

Chemistry Training Example 1: Volume-Average

February 2018

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

Training Plan

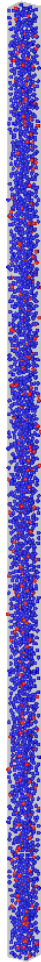
- Chemistry training will be provided in three parts
 - Lecture: Introduction to the Chemistry module
 - Volume Average Chemistry
 - Discrete Particle Chemistry
 - Example 1: Set up of training problem using Volume Average Chemistry
 - Example 2: Set up of training problem using Discrete Particle Chemistry

Steam Gasification Tube Setup

- The steam gasification system consists of
 - A narrow square tube (1 cm x 1 cm x 40 cm)
 - Tube is filled with 200 μm diameter coal particles.
 - Coal particle locations are fixed in space with a 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 at 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



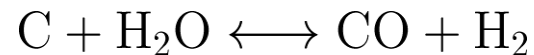
Case #1



Case #2

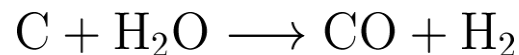
Steam Gasification Reaction

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



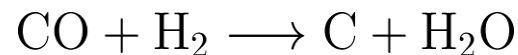
- Reaction is reversible, meaning that full reaction consists of a forward reaction and a reverse reaction.

Forward Reaction



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

Reverse Reaction



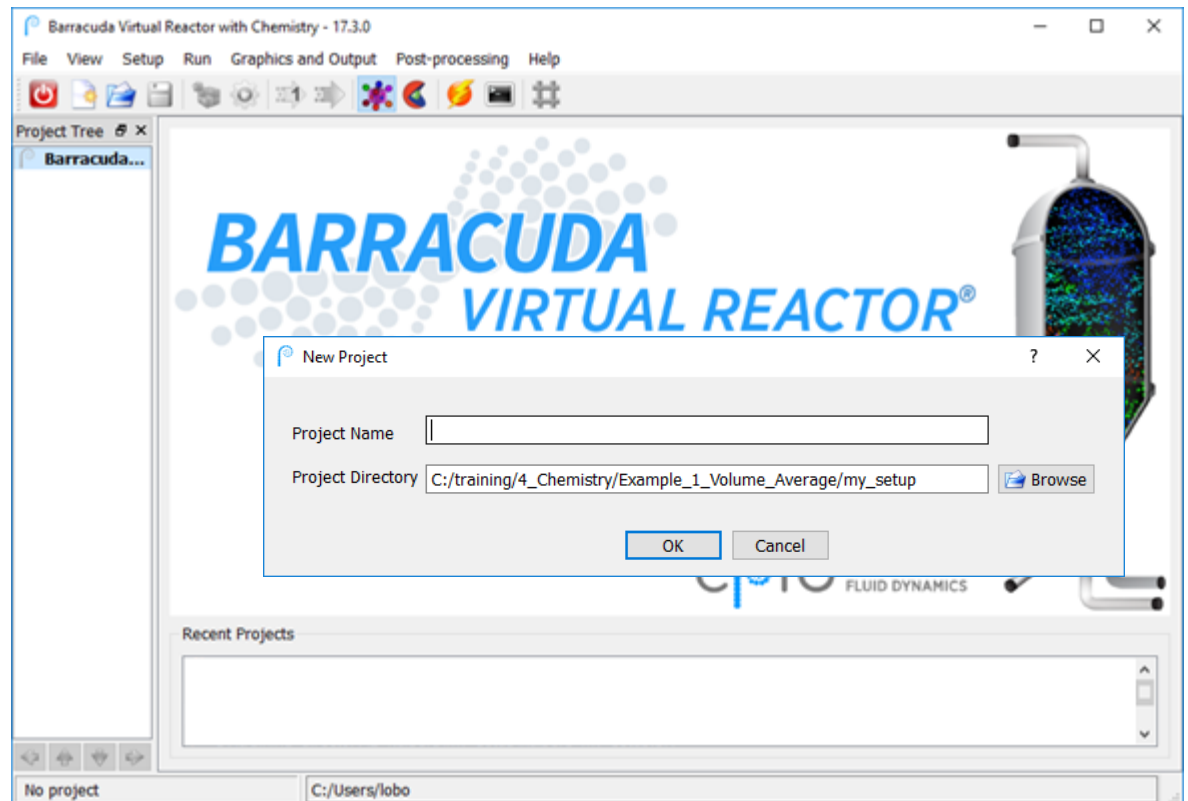
$$\frac{d[\text{H}_2\text{O}]}{dt} = \left(15.7 \frac{\text{m}^6}{\text{kg mol K}^2 \text{s}} \right) T^2 \exp \left(\frac{-33190 \text{K}}{T} \right) \rho_{\text{C}} [\text{H}_2] [\text{CO}]$$

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

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.

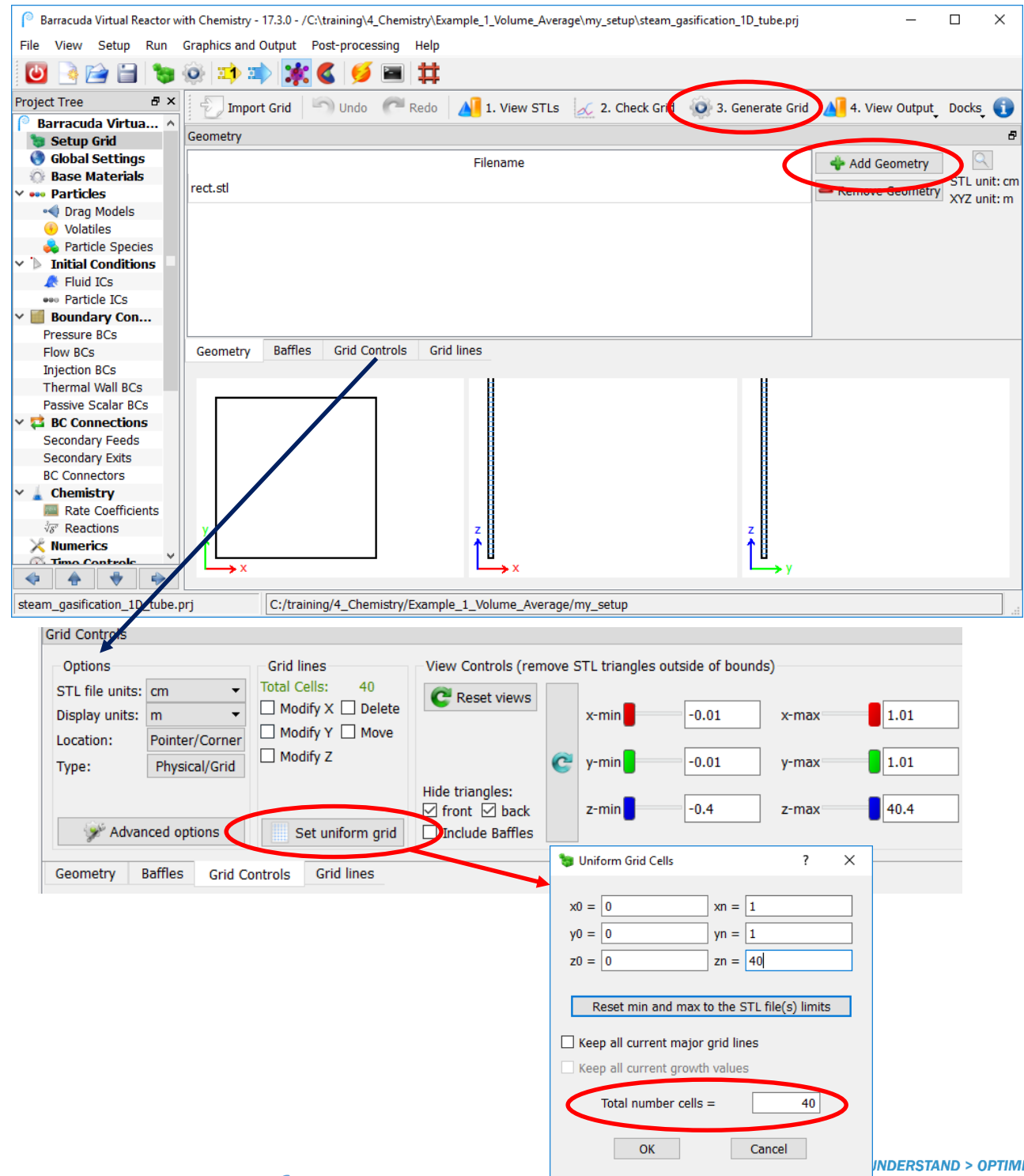
Volume Average Project File

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

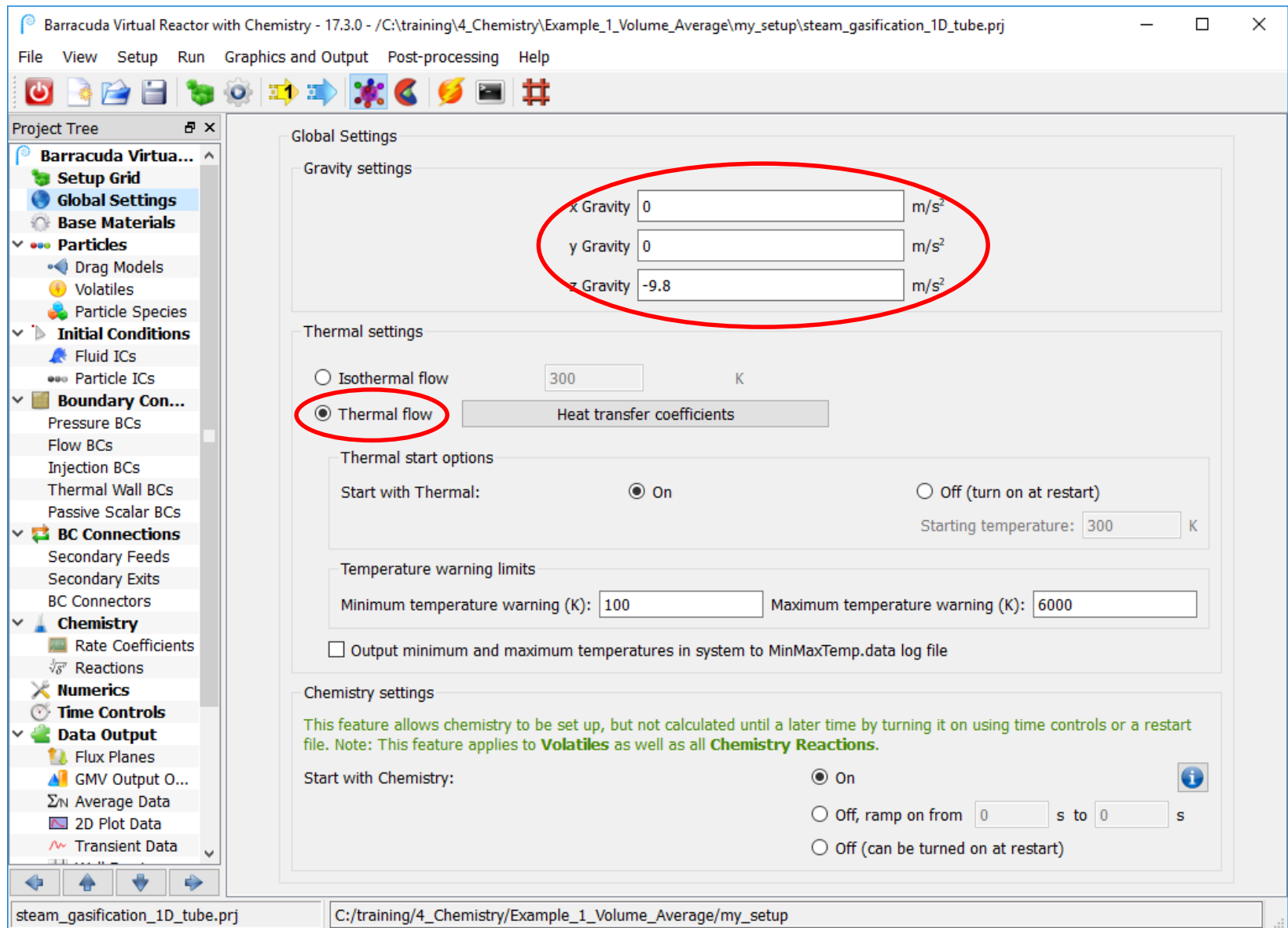


Generate the Grid

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



Global Settings



Base Materials

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

The screenshot displays the Barracuda Virtual Reactor software interface. The **Project Tree** on the left shows the **Base Materials** section selected. The **Base Materials Manager** window is open, showing the **Project Material List** and the **Material Properties Library**.

