

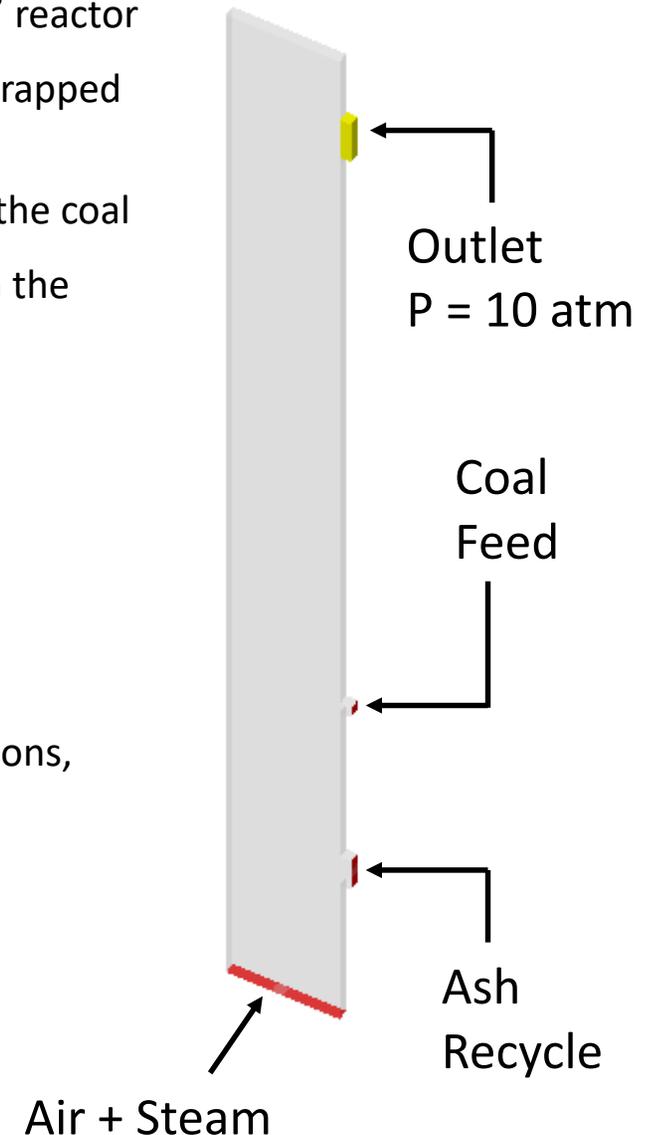
# Chemistry Training: 2D Coal Gasifier

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# Coal Gasifier 2D Reactor

- This model simulates the gasification of coal particles in a thin “2D” reactor
- The coal particles consist of carbon, ash, and volatile components trapped inside the coal
- The volatile components in the coal particles will devolatilize from the coal
- The carbon in the coal and devolatilized methane will participate in the following reactions:
  - Steam gasification:  $C + H_2O \leftrightarrow CO + H_2$
  - CO<sub>2</sub> gasification:  $C + CO_2 \leftrightarrow 2 CO$
  - Methanation:  $0.5 C + H_2 \leftrightarrow 0.5 CH_4$
  - Carbon combustion:  $2 C + O_2 \rightarrow 2 CO$
  - Water gas-shift:  $CO + H_2O \leftrightarrow CO_2 + H_2$
- Reversible reactions will be broken into forward and reverse directions, with separate reaction rates given for each direction
- Simulation includes thermal calculations

