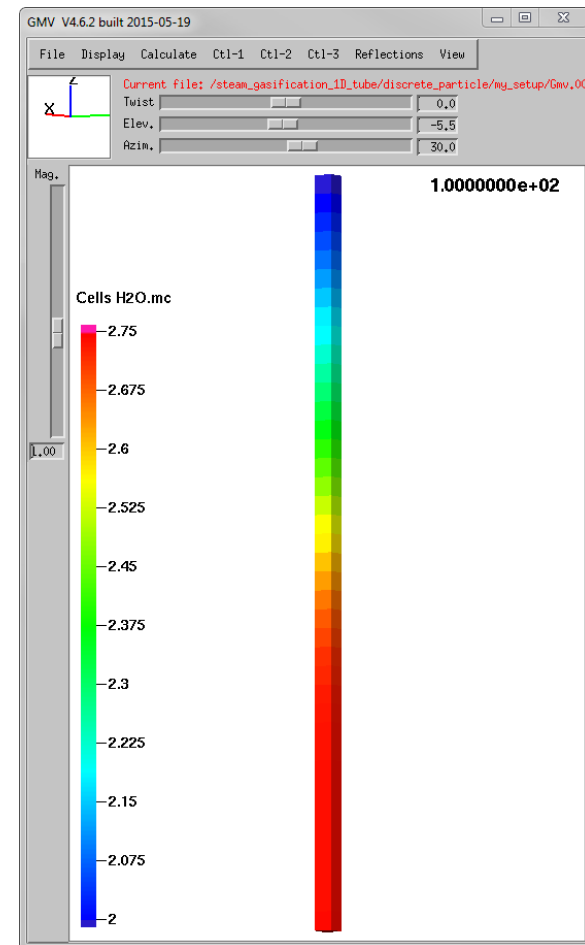
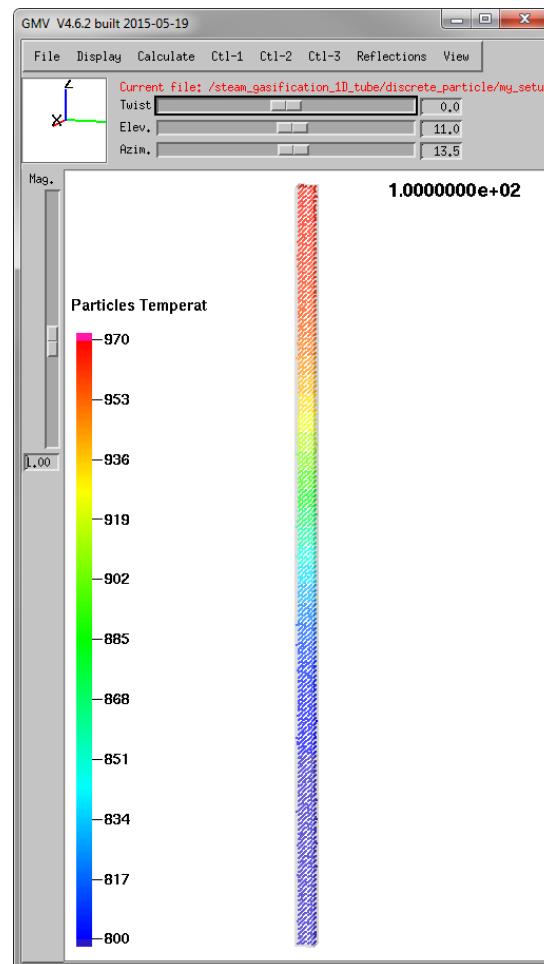
Start the Barracuda Solver

