Chemistry Training: 2D Coal Gasifier

February 2018

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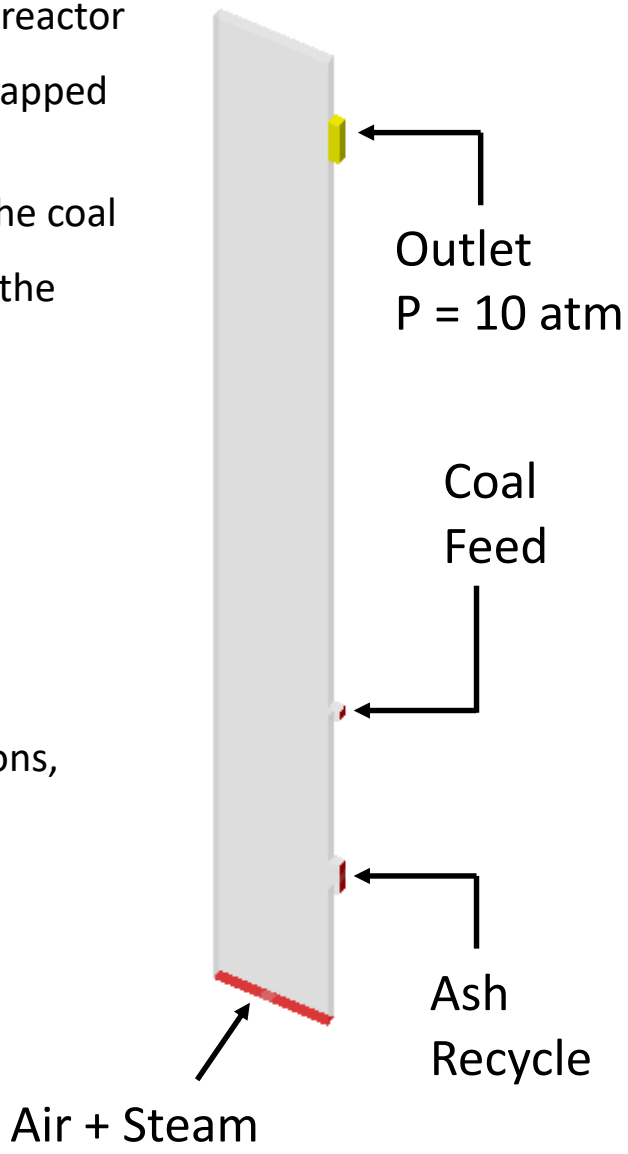
Coal Gasifier 2D Reactor

- 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: $C + H_2O \leftrightarrow CO + H_2$
  - CO2 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