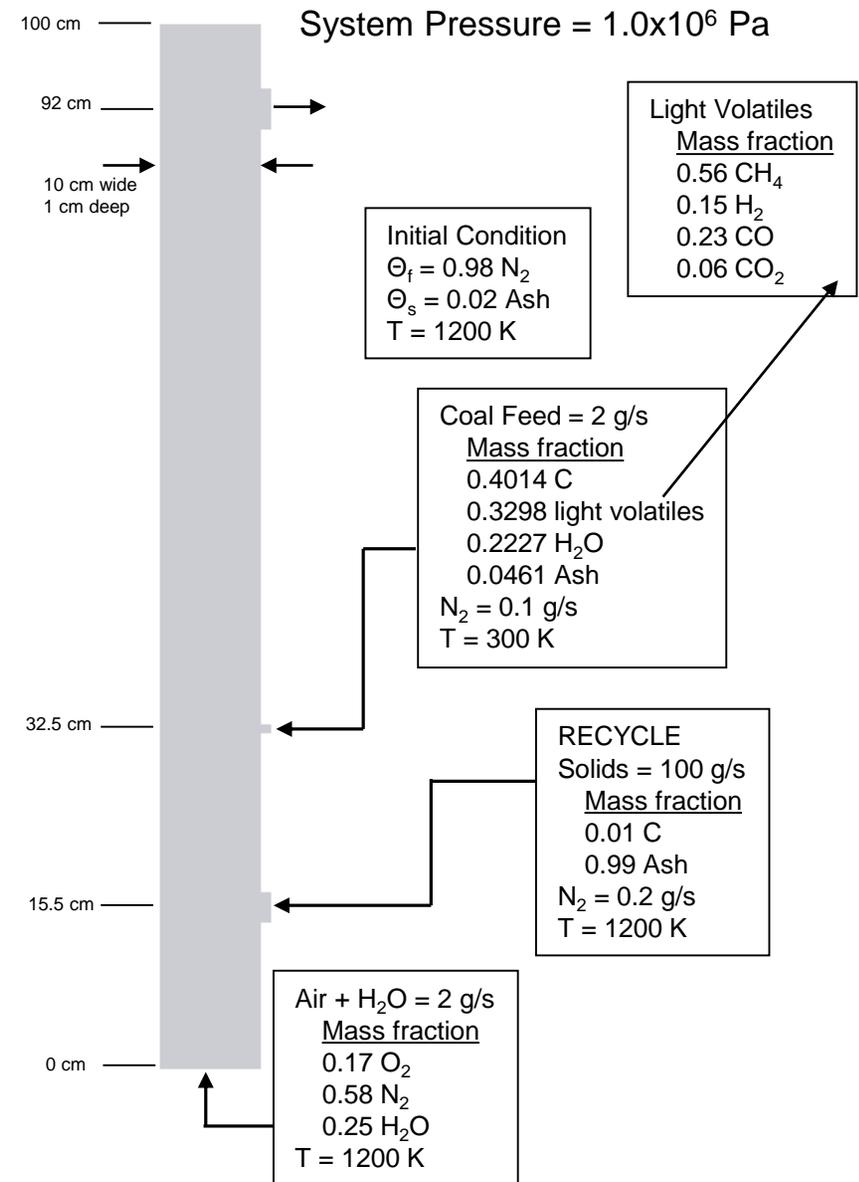


# Outline for Simulation Setup

- Use a diagram of system information to set up flow and pressure BCs
  - Discuss best ways to define fluid-only and fluid + solid flow BCs
  - How to handle different solid species, i.e. fresh coal feed and ash recycle
- Convert reaction rates from format(s) given in open literature to “Barracuda format”
  - The main source used for defining the chemistry is Syamlal et al (1992).
  - Carbon combustion is from Yoon (1978), and water gas-shift is from Bustamante (2004, 2005)
- Select GMV output variables, transient data points, and any other output data
  - Which parameters are important to monitor?
  - How do you want to display the results of the simulation?  
Verify that problem setup is correct and run the simulation.
  - View boundary conditions to make sure BCs are defined correctly
  - Look in the info.log file to verify that chemistry is set up correctly
- Briefly review results of simulation that has been previously run and post-processed

# System Diagram

- The diagram on the right summarizes the conditions for the problem flow and pressure BCs
- There are no default species for “Coal” or “Ash” in Barracuda. Use “C:1”, carbon, as coal. Copy the coal material as a starting point for “Ash”
- Notice that the Air + steam inlet is defined using the proper mass ratios of  $N_2$  and  $O_2$ , instead of the built-in “AIR” species
- For all particles, use the **default FCC size distribution** in Barracuda
- The solids feed BCs have both “C” and “Ash” being fed in. How do you specify ratios such as this?
- The mass fractions used for “Volatile Material” are based on information from Yoon (1978).
- The system is initially filled with “Ash” at a volume fraction of 0.02. It is a good idea to define this as a separate particle species so that the “Ash” fed at the flow BCs can be tracked independently



# Summary of Barracuda Rate Equations

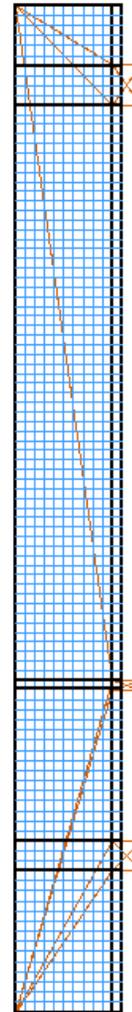
Reaction	Stoichiometric Equation	Reaction Rate Expression (mol m <sup>-3</sup> s <sup>-1</sup> )	Source
Steam gasification	C(s)+H <sub>2</sub> O → CO+H <sub>2</sub>	$r_{1,f} = 6.36m_c T \exp\left(\frac{-22,645}{T}\right)[\text{H}_2\text{O}]$	Syamlal, 1992
	CO+H <sub>2</sub> → C(s)+H <sub>2</sub> O	$r_{1,r} = 5.218 \times 10^{-4} m_c T^2 \exp\left(\frac{-6,319}{T} - 17.29\right)[\text{H}_2][\text{CO}]$	
CO <sub>2</sub> gasification	C(s)+CO <sub>2</sub> → 2CO	$r_{2,f} = 6.36m_c T \exp\left(\frac{-22,645}{T}\right)[\text{CO}_2]$	Syamlal, 1992
	2CO → C(s)+CO <sub>2</sub>	$r_{2,r} = 5.218 \times 10^{-4} m_c T^2 \exp\left(\frac{-2,363}{T} - 20.92\right)[\text{CO}]^2$	
Methanation	0.5C(s)+H <sub>2</sub> → 0.5CH <sub>4</sub>	$r_{3,f} = 6.838 \times 10^{-3} m_c T \exp\left(\frac{-8,078}{T} - 7.087\right)[\text{H}_2]$	Syamlal, 1992
	0.5CH <sub>4</sub> → 0.5C(s)+H <sub>2</sub>	$r_{3,r} = 0.755m_c T^{0.5} \exp\left(\frac{-13,578}{T} - 0.372\right)[\text{CH}_4]^{0.5}$	
Combustion	2C(s)+O <sub>2</sub> → 2CO	$r_4 = 4.34 \times 10^7 \theta_c T \exp\left(\frac{-13,590}{T}\right)[\text{O}_2]$	Yoon, 1978
Water gas- shift	CO+H <sub>2</sub> O → CO <sub>2</sub> +H <sub>2</sub>	$r_{5,f} = 7.68 \times 10^{10} \exp\left(\frac{-36,640}{T}\right)[\text{CO}]^{0.5}[\text{H}_2\text{O}]$	Bustamante, 2005
	CO <sub>2</sub> +H <sub>2</sub> → CO+H <sub>2</sub> O	$r_{5,r} = 6.4 \times 10^9 \exp\left(\frac{-39,260}{T}\right)[\text{H}_2]^{0.5}[\text{CO}_2]$	Bustamante, 2004

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 CPFDD Software, LLC, does not warrant or endorse these chemical kinetics for any purpose.

# Grid Generation

- Create a grid of about 1200 cells or less
- Show the instructor your grid before proceeding

## Grid Setup



## Completed Grid



# Define Base Materials in Project File

- Based on the summary of reactions and rate equations on the previous slide, define the materials in your project
  - Any species used in the chemical reactions must be defined in the **Project material list**
  - Air is introduced through one of the side inlets, and at the bottom inlet. In chemistry problems, you should not use the “AIR” material listed in the **Material library**, but instead use **N2** and **O2**. Then define any flow BCs for air with the correct ratio of  $N_2$  and  $O_2$
  - There is no “Ash” species included in the default **Material library**, so use solid carbon as a starting point and modify the Chemical name to create a new species called “Ash”
  - While you are importing the species from the **Material library**, check the properties to make sure they are valid. If you know better values for any of the properties, modify those properties. Also, ensure the molecular weights used will conserve mass when reacting.