Project Material List:

Chemical name	State	Description
ASH	S	SiO2 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

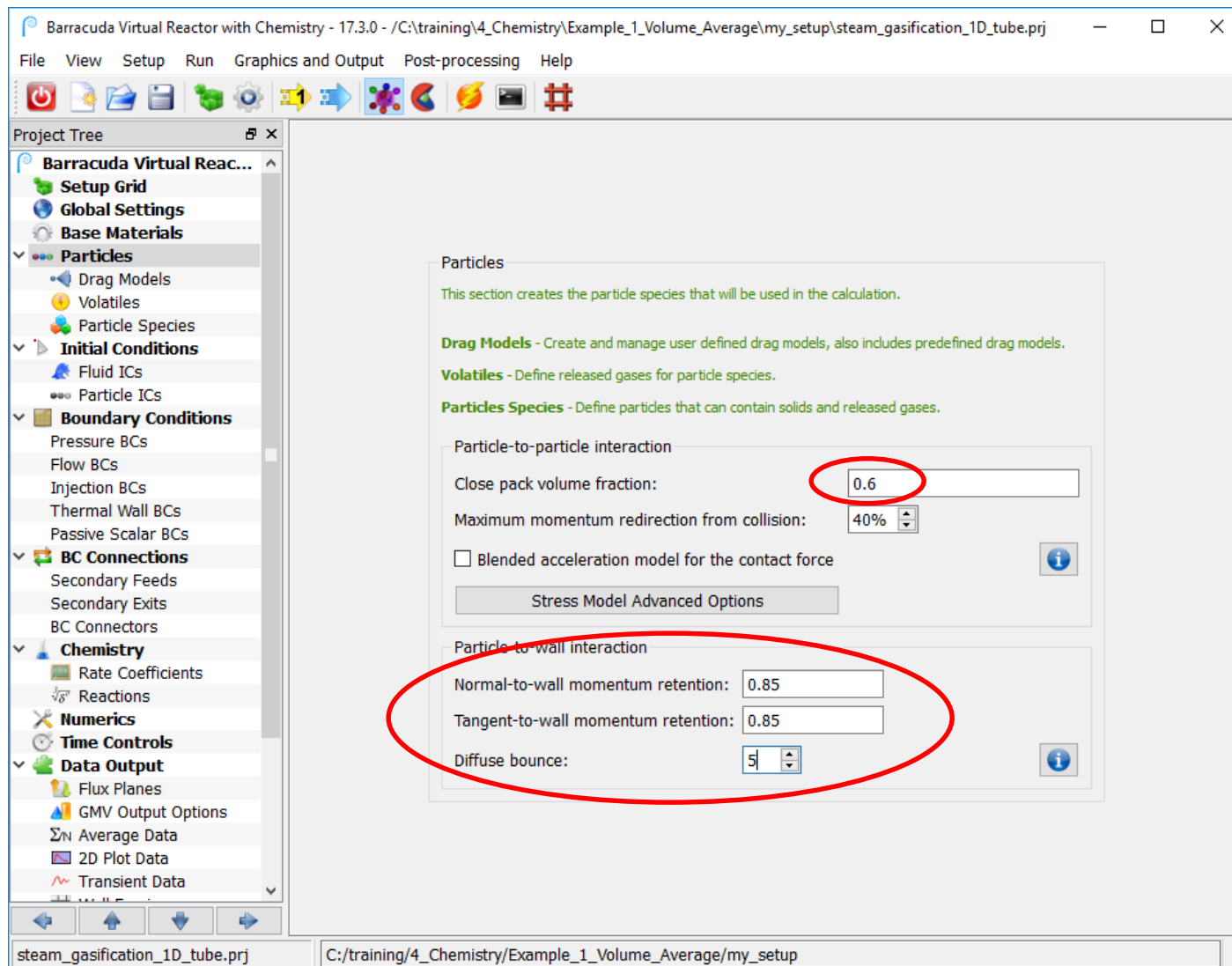
Flow Type:

☒ Compressible ☐ Incompressible (generally liquids only)

Buttons: Add, Edit, Copy, Delete, <- Import, <- Replace ->

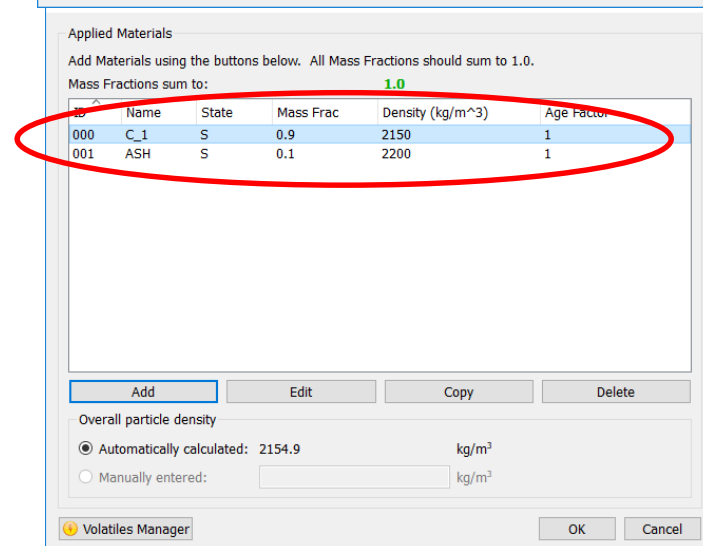
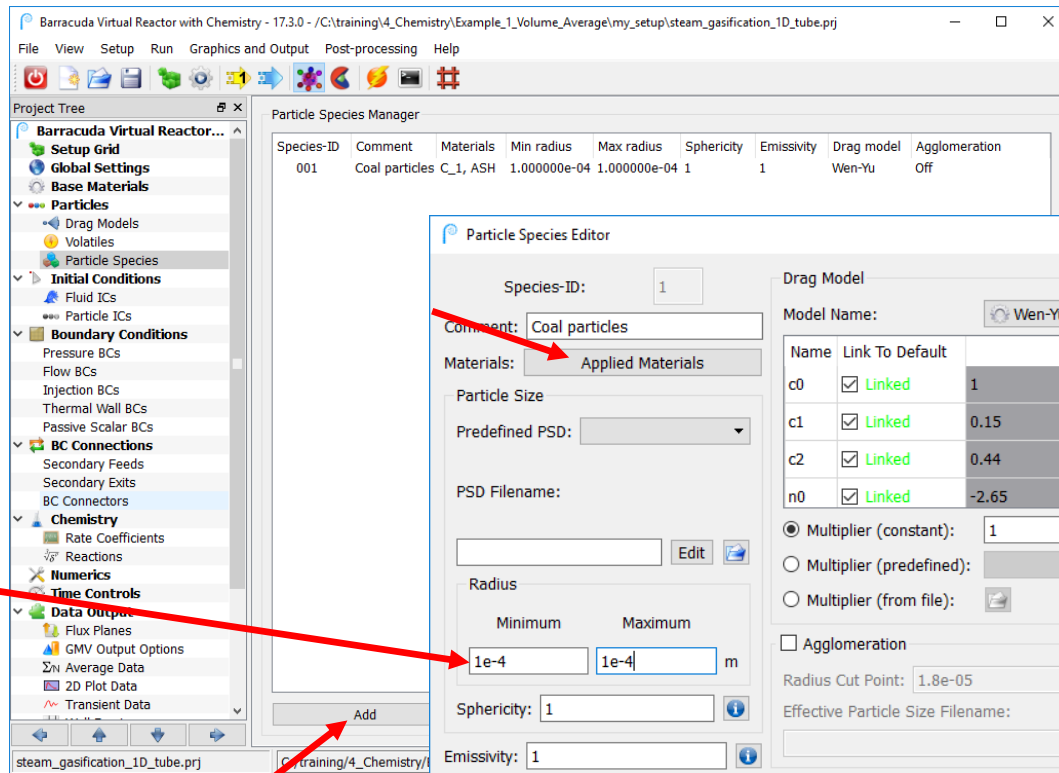
Particles

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



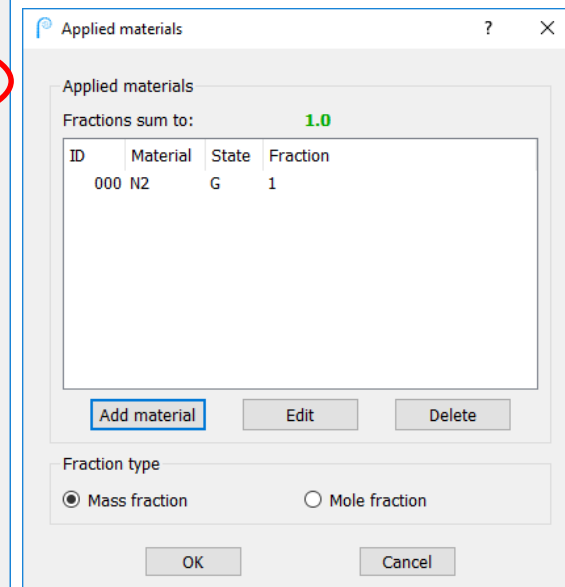
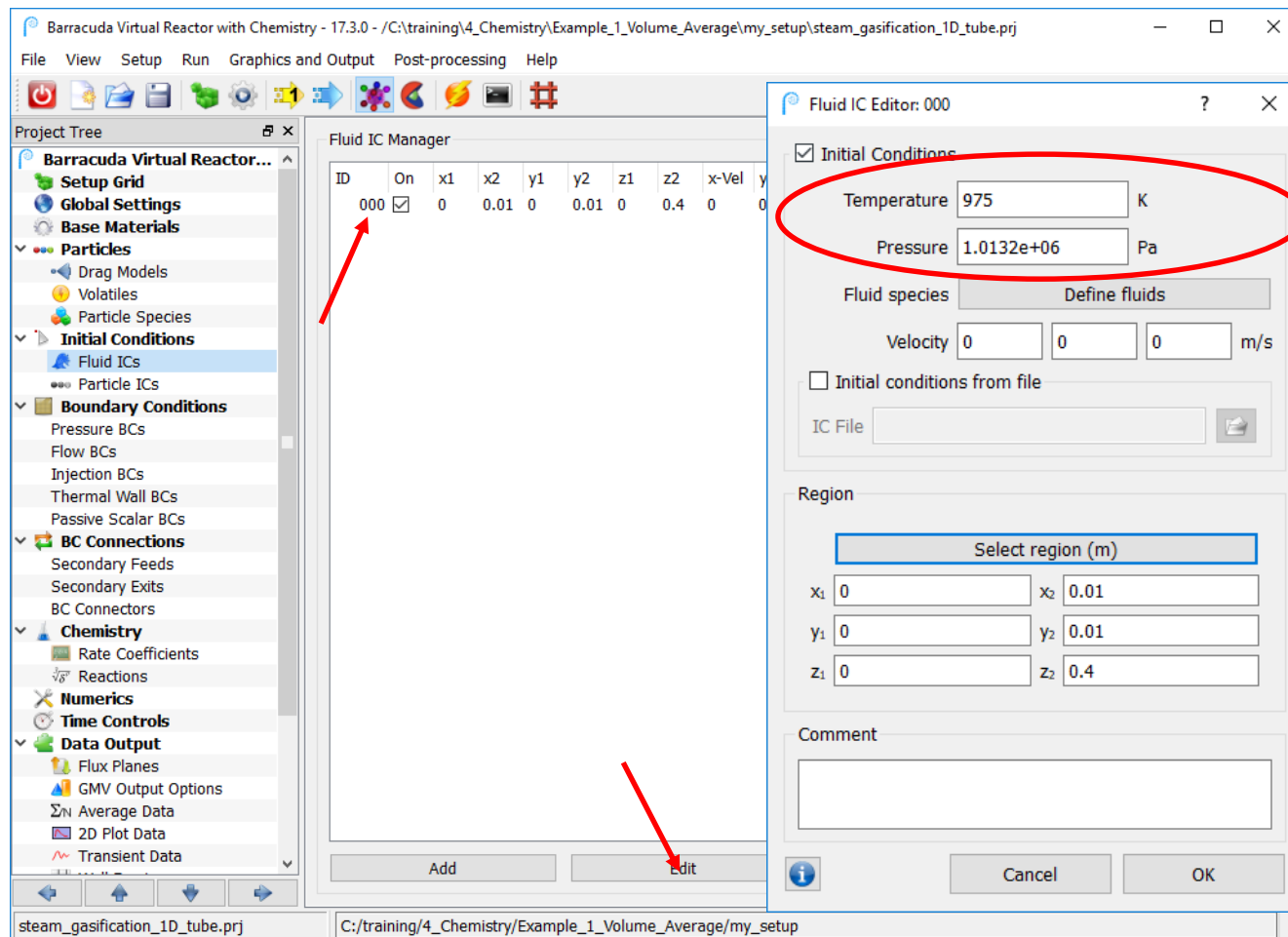
Particle Species

