

Chemistry Training Example 1: Volume-Average

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Training Plan

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

Steam Gasification Tube Setup

- The steam gasification system consists of
 - A narrow square tube (1 cm x 1 cm x 40 cm)
 - Tube is filled with 200 μm diameter coal particles.
 - Coal particle locations are fixed in space with a volume fraction of 0.4 and initial temperature of 975 K
 - Top of tube is pressurized to 10 atm.
 - Coal is assumed to be 90% carbon and 10% ash (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 #1 will be set up with volume average chemistry



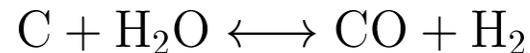
Case #1



Case #2

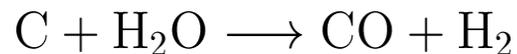
Steam Gasification Reaction

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



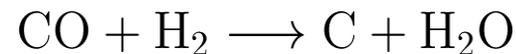
- Reaction is reversible, meaning that full reaction consists of a forward reaction and a reverse reaction.

Forward Reaction



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

Reverse Reaction



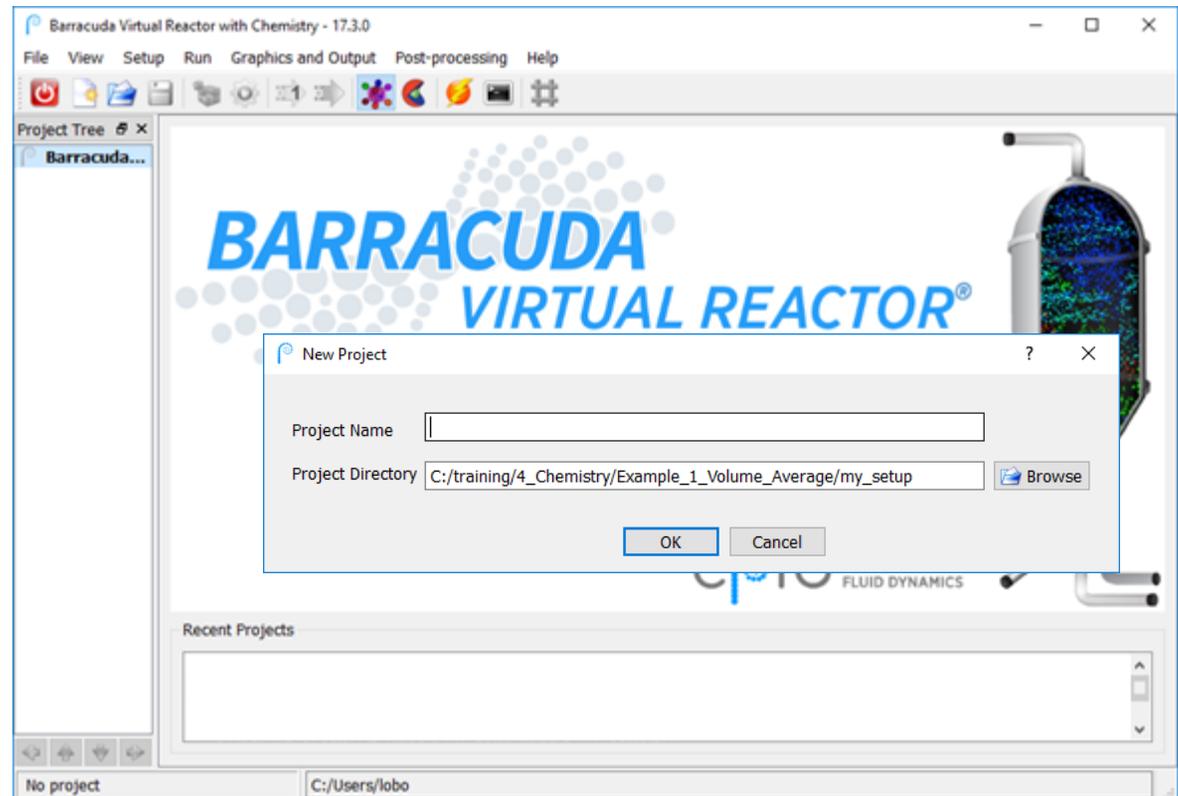
$$\frac{d[\text{H}_2\text{O}]}{dt} = \left(15.7 \frac{\text{m}^6}{\text{kg mol K}^2 \text{s}}\right) T^2 \exp\left(\frac{-33190\text{K}}{T}\right) \rho_C [\text{H}_2] [\text{CO}]$$

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

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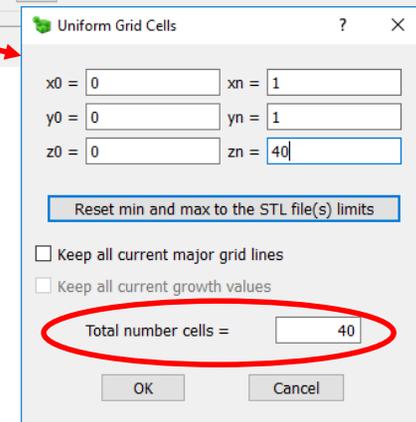
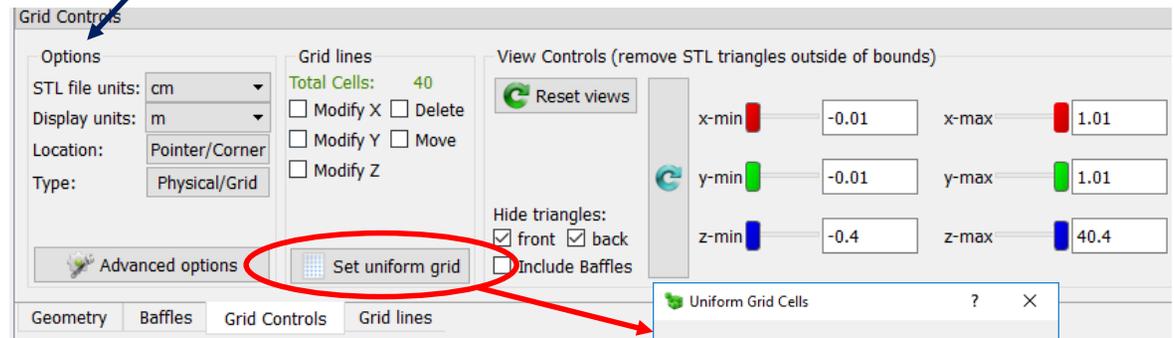
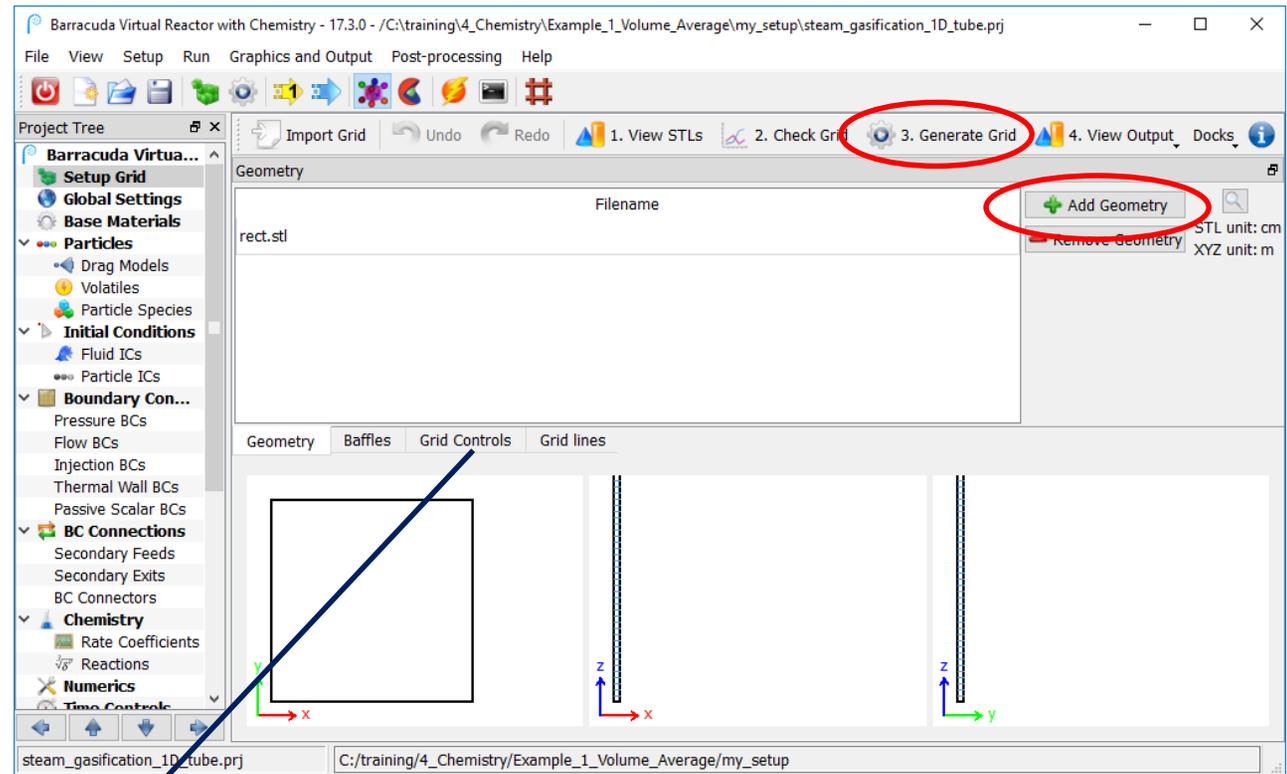
Volume Average Project File

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



Generate the Grid

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



Global Settings

The screenshot displays the Barracuda Virtual Reactor software interface. The title bar reads "Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:\training\4_Chemistry\Example_1_Volume_Average\my_setup\steam_gasification_1D_tube.prj". The menu bar includes "File", "View", "Setup", "Run", "Graphics and Output", "Post-processing", and "Help". The Project Tree on the left lists various settings categories, with "Global Settings" selected. The main panel shows the "Global Settings" configuration. Under "Gravity settings", the x, y, and z Gravity values are 0, 0, and -9.8 m/s² respectively. Under "Thermal settings", the "Thermal flow" option is selected, and the "Start with Thermal" option is set to "On". The "Starting temperature" is 300 K. The "Minimum temperature warning (K)" is 100 and the "Maximum temperature warning (K)" is 6000. The "Chemistry settings" section includes a note about setting up chemistry and a "Start with Chemistry" option set to "On".