The screenshot displays the Barracuda Virtual Reactor software interface. The main window is titled "Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/6\_Optional\_Training/3\_2D\_Gasification/my\_setup/gasifier\_2d.prj". The interface includes a menu bar (File, View, Setup, Run, Graphics and Output, Post-processing, Help) and a toolbar. The Project Tree on the left shows the project structure, with "Base Materials" selected. The Base Materials Manager window is open, showing the Project Material List table. The table has columns for Chemical name, State, and Description. The following table represents the data shown in the screenshot:

Chemical name	State	Description
Ash	S	C CARBON SOLID GRAPHITE REFEREN
C	S	C CARBON, SOLID GRAPHITE REF ELE
CH4	G	CH4 METHANE SAME AS THE ANHAR
CO	G	CO CARBON-MONOXIDE CALCULATED
CO2	G	CO2 CARBON-DIOXIDE
H2	G	H2, REF ELEMENT
H2O	G	H2O
N2	G	N2 REF ELEMENT
O2	G	O2 CALCULATED FROM ORIGINAL VA

Below the table are buttons for "Add", "Edit", "Copy", and "Delete". The Properties section shows the "Averaging method for fluid mixture properties" set to "Mole average" and "Flow Type" set to "Compressible". The Material Properties Library on the right shows a list of materials, with "Carbon" selected in the "Contains" dropdown.

# Volatiles

- **Add** the volatile materials to the project file as two separate volatile species:
  - **Name** the first species “light volatiles”
  - Set the **Specific heat** to 1000 J/Kg K
  - Select the **Release gases**: CH<sub>4</sub>, H<sub>2</sub>, CO, and CO<sub>2</sub> specifying the mass fraction of each as shown on the right
  - Set **c<sub>0</sub>** to “7.5e13”
  - Set **E** to “30000”
  - **Add** a second volatile species and name it “water”
  - Set the **Specific heat** to 1000 J/Kg K
  - Select the **Release gases**: H<sub>2</sub>O with a mass fraction of 1
  - Set **c<sub>0</sub>** to “2.2e18”
  - Set **E** to “30000”

The screenshot shows the Barracuda Virtual Reactor interface. The Project Tree on the left lists various settings like 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, Flux Planes, GMV Output Options, and Average Data. The Volatiles Manager window is open, showing a table with columns for ID, Name, Density (kg/m<sup>3</sup>), and Rate. The first entry is ID 000, Name 'light volatiles', Density 'Unspecified', and Rate '7.5e+13 e^(-30000 / T + 0)'. A 'Volatile Editor' dialog box is open for 'light volatiles', showing properties: Name: light volatiles, Specific heat (Cp): 1000 J/kg K, Heat of devolatilization at 298.15K: 0 J/kg, Release gases: CH<sub>4</sub>, H<sub>2</sub>, CO, CO<sub>2</sub>. The 'Applied materials' dialog box is also open, showing a table with columns for ID, Material, State, and Fraction. The table contains three rows: ID 000, Material CH<sub>4</sub>, State G, Fraction 0.56; ID 001, Material H<sub>2</sub>, State G, Fraction 0.15; ID 002, Material CO, State G, Fraction 0.23; ID 003, Material CO<sub>2</sub>, State G, Fraction 0.06. The 'Fractions sum to:' is 1.0. The 'Fraction type' is set to 'Mass fraction'. A red circle highlights the table content.

The screenshot shows the 'Volatile Editor' dialog box for a species named 'water'. The properties are: Name: water, Specific heat (Cp): 1000 J/kg K, Heat of devolatilization at 298.15K: 0 J/kg, Release gases: H<sub>2</sub>O. The 'Values' section shows: Rate of release:  $\frac{dm}{dt} = -k m$  [kg/s], Rate coefficient:  $k = c_0 T^{c1} p^{c2} p_i^{c3} e^{-E/T+E0}$  [1/s], c<sub>0</sub> = 2.2e+18, c<sub>1</sub> = 0, c<sub>2</sub> = 0, c<sub>3</sub> = 0, E = 30000, E<sub>0</sub> = 0. A red arrow points from the text 'Add a second volatile species and name it "water"' to the 'Name' field.

# Particle Species

- Add the **Particle Species** for the coal feed, the recycle ash, and the initial ash particles in the system
- Refer to slide # 4, if needed, for the mass fractions composition in each
- Set the density of the **Coal Feed** to "1050" kg/m<sup>3</sup>

The screenshot displays the Barracuda Virtual Reactor interface with the following components:

- Particle Species Manager:**

Species-ID	Comment	Materials	Min radius	Max radius	Sphericity	Emissivity	Drag model	Agglomeration
001	Coal Feed	C, Ash, light volatiles, water	psd_fcc.sff		1	1	Wen-Yu	Off
002	Recycle Ash	Ash, C	psd_fcc.sff		1	1	Wen-Yu	Off
003	Ash Initially in System	Ash, C	psd_fcc.sff		1	1	Wen-Yu	Off
- Applied Materials Manager (Top):**

ID	Name	State	Mass Frac	Density (kg/m <sup>3</sup> )	Age Factor
000	C	S	0.4014	2150	1
001	Ash	S	0.0461	2850	1
002	light volatiles	Volatile	0.3298	Unspecified	N/A
003	water	Volatile	0.2227	Unspecified	N/A

Overall particle density:  Manually entered: 1050 kg/m<sup>3</sup>
- Applied Materials Manager (Bottom Left):**

ID	Name	State	Mass Frac	Density (kg/m <sup>3</sup> )	Age Factor
000	Ash	S	0.99	2850	1
001	C	S	0.01	2150	1