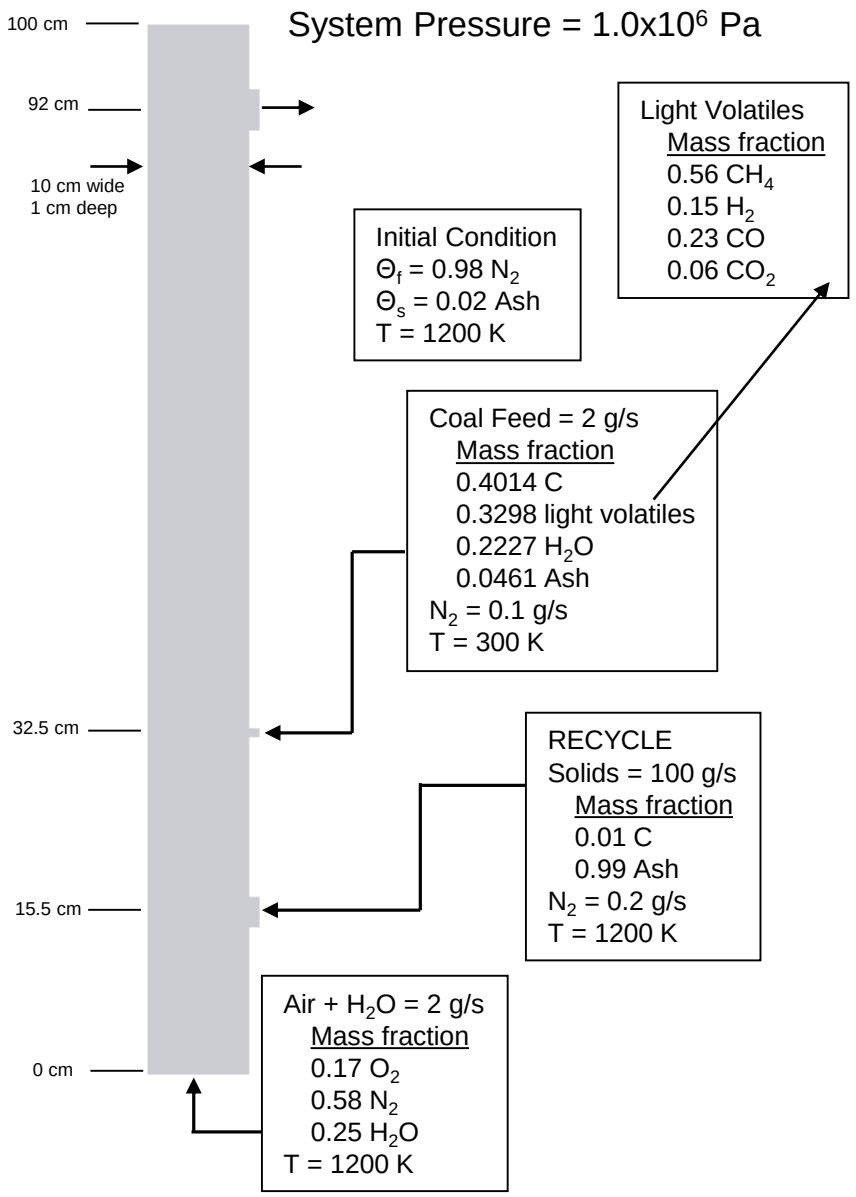


Outline for Simulation Setup

- 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

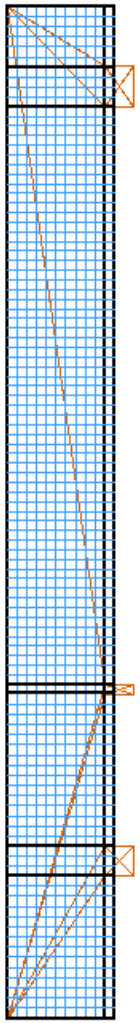
Reaction	Stoichiometric Equation	Reaction Rate Expression (mol m^{-3} s^{-1})	Source
Steam gasification	$C(s)+H_2O \rightarrow CO+H_2$	$r_{1,f} = 6.36 m_C T \exp\left(\frac{-22{,}645}{T}\right)[H_2O]$	Syamlal, 1992
	$CO+H_2 \rightarrow C(s)+H_2O$	$r_{1,r} = 5.218\times10^{-4} m_C T^2 \exp\left(\frac{-6{,}319}{T} - 17.29\right)[H_2][CO]$	
CO_2 gasification	$C(s)+CO_2 \rightarrow 2CO$	$r_{2,f} = 6.36 m_C T \exp\left(\frac{-22{,}645}{T}\right)[CO_2]$	Syamlal, 1992
	$2CO \rightarrow C(s)+CO_2$	$r_{2,r} = 5.218\times10^{-4} m_C T^2 \exp\left(\frac{-2{,}363}{T} - 20.92\right)[CO]^2$	
Methanation	$0.5C(s)+H_2 \rightarrow 0.5CH_4$	$r_{3,f} = 6.838\times10^{-3} m_C T \exp\left(\frac{-8{,}078}{T} - 7.087\right)[H_2]$	Syamlal, 1992
	$0.5CH_4 \rightarrow 0.5C(s)+H_2$	$r_{3,r} = 0.755 m_C T^{0.5} \exp\left(\frac{-13{,}578}{T} - 0.372\right)[CH_4]^{0.5}$	
Combustion	$2C(s)+O_2 \rightarrow 2CO$	$r_4 = 4.34\times10^{7} \theta_C T \exp\left(\frac{-13{,}590}{T}\right)[O_2]$	Yoon, 1978
Water gas- shift	$CO+H_2O \rightarrow CO_2+H_2$	$r_{5,f} = 7.68\times10^{10} \exp\left(\frac{-36{,}640}{T}\right)[CO]^{0.5}[H_2O]$	Bustamante, 2005
	$CO_2+H_2 \rightarrow CO+H_2O$	$r_{5,r} = 6.4\times10^{9} \exp\left(\frac{-39{,}260}{T}\right)[H_2]^{0.5}[CO_2]$	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 CPFD Software, LLC, does not warrant or endorse these chemical kinetics for any purpose.

