

Chemistry Training Example 2: Discrete Particle

February 2018

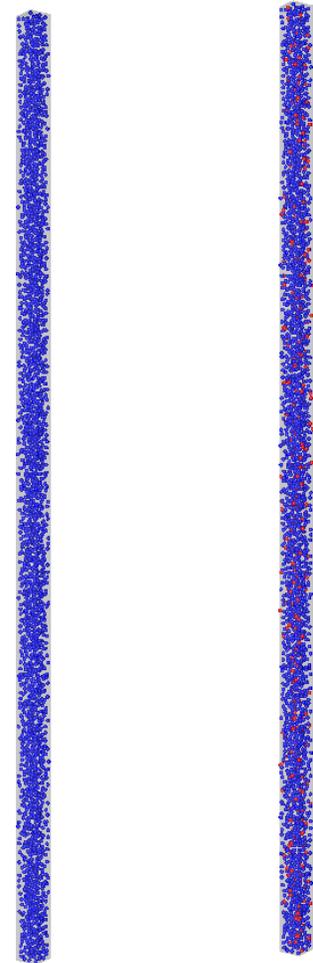
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Training Plan

- 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 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

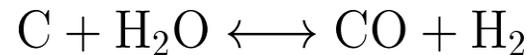


Case #1

Case #2

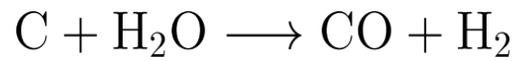
Steam Gasification Reaction

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



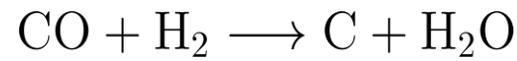
- Reaction is reversible, meaning that full reaction consists of a forward reaction and a reverse reaction.

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**.

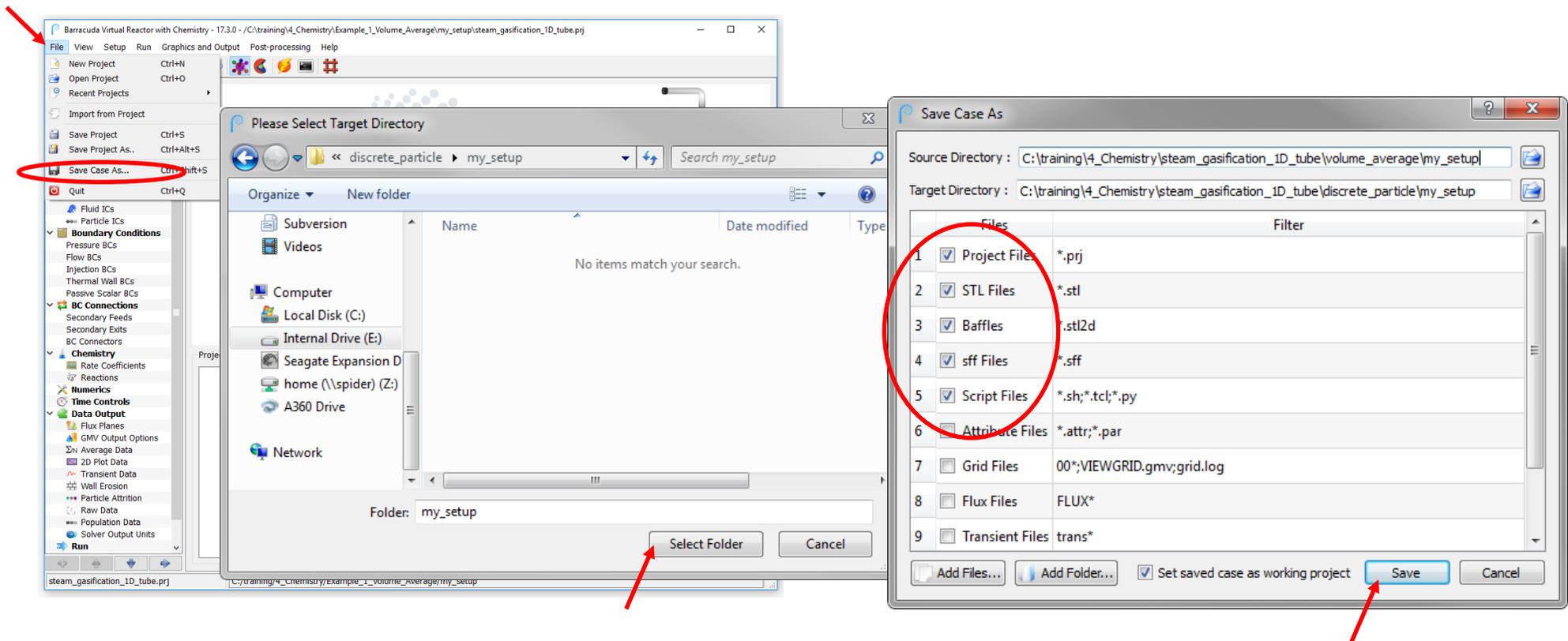
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Modifications to Project Setup

- 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**

The screenshot shows the Barracuda Virtual Reactor interface. The Project Tree on the left lists various settings, with 'Particle Species' selected. The Particle Species Manager window displays a table of species:

Species-ID	Comment	Materials	Min radius	Max radius	Sphericity	Emissivity	Drag model	Agglomeration
001	Coal particles	C:1, ASH	1.000000e-04	1.000000e-04	1	1	Wen-Yu	Off
002	Small coal particles	C:1, ASH	1.000000e-05	1.000000e-05	1	1	Wen-Yu	Off

The Particle Species Editor window is open for species 002. The 'Comment' field is set to 'Small coal particles' and the 'Radius' (Minimum and Maximum) is set to '1e-05 m'. The 'Drag Model' is set to 'Wen-Yu'. The 'Multiplier (constant)' is set to 1. The 'Agglomeration' checkbox is unchecked. The 'Radius Cut Point' is set to 1.8e-05 m. The 'OK' button is highlighted with a red arrow.