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



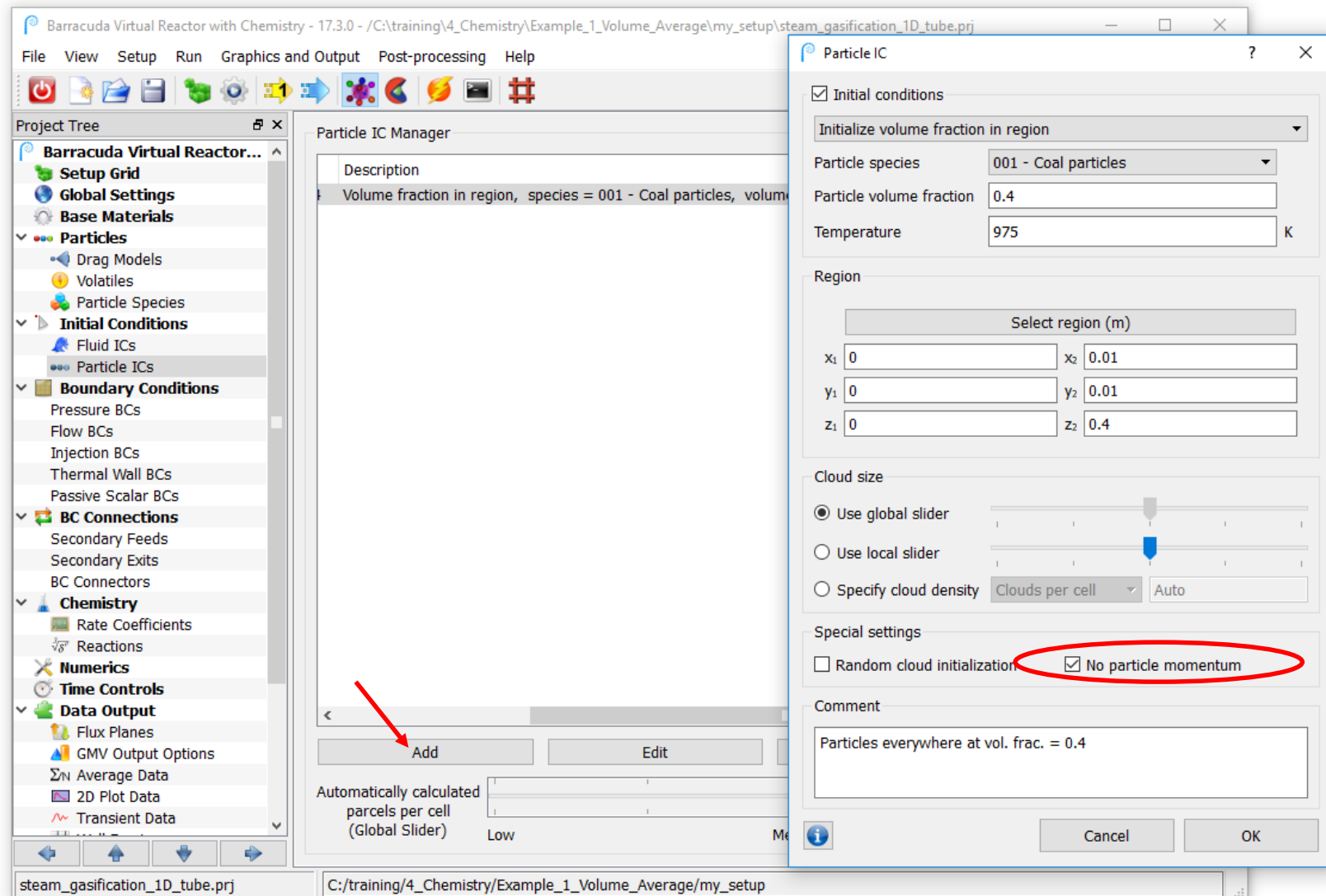
Fluid Initial Conditions

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



Particle Initial Conditions

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



Pressure Boundary Conditions

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

The screenshot displays the Barracuda Virtual Reactor software interface. The **Pressure BC Manager** window shows a list of boundary conditions with ID 000, direction z, and region x1=0, x2=0.01, y1=0, y2=0.01, z1=0.39, z2=0.4. The **Pressure BC Editor** window is open for this boundary condition, showing the following settings:

- Region:** Direction: z
- Fluid behavior at boundary:** Specify values: 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 (circled in red)
- Particle behavior at boundary:** No particle exit (selected)
- Properties:** Fluid properties if inflow: Interior cell values, Applied fluid species: Define fluid species (circled in red)

The **Applied materials** dialog box is also open, showing the following table:

ID	Material	State	Fraction
000	N2	G	1

The **Fraction type** is set to Mass fraction.

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”

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

Flow direction

☐ x-direction flow
☐ y-direction flow
☒ z-direction flow

x/y/z variation angle: 50 degrees

Flux plane options

Flux plane name: FLUXBC_flow_inlet

Gas species flow plane behavior

Mass Fraction

☐ Subdivide by radius Radius divisions: 5
☐ Output raw particle data

Comment

Flow BC inlet at bottom of tube

Behavior at boundary

Fluid behavior at boundary

☒ Use transient fluid flow file
☐ Use BC Connector data
☐ Specify values

Velocity flow: 0 m/s
Pressure: 0 Pa
Temp: 0 K

Particle behavior at boundary

☐ Use transient particle flow file
☐ Use BC Connector data
☒ No particle exit
☐ Particle exit flow

Particle radius (m) range allowed to exit: Min = 0 to Max = UNLIMITED

Particle exit control (Off)

☐ Particle feed (Slip and volume fraction)
☐ Particle feed (Slip and mass flux)
☐ Particle feed (Slip and mass flow rate)

Edit particle feed
Particle feed control

Fluid composition

Applied fluids: Define fluids

Transient fluid and particle flow file

SFF file: flow_bc_velocity_inlet.sff

Edit

OK

Applied materials

Applied materials

Fractions sum to: 1.0

ID	Material	State	Fraction
000	H2O	G	1

Add material Edit Delete

Fraction type

☒ Mass fraction ☐ Mole fraction

OK Cancel

Flow Boundary Conditions Editor

	Time (s)	Velocity (m/s)	Temperature (K)	Pressure (Pa)
1	0	0.01	800	1.01325e6
2				

Add Row Delete Row Check Data Graph Update Simulation

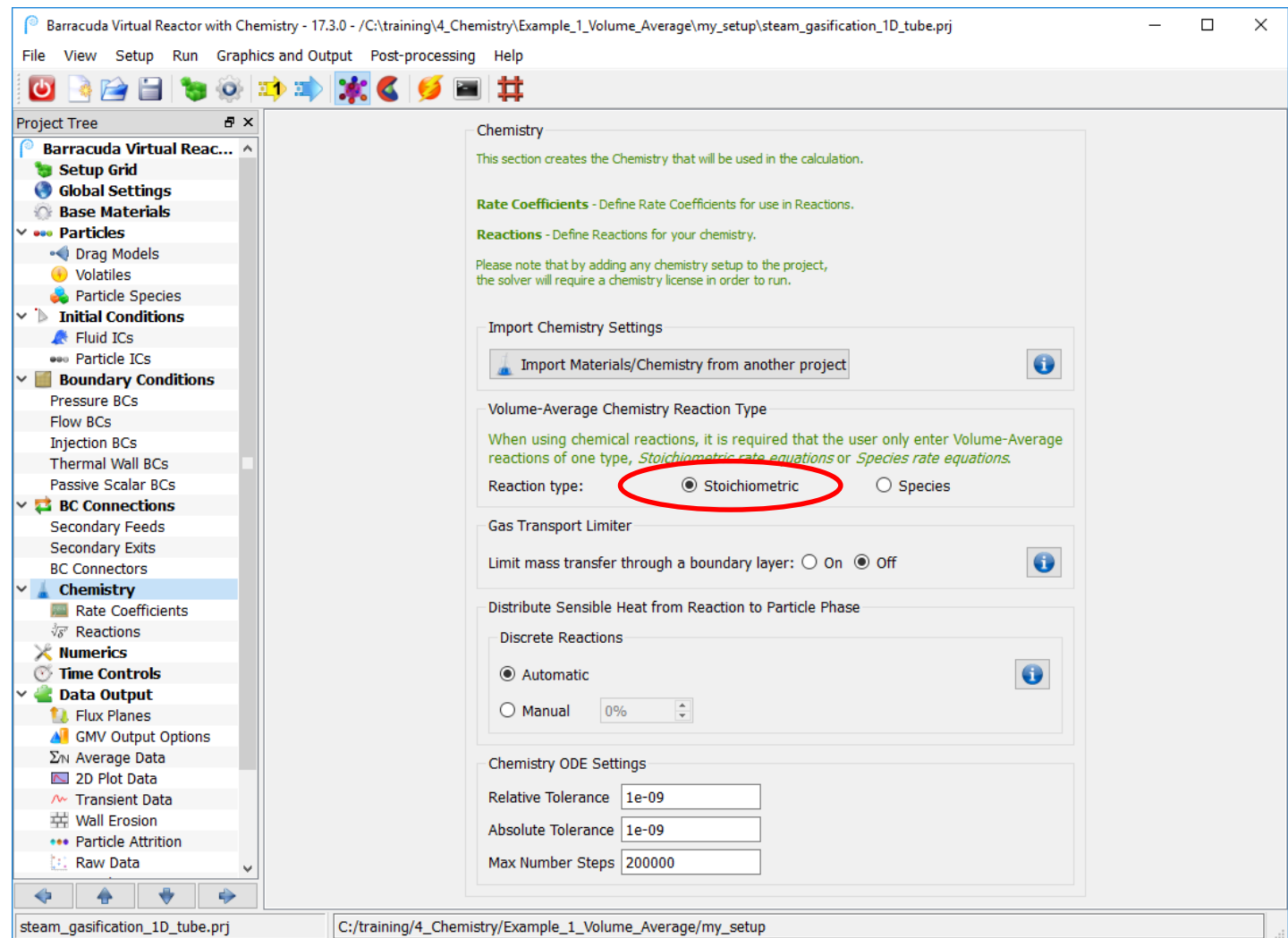
File: flow_bc_velocity_inlet.sff Save Save As Close