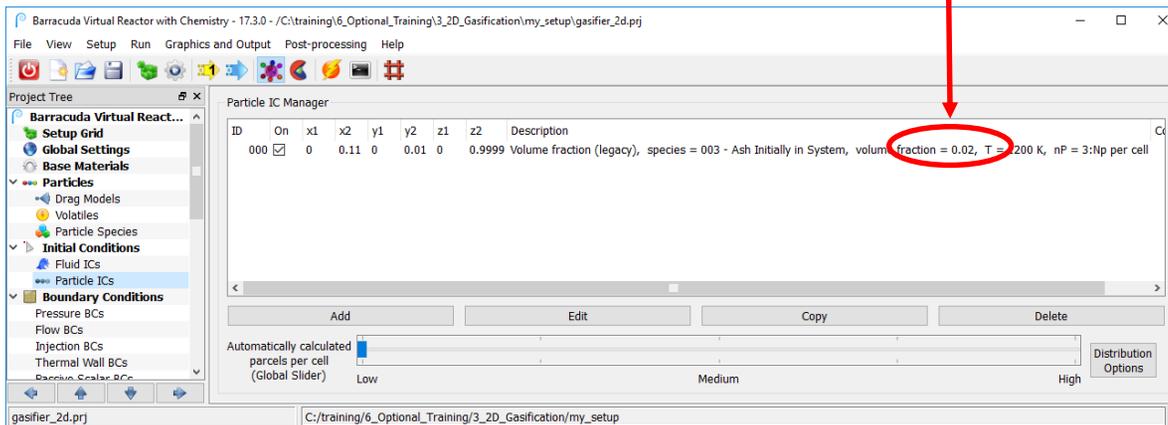
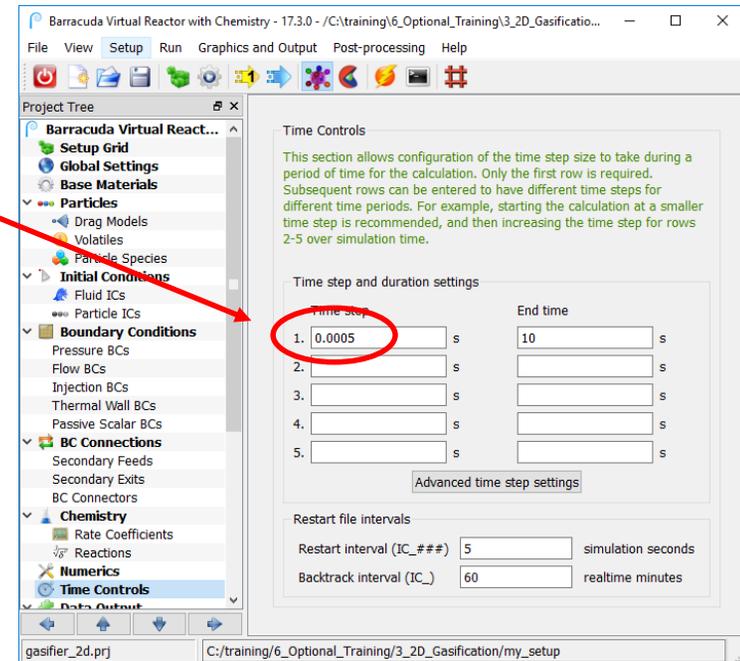
Overall particle density:  Automatically calculated: 2840.75 kg/m<sup>3</sup>
- Applied Materials Manager (Bottom Right):**

ID	Name	State	Mass Frac	Density (kg/m <sup>3</sup> )	Age Factor
000	Ash	S	0.99	2850	1
001	C	S	0.01	2150	1

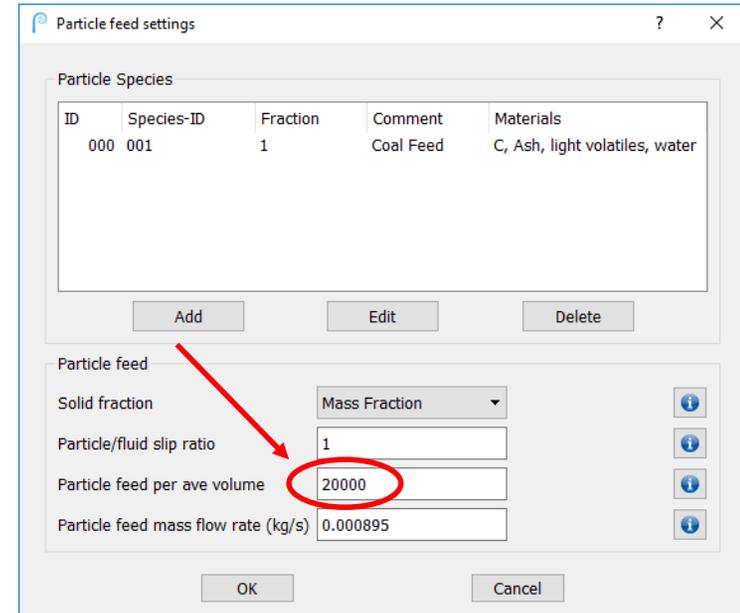
Overall particle density:  Automatically calculated: 2840.75 kg/m<sup>3</sup>

# Some Finer Points in this Project

- The solution of the chemistry ODEs is what limits the time-step in this simulation. While the simulation is running, notice that the CFL is near unity. However, if you increase the time-step too much, the ODE solver will fail and the simulation will stop
- Since the initial particle volume fraction is low (0.02), a low nP can be used for the particle initialization



- Because the mass flow rate of particles at the coal feed flow BC is fairly low, it is necessary to use a high nP (number of particles per cell) to ensure that enough computational particles are introduced. The same applies to the recycle ash stream. Discuss this with your instructor.



# Define Rate Coefficients

- Define the reaction rate coefficients  $k_0$ -  $k_8$
- Refer to slide #5 for reaction rate equations
- Remember to define the solids dependence of the reaction rate. It should only depend on carbon

Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/6\_Optional\_Training/3\_2D\_Gasification/my\_setup/gasifier\_2d.prj

File View Setup Run Graphics and Output Post-processing Help

Project Tree

- Barracuda Virtual React...
- 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

Chemistry Rate Coefficients Manager

ID	Name	Reaction Type	Coefficient Type	Expression	Comment
00	k0	Volume-Average	Arrhenius Chem Rate	$1.272 T^1 e^{(-22645 / T)} m_C^1$	
01	k1	Volume-Average	Arrhenius Chem Rate	$0.00010436 T^2 e^{(-6319 / T + -17.29)} m_C^1$	
02	k2	Volume-Average	Arrhenius Chem Rate	$1.272 T^1 e^{(-22645 / T)} m_C^1$	
03	k3	Volume-Average	Arrhenius Chem Rate	$0.00010436 T^2 e^{(-2363 / T + -20.92)} m_C^1$	
04	k4	Volume-Average	Arrhenius Chem Rate	$0.001368 T^1 e^{(-8078 / T + -7.087)} m_C^1$	
05	k5	Volume-Average	Arrhenius Chem Rate	$0.151 T^{0.5} e^{(-13578 / T + -0.372)} m_C^1$	
06	k6	Volume-Average	Arrhenius Chem Rate	$1.47e+08 T^1 e^{(-13590 / T)} vf_C^1$	
07	k7	Volume-Average	Arrhenius Chem Rate	$7.68e+10 e^{(-36640 / T)}$	
08	k8	Volume-Average	Arrhenius Chem Rate	$6.4e+09 e^{(-39260 / T)}$	

Add Edit Copy Delete

gasifier\_2d.prj C:/training/6\_Optional\_Training/3\_2D\_Gasification/my\_setup

# Define Chemical Reactions

- Define the chemical reactions and their rates. Refer to slide # 6 for reaction rate equations
- In the **Chemistry** tab, make sure that **Stoichiometric** reaction mode is selected
- Also make sure that **Gas species units** are set to mol/m<sup>3</sup>