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**

The screenshot displays the Barracuda Virtual Reactor software interface. The main window shows a project tree on the left with categories like Global Settings, Base Materials, Particles, Initial Conditions, Boundary Conditions, BC Connections, Chemistry, Numerics, Time Controls, and Data Output. The 'Boundary Conditions' section is expanded, showing 'Pressure BCs'. A 'Pressure BC Manager' table lists a boundary with ID '000', direction 'z', and coordinates (0, 0.01, 0, 0.0). The 'Pressure BC Editor' dialog box is open, showing the 'Particle behavior at boundary' section with the 'Particle out flow' option selected. The 'Fluid behavior at boundary' section has 'Specify values' selected, with fields for Area fraction (1), Pressure (1.0132e+06 Pa), Temperature (975 K), and K-factor (0). The 'Flux plane options' section has 'Flux file name' set to 'FLUXBC_pressure_outlet' and 'Gas species flux plane behavior' set to 'Mass Fraction'. The 'Comment' field contains '10 atm pressure at outlet'. The 'OK' button is highlighted with a red arrow.

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

Fluid behavior at boundary

Pressure file: [] Edit

Specify values:

Area fraction: 1

Pressure: 1.0132e+06 Pa

Temperature: 975 K

K-factor: 0

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)

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

Applied fluid species: Define fluid species

OK Cancel

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”

The screenshot displays the 'Flow BC Editor' interface. The main window shows the 'Flow boundary condition' settings for a region. The 'Particle feed settings' dialog is open, showing the following table:

ID	Species-ID	Fraction	Comment	Materials
000	002	1	Small coal particles	C:1, ASH

The 'Particle feed' section in the dialog shows the following values:

- Solid fraction: Mass Fraction
- Particle/fluid slip ratio: 1
- Particle feed per average volume: 125
- Particle feed volume fraction: 0.1

The 'Species Editor' dialog is also open, showing the 'Project species list' table:

Species-ID	Comment	Materials
001	Coal par...	C:1, ASH
002	Small co...	C:1, ASH

The 'Particle mixture fraction' is set to 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**

Flow BC Editor

Flow boundary condition

Region

Select region (m)

x₁ 0 x₂ 0.01

y₁ 0 y₂ 0.01

z₁ 0 z₂ 0.01

Flux plane options

Flux plane name: FLUXBC_flow_inlet

Gas species flux plane behavior:

Mass Fraction

Subdivide by radius Radius divisions 5

Output raw particle data

Comment

Flow BC inlet at bottom of tube

	Time (s)	Velocity (m/s)	Temperature (K)	Pressure (Pa)	Particle Feed	Number Density Manual
1	0	0.01	800	1.01325e6	On	1.75
2					On	

File: flow_bc_velocity_inlet.sff

Save Save As Close

Fluid composition

Applied fluids: Define fluids

Particle feed (Slip and mass flow rate)

Edit particle feed

Particle feed control

Transient fluid and particle flow file

SFF file: flow_bc_velocity_inlet.sff

Edit

OK Cancel

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**

The screenshot shows the Barracuda Virtual Reactor software interface. The main window is titled "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". The interface includes a menu bar (File, View, Setup, Run, Graphics and Output, Post-processing, Help) and a toolbar with various icons. On the left is a "Project Tree" with categories like Setup Grid, Global Settings, Base Materials, Particles, Initial Conditions, Boundary Conditions, BC Connections, Chemistry, Numerics, Time Controls, and Data Output. The "Chemistry" category is expanded, showing "Rate Coefficients" and "Reactions". The "Reactions" sub-category is selected, displaying the "Chemistry Reactions Manager" window. This window contains a table with the following data:

ID	Reaction Type	Rate	Equation	Comment
00 VA	Stoichiometric	Equation: $C_1(S) + H_2O \Rightarrow CO + H_2$ R00 = $(k0[H_2O])$		
01 VA	Stoichiometric	Equation: $CO + H_2 \Rightarrow C_1(S) + H_2O$ R01 = $(k1[H_2][CO])$		

At the bottom of the "Chemistry Reactions Manager" window, there is a toolbar with buttons for "Add", "Edit", "Copy", and "Delete". The "Delete" button is circled in red. The status bar at the bottom of the software window shows the file path: "discrete_particle_steam_gasification_1D_tube.prj C:/training/4_Chemistry/Example_2_Discrete_Particle/my_setup".

Deleting Existing Rate Coefficients

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

The screenshot shows the Barracuda Virtual Reactor software interface. The main window is titled "Chemistry Rate Coefficients Manager" and contains a table with the following data:

ID	Name	Reaction Type	Coefficient Type	Expression	Comment
00	k0	Volume-Average	Arrhenius Chem Rate	$219 T^{11} e^{(-22645 / T)}$	$m_{C_1}^{11}$
01	k1	Volume-Average	Arrhenius Chem Rate	$15.7 T^{12} e^{(-33190 / T)}$	$m_{C_1}^{12}$

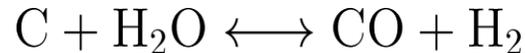
The "Delete" button at the bottom right of the table is circled in red. The Project Tree on the left shows the "Chemistry" folder expanded, with "Rate Coefficients" selected.

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)

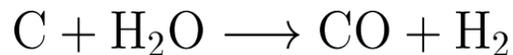
Steam Gasification Chemistry

- Recall that the chemical reaction being modeled is:



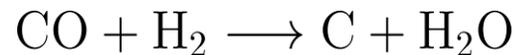
- In Barracuda, a reversible reaction is defined by splitting it into the forward and reverse reactions, defining a reaction rate for both the forward and reverse directions

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

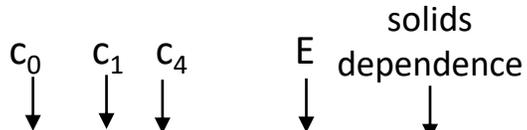
$$\begin{aligned} \frac{d[H_2O]}{dt} &= 1 \frac{d[C(s)]}{dt} \\ \frac{d[CO]}{dt} &= -1 \frac{d[C(s)]}{dt} \\ \frac{d[H_2]}{dt} &= -1 \frac{d[C(s)]}{dt} \end{aligned}$$

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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**

Chemistry Rate Coefficients Manager

ID	Name	Reaction Type	Coefficient Type	Expression
00	k0	Discrete	Arrhenius Chem Rate	219 T^1 theta_f^1 e^{-22645/T} m_{C:1}