Global Settings

Gravity settings

x Gravity 0 m/s²

y Gravity 0 m/s²

z Gravity -9.8 m/s²

Thermal settings

Isothermal flow 300 K

Thermal flow Heat transfer coefficients

Thermal start options

Start with Thermal: On Off (turn on at restart)

Starting temperature: 300 K

Temperature warning limits

Minimum temperature warning (K): 100 Maximum temperature warning (K): 6000

Output minimum and maximum temperatures in system to MinMaxTemp.data log file

Chemistry settings

This feature allows chemistry to be set up, but not calculated until a later time by turning it on using time controls or a restart file. Note: This feature applies to **Volatiles** as well as all **Chemistry Reactions**.

Start with Chemistry: On Off, ramp on from 0 s to 0 s Off (can be turned on at restart)

Base Materials

- For each species that you want to use in your project, highlight it in the **Material Properties Library** pane, then click **Import** to add it to the **Project Material List**
- Import **SiO2_2 QUARTZ (HQZ)**, then select it on the **Project material list**, click **Edit**, and rename it “ASH”
- Choose **Compressible Flow** to add multiple fluids

The screenshot shows the 'Base Materials Manager' window in the Barracuda Virtual Reactor software. The window title is 'Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/4_Chemistry/Example_1_Volume_Average/my_setup/steam_gasification_ID_tube.prj'. The interface includes a 'Project Tree' on the left, a 'Project Material List' table, a 'Material Properties Library' on the right, and a 'Properties' section at the bottom.

Project Material List

Chemical name	State	Description
ASH	S	SI02 QUARTZ. (HQZ) COMMON S
C_1	S	C CARBON. SOLID GRAPHITE REF
CO	G	CO CARBON MONOXIDE
H2	G	H2 HYDROGEN. REF ELEMENT
H2O	G	H2O STEAM
N2	G	N2 NITROGEN. REF ELEMENT

Material Properties Library

Chemical name	State	Description
AIR	G	AIR CALCULATED FROM
Al	S	Al REF ELEMENT (S)
Al	L	Al REF ELEMENT (L)
Al	G	Al
Al2O	G	Al2O DIALUMINUM MON
Al2O2	G	Al2O2
Al2O3	S	Al2O3 ALUMINUM OXIDE
Al2O3	L	Al2O3 ALUMINUM OXIDE
Al2O3	G	Al2O3 ALUMINUM OXIDE
AlH	G	AlH
AlHO2	G	AlO2H ALUMINUM HYDR
AlO	G	AlO
AlO2	G	AlO2 ALUMINUM OXIDE
AlOH	G	AlOH
Ar	G	Ar ARGON. REF ELEMEN
Ar_plus	G	AR+
B	G	B
B	L	B
B2	G	B2
B2O	G	B2O
B2O2	G	B2O2 (BO)2
B2O3	L	B2O3 LIQUID DIBORON

Properties

Averaging method for fluid mixture properties (applies to viscosity, thermal conductivity, and mass diffusivity):

Mole average Mass average

Flow Type

Compressible Incompressible (generally liquids only)

β : 0 Pref: 0

Particles

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

The screenshot shows the Barracuda Virtual Reactor software interface. The Project Tree on the left lists various settings categories, with 'Particles' expanded. The main panel displays the 'Particles' settings, including 'Close pack volume fraction' (0.6) and 'Particle-to-wall interaction' settings (Normal-to-wall momentum retention: 0.85, Tangent-to-wall momentum retention: 0.85, Diffuse bounce: 5). The 'Close pack volume fraction' field is circled in red, and the 'Particle-to-wall interaction' section is also circled in red.

Project Tree

- Barracuda Virtual Reac...
- 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

Particles

This section creates the particle species that will be used in the calculation.

Drag Models - Create and manage user defined drag models, also includes predefined drag models.

Volatiles - Define released gases for particle species.

Particles Species - Define particles that can contain solids and released gases.

Particle-to-particle interaction

Close pack volume fraction: 0.6

Maximum momentum redirection from collision: 40%

Blended acceleration model for the contact force

Stress Model Advanced Options

Particle-to-wall interaction

Normal-to-wall momentum retention: 0.85

Tangent-to-wall momentum retention: 0.85

Diffuse bounce: 5

Particle Species

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

The screenshot shows the Barracuda Virtual Reactor software interface. The main window displays the 'Particle Species Manager' with a table of species. The 'Particle Species Editor' window is open, showing configuration options for a new species. Red arrows highlight the 'Add' button in the Particle Species Manager and the 'Applied Materials' button in the Particle Species Editor.

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

The Particle Species Editor dialog box is shown. The 'Applied Materials' button is highlighted with a red arrow. The 'Drag Model' section shows the 'Wen-Yu' model selected. The 'Multiplier (constant)' is set to 1. The 'Radius' section shows 'Minimum' and 'Maximum' values both set to 1e-4 m.

The Applied Materials dialog box is shown. A table of materials is displayed, with the first two rows (C_1 and ASH) circled in red. The 'Mass Fractions sum to:' field is set to 1.0.

ID	Name	State	Mass Frac	Density (kg/m ³)	Age Factor
000	C_1	S	0.9	2150	1
001	ASH	S	0.1	2200	1

Fluid Initial Conditions

- For the fluid initial condition, fill the tube with 100% N₂, at a pressure of 10 atm and a temperature of 975 K

The screenshot shows the Barracuda Virtual Reactor software interface. The Project Tree on the left lists various settings, with 'Initial Conditions' expanded to show 'Fluid ICs'. The 'Fluid IC Manager' window displays a table with the following data:

ID	On	x1	x2	y1	y2	z1	z2	x-Vel	y-Vel	z-Vel
000	<input checked="" type="checkbox"/>	0	0.01	0	0.01	0	0.4	0	0	0

A red arrow points to the '000' ID in the table. The 'Fluid IC Editor: 000' dialog box is open, showing the following settings:

- Initial Conditions
- Temperature: 975 K
- Pressure: 1.0132e+06 Pa
- Fluid species: Define fluids
- Velocity: 0 m/s
- Initial conditions from file
- IC File: [empty]
- Region: Select region (m)
- x₁: 0, x₂: 0.01
- y₁: 0, y₂: 0.01
- z₁: 0, z₂: 0.4
- Comment: [empty]

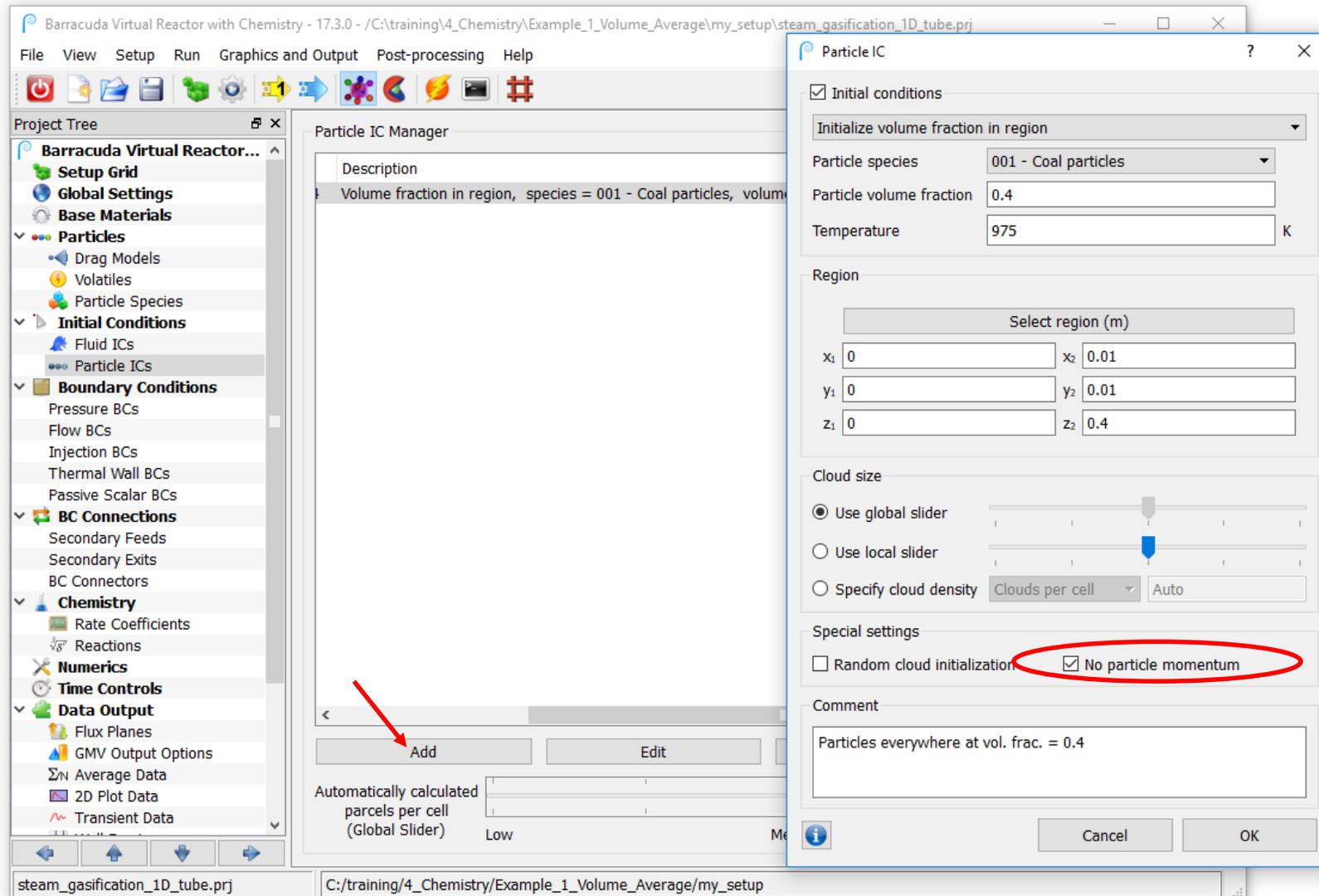
A red arrow points to the 'Edit' button at the bottom of the Fluid IC Manager. The 'Applied materials' dialog box is also visible, showing a table with the following data:

ID	Material	State	Fraction
000	N2	G	1

The 'Applied materials' dialog box also shows 'Fractions sum to: 1.0' and 'Mass fraction' selected.

Particle Initial Conditions

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



Pressure Boundary Conditions

- Define the fluid species for the Pressure BC as 100% N₂
- Be sure to enter the **Flux plane name** as “FLUXBC_pressure_outlet”

The screenshot displays the Barracuda Virtual Reactor software interface. The main window shows the Project Tree on the left, the Pressure BC Manager in the center, and the Pressure BC Editor on the right. The Pressure BC Editor is configured for a pressure boundary condition with the following settings:

- Region: Direction: z
- Fluid behavior at boundary: Specify values (selected)
- Area fraction: 1
- Pressure: 1.0132e+06 Pa
- Temperature: 975 K
- K-factor: 0
- Flux plane options: Flux file name: FLUXBC_pressure_outlet
- Gas species flux plane behavior: Mass Fraction
- Comment: 10 atm pressure at outlet

The 'Applied materials' dialog is also shown, listing the applied materials:

ID	Material	State	Fraction
000	N2	G	1

Flow Boundary Conditions

- For the **Flow BC**, use a velocity file to specify the flow of fluid into the bottom of the tube. Feed 0.01 m/s H₂O, at T = 800 K and P = 10 atm
- Remember to save the velocity file before closing the file window
- In the **Applied materials** window, select 100% H₂O
- Be sure to enter the **Flux plane name** as “FLUXBC_flow_inlet”

The Flow BC Editor window is configured for a z-direction flow. The region is defined by x1=0, x2=0.01, y1=0, y2=0.01, z1=0, and z2=0.01. The flow direction is set to z-direction flow. The fluid behavior at the boundary is set to 'Use transient fluid flow file'. The velocity flow is set to 0 m/s, pressure to 0 Pa, and temperature to 0 K. The flux plane name is 'FLUXBC_flow_inlet'. The SFF file is 'flow_bc_velocity_inlet.sff'.

The Applied materials window shows a table with one material: H2O (ID 000, State G, Fraction 1). The fractions sum to 1.0. The fraction type is set to Mass fraction.

ID	Material	State	Fraction
000	H2O	G	1

The Flow Boundary Conditions Editor window shows a table with one row of conditions: Time (s) 1.0, Velocity (m/s) 0.01, Temperature (K) 800, and Pressure (Pa) 1.01325e6.

Time (s)	Velocity (m/s)	Temperature (K)	Pressure (Pa)
1.0	0.01	800	1.01325e6

Adding Chemical Reactions

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

Chemistry

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

The screenshot shows the Barracuda Virtual Reactor software interface. The main window title is "Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/4_Chemistry/Example_1_Volume_Average/my_setup/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 the following structure:

- Barracuda Virtual Reac...
- 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

The main panel displays the "Chemistry" settings. It includes the following sections:

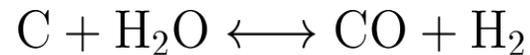
- Chemistry**: This section creates the Chemistry that will be used in the calculation.
 - Rate Coefficients** - Define Rate Coefficients for use in Reactions.
 - Reactions** - Define Reactions for your chemistry.

Please note that by adding any chemistry setup to the project, the solver will require a chemistry license in order to run.
- Import Chemistry Settings**: Includes a button "Import Materials/Chemistry from another project".
- Volume-Average Chemistry Reaction Type**: Includes a note: "When using chemical reactions, it is required that the user only enter Volume-Average reactions of one type, *Stoichiometric rate equations* or *Species rate equations*." The "Reaction type" is set to Stoichiometric and Species.
- Gas Transport Limiter**: Includes a setting "Limit mass transfer through a boundary layer: On Off".
- Distribute Sensible Heat from Reaction to Particle Phase**: Includes a setting "Discrete Reactions" with Automatic and Manual (0%).
- Chemistry ODE Settings**: Includes input fields for "Relative Tolerance" (1e-09), "Absolute Tolerance" (1e-09), and "Max Number Steps" (200000).

The status bar at the bottom shows the file name "steam_gasification_1D_tube.prj" and the path "C:/training/4_Chemistry/Example_1_Volume_Average/my_setup".

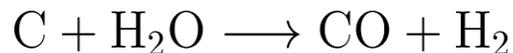
Chemistry

- Recall that the chemical reaction being modeled is:



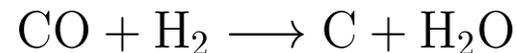
- In Barracuda, a reversible reaction is defined by splitting it into the forward and reverse reactions, defining a reaction rate for both the forward and reverse directions

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

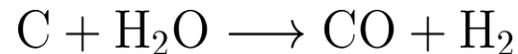


$$\frac{d[\text{H}_2\text{O}]}{dt} = \left(15.7 \frac{\text{m}^6}{\text{kg mol K}^2 \text{s}} \right) T^2 \exp \left(\frac{-33190\text{K}}{T} \right) \rho_{\text{C}} [\text{H}_2] [\text{CO}]$$

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Forward Reaction Rate

- Since we selected **Stoichiometric** on the main chemistry page, we will be able to specify the forward reaction by the stoichiometric equation:



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

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

- In Barracuda:

Reaction rate expression: $r_{\text{forward}} = k_0 [\text{H}_2\text{O}]$

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

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

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

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Creating the Forward Rate Coefficient

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

The screenshot displays the Barracuda Virtual Reactor interface. The Project Tree on the left shows the 'Chemistry' section expanded to 'Rate Coefficients'. The 'Add' button at the bottom of the 'Rate Coefficients' list is highlighted with a red arrow. The 'Chemistry Rate Coefficients Manager' window is open, showing a table with columns for ID, Name, Reaction Type, Coefficient Type, and Expression. The 'Chemistry Coefficient Editor' dialog box is also open, showing the 'Coefficient Properties' section. The 'Type' is set to 'Arrhenius Chem Rate'. The 'Coefficient is for reaction type' section has 'Volume-Average' selected with a red circle around it. The 'Equation' is $k_0 = 1$. The 'Values' section shows $C_0 = 1$, $C_1 = 0$, $C_2 = 0$, $C_3 = 0$, $C_4 = 0$, $C_5 = 0$, $E = 0$, and $E_0 = 0$. The 'Temperature weighting' section shows 'Fluid weighting factor' and 'Particle weighting factor' both set to 0.50. The 'Comment' field is empty. The 'OK' button is highlighted.