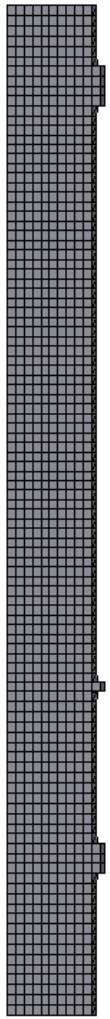
Grid Generation

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

Grid Setup

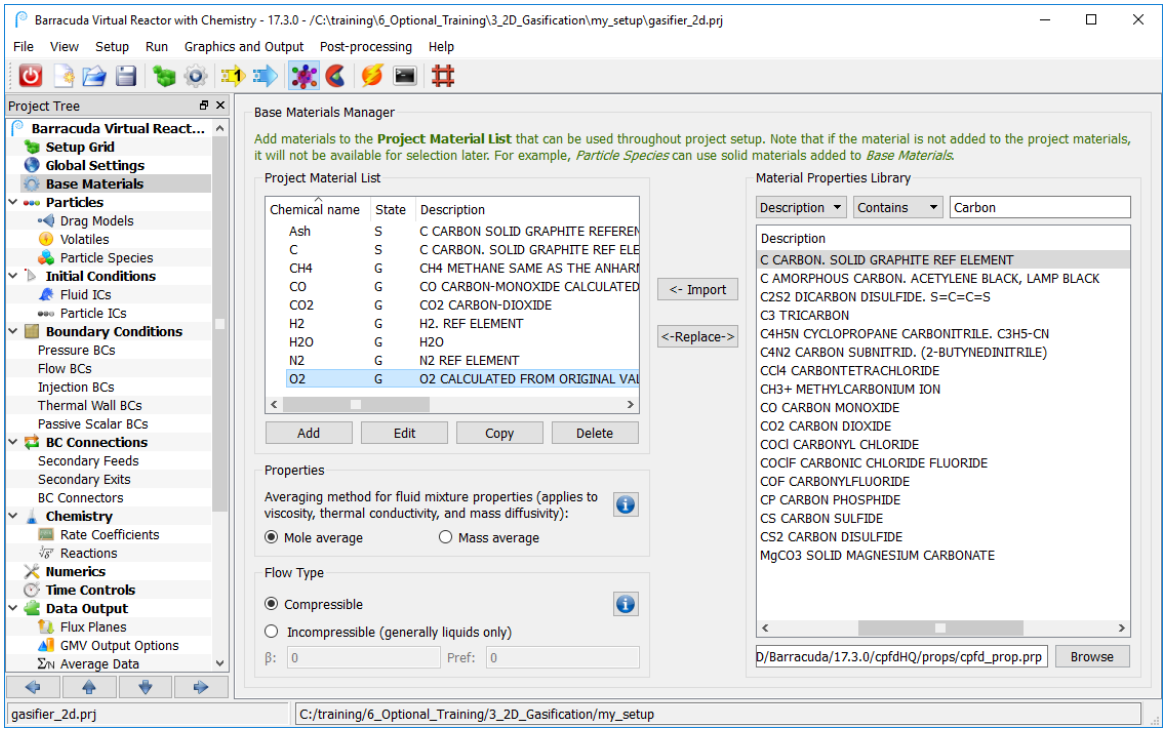


Completed Grid



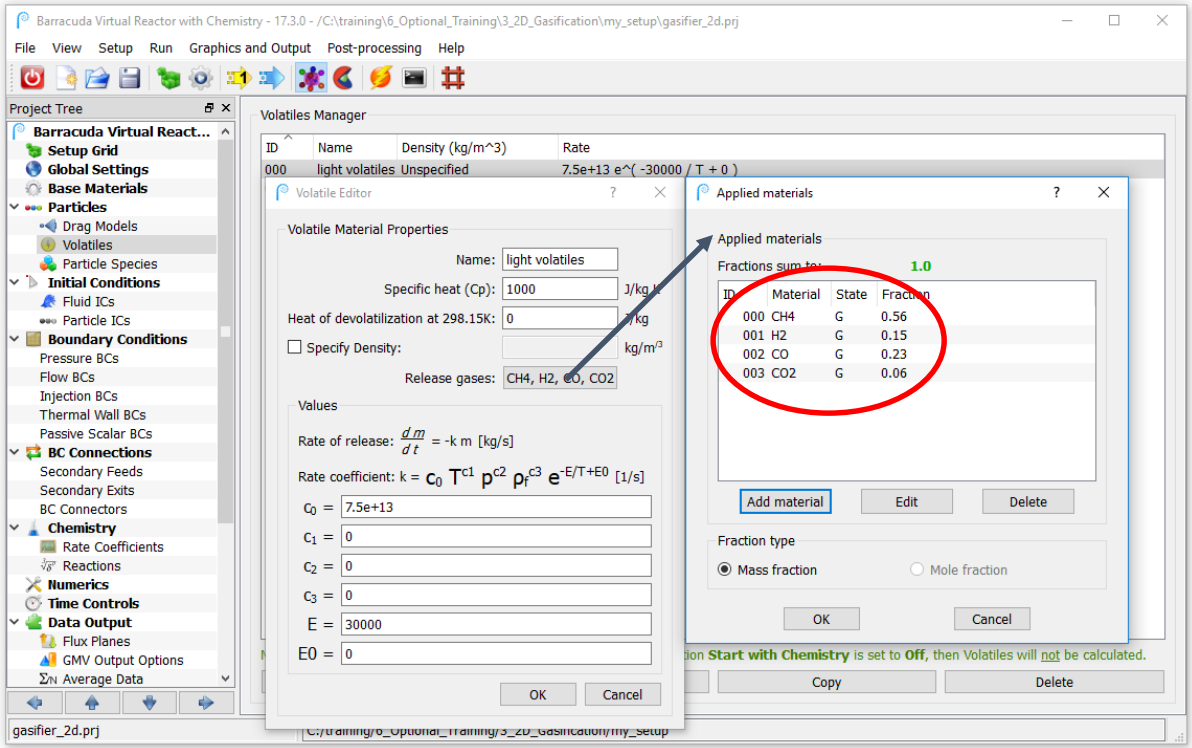
Define Base Materials in Project File

- 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.