The screenshot shows the Barracuda Virtual Reactor software interface. The main window is titled "Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/6\_Optional\_Training/3\_2D\_Gasification/my\_setup/gasifier\_2d.prj". The interface includes a menu bar (File, View, Setup, Run, Graphics and Output, Post-processing, Help) and a toolbar. The Project Tree on the left shows the following structure:

- Barracuda Virtual React...
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  - Drag Models
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  - Transient Data

The Chemistry Reactions Manager window is open, displaying a table of reactions:

ID	Reaction Type	Rate	Equation	Comment
00	VA: Stoichiometric	Equation: $C(S) + H_2O \Rightarrow CO + H_2$ R00 = $(k0[H_2O])$		
01	VA: Stoichiometric	Equation: $CO + H_2 \Rightarrow C(S) + H_2O$ R01 = $(k1[H_2][CO])$		
02	VA: Stoichiometric	Equation: $C(S) + CO_2 \Rightarrow 2 CO$ R02 = $(k2[CO_2])$		
03	VA: Stoichiometric	Equation: $2 CO \Rightarrow C(S) + CO_2$ R03 = $(k3[CO]^2)$		
04	VA: Stoichiometric	Equation: $0.5 C(S) + H_2 \Rightarrow 0.5 CH_4$ R04 = $(k4[H_2])$		
05	VA: Stoichiometric	Equation: $0.5 CH_4 \Rightarrow 0.5 C(S) + H_2$ R05 = $(k5[CH_4]^{0.5})$		
06	VA: Stoichiometric	Equation: $2 C(S) + O_2 \Rightarrow 2 CO$ R06 = $(k6[O_2])$		
07	VA: Stoichiometric	Equation: $CO + H_2O \Rightarrow CO_2 + H_2$ R07 = $(k7[CO]^{0.5}[H_2O])$		
08	VA: Stoichiometric	Equation: $CO_2 + H_2 \Rightarrow CO + H_2O$ R08 = $(k8[H_2]^{0.5}[CO_2])$		

The interface also includes buttons for Add, Edit, Copy, and Delete, and a status bar at the bottom showing the file name "gasifier\_2d.prj" and the path "C:/training/6\_Optional\_Training/3\_2D\_Gasification/my\_setup".

# Select GMV Output Options

Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/6\_Optional\_Training/3\_2D\_Gasification/my\_setup/gasifier\_2d.prj

File View Setup Run Graphics and Output Post-processing Help

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General Mesh View Data Output Options

Please select Eulerian and Lagrangian data for export to the General Mesh Viewer (GMV). Only data selected here can be viewed during post-processing. Values inside parenthesis are the **field names** of the variables within GMV.

Output file interval

Plot interval: 0.02 s Number of files produced using current end time of 10s: 502

Eulerian (Cell) Output Data

<input checked="" type="checkbox"/> Particle volume fraction (p-volFra)	<input type="checkbox"/> Particle bulk density (p-dens)	<input type="checkbox"/> dp/dx (dp/dx)
<input checked="" type="checkbox"/> Fluid velocity (U, V, W)	<input type="checkbox"/> Turbulent viscosity (ViscTurb)	<input type="checkbox"/> dp/dy (dp/dy)
<input type="checkbox"/> Particle velocity (P_[xyz]Vel)	<input type="checkbox"/> CFL (CFL)	<input checked="" type="checkbox"/> dp/dz (dp/dz)
<input checked="" type="checkbox"/> Pressure (Pressure)	<input type="checkbox"/> Particle species (Species)	<input checked="" type="checkbox"/> Particle mass flux (P_
<input type="checkbox"/> Dynamic pressure (DynPres)	<input checked="" type="checkbox"/> Fluid temperature (f-Temp)	<input checked="" type="checkbox"/> Fluid mass flux (F_[xyz]Mass)
<input checked="" type="checkbox"/> Fluid density (f-dens)	<input checked="" type="checkbox"/> Particle temperature (p-Temp)	<input type="checkbox"/> Wall heat transfer (wallHeat)
<input type="checkbox"/> Cell indices (i, j, k)	<input type="checkbox"/> Cell volume (cellVol)	

Lagrangian (Particle) Output Data

<input checked="" type="checkbox"/> Particle volume fraction (VolFrac)	<input checked="" type="checkbox"/> Particle material (Material)	<input checked="" type="checkbox"/> Velocity (vel[xyz])
<input checked="" type="checkbox"/> Particle speed (Speed)	<input type="checkbox"/> Particle density (Density)	<input type="checkbox"/> Residence time (ResTime)
<input checked="" type="checkbox"/> Particle radius in microns (rad)	<input checked="" type="checkbox"/> Particle species (Species)	<input checked="" type="checkbox"/> Residence time by species (ResTime##)
<input type="checkbox"/> Constant color (Particle)	<input type="checkbox"/> Unique particle ID (pid)	<input checked="" type="checkbox"/> Temperature (Temperat)
<input type="checkbox"/> Drag (drag)	<input type="checkbox"/> Liquid fraction total (liqFrac)	<input type="checkbox"/> Liquid mass total (liqMass)
<input type="checkbox"/> Cloud mass (cldMass)	<input type="checkbox"/> Particles per cloud (npCloud)	<input type="checkbox"/> Particle mass (mass)

Gas Species

<input type="radio"/> Mass fraction (<species>.mf)	<input type="radio"/> Mole fraction (<species>.nf)
<input checked="" type="radio"/> Mass concentration (<species>.mc)	<input type="radio"/> Mole concentration (<species>.nc)

Options

- Compress graphics output (not common)
- Generate predefined GMV attribute files

Map particle temperature to the grid

# Select Transient Data Points

- Select the desired transient data
- Suggested transient data type includes:
  - p Vol Frac
  - Fluid temp
  - Gas mole conc
  - Stoich eq rate
- Suggested transient data points include:
  - $x = 0.095$
  - $y = 0.0$
  - $z = 0.325$  to  $z = 0.92$  at reasonable intervals

The screenshot shows the 'Transient Data Output' window in the Barracuda Virtual Reactor software. The window title is 'Barracuda Virtual Reactor with Chemistry - 17.3.0 - /C:/training/6\_Optional\_Training/3\_2D\_Gasification/my\_setup/gasifier\_2d.prj'. The 'Project Tree' on the left shows the following structure:

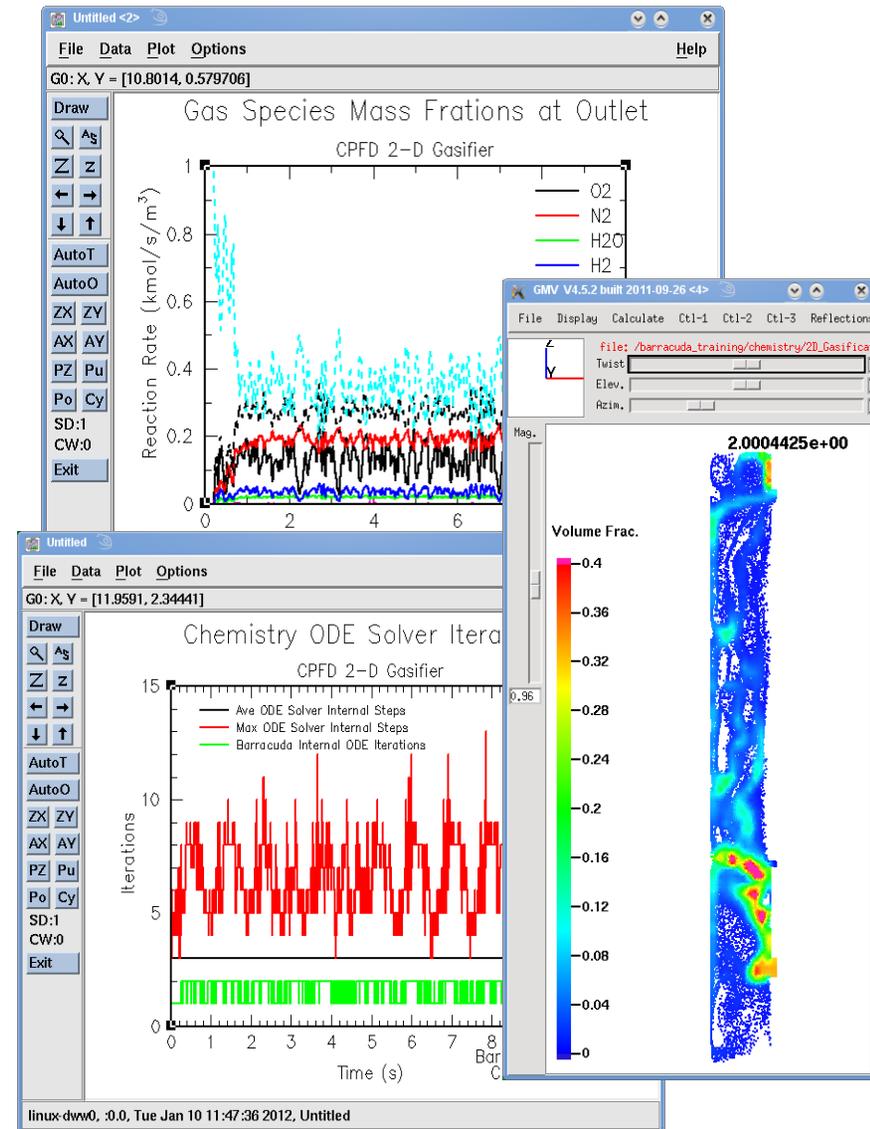
- Barracuda Virtual R...
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  - Flux Planes
  - GMV Output Options
  - Average Data
  - 2D Plot Data
  - Transient Data
  - Wall Erosion
  - Particle Attrition
  - Raw Data
  - Population Data
  - Solver Output Units
- Run
- Post-Run
- Plot Manager

The 'Transient Data Output' window shows the following table:

Type		x (m) / i	y (m) / j	z (m) / k	Comment
p Vol Frac	xyz	0.095	0	0.325	
Fluid temp	xyz	0.095	0	0.325	
Gas mole conc	xyz	0.095	0	0.325	
Stoich eq rate	xyz	0.095	0	0.325	
p Vol Frac	xyz	0.095	0	0.1	
Fluid temp	xyz	0.095	0	0.1	
Gas mole conc	xyz	0.095	0	0.1	
Stoich eq rate	xyz	0.095	0	0.1	
p Vol Frac	xyz	0.095	0	0.15	
Fluid temp	xyz	0.095	0	0.15	
Gas mole conc	xyz	0.095	0	0.15	
Stoich eq rate	xyz	0.095	0	0.15	
p Vol Frac	xyz	0.095	0	0.2	
Fluid temp	xyz	0.095	0	0.2	
Gas mole conc	xyz	0.095	0	0.2	
Stoich eq rate	xyz	0.095	0	0.2	
p Vol Frac	xyz	0.095	0	0.4	
Fluid temp	xyz	0.095	0	0.4	
Gas mole conc	xyz	0.095	0	0.4	
Stoich eq rate	xyz	0.095	0	0.4	
p Vol Frac	xyz	0.095	0	0.5	
Fluid temp	xyz	0.095	0	0.5	
Gas mole conc	xyz	0.095	0	0.5	
Stoich eq rate	xyz	0.095	0	0.5	
p Vol Frac	xyz	0.095	0	0.6	
Fluid temp	xyz	0.095	0	0.6	
Gas mole conc	xyz	0.095	0	0.6	
Stoich eq rate	xyz	0.095	0	0.6	