Chemistry Coefficient Editor

Name: k0
 Type: Arrhenius Chem Rate
 Coefficient is for reaction type: Volume-Average Discrete
 Equation: $C_0 T^{C_1} p^{C_2} \rho_f^{C_3} \Theta_f^{C_4} (Np/Vol)^{C_5} e^{-E/T+E0} \{type_s\}$
 $k_0 = 219 T^1 \Theta_f^1 e^{-22645/T} m_{C:1}$

Values:

$C_0 = 219$
 $C_1 = 1$ Temperature unit: K
 $C_2 = 0$ Pressure unit: Pa
 $C_3 = 0$ Density unit: kg/m^3
 $C_4 = 1$
 $C_5 = 0$
 $E = 22645$
 $E0 = 0$

type_s = Solids Dependence
 Diameter unit: m
 Mass unit: kg
 Area unit: m^2

Temperature Weighting
 Fluid weighting factor: 0.50
 Particle weighting factor: 0.50

Comment

Buttons: Add, Edit, OK, Cancel

Solids Dependence

Species List

ID	Chemical Name	State	Type	Exponent
00	C:1	S	mass	1

Material coefficient type: mass
 Exponent on material: 1

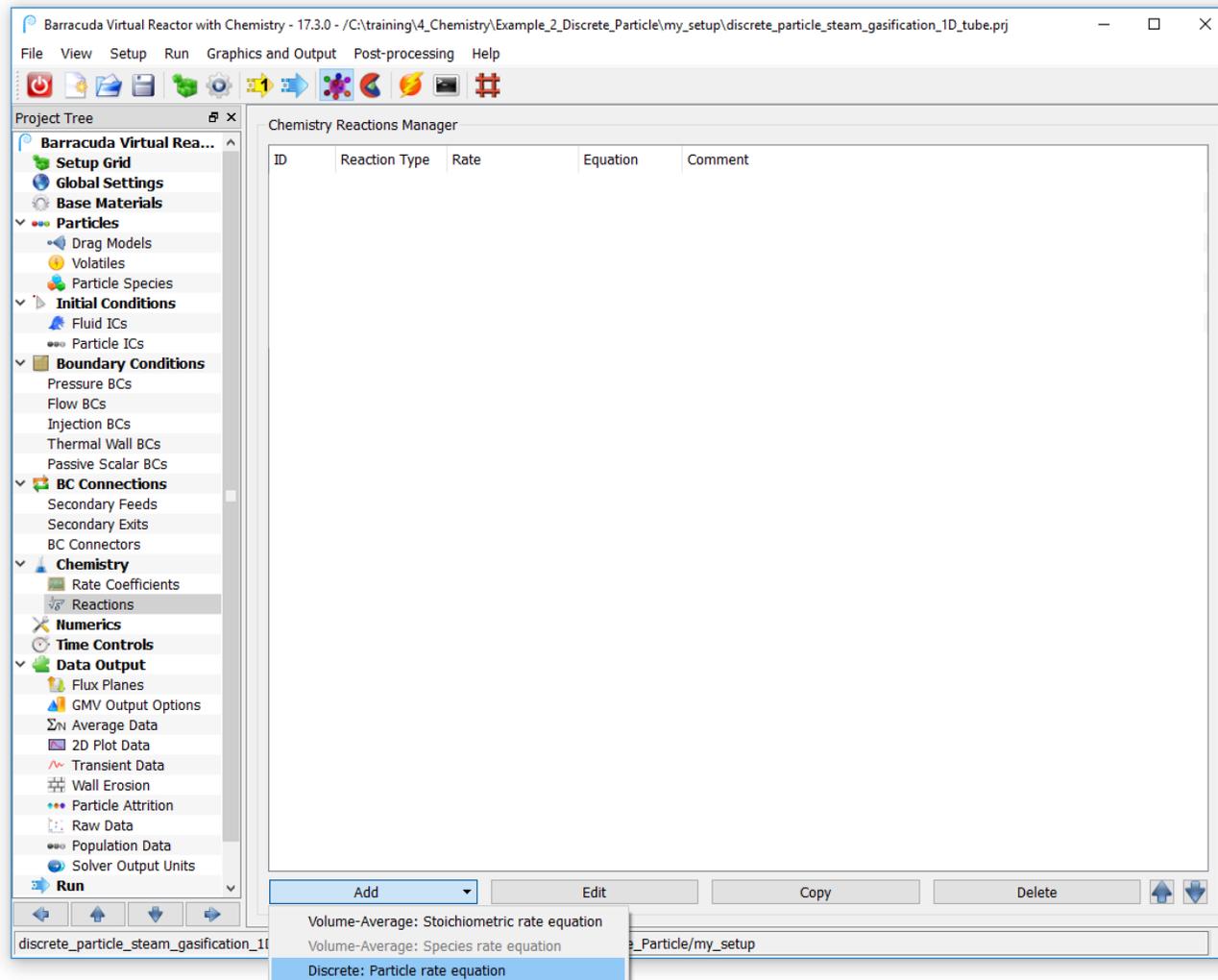
Solid Project Species List

Chemical Name	State	Description
all	S	Add all solids as a...
SiO2	S	SIO2 QUARTZ / (H...
C:1	S	C CARBON, SOLID