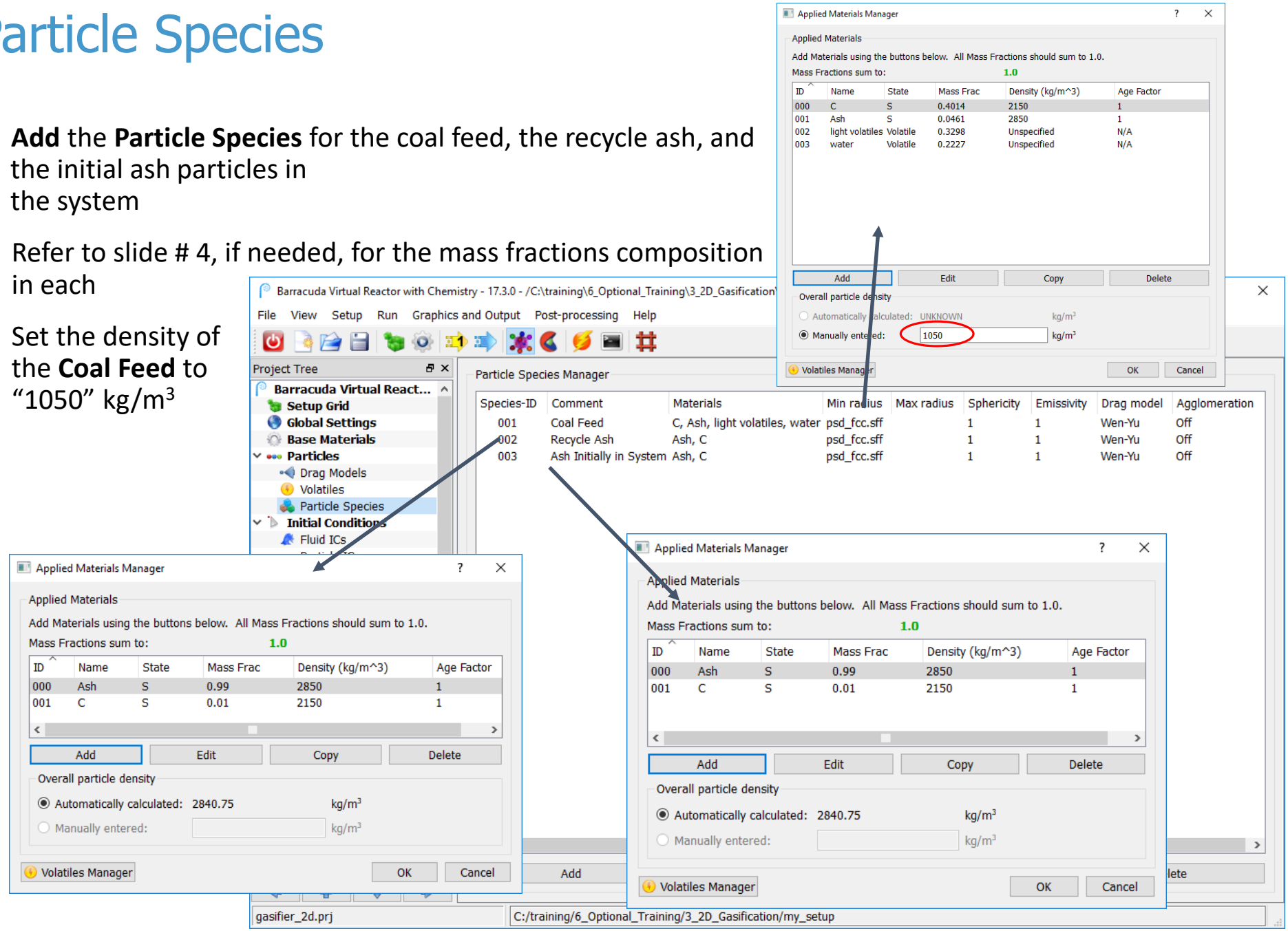
Volatiles

- **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_4, H_2, CO, and CO_2 specifying the mass fraction of each as shown on the right
  - Set $\mathbf{c_o}$ 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_2O with a mass fraction of 1
  - Set $\mathbf{c_o}$ to “2.2e18”
  - Set **E** to “30000”