Adding Chemical Reactions

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

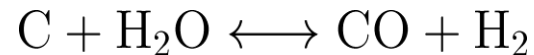
Chemistry

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



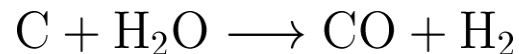
Chemistry

- Recall that the chemical reaction being modeled is:



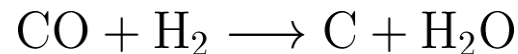
- In Barracuda, a reversible reaction is defined by splitting it into the forward and reverse reactions, defining a reaction rate for both the forward and reverse directions

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

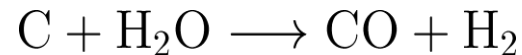


$$\frac{d[\text{H}_2\text{O}]}{dt} = \left(15.7 \frac{\text{m}^6}{\text{kg mol K}^2 \text{s}} \right) T^2 \exp \left(\frac{-33190 \text{K}}{T} \right) \rho_{\text{C}} [\text{H}_2] [\text{CO}]$$

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

Forward Reaction Rate

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



- 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

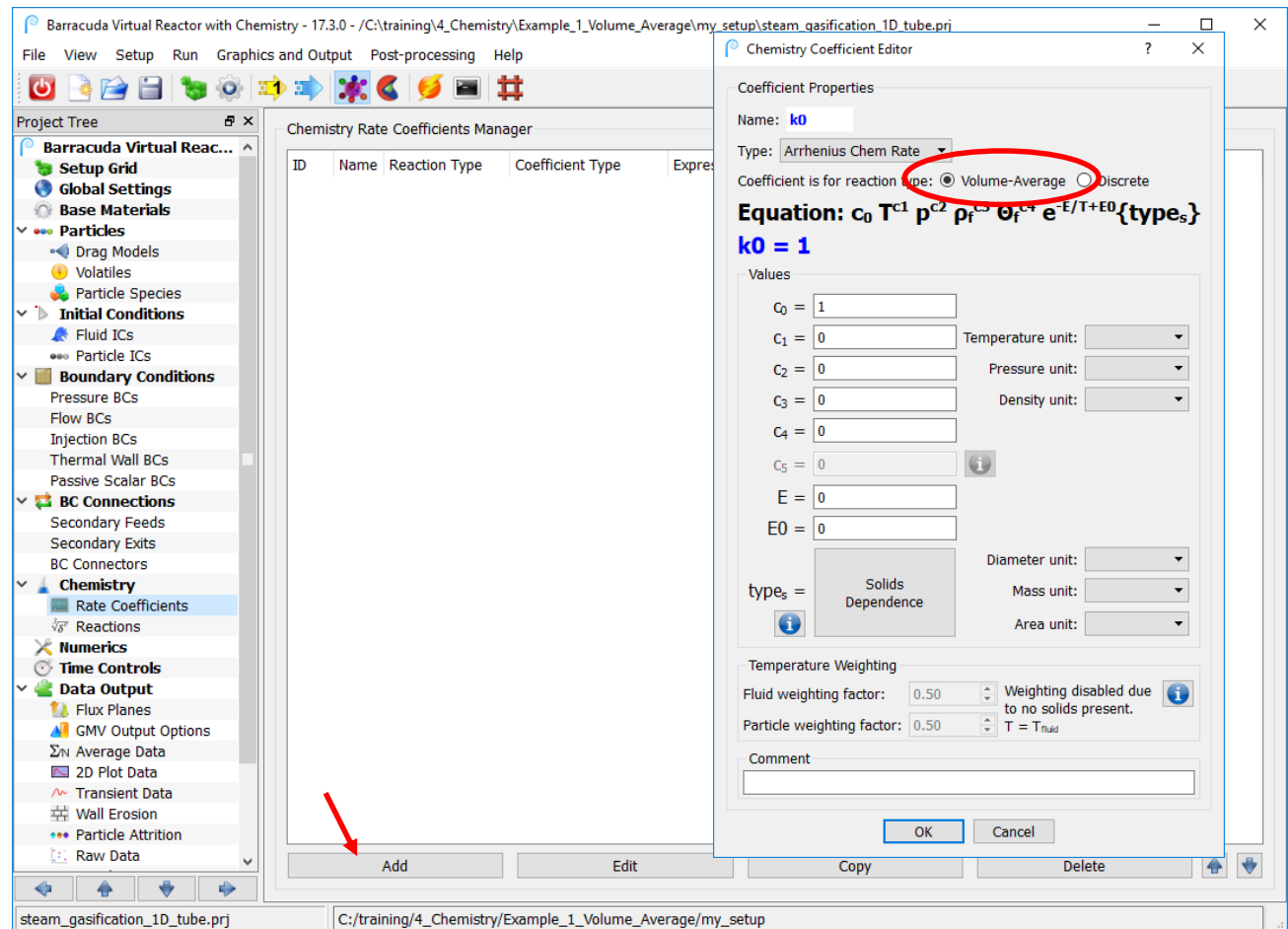
Rate coefficient: $k_0 = 219T \exp \left(\frac{-22645}{T} \right) \rho_{\text{C}}$

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

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.

Creating the Forward Rate Coefficient

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



Forward Rate Coefficients

- Enter the equation for k0 as follows:

C_0 C_1 E solids dependence
 \downarrow \downarrow \downarrow \downarrow

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

Chemistry Coefficient Editor

Coefficient Properties

Name: **k0**

Type: Arrhenius Chem Rate

Coefficient is for reaction type: ☒ Volume-Average ☐ Discrete

Equation: $c_0 T^{c_1} p^{c_2} \rho_f^{c_3} \theta_f^{c_4} e^{-E/T+E0} \{type_s\}$

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

Values

$C_0 =$ 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

$type_s =$ Solids Dependence

Diameter unit:

Mass unit: kg/m^3

Area unit:

Temperature Weighting

Fluid weighting factor: 0.50

Particle weighting factor: 0.50

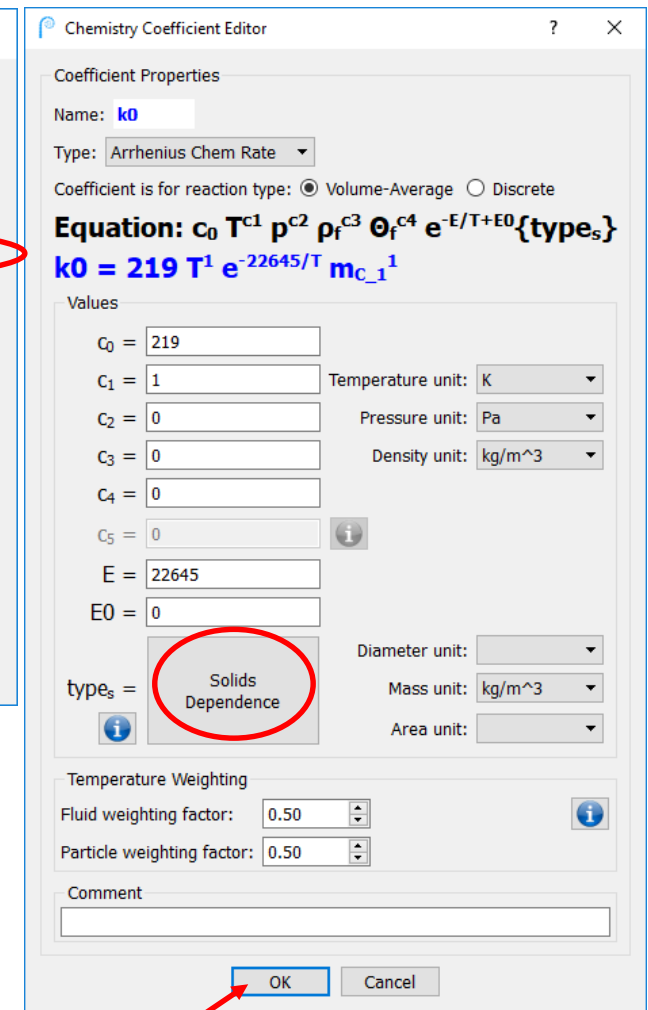
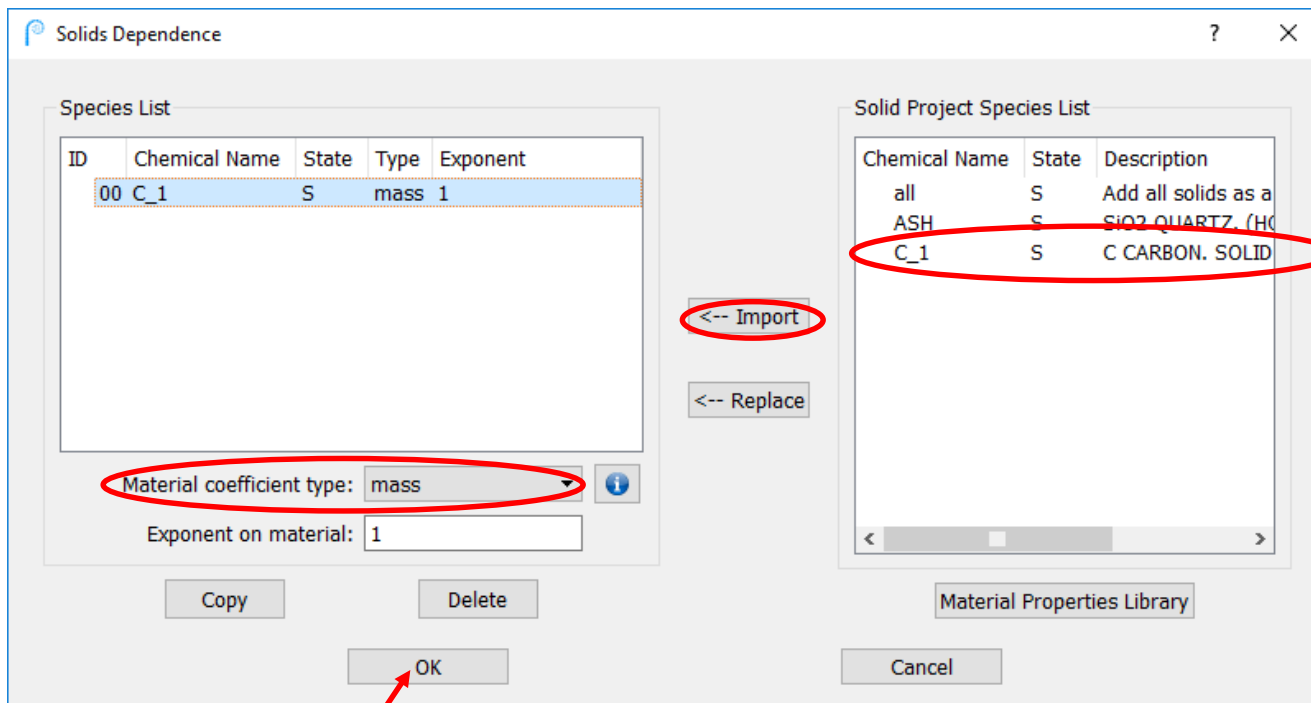
Comment

OK Cancel

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.