Buttons: Import, Replace, Copy, Delete, OK, Cancel

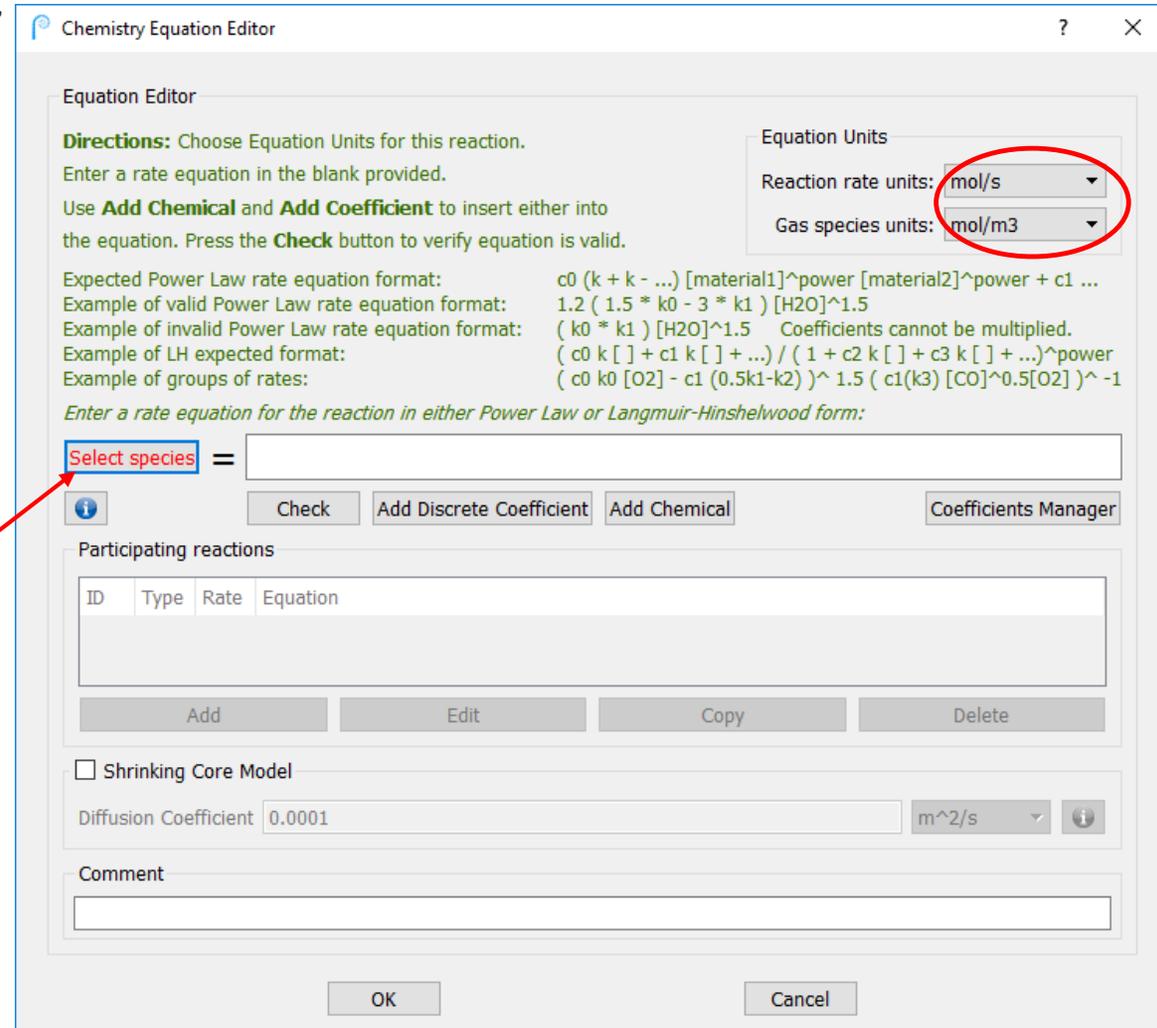
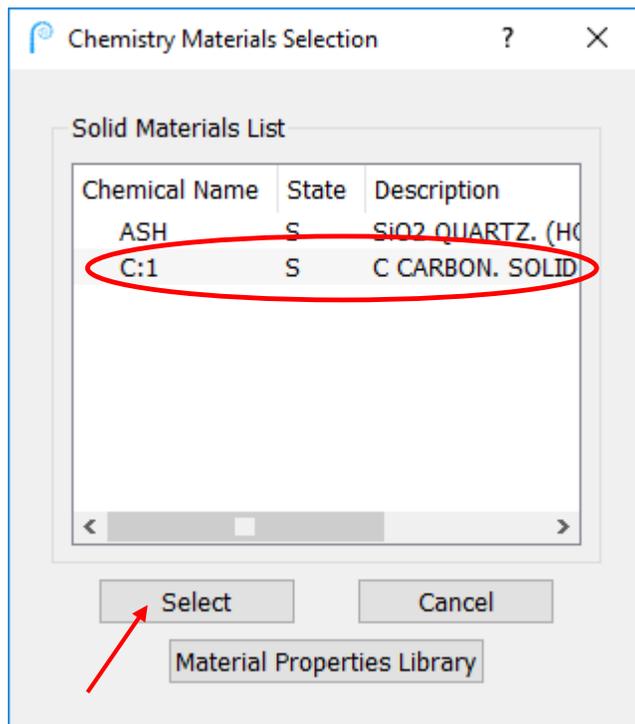
Creating the Forward Reaction

- 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 image shows three overlapping windows from a software interface:

- Chemistry Equation Editor:** The main window where the rate equation $d[C:1(S)]/dt = (-1k_0[H_2O])$ is entered. The **Add Discrete Coefficient** and **Add Chemical** buttons are circled in red. The **Equation Units** are set to **mol/s** and **Gas species units** to **mol/m3**. A **Check** button is also visible.
- Chemistry Coefficient Selection:** A window titled "Chemistry Rate Coefficients Manager" showing a table with one entry:

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

 A red arrow points to the "k0" name.
- Chemistry Materials Selection:** A window titled "Gas Materials List" showing a table:

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

 A red arrow points to the "H2O" entry. Below the table are **Select** and **Cancel** buttons, and a **Material Properties Library** button.

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**

The screenshot illustrates the software workflow for adding a reaction. In the **Chemistry Equation Editor**, the **Participating reactions** table is empty. The **Add** button is highlighted with a red arrow. The **Chemistry Product Editor** dialog is open, showing the equation $d[\text{C:1(S)}]/dt = 1$. The coefficient **1** is circled in red. The **Chemistry Materials Selection** dialog is also open, showing a list of materials. The material **C:1** is selected and highlighted in blue. A red arrow points from the **Select** button in the **Chemistry Materials Selection** dialog back to the **Chemistry Product Editor** dialog.

ID	Type	Rate	Equation

Chemical Name	State	Description
ASH	S	SI02 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...

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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**

The screenshot shows the 'Chemistry Equation Editor' window. At the top, there are instructions: '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.' Below this, there are examples of rate equations and a text box for entering a rate equation: $d[\text{C}:1(\text{S})]/dt = (-1k_0[\text{H}_2\text{O}])$. A 'Chemistry Product Editor' dialog is open over this, with 'Directions: Click on the buttons to select a chemical species and coefficient. Enter a constant in the text box if needed.' The dialog shows a coefficient of -1 being entered for the species C:1(S). A 'Chemistry Materials Selection' dialog is also open, showing a list of materials with CO selected. The 'Add' button in the main window is highlighted with a red arrow.