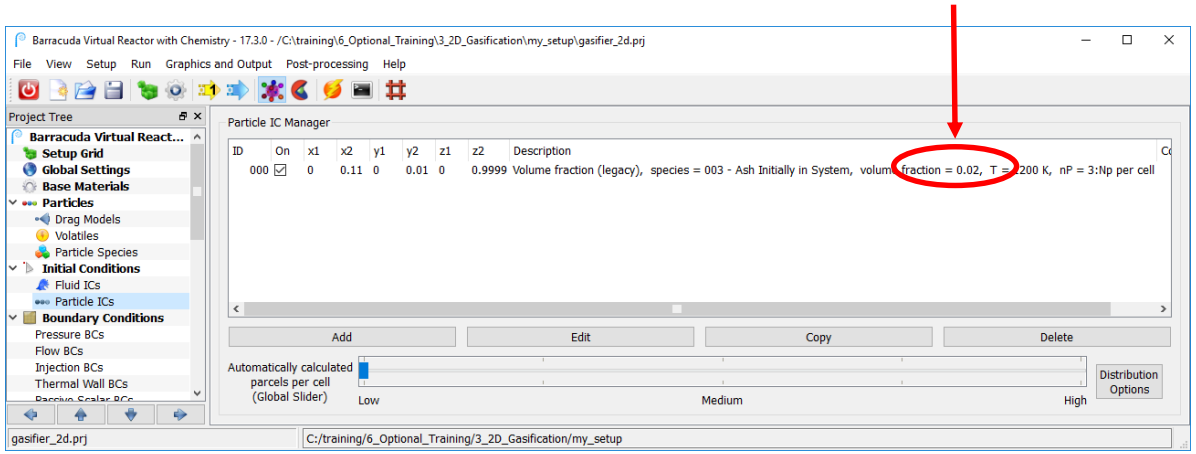
Particle Species

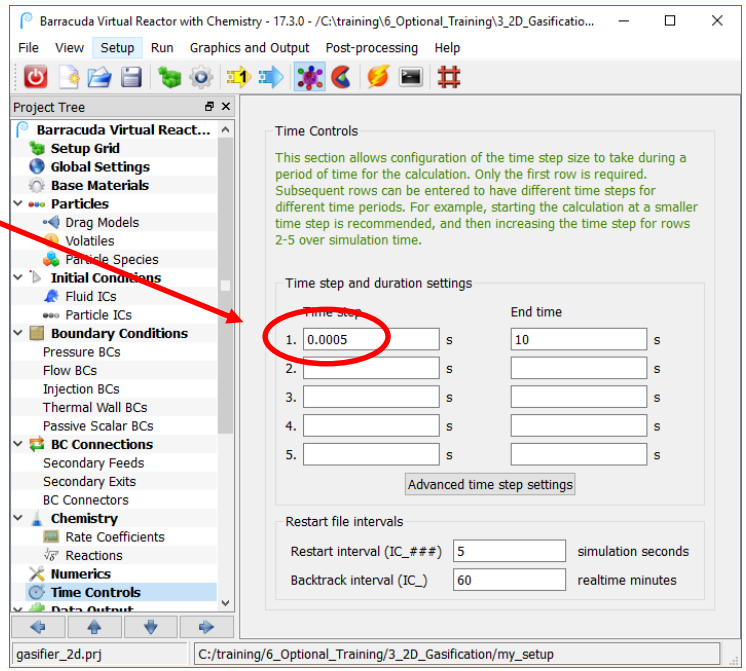
- **Add** the **Particle Species** for the coal feed, the recycle ash, and the initial ash particles in the system
- Refer to slide # 4, if needed, for the mass fractions composition in each
- Set the density of the **Coal Feed** to "1050" kg/m^3