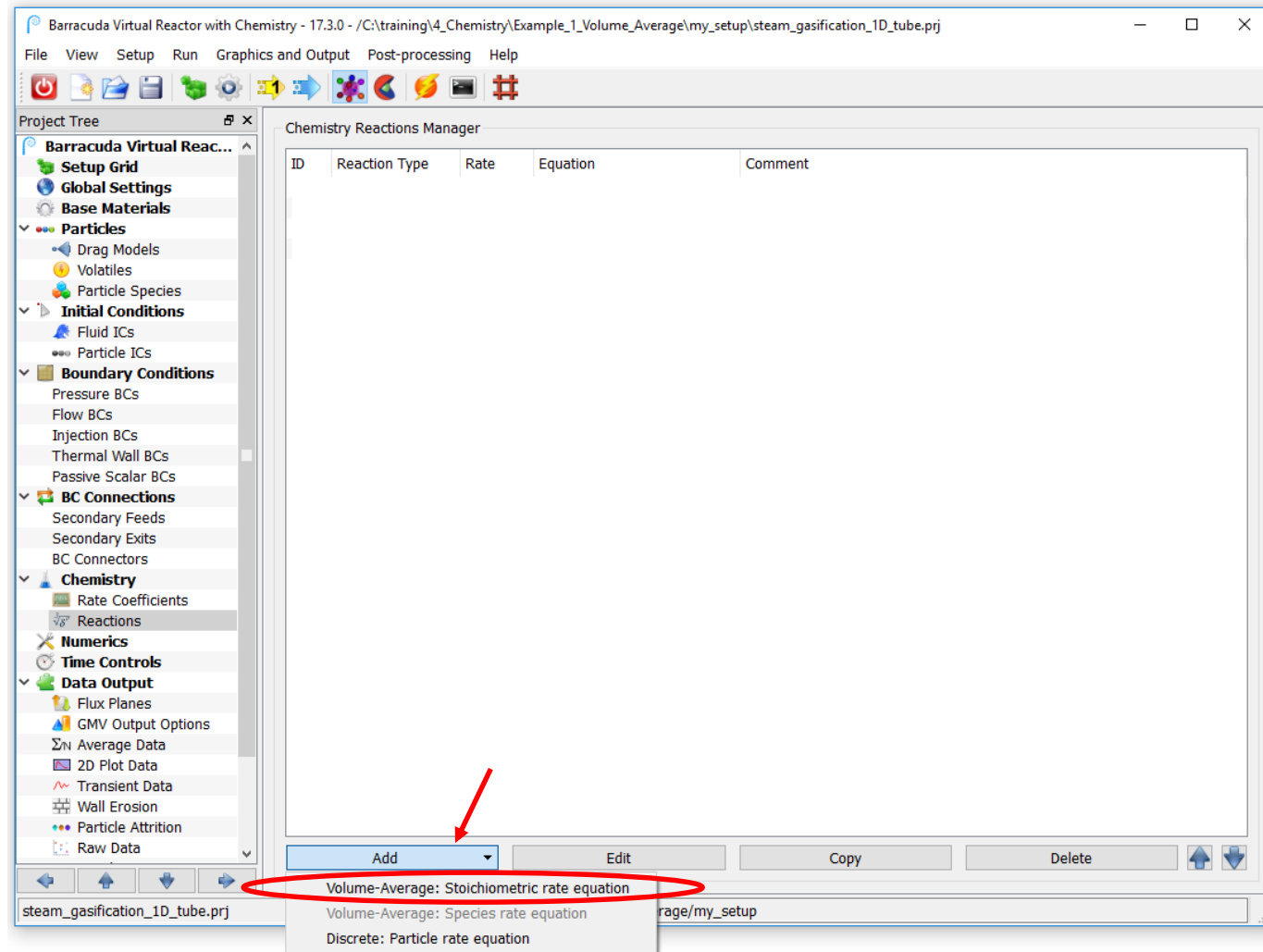
Rate Coefficients: Solids Term

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



Creating the Forward Reaction

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



Specifying the Forward Reaction Stoichiometry

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

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 i 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:
 Gas species units:

Enter a stoichiometric reaction:

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

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

$R00 = (k0[\text{H2O}])$

Comment

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

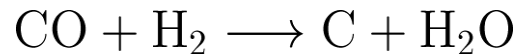
The screenshot shows the Barracuda Virtual Reactor software interface. The main window is titled "Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/4_Chemistry/Example_1_Volume_Average/my_setup/steam_gasification_1D_tube.prj". The interface includes a menu bar (File, View, Setup, Run, Graphics and Output, Post-processing, Help) and a toolbar. On the left is a "Project Tree" with various settings categories. The "Chemistry Reactions Manager" window is open, displaying a table of reactions. The first reaction is highlighted with a red oval.

ID	Reaction Type	Rate	Equation	Comment
00	VA: Stoichiometric	Equation: $C_1(S) + H_2O \Rightarrow CO + H_2$ R00 = $(k_0[H_2O])$		

At the bottom of the "Chemistry Reactions Manager" window, there are buttons for "Add", "Edit", "Copy", and "Delete".

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 CPFD 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:

$$\begin{array}{ccccccc} c_0 & c_1 & E & \text{solids dependence} \\ \downarrow & \downarrow & \downarrow & \downarrow \\ k_1 = 15.7 T^2 \exp(-33190/T) m_{C:1} \end{array}$$

- 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 Barracuda Virtual Reactor software interface. The Project Tree on the left includes sections 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, showing Rate Coefficients, Reactions, and Numerics. The Chemistry Rate Coefficients Manager table shows a single entry for k1 with a Volume-Average reaction type. The Chemistry Coefficient Editor dialog box is open, showing the equation $k_1 = 15.7 T^2 e^{-33190/T} m_{C:1}^1$. The dialog box includes fields for C0, C1, C2, C3, C4, C5, E, and E0, as well as units for temperature, pressure, density, diameter, mass, and area. The Volume-Average radio button is selected, and the Solids Dependence button is highlighted with a red arrow.

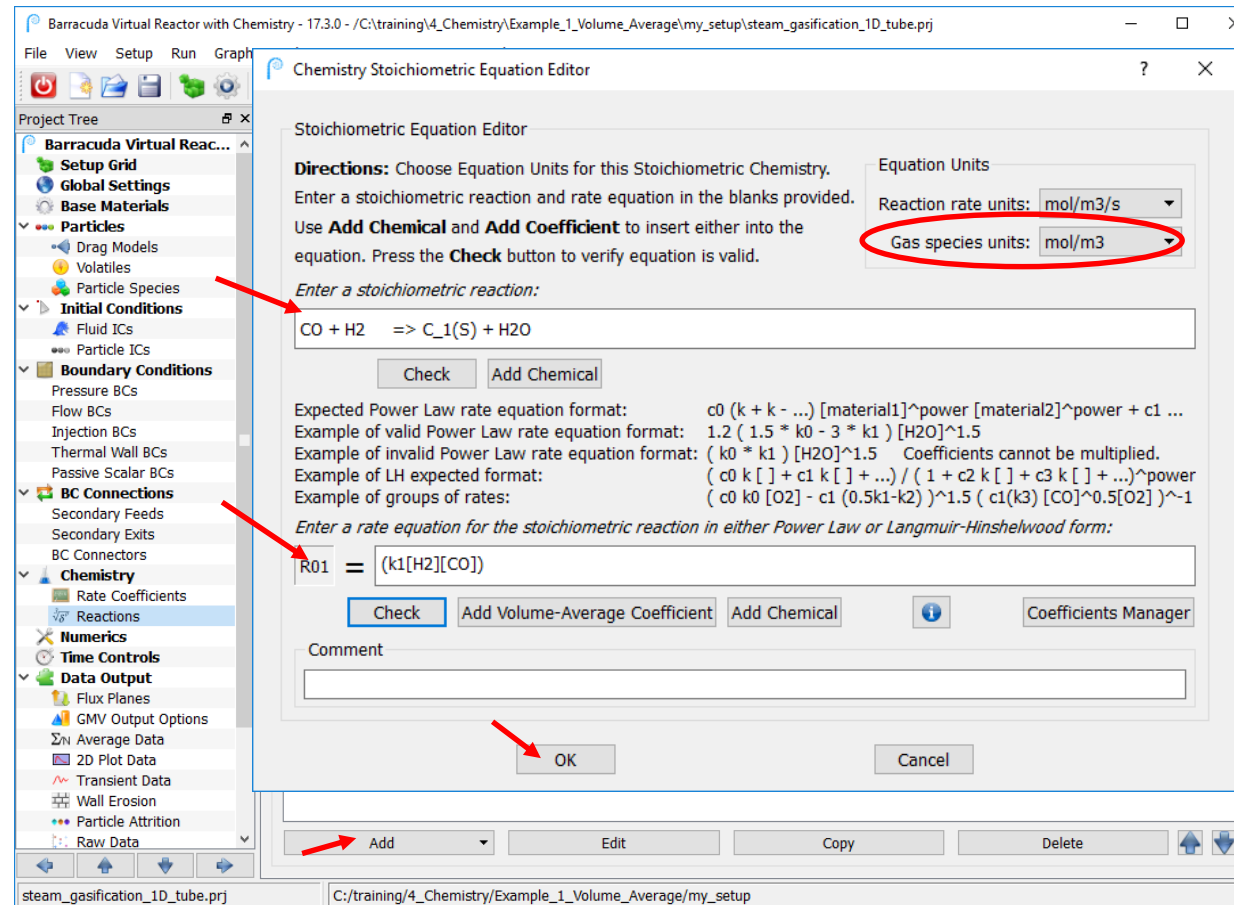
The chemical kinetics shown are for demonstration or education purpose only and have not been validated, nor are they recommended for any application. Development, validation, and use of chemical kinetics is the User's responsibility, and CPFD Software, LLC, does not warrant or endorse these chemical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

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:

$$R01 = k_1[\text{H}_2][\text{CO}]$$
- 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 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

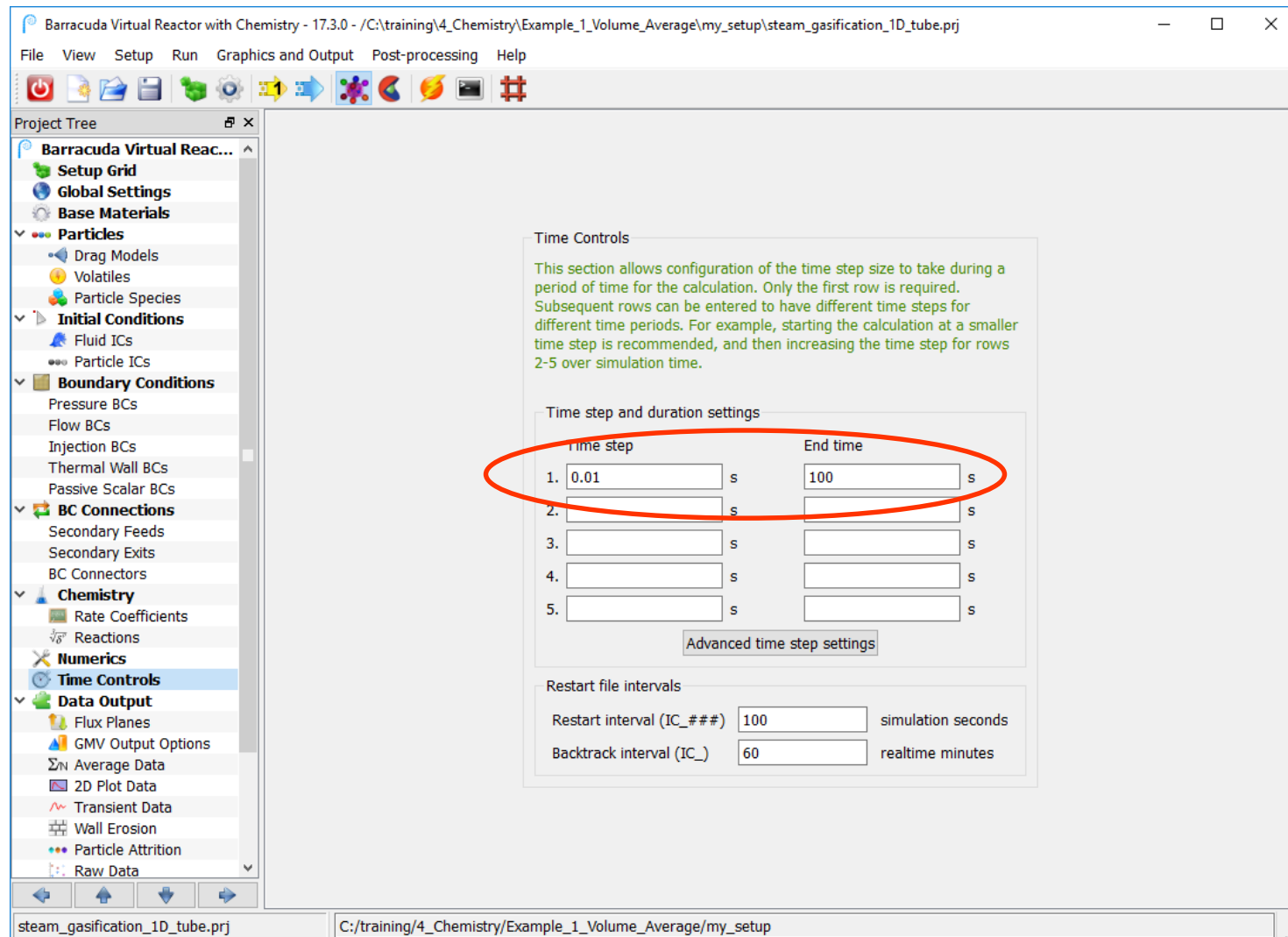
The screenshot shows the Barracuda Virtual Reactor software interface. The main window is titled "Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/4_Chemistry/Example_1_Volume_Average/my_setup/steam_gasification_1D_tube.prj". The interface includes a menu bar (File, View, Setup, Run, Graphics and Output, Post-processing, Help) and a toolbar with various icons. On the left is a "Project Tree" with a hierarchical list of settings: Setup Grid, Global Settings, Base Materials, Particles (with sub-items: Drag Models, Volatiles, Particle Species), Initial Conditions (with sub-items: Fluid ICs, Particle ICs), Boundary Conditions (with sub-items: Pressure BCs, Flow BCs, Injection BCs, Thermal Wall BCs, Passive Scalar BCs), BC Connections (with sub-items: Secondary Feeds, Secondary Exits, BC Connectors), Chemistry (with sub-items: Rate Coefficients, Reactions), Numerics, Time Controls, and Data Output (with sub-items: Flux Planes, GMV Output Options, Average Data, 2D Plot Data, Transient Data, Wall Erosion, Particle Attrition, Raw Data). The "Reactions" sub-item under "Chemistry" is selected. The main panel, titled "Chemistry Reactions Manager", displays a table of reactions:

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 reaction with ID 01 is circled in red. At the bottom of the main panel are buttons for "Add", "Edit", "Copy", and "Delete". 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".

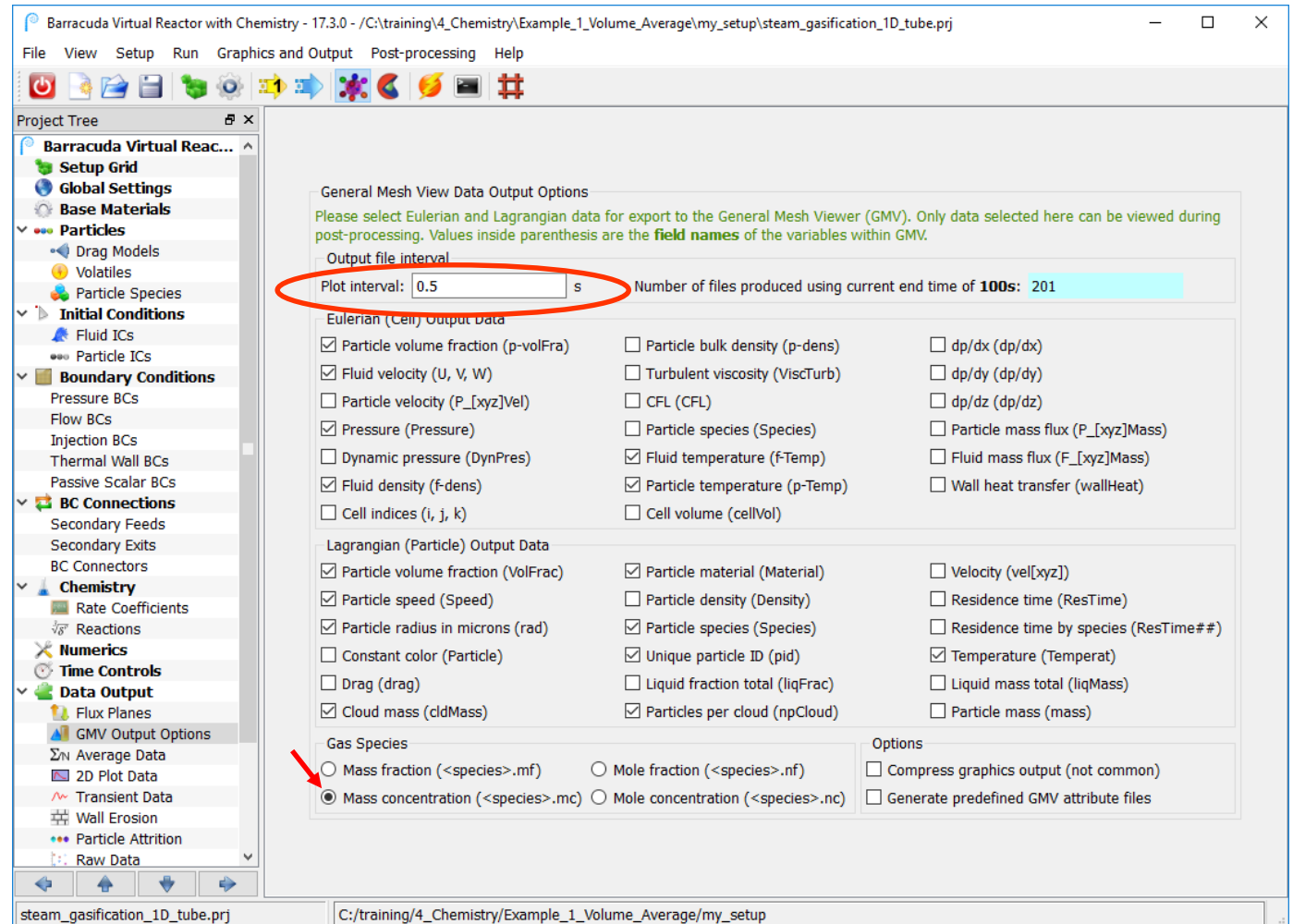
Time Controls

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



GMV Output Options

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



Select 2D Data

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

2D Plot Output

2D Plot Data

- ☐ Plot xy k-index nz/2
- ☐ Plot xz j-index ny/2
- ☐ Plot yx k-index nz/2
- ☐ Plot yz i-index nx/2
- ☒ Plot xz j-index ny/2
- ☐ Plot zy i-index nx/2
- ☐ Include boundary data in 2D plot

Plot Interval Options

Time interval 50 s

If plot interval = 0, use mesh viewer interval.

Max # of columns: 29

2D Data to Display

- ☐ Fluid volume fraction
- ☐ Particle volume fraction
- ☒ Pressure
- ☐ Fluid velocity
- ☐ Particle velocity
- ☒ Fluid temperature
- ☒ Particle temperature
- ☐ Fluid mass flux
- ☐ Solid mass flux
- ☐ Passive scalar
- ☒ Fluid density
- ☐ Particle density
- ☐ Gas species chemical reaction rate
- ☐ Ave particle volume fraction
- ☐ Ave pressure
- ☐ Ave fluid velocity
- ☐ Ave particle velocity
- ☐ Ave fluid temperature
- ☐ Ave particle temperature
- ☐ Ave fluid mass flux
- ☐ Ave solid mass flux
- ☒ Stoichiometric equation rate
- ☐ Liquid concentration

Output Gas Species

- ☒ Gas species
- ☐ Ave gas species

Output Format

- ☐ Mass fraction
- ☐ Mass concentration
- ☐ Mole fraction
- ☒ Mole concentration

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

- For transient data, choose the options shown below

Barracuda Virtual Reactor - 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 Reactor
 - 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

Transient Data Output

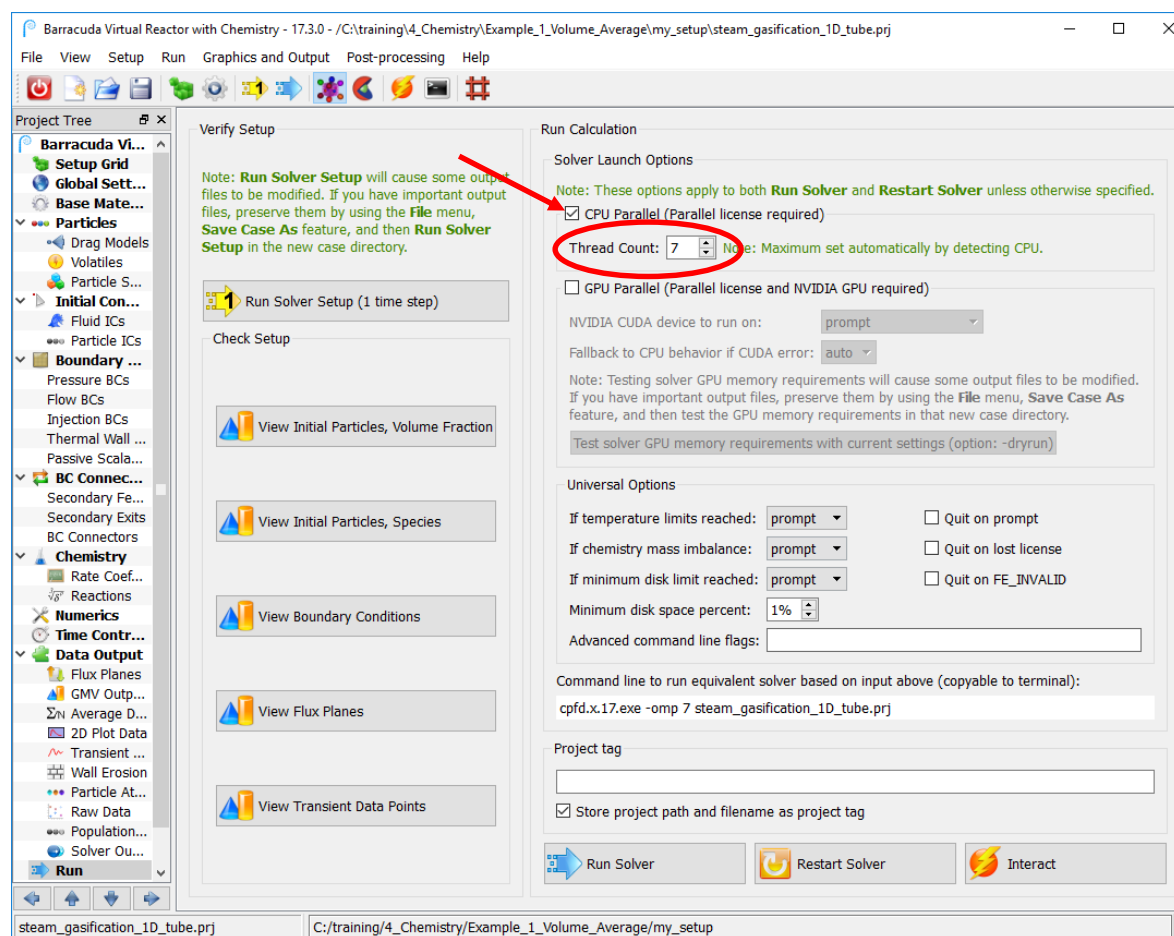
Output file name: trans.data

Type	Node	x (m) / i	y (m) / j	z (m) / k	Comment
p Vol Frac	1	1	20		
Particle temp	1	1	20		
Gas mass frac	1	1	20		
Gas mole frac	1	1	20		
Gas mass conc	1	1	20		
Gas mole conc	1	1	20		
Stoich eq rate	1	1	20		
Fluid temp	1	1	20		
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				
	xyz				