Forward Rate Coefficients

- Enter the equation for k0 as follows:

$$\begin{array}{cccc}
 C_0 & C_1 & E & \text{solids dependence} \\
 \downarrow & \downarrow & \downarrow & \downarrow \\
 k_0 = 219 T^1 \exp(-22645/T) m_{C_1}
 \end{array}$$
- Parameters with values of zero will be ignored by the solver. For example, if c2 is set to zero, then the pressure term will not be evaluated by the solver during the simulation
- Be sure to enter the units for temperature, pressure, density, mass, etc. as shown on the right
- Note that a positive value for “E” is entered since the GUI already includes a negative sign in the formula for the activation energy and that it has units of (K)
- There is no universal gas constant, “R”, in the denominator of the activation energy term

The screenshot shows the 'Chemistry Coefficient Editor' window. The 'Coefficient Properties' section includes:

- Name: **k0**
- Type: **Arrhenius Chem Rate**
- Coefficient is for reaction type: Volume-Average Discrete
- Equation: $c_0 T^{c_1} p^{c_2} \rho_f^{c_3} \theta_f^{c_4} e^{-E/T+E0} \{type_s\}$
- Equation: $k_0 = 219 T^1 e^{-22645/T} m_{C_1}^1$

The 'Values' section contains input fields for:

- $C_0 = 219$
- $C_1 = 1$
- $C_2 = 0$
- $C_3 = 0$
- $C_4 = 0$
- $C_5 = 0$
- $E = 22645$
- $E0 = 0$
- Temperature unit: **K**
- Pressure unit: **Pa**
- Density unit: **kg/m^3**
- Diameter unit: (empty)
- Mass unit: **kg/m^3**
- Area unit: (empty)
- $type_s =$ **Solids Dependence**

The 'Temperature Weighting' section includes:

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

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

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Rate Coefficients: Solids Term

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

Solids Dependence

ID	Chemical Name	State	Type	Exponent
00	C_1	S	mass	1

Material coefficient type: **mass**

Exponent on material: 1

<-- Import

<-- Replace

OK

Chemistry Coefficient Editor

Coefficient Properties

Name: **k0**

Type: Arrhenius Chem Rate

Coefficient is for reaction type: Volume-Average Discrete

Equation: $c_0 T^{c1} p^{c2} \rho_f^{c3} \theta_f^{c4} e^{-E/T+E0} \{type_s\}$

$k_0 = 219 T^1 e^{-22645/T} m_{C_1}^1$

Values

$C_0 = 219$

$C_1 = 1$ Temperature unit: K

$C_2 = 0$ Pressure unit: Pa

$C_3 = 0$ Density unit: kg/m³

$C_4 = 0$

$C_5 = 0$

$E = 22645$

$E0 = 0$

type_s = **Solids Dependence**

Temperature Weighting

Fluid weighting factor: 0.50

Particle weighting factor: 0.50

Comment

OK

Creating the Forward Reaction

- Start by entering the chemical equation for the forward reaction
- Under **Reactions** click **Add** → **Volume-Average:**
Stoichiometric rate equation to define the chemical reaction and its reaction rate

The screenshot shows the Barracuda Virtual Reactor software interface. The main window is titled "Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/v4_Chemistry/Example_1_Volume_Average/my_setup/steam_gasification_1D_tube.prj". The interface includes a menu bar (File, View, Setup, Run, Graphics and Output, Post-processing, Help) and a toolbar. On the left is a "Project Tree" with various settings categories like 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 to show "Reactions". The main area is the "Chemistry Reactions Manager" window, which contains a table with columns for ID, Reaction Type, Rate, Equation, and Comment. At the bottom of this window, there are buttons for "Add", "Edit", "Copy", and "Delete". The "Add" button is highlighted with a red circle, and a dropdown menu is open below it, showing three options: "Volume-Average: Stoichiometric rate equation", "Volume-Average: Species rate equation", and "Discrete: Particle rate equation". A red arrow points to the "Add" button.

Specifying the Forward Reaction Stoichiometry

- Define the stoichiometric reaction by either:
 - Typing directly into the text box using the chemical names needed to match the name in the materials library, i.e. carbon needs to be entered as "C_1"
 - Clicking in the text box to place your cursor in the appropriate position, then using the Add Chemical button
- With either method, you will need to type in the "+" signs and coefficients for each species. The characters "=>" represent the forward direction for the reaction
- Set the **Gas species units** to mol/m³

Chemistry Stoichiometric Equation Editor

Stoichiometric Equation Editor

Directions: Choose Equation Units for this Stoichiometric Chemistry. Enter a stoichiometric reaction and rate equation in the blanks provided. Use **Add 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/m³/s
Gas species units: mol/m³

Enter a stoichiometric reaction:
C_1(S) + H2O => CO + H2

Check Add Chemical

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 stoichiometric reaction in either Power Law or Langmuir-Hinshelwood form:
R00 = (k0[H2O])

Check Add Volume-Average Coefficient Add Chemical Coefficients Manager

Comment

OK Cancel

Specifying the Forward Reaction Rate

- To enter the rate equation for the reaction, click **Add Volume-Average Coefficient** and select k_0 , then click **Add Chemical** and select **H2O**
- Use the **Check** buttons to verify that both the chemical equation and the rate equation are formatted properly
- Click **OK**

Chemistry Stoichiometric Equation Editor

Stoichiometric Equation Editor

Directions: Choose Equation Units for this Stoichiometric Chemistry. Enter a stoichiometric reaction and rate equation in the blanks provided. Use **Add 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/m3/s
Gas species units: mol/m3

Enter a stoichiometric reaction:
C_1(S) + H2O => CO + H2

Check Add Chemical

Expected Power Law rate equation format: $c_0 (k + k - \dots) [\text{material1}]^{\text{power}} [\text{material2}]^{\text{power}} + c_1 \dots$
Example of valid Power Law rate equation format: $1.2 (1.5 * k_0 - 3 * k_1) [\text{H}_2\text{O}]^{1.5}$
Example of invalid Power Law rate equation format: $(k_0 * k_1) [\text{H}_2\text{O}]^{1.5}$ Coefficients cannot be multiplied.
Example of LH expected format: $(c_0 k [] + c_1 k [] + \dots) / (1 + c_2 k [] + c_3 k [] + \dots)^{\text{power}}$
Example of groups of rates: $(c_0 k_0 [\text{O}_2] - c_1 (0.5k_1 - k_2))^{\wedge}1.5 (c_1(k_3) [\text{CO}]^{\wedge}0.5[\text{O}_2])^{\wedge}-1$

Enter a rate equation for the stoichiometric reaction in either Power Law or Langmuir-Hinshelwood form:
R00 = (k0[H2O])

Check Add Volume-Average Coefficient Add Chemical ⓘ Coefficients Manager

Comment

OK Cancel

Forward Reaction Rate

- The forward reaction rate equation is now complete:
 - Rate coefficient and units
 - Stoichiometric chemical equation
 - Reaction rate equation
 - Reaction rate and concentration units

Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:\training\4_Chemistry\Example_1_Volume_Average\my_setup\steam_gasification_1D_tube.prj

File View Setup Run Graphics and Output Post-processing Help

Project Tree

- Barracuda Virtual Reac...
- 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

Chemistry Reactions Manager

ID	Reaction Type	Rate	Equation	Comment
00 VA:	Stoichiometric	Equation: R00 = (k0[H2O])	$C_1 (S) + H_2O \Rightarrow CO + H_2$	

steam_gasification_1D_tube.prj C:/training/4_Chemistry/Example_1_Volume_Average/my_setup

Reverse Reaction Rate

- We will be able to specify the reverse reaction by the stoichiometric equation.



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

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

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

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

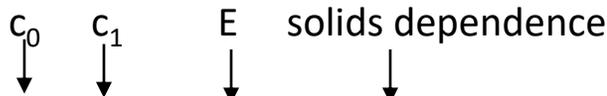
Rate coefficient: $k_1 = 15.7 T^2 \exp\left(\frac{-33190}{T}\right) \rho_C$

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

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

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:



- Check that **Volume-Average** is selected and that units are selected for temperature, pressure, density, mass, etc.
- Remember to click on **Solids Dependence** to select **C_1** and set **Material coefficient type** to **mass**

The screenshot shows the 'Chemistry Rate Coefficients Manager' window with a table containing one entry: ID 01, Name k1, Reaction Type Volume-Average, and Coefficient Type Arrhenius. A red arrow points to the 'Add' button at the bottom of this window.

The 'Chemistry Coefficient Editor' dialog box is open, showing the following settings:

- Name:** k1
- Type:** Arrhenius Chem Rate
- Coefficient is for reaction type:** Volume-Average Discrete
- Equation:** $k_1 = 15.7 T^2 e^{-33190/T} m_{C:1}$
- Values:**
 - C₀ = 15.7
 - C₁ = 2
 - C₂ = 0
 - C₃ = 0
 - C₄ = 0
 - C₅ = 0
 - E = 33190
 - E0 = 0
- Units:**
 - Temperature unit: K
 - Pressure unit: Pa
 - Density unit: kg/m³
 - Mass unit: kg/m³
 - Area unit: (empty)
- Temperature Weighting:**
 - Fluid weighting factor: 0.50
 - Particle weighting factor: 0.50
- type_s:** Solids Dependence (indicated by a red arrow)
- Comment:** (empty text box)

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Chemical Equations: Reverse Reaction

- Define the stoichiometric equation for the reverse reaction:
 $\text{CO} + \text{H}_2 \rightarrow \text{C} + \text{H}_2\text{O}$
- Enter the rate equation for the reverse reaction as follows:
 $R_{01} = k_1[\text{H}_2][\text{CO}]$
- Set **Gas species units** to “mol/m³”
- Use the **Check** buttons to verify that both the chemical equation and the rate equation are formatted properly
- Click **OK** when finished

The screenshot shows the 'Chemistry Stoichiometric Equation Editor' dialog box in the Barracuda Virtual Reactor software. The dialog box is titled 'Chemistry Stoichiometric Equation Editor' and contains the following fields and buttons:

- Stoichiometric Equation Editor**:
 - Directions:** Choose Equation Units for this Stoichiometric Chemistry. Enter a stoichiometric reaction and rate equation in the blanks 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/m3/s; Gas species units: mol/m3 (circled in red).
 - Enter a stoichiometric reaction:** CO + H2 => C_1(S) + H2O
 - Buttons:** Check, Add Chemical
 - Expected Power Law rate equation format:** $c_0 (k + k - \dots) [\text{material1}]^{\text{power}} [\text{material2}]^{\text{power}} + c_1 \dots$
 - Example of valid Power Law rate equation format:** $1.2 (1.5 * k_0 - 3 * k_1) [\text{H}_2\text{O}]^{1.5}$
 - Example of invalid Power Law rate equation format:** $(k_0 * k_1) [\text{H}_2\text{O}]^{1.5}$ Coefficients cannot be multiplied.
 - Example of LH expected format:** $(c_0 k [] + c_1 k [] + \dots) / (1 + c_2 k [] + c_3 k [] + \dots)^{\text{power}}$
 - Example of groups of rates:** $(c_0 k_0 [\text{O}_2] - c_1 (0.5k_1 - k_2))^{\wedge} 1.5 (c_1 (k_3) [\text{CO}]^{\wedge} 0.5 [\text{O}_2])^{\wedge} -1$
 - Enter a rate equation for the stoichiometric reaction in either Power Law or Langmuir-Hinshelwood form:** R01 = (k1[H2][CO])
 - Buttons:** Check, Add Volume-Average Coefficient, Add Chemical, Coefficients Manager
 - Comment:** (empty text box)
 - Buttons:** OK, Cancel
- Buttons:** Add, Edit, Copy, Delete

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

Reverse Reaction

- The reverse reaction is now complete

The screenshot shows the Barracuda Virtual Reactor interface. The 'Chemistry Reactions Manager' window is open, displaying a table of reactions. The reverse reaction (R01) is highlighted with a red circle.