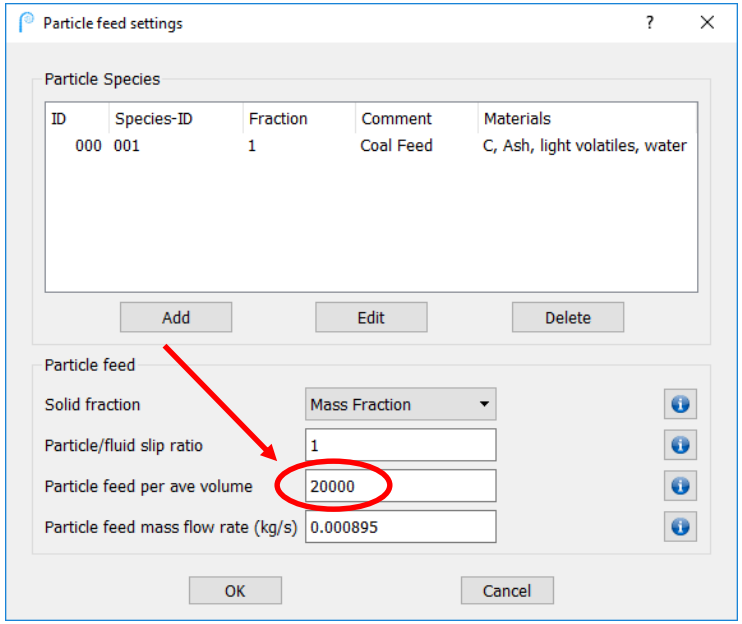


Some Finer Points in this Project

- 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



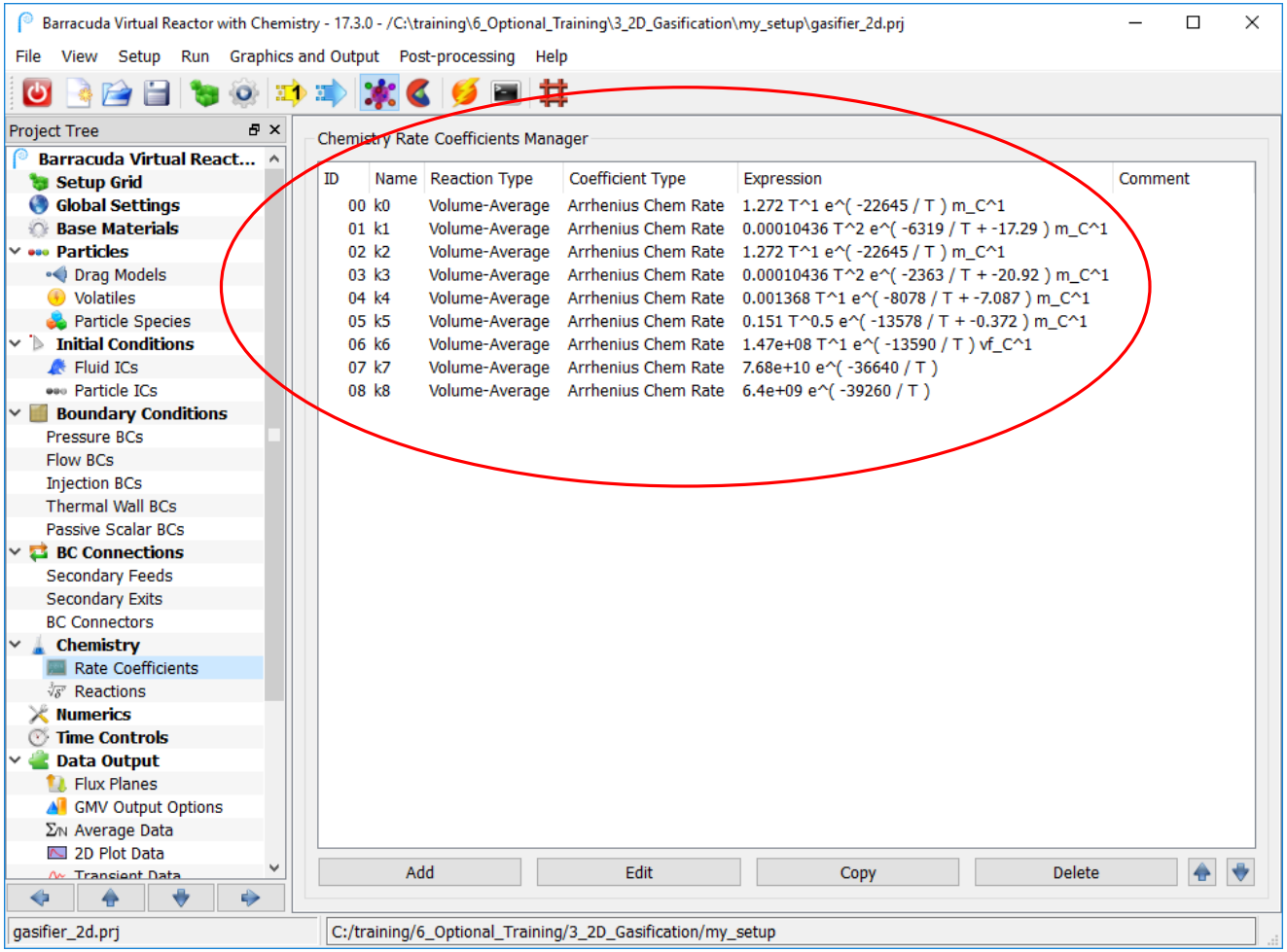




- Because the mass flow rate of particles at the coal feed flow BC is fairly low, it is necessary to use a high nP (number of particles