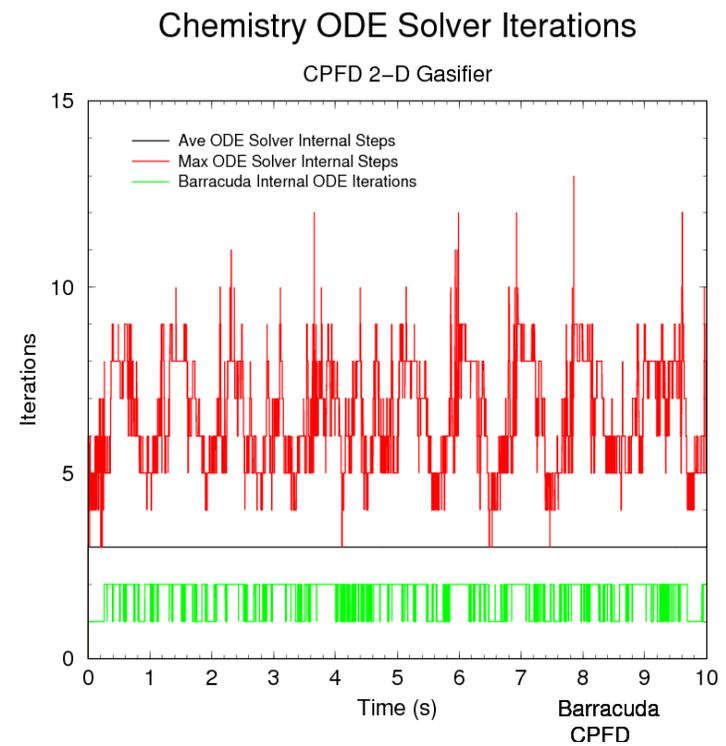
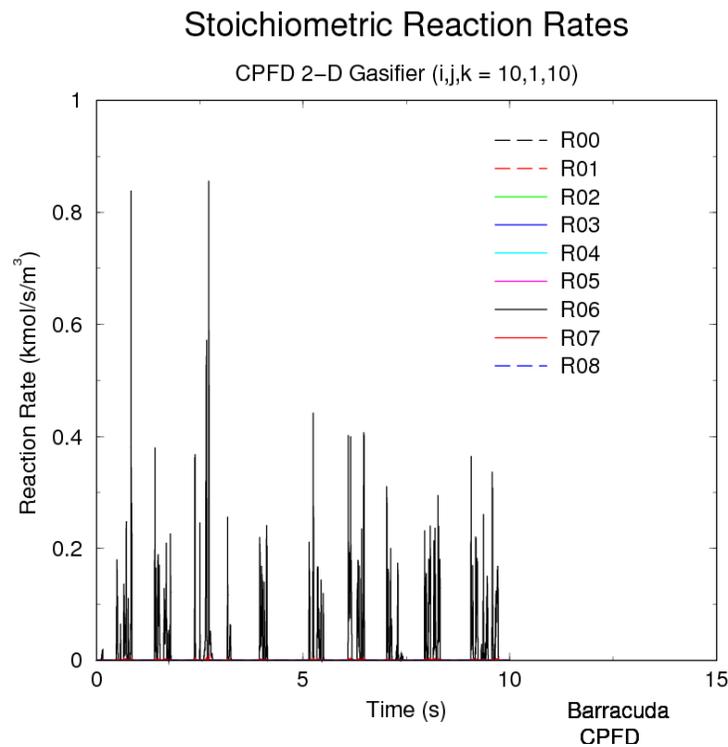
# Start and Monitor the Simulation

- Save your project file and start the Barracuda simulation
- How do you know if the simulation is running correctly, i.e. that flow BCs were defined as you intended, that chemistry is occurring, etc.?
- Barracuda outputs several useful text files with data about the simulation
  - For mass flow rates at flow BCs, use the flux plane files to confirm correct setup
  - For chemistry, use transient data points to monitor reaction rates. Use the last three columns in the history.log file to verify that the ODE solver is running acceptably
- Also, you can visually inspect the simulation using Gmv post-processing techniques
  - Explore some of the early Gmv.00\* output files with Gmv to make sure that things look as expected. Make sure that all necessary variables are being output to the Gmv files



# Chemistry Data and ODE Solver Info

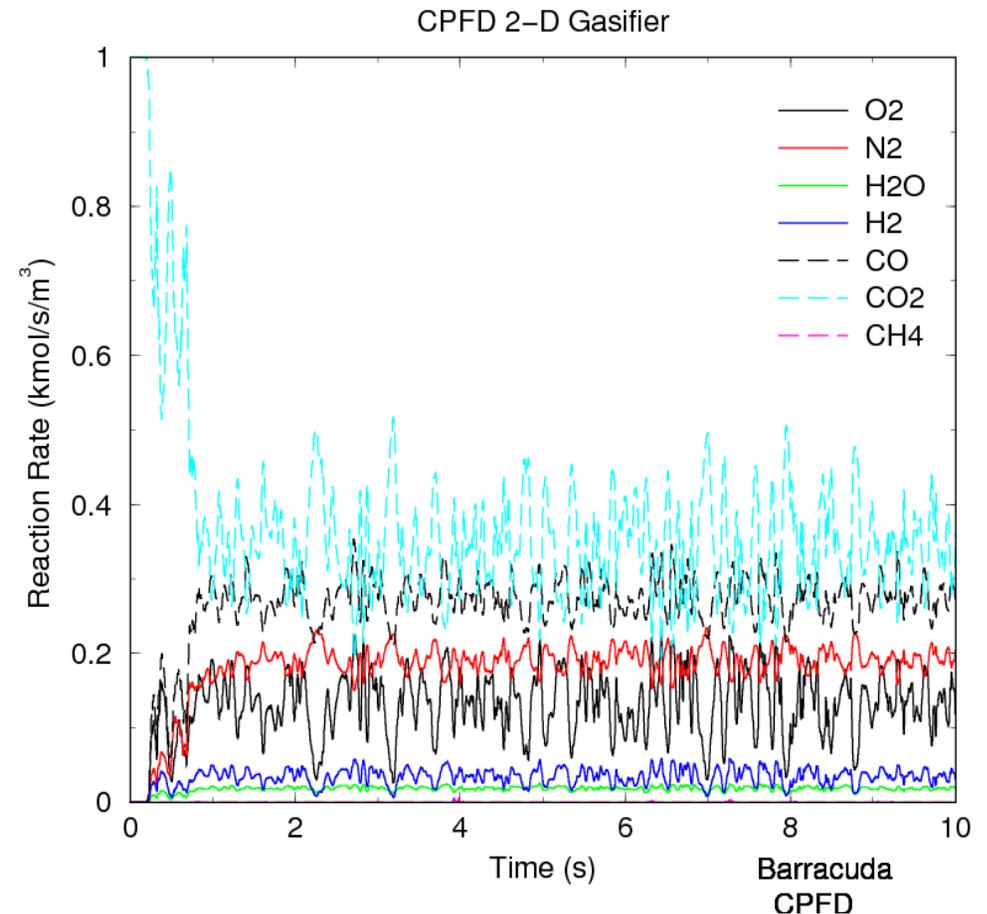
- The plots below show information about the performance of chemical reactions
  - On the left, the stoichiometric reaction rates are shown for the 9 reactions. This data is contained in trans.data files. R06 and R07 seem to dominate the system
  - On the right, information from history.log is plotted to show how the ODE solver performed over the course of the simulation