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



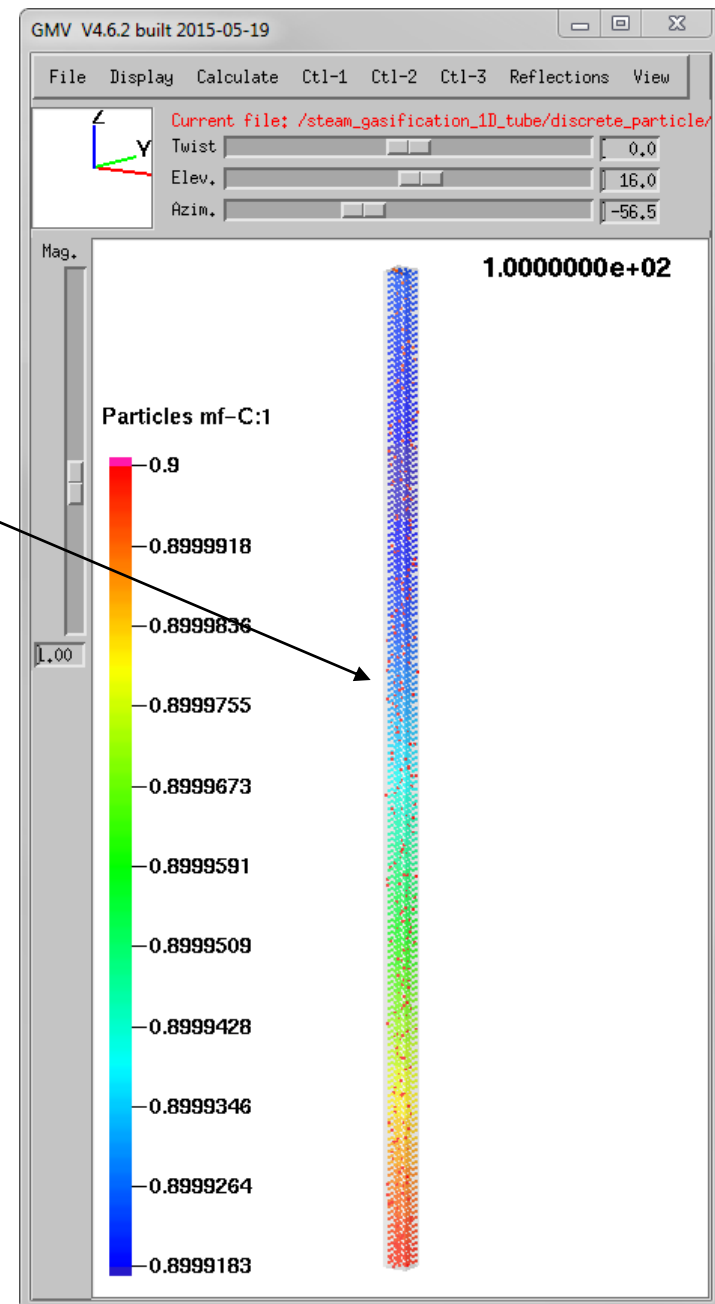
Post Processing

- 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**



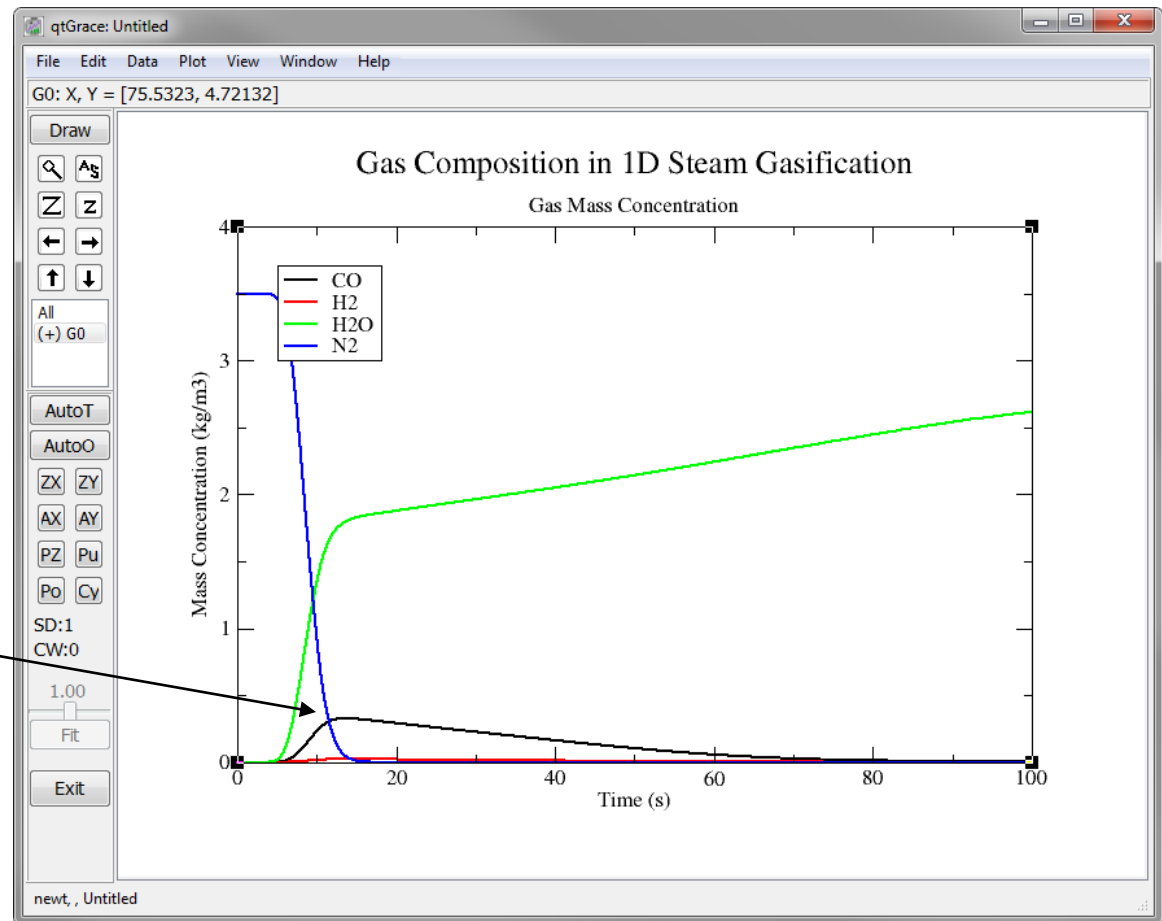
Post Processing