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

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

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Specifying Participating Reactions

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

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

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

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

$d[\text{C}:1(\text{S})]/dt = (-1k_0[\text{H}_2\text{O}])$

Check Add Discrete Coefficient Add Chemical Coefficients Manager

Participating reactions

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

Add Edit Copy Delete

Shrinking Core Model
Diffusion Coefficient 0.0001 m²/s

Comment

OK Cancel

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Forward Reaction Rate

- The forward reaction rate equation is now complete

The screenshot shows the Barracuda Virtual Reactor software interface. The main window is titled "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". The "Chemistry Reactions Manager" window is open, displaying a table of reactions. A red circle highlights the reaction with ID 00, which is a Discrete reaction with the rate equation $d[C:1(S)]/dt = (-1k_0[H_2O])$. The table also shows reactions for $d[H_2O(G)]/dt = 1 d[C:1(S)]/dt$, $d[CO(G)]/dt = -1 d[C:1(S)]/dt$, and $d[H_2(G)]/dt = -1 d[C:1(S)]/dt$.

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		$d[H_2(G)]/dt = -1 d[C:1(S)]/dt$		

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

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

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:

$$k_1 = 15.7 T^2 \Theta_f^1 \exp(-33190/T) m_{C:1}$$
- 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 main window is titled "Barracuda Virtual Reactor with Chemistry - 17.3.0". The "Chemistry Rate Coefficients Manager" window is open, showing a table with columns for ID, Name, Reaction Type, and Coefficient. The "Add" button is highlighted with a red arrow. The "Chemistry Coefficient Editor" window is also open, showing the "Coefficient Properties" for a coefficient named "k1". The "Type" is set to "Arrhenius Chem Rate". The "Coefficient is for reaction type" is set to "Discrete". The "Equation" is $k_1 = 15.7 T^2 \Theta_f^1 \exp(-33190/T) m_{C:1}$. The "Values" section shows $C_0 = 15.7$, $C_1 = 2$, $C_2 = 0$, $C_3 = 0$, $C_4 = 1$, $C_5 = 0$, $E = 33190$, and $E_0 = 0$. The "type_s" dropdown is set to "Solids Dependence". The "Temperature Weighting" section shows "Fluid weighting factor" and "Particle weighting factor" both set to 0.50. The "Comment" field is empty. The "OK" and "Cancel" buttons are at the bottom.

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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 shows the **Chemistry Equation Editor** window. The **Equation Editor** section contains the following text:

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

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

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

Buttons: Check, Add Discrete Coefficient, Add Chemical, Coefficients Manager

Participating reactions table:

ID	Type	Rate	Equation
----	------	------	----------

Buttons: Add, Edit, Copy, Delete

Shrinking Core Model

Diffusion Coefficient: 0.0001 m²/s

Comment:

Buttons: OK, Cancel

Bottom bar: Add, Edit, Copy, Delete

Status bar: discrete_particle_steam_gasification_1D_tube.prj 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**

The image shows two overlapping software windows. The background window is the 'Chemistry Equation Editor'. It has a 'Participating reactions' table with columns for ID, Type, Rate, and Equation. Below the table are buttons for 'Add', 'Edit', 'Copy', and 'Delete'. A red arrow points to the 'Add' button. The foreground window is the 'Chemistry Product Editor'. It contains a text input field with the equation $d[\text{H}_2\text{O}(\text{G})]/dt = 1 \frac{d[\text{C}:1(\text{S})]}{dt}$. The terms $d[\text{H}_2\text{O}(\text{G})]/dt$ and the coefficient '1' are circled in red. Below the input field are 'OK' and 'Cancel' buttons, with a red arrow pointing to the 'OK' button.

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

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

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

Check Add Discrete Coefficient Add Chemical Coefficients Manager

Participating reactions

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

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

The screenshot shows the Barracuda Virtual Reactor software interface. The main window is titled "Chemistry Reactions Manager" and displays a table of reactions. The table has the following columns: ID, Reaction Type, Rate, Equation, and Comment. The reaction with ID 01 is highlighted with a red circle. The reaction is a Discrete reaction with the rate equation $d[C:1(S)]/dt = (k_1[H_2][CO])$. The software interface also includes a Project Tree on the left and a menu bar at the top.

ID	Reaction Type	Rate	Equation	Comment
00	Discrete	$d[C:1(S)]/dt =$	$(-1k_0[H_2O])$	
01	Discrete	$d[C:1(S)]/dt =$	$(k_1[H_2][CO])$	
02		$d[H_2O(G)]/dt =$	$1 d[C:1(S)]/dt$	
01		$d[CO(G)]/dt =$	$-1 d[C:1(S)]/dt$	
02		$d[H_2(G)]/dt =$	$-1 d[C:1(S)]/dt$	

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

The screenshot shows the Barracuda Virtual Reactor software interface. The Project Tree on the left is expanded to 'Data Output' > 'GMV Output Options'. The main window displays the 'General Mesh View Data Output Options' dialog box. The 'Output file interval' section shows a 'Plot interval' of 0.5 s and 'Number of files produced using current end time of 100s: 201'. The 'Eulerian (Cell) Output Data' section has several checked options: Particle volume fraction (p-volFra), Fluid velocity (U, V, W), Pressure (Pressure), Fluid density (f-dens), and Cell indices (i, j, k). The 'Lagrangian (Particle) Output Data' section has several checked options: Particle volume fraction (VolFrac), Particle speed (Speed), Particle radius in microns (rad), Particle material (Material), Particle species (Species) (highlighted with a red circle), Unique particle ID (pid), Cloud mass (cldMass), and Particles per cloud (npCloud). The 'Gas Species' section has 'Mass concentration (<species>.mc) selected. The 'Options' section has 'Compress graphics output (not common)' and 'Generate predefined GMV attribute files' unchecked.