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

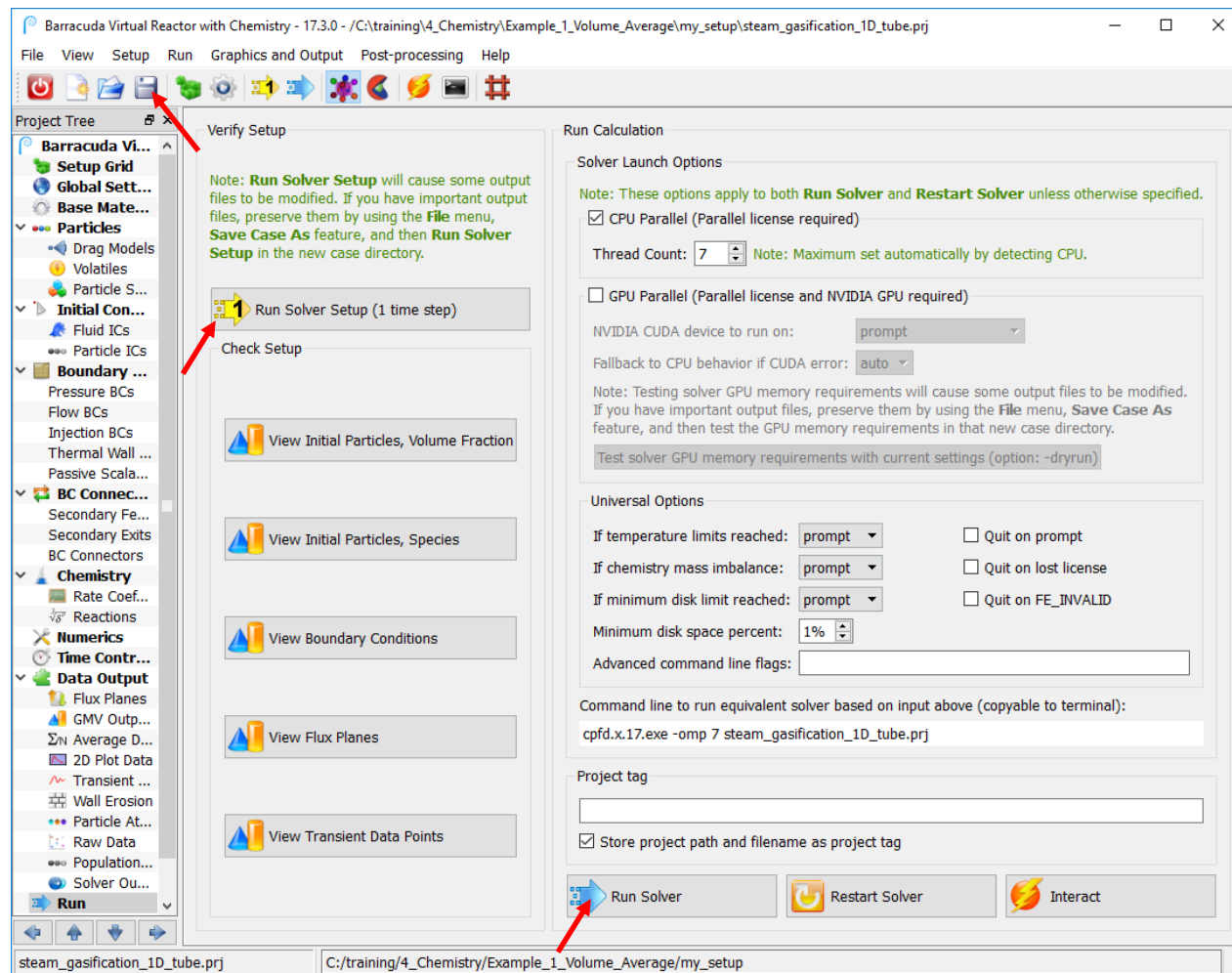
Set CPU Parallel

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



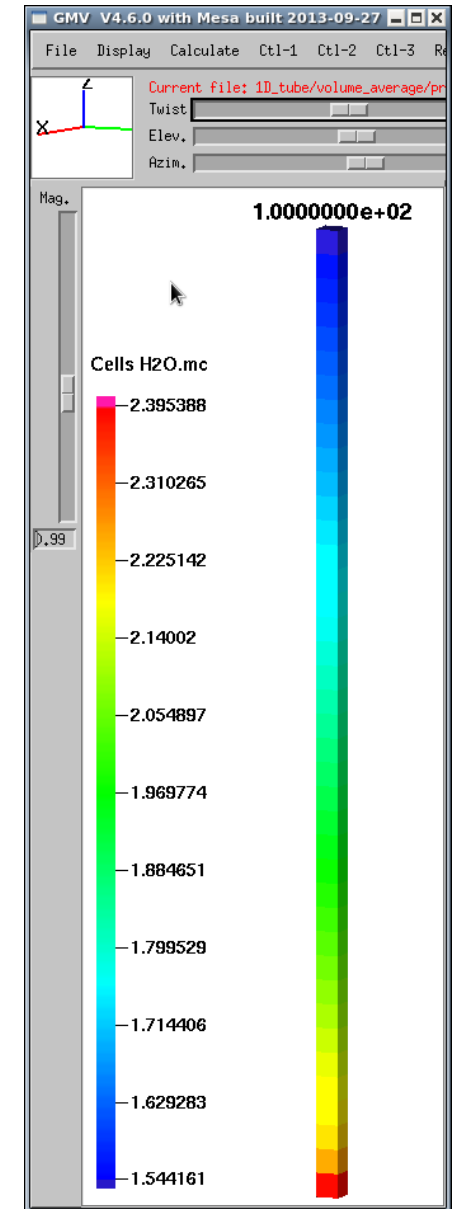
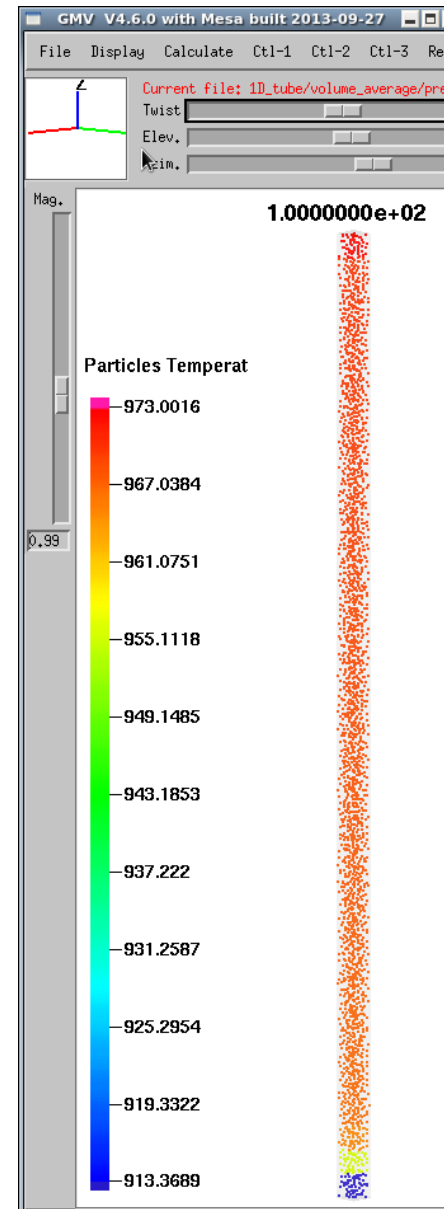
Start the Barracuda Solver

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



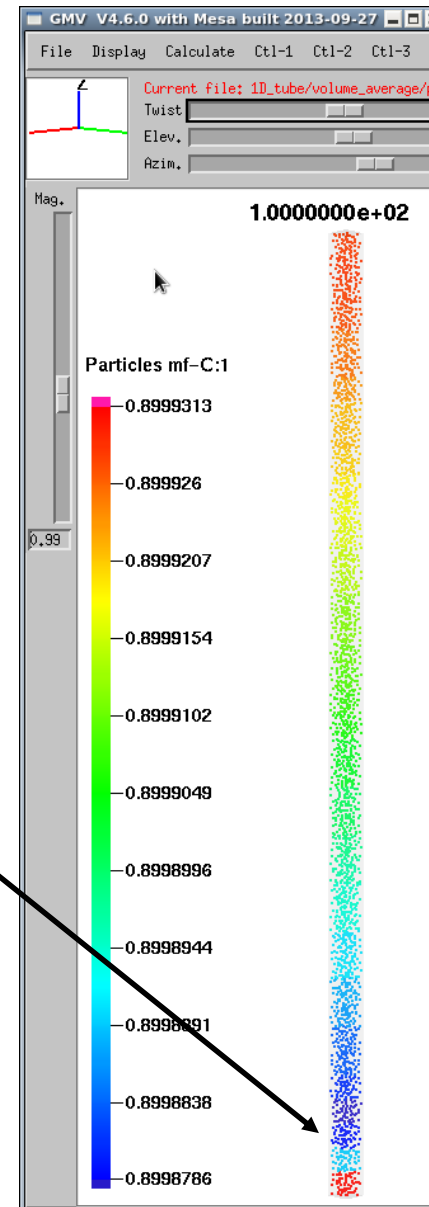
Post Processing

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



Post Processing

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

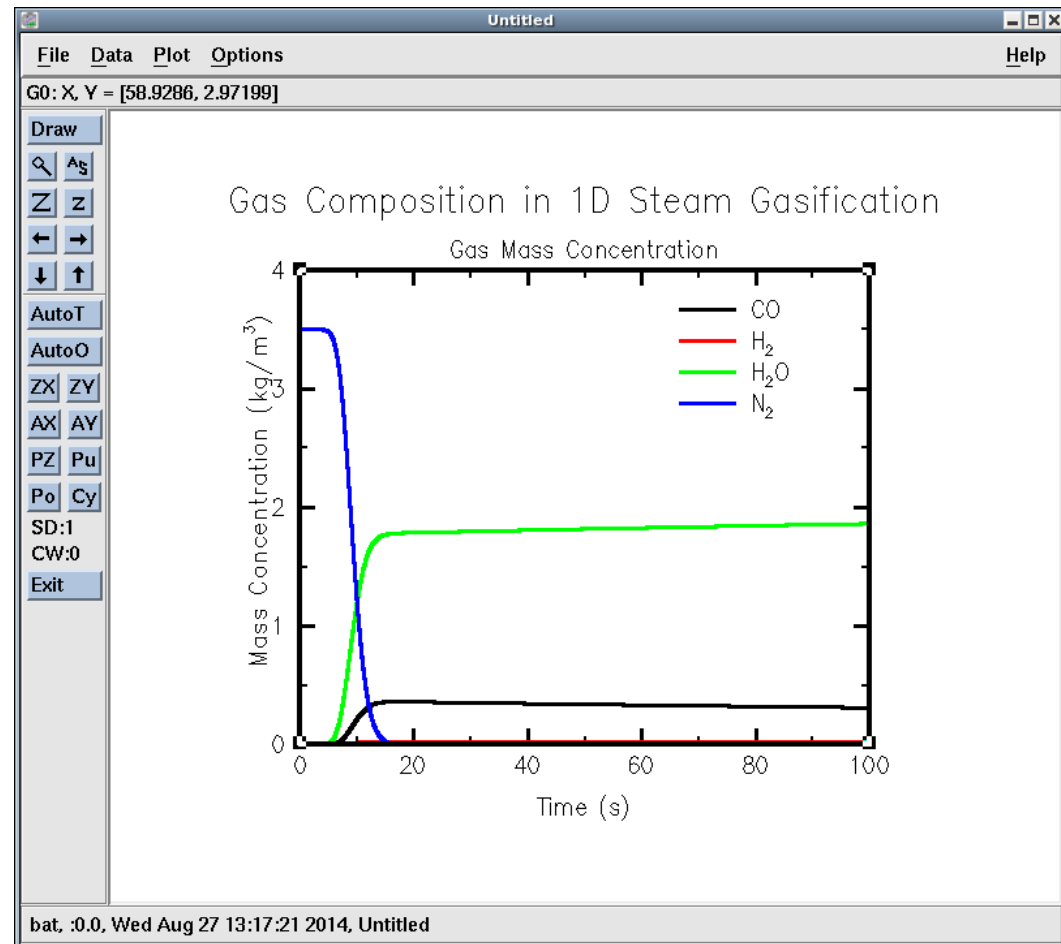


Plotting Transient Data

- Make a plot of the mass concentration of all gas species versus time in Plot Manager
 - Hint: refer to the Kuipers post processing exercise in plotting
 - Data is in the **trans.data00** file
 - The plot shows the gas concentrations in the cell containing the transient data ($z \sim 0.2$ 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 C0 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 C0 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 C0 (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 C0 (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