per cell) to ensure that enough computational particles are introduced. The same applies to the recycle ash stream. Discuss this with your instructor.

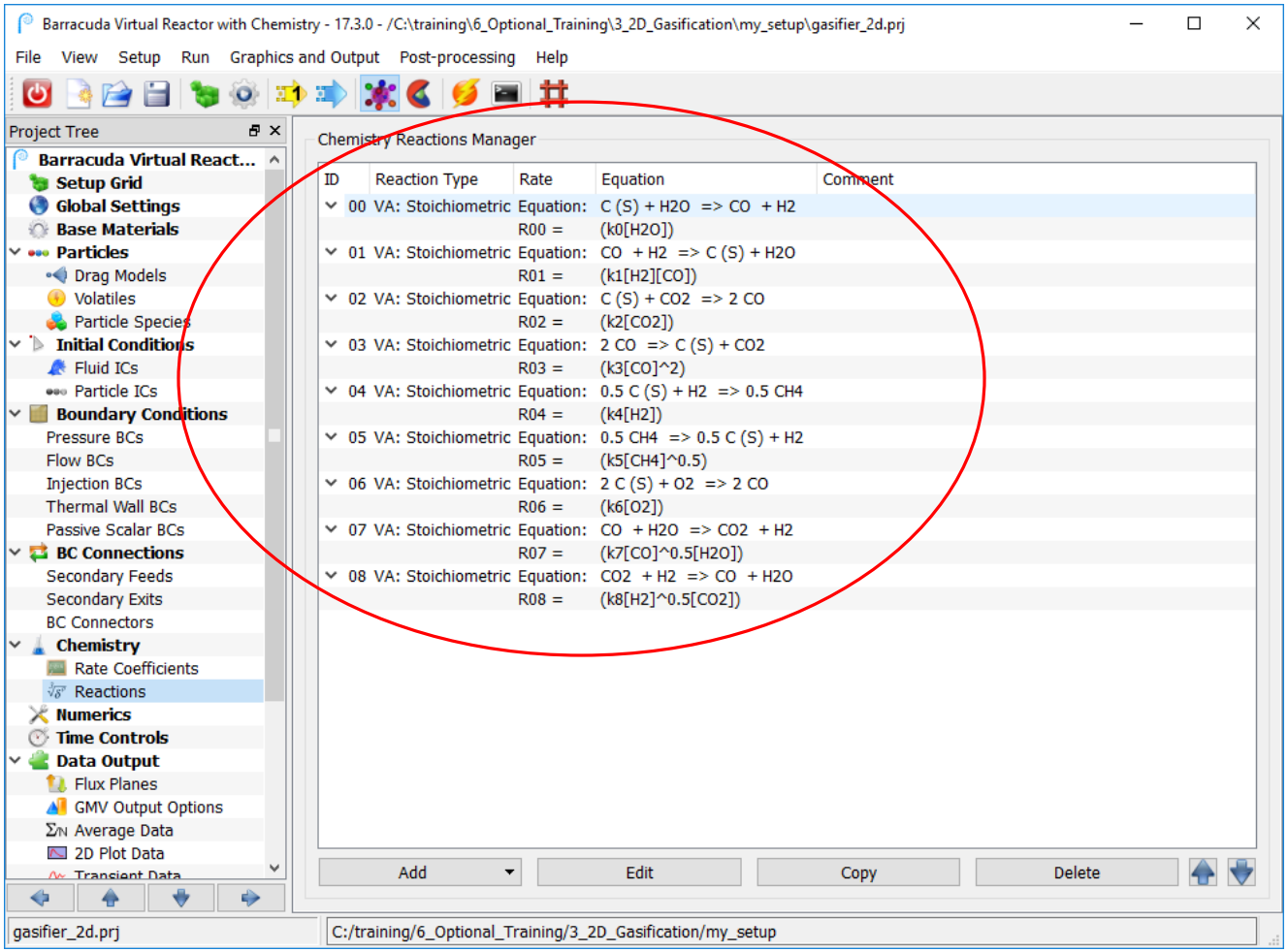
Define Rate Coefficients

- Define the reaction rate coefficients k_o- 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