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

The interface includes a Project Tree on the left with categories like Setup Grid, Global Settings, Base Materials, Particles, Initial Conditions, Boundary Conditions, BC Connections, Chemistry, Numerics, Time Controls, and Data Output. The bottom status bar shows the file name 'steam_gasification_1D_tube.prj' and the path 'C:/training/4_Chemistry/Example_1_Volume_Average/my_setup'.

Time Controls

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

The screenshot shows the Barracuda Virtual Reactor software interface. The 'Time Controls' window is open, displaying the following configuration:

Time Controls
This section allows configuration of the time step size to take during a period of time for the calculation. Only the first row is required. Subsequent rows can be entered to have different time steps for different time periods. For example, starting the calculation at a smaller time step is recommended, and then increasing the time step for rows 2-5 over simulation time.

Time step and duration settings

	Time step	End time
1.	0.01 s	100 s
2.		
3.		
4.		
5.		

Advanced time step settings

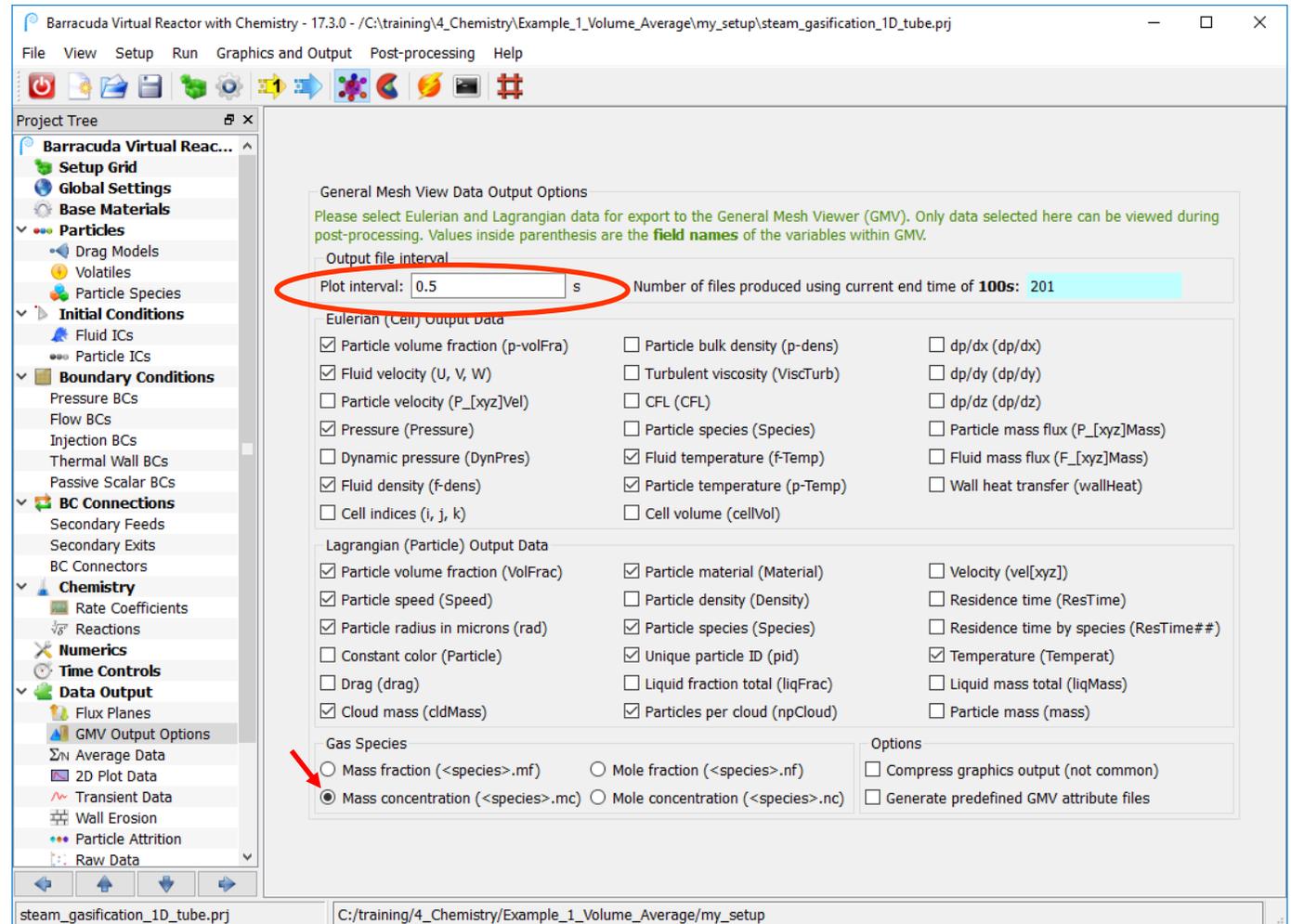
Restart file intervals

Restart interval (IC_###)	100	simulation seconds
Backtrack interval (IC_)	60	realtime minutes

The first row of the 'Time step and duration settings' table is circled in red, indicating the required input for the time step (0.01 s) and end time (100 s).

GMV Output Options

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



Select 2D Data

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_1_Volume_Average/my_setup/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 Data Output section is expanded, showing options for Flux Planes, GMV Output Options, Average Data, 2D Plot Data, Transient Data, Wall Erosion, Particle Attrition, and Raw Data. The 2D Plot Data section is selected, showing a list of plot options with checkboxes and input fields for indices. The 2D Data to Display section is also visible, showing a list of data types with checkboxes. The 2D Plot Output settings are as follows:

Plot Option	Index	Value
<input type="checkbox"/> Plot xy	k-index	nz/2
<input type="checkbox"/> Plot xz	j-index	ny/2
<input type="checkbox"/> Plot yx	k-index	nz/2
<input type="checkbox"/> Plot yz	i-index	nx/2
<input checked="" type="checkbox"/> Plot zx	j-index	ny/2
<input type="checkbox"/> Plot zy	i-index	nx/2

Plot Interval Options:

- Time interval: 50 s
- If plot interval = 0, use mesh viewer interval.
- Max # of columns: 29

2D Data to Display:

Data Type	Checked
Fluid volume fraction	<input type="checkbox"/>
Particle volume fraction	<input type="checkbox"/>
Pressure	<input checked="" type="checkbox"/>
Fluid velocity	<input type="checkbox"/>
Particle velocity	<input type="checkbox"/>
Fluid temperature	<input checked="" type="checkbox"/>
Particle temperature	<input checked="" type="checkbox"/>
Fluid mass flux	<input type="checkbox"/>
Solid mass flux	<input type="checkbox"/>
Passive scalar	<input type="checkbox"/>
Fluid density	<input checked="" type="checkbox"/>
Particle density	<input type="checkbox"/>
Gas species chemical reaction rate	<input type="checkbox"/>
Ave particle volume fraction	<input type="checkbox"/>
Ave pressure	<input type="checkbox"/>
Ave fluid velocity	<input type="checkbox"/>
Ave particle velocity	<input type="checkbox"/>
Ave fluid temperature	<input type="checkbox"/>
Ave particle temperature	<input type="checkbox"/>
Ave fluid mass flux	<input type="checkbox"/>
Ave solid mass flux	<input type="checkbox"/>
Stoichiometric equation rate	<input checked="" type="checkbox"/>
Liquid concentration	<input type="checkbox"/>

Output Gas Species:

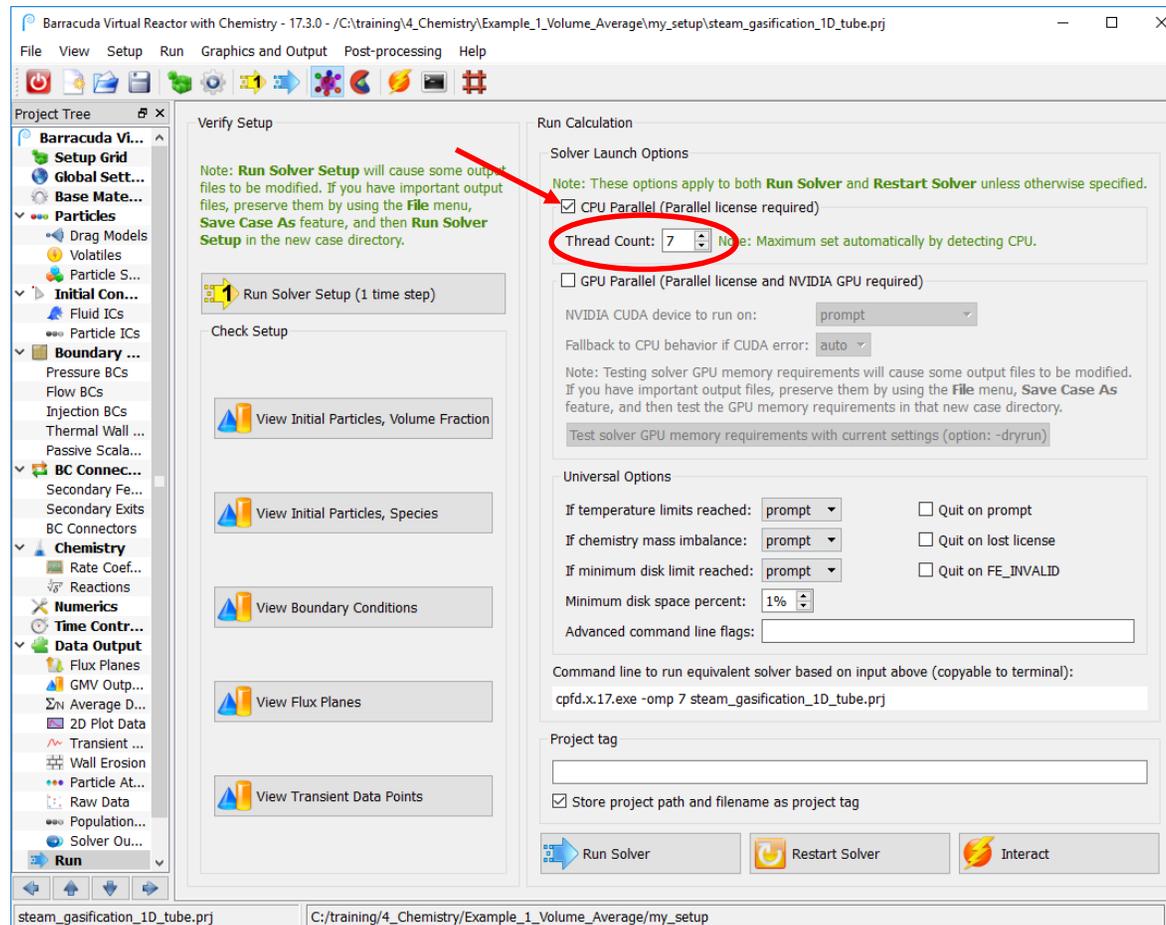
- Gas species
- Ave gas species

Output Format:

- Mass fraction
- Mole fraction
- Mole concentration

Set CPU Parallel

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



Start the Barracuda Solver

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

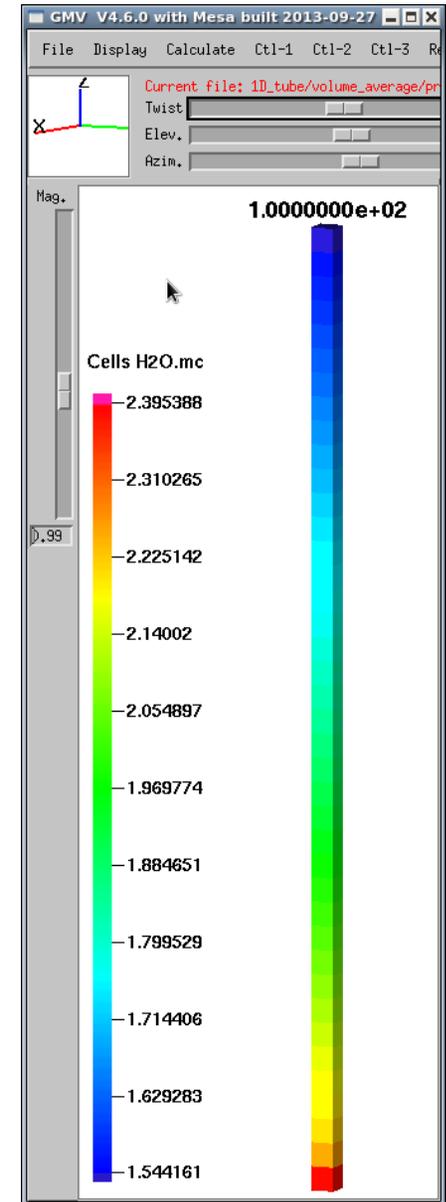
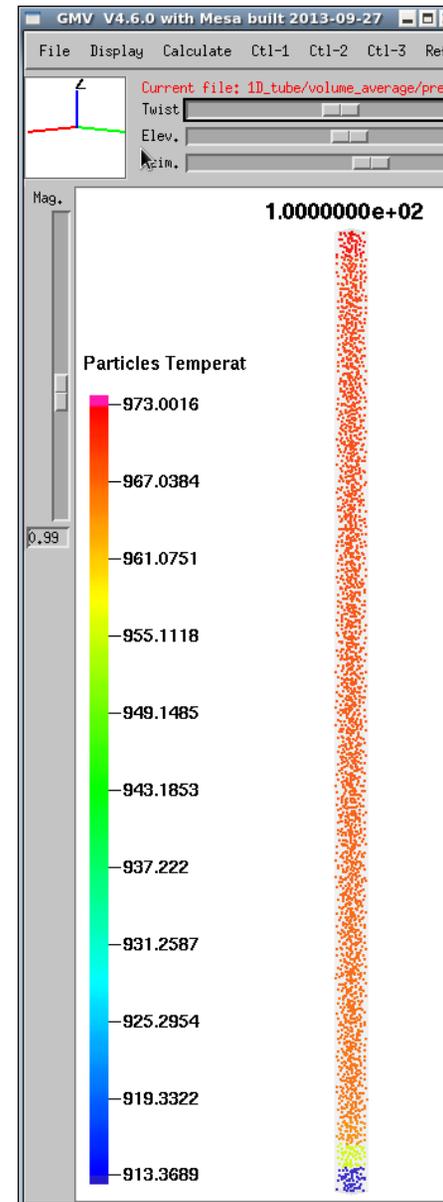
The screenshot displays the Barracuda Virtual Reactor software interface. The window title is "Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/4_Chemistry/Example_1_Volume_Average/my_setup/steam_gasification_1D_tube.prj". The interface is divided into several panels:

- Project Tree:** Located on the left, it shows a hierarchical view of the simulation setup, including "Setup Grid", "Global Sett...", "Base Mate...", "Particles", "Initial Con...", "Boundary ...", "BC Connec...", "Chemistry", "Numerics", "Time Contr...", and "Data Output".
- Verify Setup:** The central panel, which contains 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 the note is a prominent button labeled "1 Run Solver Setup (1 time step)", which is highlighted with a red arrow.
- Run Calculation:** The right panel, containing "Solver Launch Options" (with "CPU Parallel" checked and "Thread Count" set to 7), "Universal Options" (with various prompts and checkboxes), and a "Run Solver" button at the bottom, also highlighted with a red arrow.

The status bar at the bottom shows the current project file "steam_gasification_1D_tube.prj" and the working directory "C:/training/4_Chemistry/Example_1_Volume_Average/my_setup".