# Gas Species Mass Fractions at Outlet

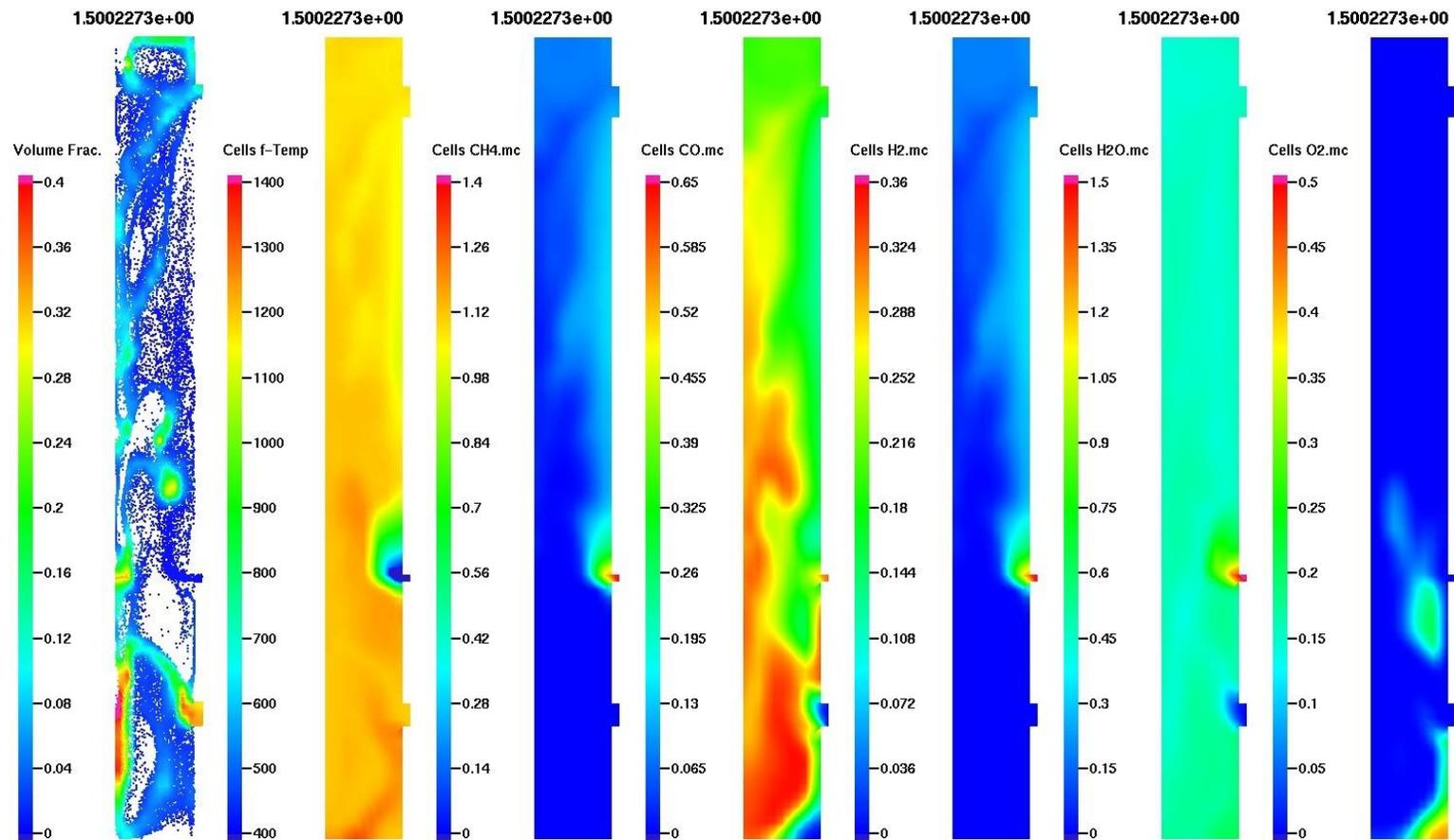
- The plot shows gas mass fraction data for the pressure outlet at the top of the vessel
- In an experimental unit, this would likely be the location with instrumentation to measure the outlet composition of the various gas species
- This data is collected in a FLUXBC\_ file for the pressure BC and written for every time step
- The simulation arrives at a fairly “steady state” by about 2 seconds. The gas concentrations do not change significantly after this time

## Gas Species Mass Fractions at Outlet



# Post-Processing the Results

- GMV allows you to visualize what is happening inside the vessel. The particle behavior is complex, the fluid temperature varies, and the chemical reactions cause the gas species to interact in complex ways



# Conclusions for 2D Gasifier Example

- This example shows how the complexity of a simulation can increase significantly when multiple chemical reactions and multi-fluid / solids flow BCs are used, even in a simple geometry
  - Setting up the chemistry in Barracuda is not difficult. It is more challenging to make sure that you have good reaction rate expressions to model the chemistry accurately
  - The diagram provided in this example gave all flow rates in Barracuda SI units, but usually you will have to interpret boundary condition information from less consistent sources. Defining multi-component flow BCs requires care with conversions and mass fraction calculations, so be sure to verify with flux plane data that you are getting the flow rates you expect for each species.
  - The Barracuda simulation provides a great deal of information about the system
  - Particle and fluid flow behavior, as well as the dynamic nature of gas species concentrations, can be visualized with GMV
  - Quantitative data is available in several forms, including flux plane data, transient data points, and 2-D data files. These files provide valuable information that would be very difficult (and sometimes impossible) to obtain experimentally.

# References

- References:
  - Syamlal, M., and Bisset, L.A., 1992, "METC Gasifier Advanced Simulation (MGAS) Model", DOE/METC--92/4108, DE92 001111
  - Wen, C.Y., Chen, H., and Onozaki, M., 1982, "User's Manual for Computer Simulation and Design of the Moving Bed Coal Gasifier", DOE/MC/16474-1390, NTIS/DE83009533
  - Yoon, H., Wei, J., and Denn, M., 1978, "A Model for Moving-Bed Coal Gasification Reactors", AIChE Journal, Vol. 24, No. 5
  - Bustamante, et al., "Uncatalyzed and Wall-Catalyzed Forward Water-Gas Shift Reaction Kinetics", presented in AIChE Journal, March 2005
  - Bustamante, et al., "Kinetics of the Homogeneous Reverse Water-Gas Shift Reaction at High Temperature", presented in AIChE Journal, April 2004
- The computational particle fluid dynamic (CPFD) numerical method was developed by D. Snider at CPFD Software, LLC