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**

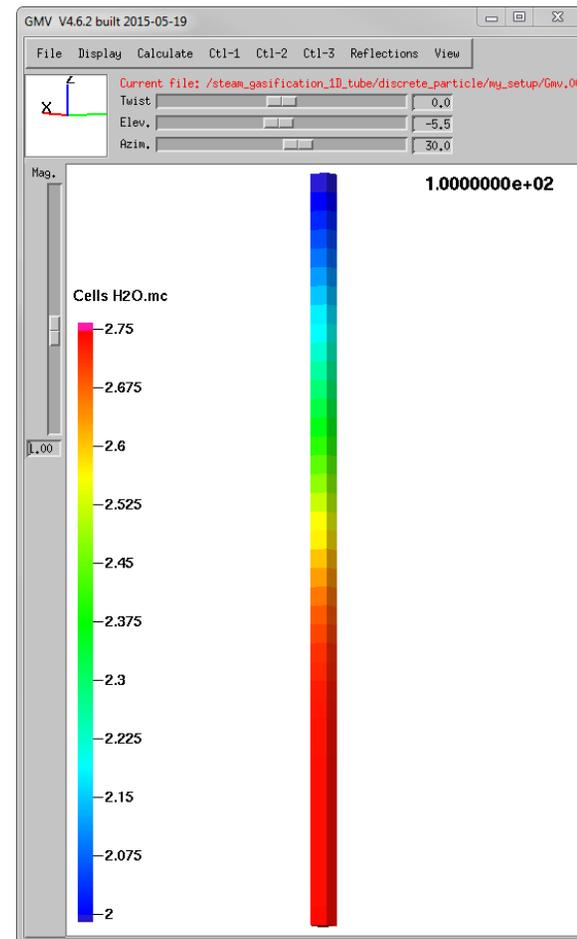
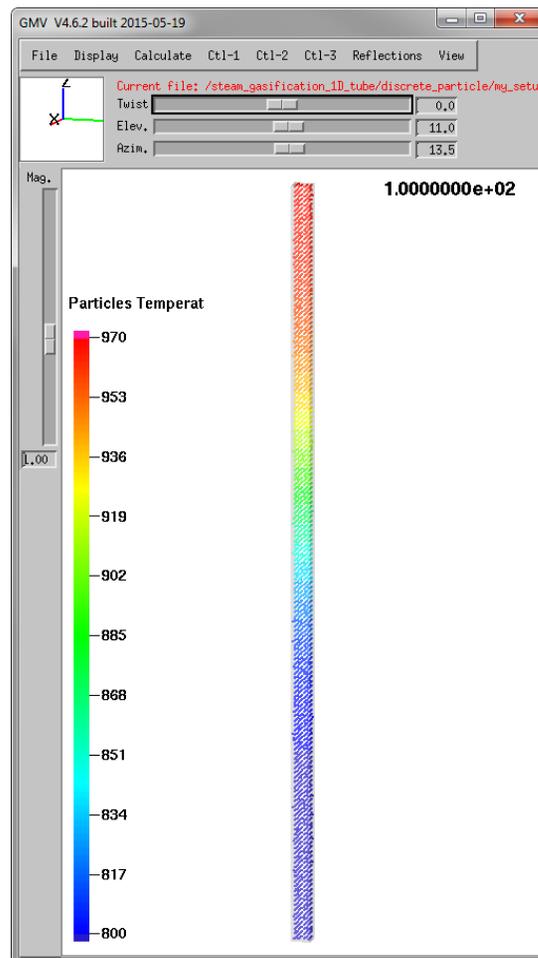
The screenshot displays the Barracuda Virtual Reactor software interface. The window title is "Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/4_Chemistry/Example_2_Discrete_Particle/my_setup/discrete_particle_steam_gasification_1D_tube.prj". The interface is divided into several panels:

- Project Tree:** Located on the left, it shows a hierarchical view of the project setup, including "Barracuda Virt...", "Setup Grid", "Global Sett...", "Base Materials", "Particles", "Initial Condit...", "Boundary C...", "BC Connect...", "Chemistry", "Numerics", "Time Controls", and "Data Output".
- Verify Setup:** The central panel displays a note: "Note: Run Solver Setup will cause some output files to be modified. If you have important output files, preserve them by using the File menu, Save Case As feature, and then Run Solver Setup in the new case directory." Below this note is a button labeled "1 Run Solver Setup (1 time step)".
- Run Calculation:** The right panel contains "Solver Launch Options" (with checkboxes for CPU and GPU parallel), "Universal Options" (with dropdowns for temperature, chemistry, and disk limits), and a "Run Solver" button. A red arrow points to the "Run Solver" button.

At the bottom of the interface, the status bar shows the current project path: "discrete_particle_steam_gasification_1D_tube.prj | C:/training/4_Chemistry/Example_2_Discrete_Particle/my_setup".