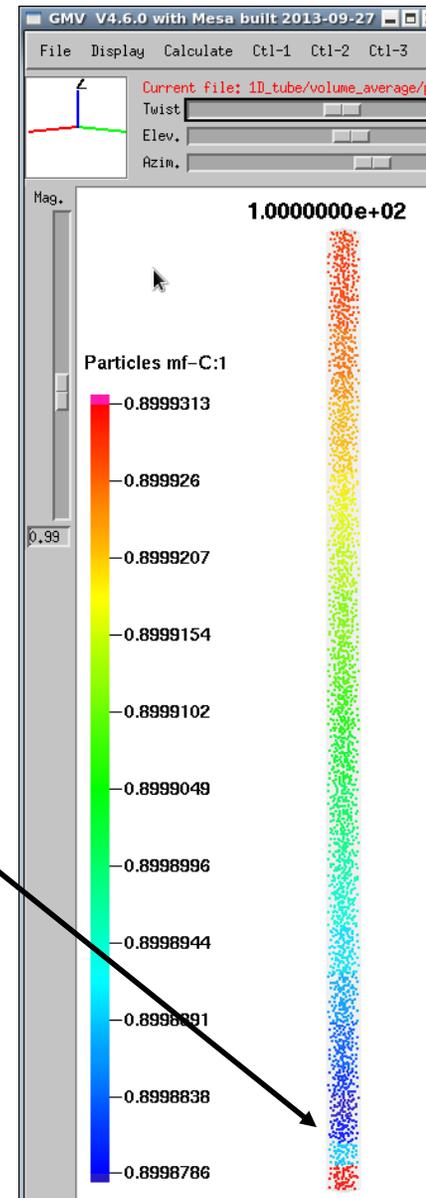
Post Processing

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



Post Processing

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

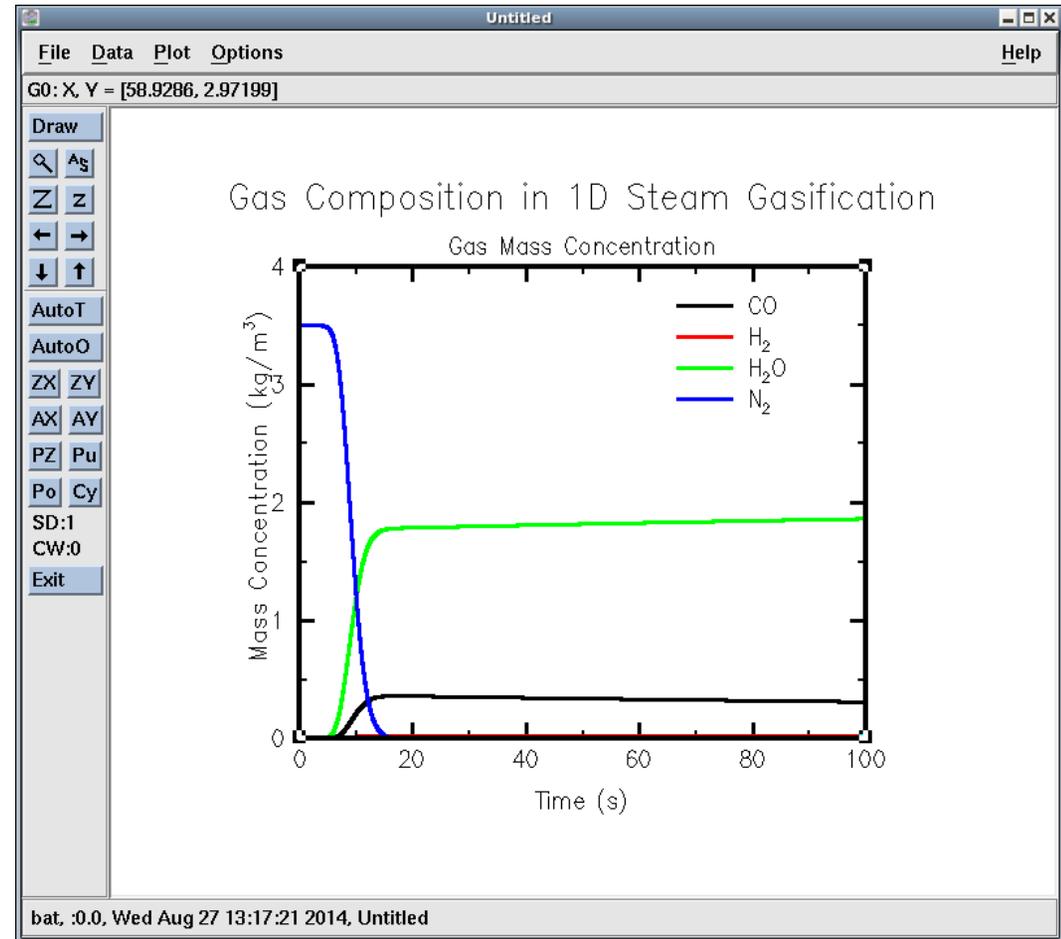


Plotting Transient Data

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

```

File
#Mon Jan 2 13:13:53 2012
#
# Barracuda release 15.0.
# Solver version 15.0.x107. Build date Wed Nov 16 22:59:58 MST 2011.
# Compiled with c++ x86 64
# 1 Time (s)
# 2 Particle volume fraction          at ( 1 1
# 3 Particle temperature (K)         at ( 1 1
# 4 Mass fraction CO                 at ( 1 1
# 5 Mass fraction H2                 at ( 1 1
# 6 Mass fraction H2O                at ( 1 1
# 7 Mass fraction N2                 at ( 1 1
# 8 Mole fraction CO                 at ( 1 1
# 9 Mole fraction H2                 at ( 1 1
# 10 Mole fraction H2O               at ( 1 1
# 11 Mole fraction N2                at ( 1 1
# 12 Mass concentration CO           (kg/m^3) at ( 1 1
# 13 Mass concentration H2           (kg/m^3) at ( 1 1
# 14 Mass concentration H2O          (kg/m^3) at ( 1 1
# 15 Mass concentration N2           (kg/m^3) at ( 1 1
# 16 Mole concentration CO           (mol/m^3) at ( 1 1
    
```



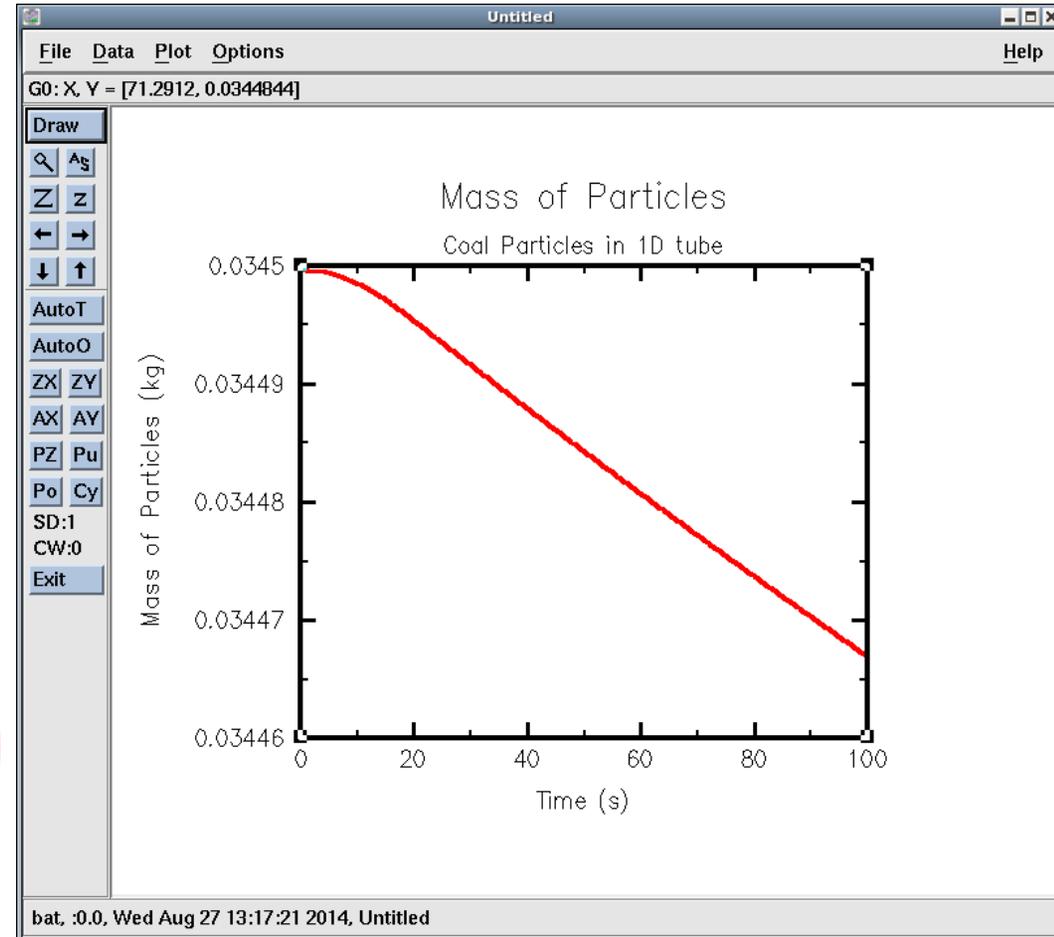
N_2 concentration goes to zero as H_2O is fed into the system and H_2 and CO are produced. All N_2 initially in tube is pushed out.