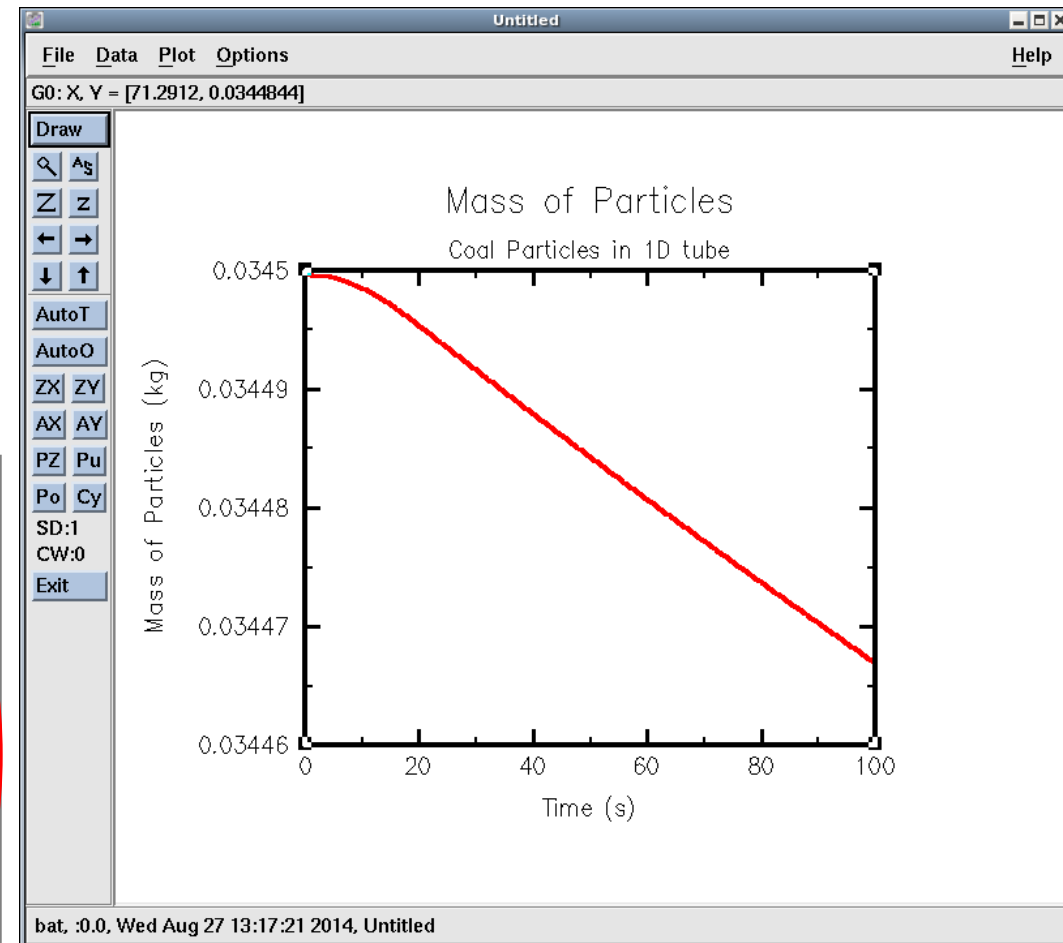
- Next, make a plot of the mass of coal particles versus time in Plot Manager
 - Hint: Data is in the **history.log** file

Barracuda CPFD editor

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	QL	pMass
#	s	s	itr	err	itr	err	itr	err	itr	err	itr	err	itr	err	itr	err	kg
0.00000e+00	1.000e-04	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	3.44765e-02
# Dumping Gmv.000000																	
1.00000e-04	1.000e-04	0.000e+00	8.73e-11	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	5.92e-09	0.000e+00	2.14e-08	0.000e+00	7.35e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
2.00000e-04	1.000e-04	0.000e+00	9.77e-11	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	3.38e-09	0.000e+00	2.28e-08	0.000e+00	6.54e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
3.00000e-04	1.000e-04	0.000e+00	1.03e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	8.26e-10	0.000e+00	2.25e-08	0.000e+00	6.38e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
4.00000e-04	1.000e-04	0.000e+00	1.18e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	3.02e-10	0.000e+00	2.20e-08	0.000e+00	6.22e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
5.00000e-04	1.000e-04	0.000e+00	1.34e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	1.39e-10	0.000e+00	2.15e-08	0.000e+00	6.40e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
6.00000e-04	1.000e-04	0.000e+00	1.49e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	1.81e-10	0.000e+00	2.09e-08	0.000e+00	6.58e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
7.00000e-04	1.000e-04	0.000e+00	1.64e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	2.06e-10	0.000e+00	2.02e-08	0.000e+00	6.75e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
8.00000e-04	1.000e-04	0.000e+00	1.79e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	2.14e-10	0.000e+00	1.95e-08	0.000e+00	6.90e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
9.00000e-04	1.000e-04	0.000e+00	1.94e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	2.80e-10	0.000e+00	1.88e-08	0.000e+00	7.03e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
1.00000e-03	1.000e-04	0.000e+00	2.08e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	4.02e-10	0.000e+00	1.81e-08	0.000e+00	7.15e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
1.10000e-03	1.000e-04	0.000e+00	2.23e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	4.89e-10	0.000e+00	1.73e-08	0.000e+00	7.27e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
1.20000e-03	1.000e-04	0.000e+00	2.37e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	5.43e-10	0.000e+00	1.66e-08	0.000e+00	7.38e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
1.30000e-03	1.000e-04	0.000e+00	2.50e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	5.74e-10	0.000e+00	1.59e-08	0.000e+00	7.48e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
1.40000e-03	1.000e-04	0.000e+00	2.63e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	5.91e-10	0.000e+00	1.52e-08	0.000e+00	7.59e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
1.50000e-03	1.000e-04	0.000e+00	2.76e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	6.01e-10	0.000e+00	1.46e-08	0.000e+00	7.68e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
1.60000e-03	1.000e-04	0.000e+00	2.88e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	6.07e-10	0.000e+00	1.39e-08	0.000e+00	7.77e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
1.70000e-03	1.000e-04	0.000e+00	3.00e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	6.09e-10	0.000e+00	1.32e-08	0.000e+00	7.85e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
1.80000e-03	1.000e-04	0.000e+00	3.12e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	6.09e-10	0.000e+00	1.26e-08	0.000e+00	7.93e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
1.90000e-03	1.000e-04	0.000e+00	3.23e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	6.04e-10	0.000e+00	1.20e-08	0.000e+00	8.00e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02
2.00000e-03	1.000e-04	0.000e+00	3.33e-10	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	5.97e-10	0.000e+00	1.14e-08	0.000e+00	8.07e-11	0.000e+00	0.000e+00	0.000e+00	3.44766e-02

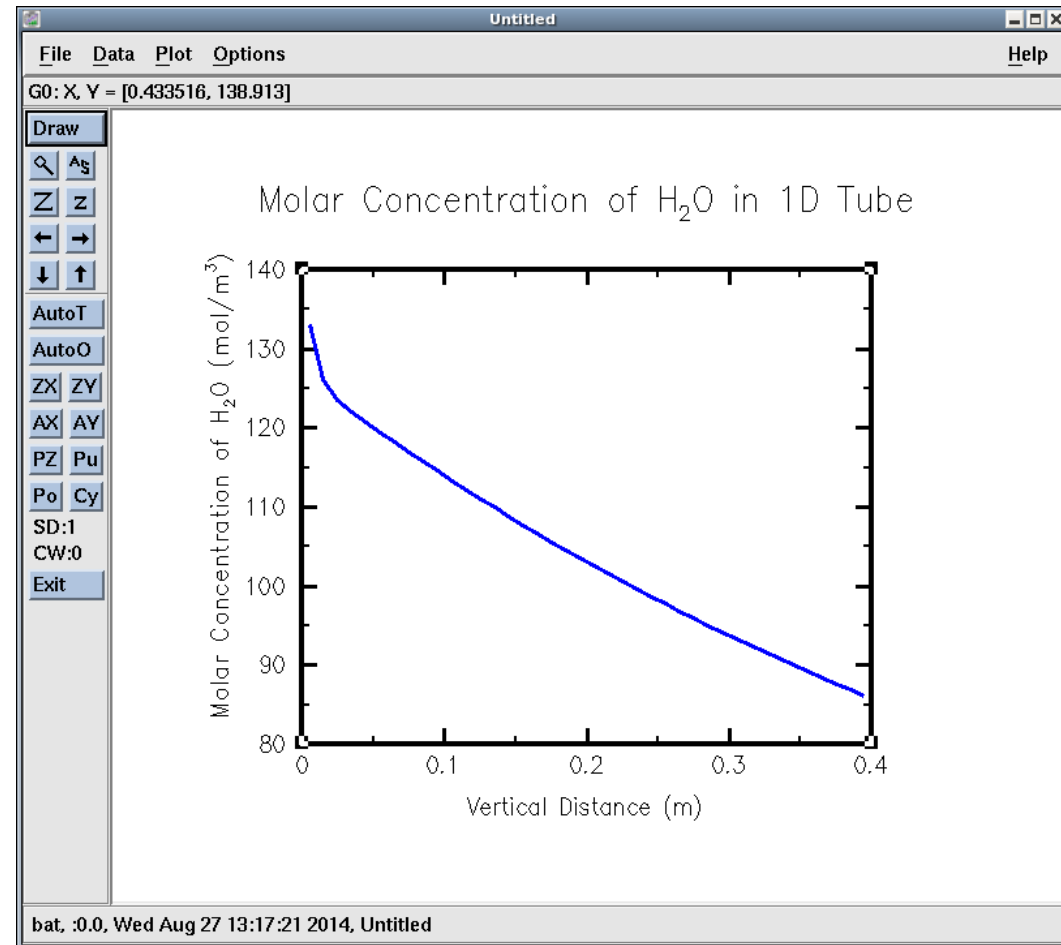
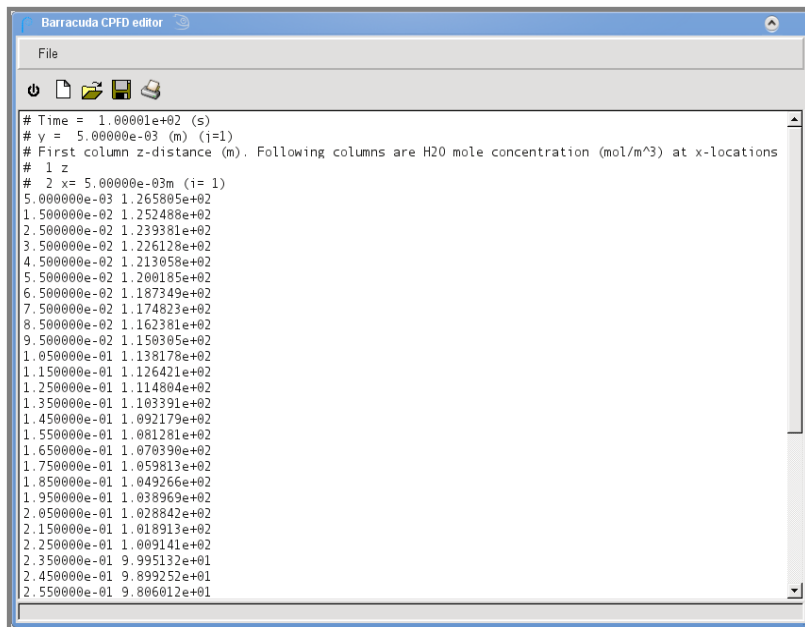


The solids mass in the system decreases as carbon is consumed in the reaction.

Plotting 2D Data

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

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



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

Summary

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