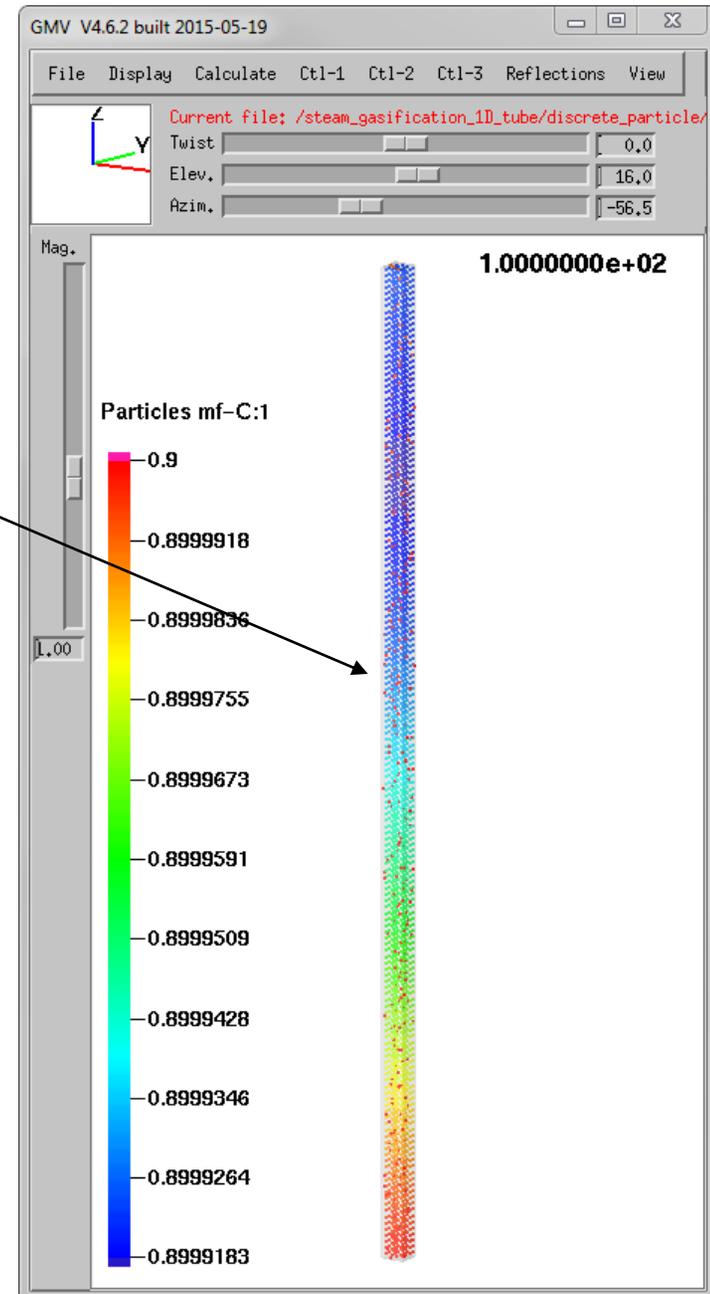
Post Processing

- 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**



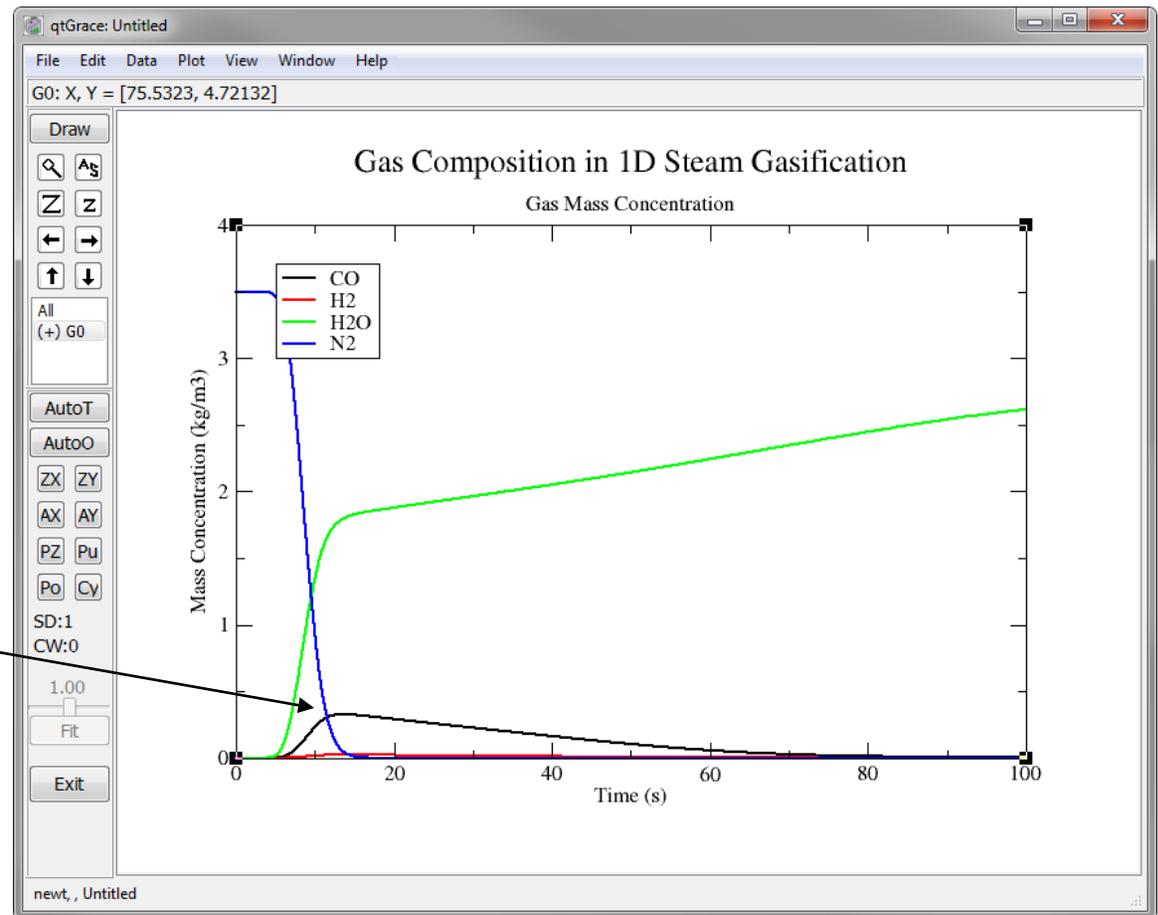
Post Processing

- 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?