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

```

# Barracuda release 15.0
# Solver version 15.0.x107. Build date Wed Nov 16 22:59:58 MST 2011.
# Compiled with c++ x86_64
#
# 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
# t dt Vol Vol u u v v w w h h p p CFL QI pMass
# s s itr err itr err itr err itr err itr err itr err err err kr
0.00000e+00 1.000e-04 000 0.00e+00 000 0.00e+00 000 0.00e+00 000 0.00e+00 000 0.00e+00 000 0.00e+00 0.000 0.000 3.44765e-02
# Dumping Gmv.00000
1.00000e-04 1.000e-04 002 8.73e-11 000 0.00e+00 000 0.00e+00 001 5.92e-09 002 2.14e-08 000 7.35e-11 0.000 0.000 3.44765e-02
2.00000e-04 1.000e-04 002 9.77e-11 000 0.00e+00 000 0.00e+00 001 3.38e-09 002 2.28e-08 000 6.54e-11 0.000 0.000 3.44765e-02
3.00000e-04 1.000e-04 002 1.03e-10 000 0.00e+00 000 0.00e+00 001 8.26e-10 002 2.25e-08 000 6.20e-11 0.000 0.000 3.44765e-02
4.00000e-04 1.000e-04 002 1.18e-10 000 0.00e+00 000 0.00e+00 001 3.02e-10 002 2.20e-08 000 6.22e-11 0.000 0.000 3.44765e-02
5.00000e-04 1.000e-04 002 1.24e-10 000 0.00e+00 000 0.00e+00 001 1.39e-10 002 2.15e-08 000 6.40e-11 0.000 0.000 3.44765e-02
6.00000e-04 1.000e-04 002 1.49e-10 000 0.00e+00 000 0.00e+00 001 1.81e-10 002 2.09e-08 000 6.58e-11 0.000 0.000 3.44765e-02
7.00000e-04 1.000e-04 002 1.54e-10 000 0.00e+00 000 0.00e+00 001 2.06e-10 002 2.02e-08 000 6.75e-11 0.000 0.000 3.44765e-02
8.00000e-04 1.000e-04 002 1.79e-10 000 0.00e+00 000 0.00e+00 001 2.14e-10 002 1.95e-08 000 6.90e-11 0.000 0.000 3.44765e-02
9.00000e-04 1.000e-04 002 1.94e-10 000 0.00e+00 000 0.00e+00 001 2.80e-10 002 1.88e-08 000 7.03e-11 0.000 0.000 3.44765e-02
1.00000e-03 1.000e-04 002 2.08e-10 000 0.00e+00 000 0.00e+00 001 4.02e-10 002 1.81e-08 000 7.15e-11 0.000 0.000 3.44765e-02
1.10000e-03 1.000e-04 002 2.23e-10 000 0.00e+00 000 0.00e+00 001 4.89e-10 002 1.73e-08 000 7.27e-11 0.000 0.000 3.44765e-02
1.20000e-03 1.000e-04 002 2.37e-10 000 0.00e+00 000 0.00e+00 001 5.43e-10 002 1.66e-08 000 7.38e-11 0.000 0.000 3.44765e-02
1.30000e-03 1.000e-04 002 2.50e-10 000 0.00e+00 000 0.00e+00 001 5.74e-10 002 1.59e-08 000 7.48e-11 0.000 0.000 3.44765e-02
1.40000e-03 1.000e-04 002 2.63e-10 000 0.00e+00 000 0.00e+00 001 5.91e-10 002 1.52e-08 000 7.59e-11 0.000 0.000 3.44765e-02
1.50000e-03 1.000e-04 002 2.76e-10 000 0.00e+00 000 0.00e+00 001 6.01e-10 002 1.46e-08 000 7.68e-11 0.000 0.000 3.44765e-02
1.60000e-03 1.000e-04 002 2.88e-10 000 0.00e+00 000 0.00e+00 001 6.07e-10 002 1.39e-08 000 7.77e-11 0.000 0.000 3.44765e-02
1.70000e-03 1.000e-04 002 3.00e-10 000 0.00e+00 000 0.00e+00 001 6.09e-10 002 1.32e-08 000 7.85e-11 0.000 0.000 3.44765e-02
1.80000e-03 1.000e-04 002 3.12e-10 000 0.00e+00 000 0.00e+00 001 6.09e-10 002 1.26e-08 000 7.93e-11 0.000 0.000 3.44765e-02
1.90000e-03 1.000e-04 002 3.23e-10 000 0.00e+00 000 0.00e+00 001 6.04e-10 002 1.20e-08 000 8.00e-11 0.000 0.000 3.44765e-02
2.00000e-03 1.000e-04 002 3.33e-10 000 0.00e+00 000 0.00e+00 001 5.97e-10 002 1.14e-08 000 8.07e-11 0.000 0.000 3.44765e-02
    
```

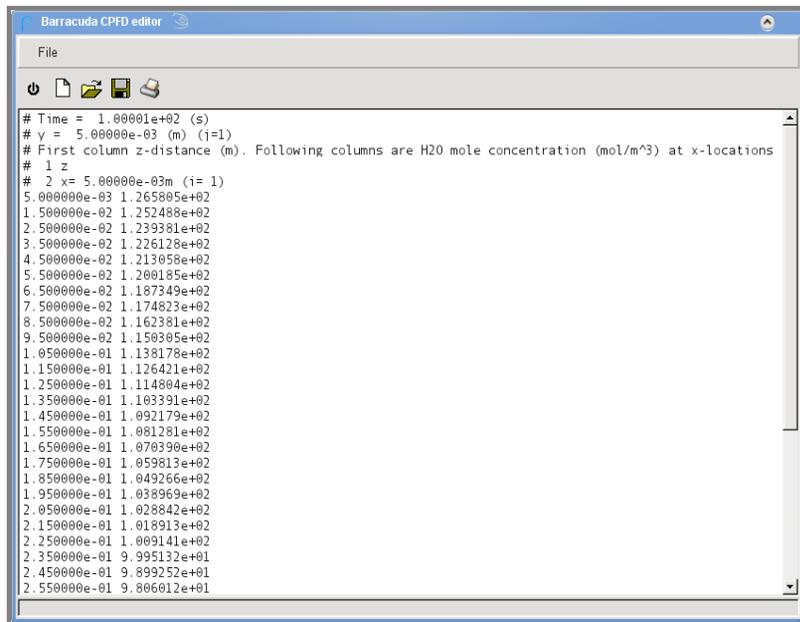


The solids mass in the system decreases as carbon is consumed in the reaction.

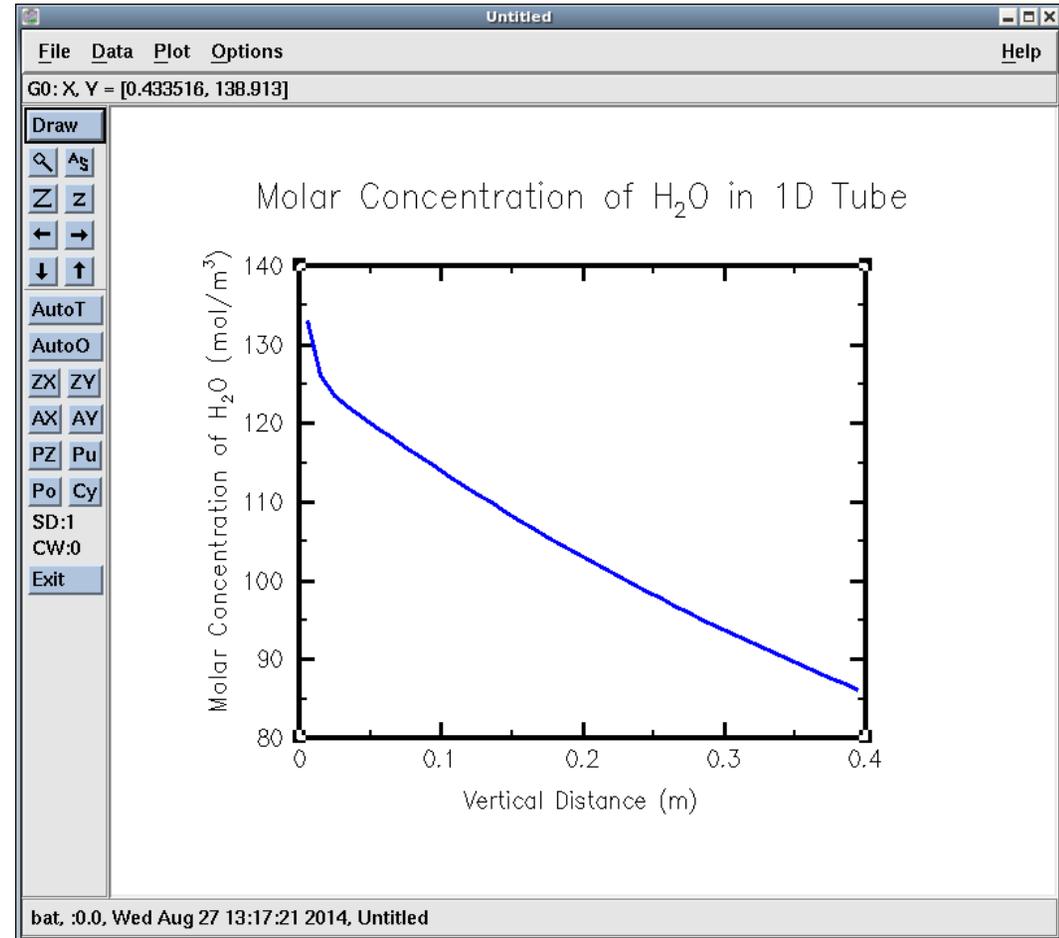
Plotting 2D Data

- Make a plot of the molar concentration of H₂O versus vertical distance in Plot Manager
 - Hint: Data is in the **H2O_zx_MoleConc_00100.003.dat** file

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



```
# Time = 1.00001e+02 (s)
# y = 5.00000e-03 (m) (j=1)
# First column z-distance (m). Following columns are H2O mole concentration (mol/m^3) at x-locations
# 1 z
# 2 x= 5.00000e-03m (i= 1)
5.000000e-03 1.265805e+02
1.500000e-02 1.252488e+02
2.500000e-02 1.239381e+02
3.500000e-02 1.226128e+02
4.500000e-02 1.213058e+02
5.500000e-02 1.200185e+02
6.500000e-02 1.187349e+02
7.500000e-02 1.174823e+02
8.500000e-02 1.162381e+02
9.500000e-02 1.150305e+02
1.050000e-01 1.138178e+02
1.150000e-01 1.126421e+02
1.250000e-01 1.114804e+02
1.350000e-01 1.103391e+02
1.450000e-01 1.092179e+02
1.550000e-01 1.081281e+02
1.650000e-01 1.070390e+02
1.750000e-01 1.059813e+02
1.850000e-01 1.049266e+02
1.950000e-01 1.038969e+02
2.050000e-01 1.028842e+02
2.150000e-01 1.018913e+02
2.250000e-01 1.009141e+02
2.350000e-01 9.995132e+01
2.450000e-01 9.899252e+01
2.550000e-01 9.806012e+01
```



The concentration of H₂O is highest at the bottom of the tube.

Summary

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