- 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?



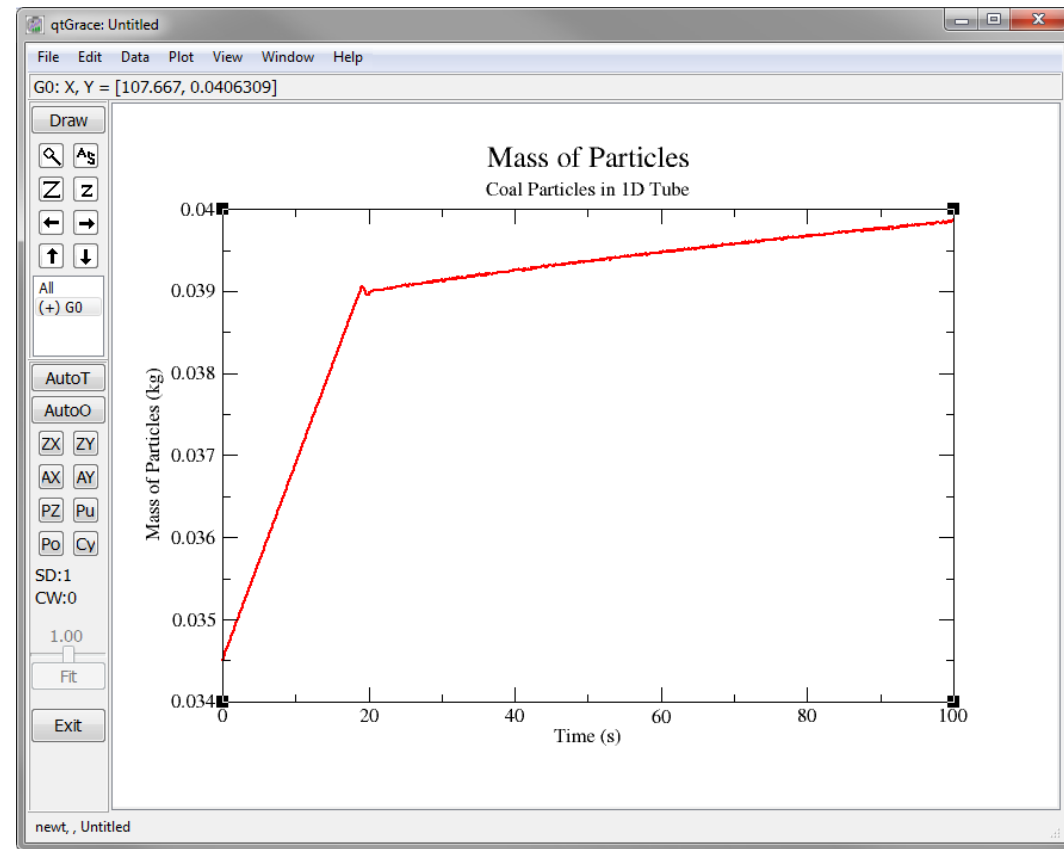
Plotting Transient Data

- 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 ($z \sim 0.2$ 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.