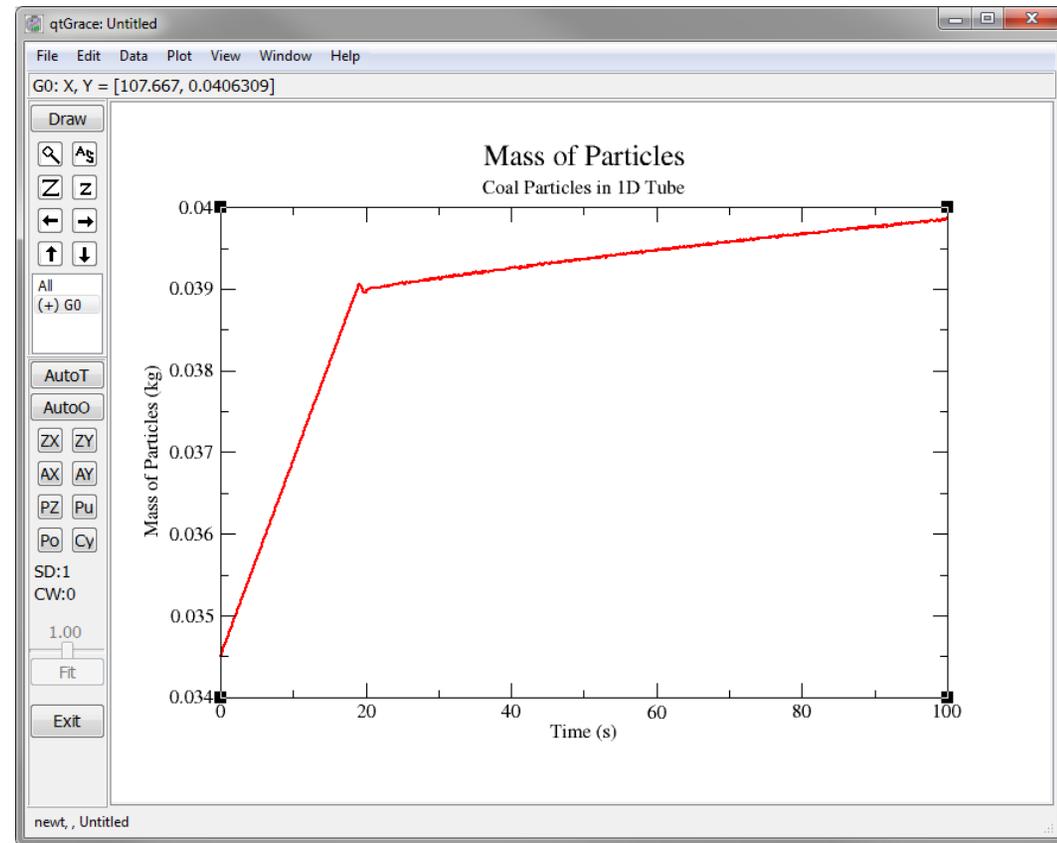
Plotting Transient Data

- 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.



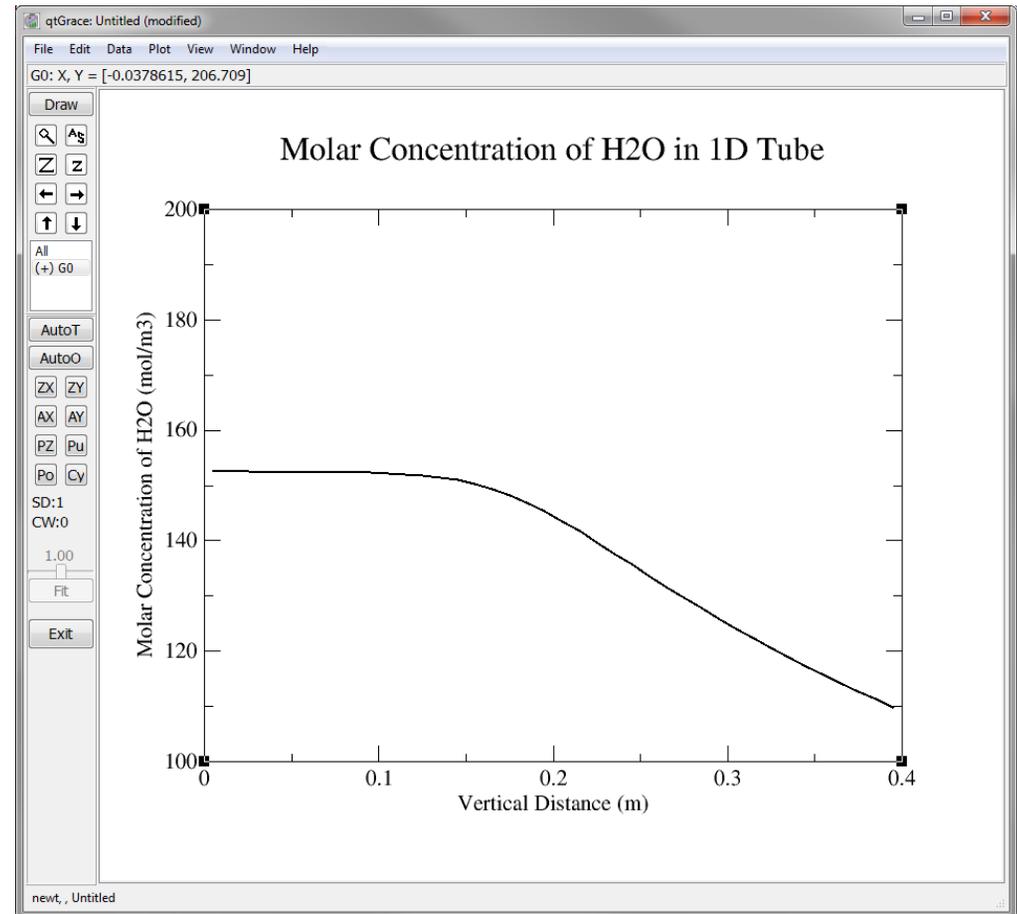
Plotting Transient Data

- 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

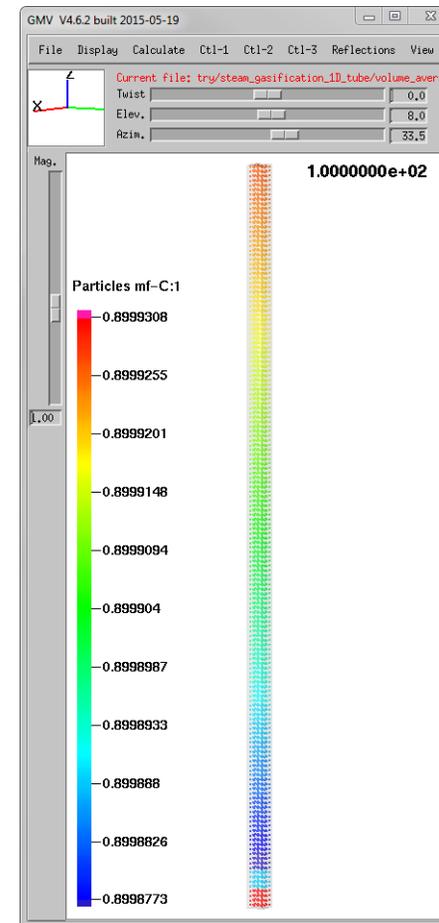
- Make a plot of the molar concentration of H₂O versus vertical distance in Plot Manager
 - Hint: Data is in the **H2O_zxMoleConc_00100.000.dat** file
- The concentration of H₂O is highest at the bottom of the tube.



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