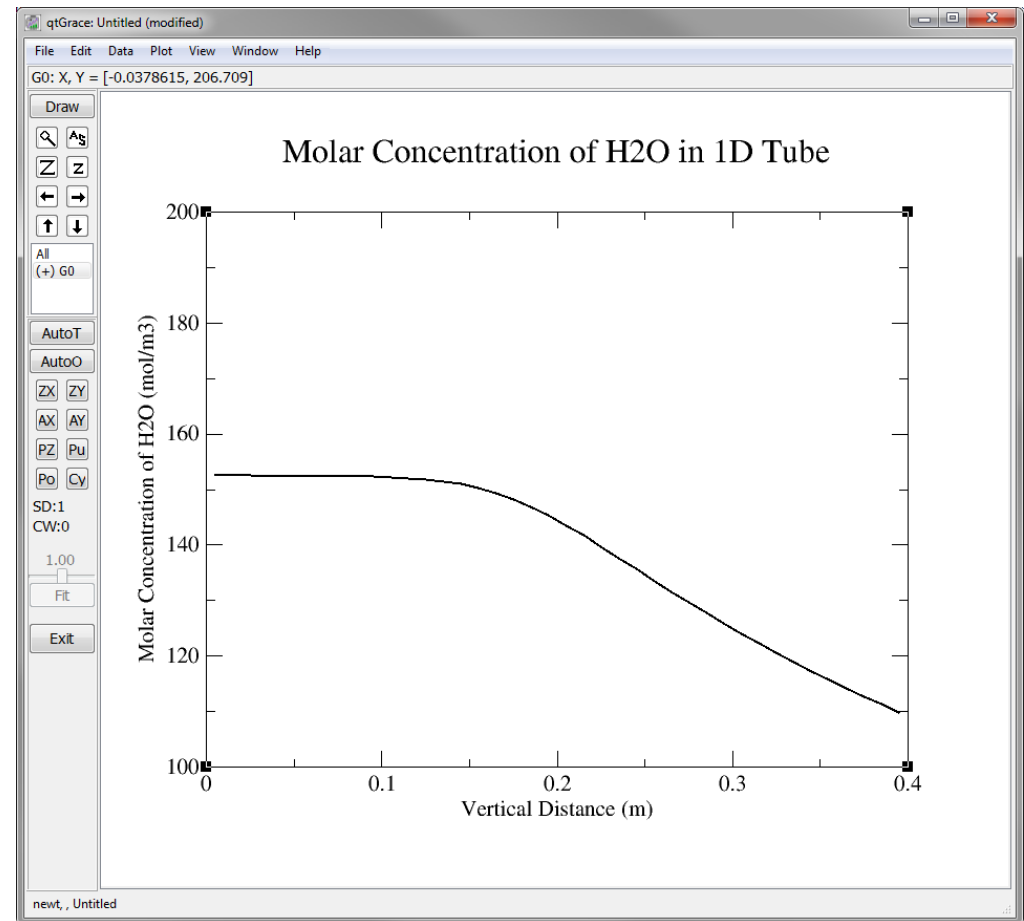
Plotting Transient Data

- 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

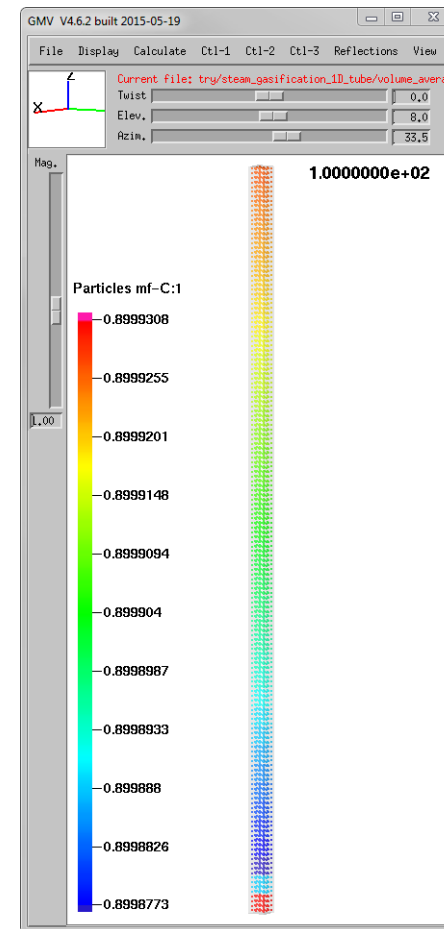
- Make a plot of the molar concentration of H_2O versus vertical distance in Plot Manager
 - Hint: Data is in the **H2O_zxMoleConc_00100.000.dat** file
- The concentration of H_2O is highest at the bottom of the tube.



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