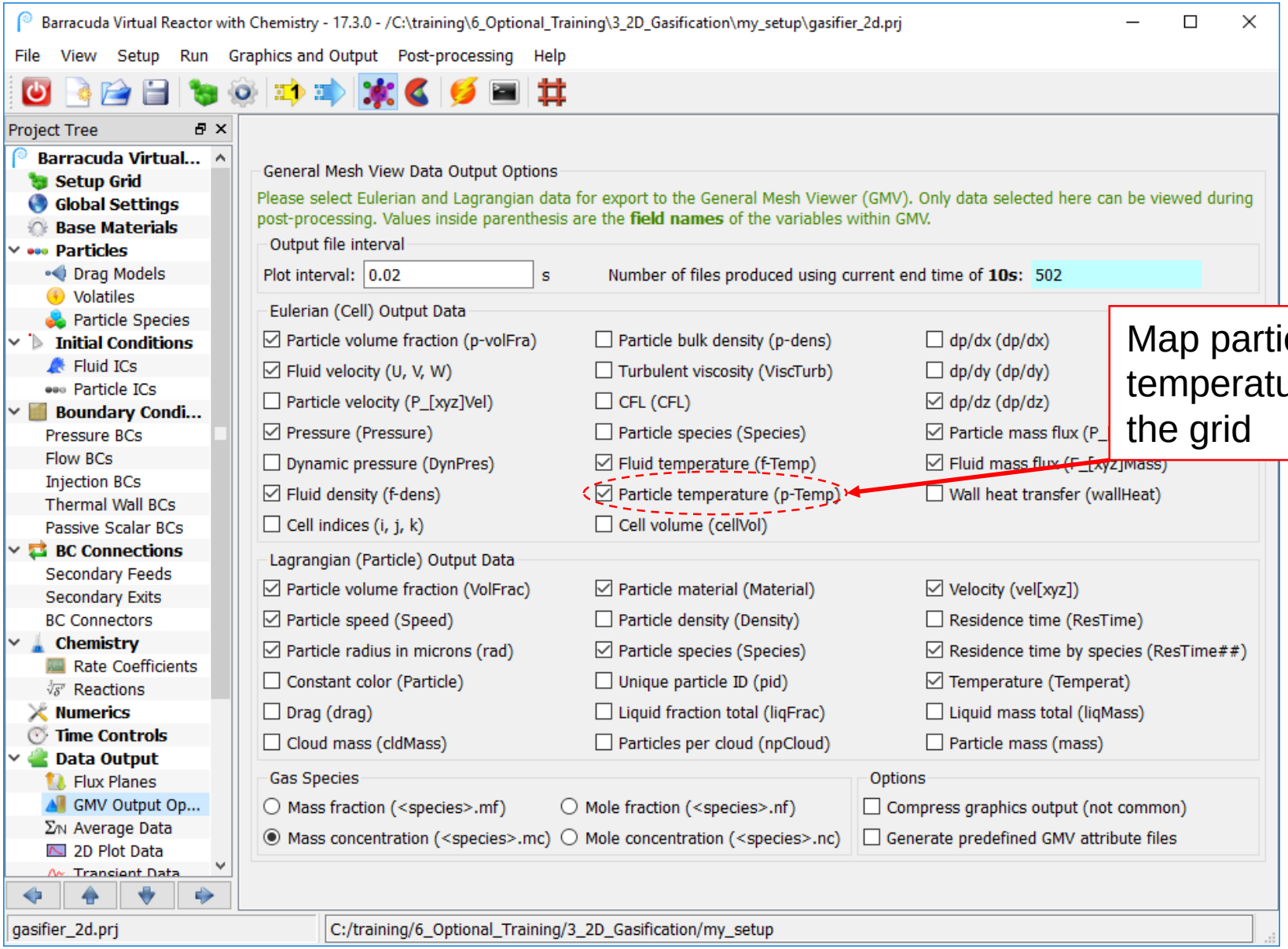


Define Chemical Reactions

- 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^3



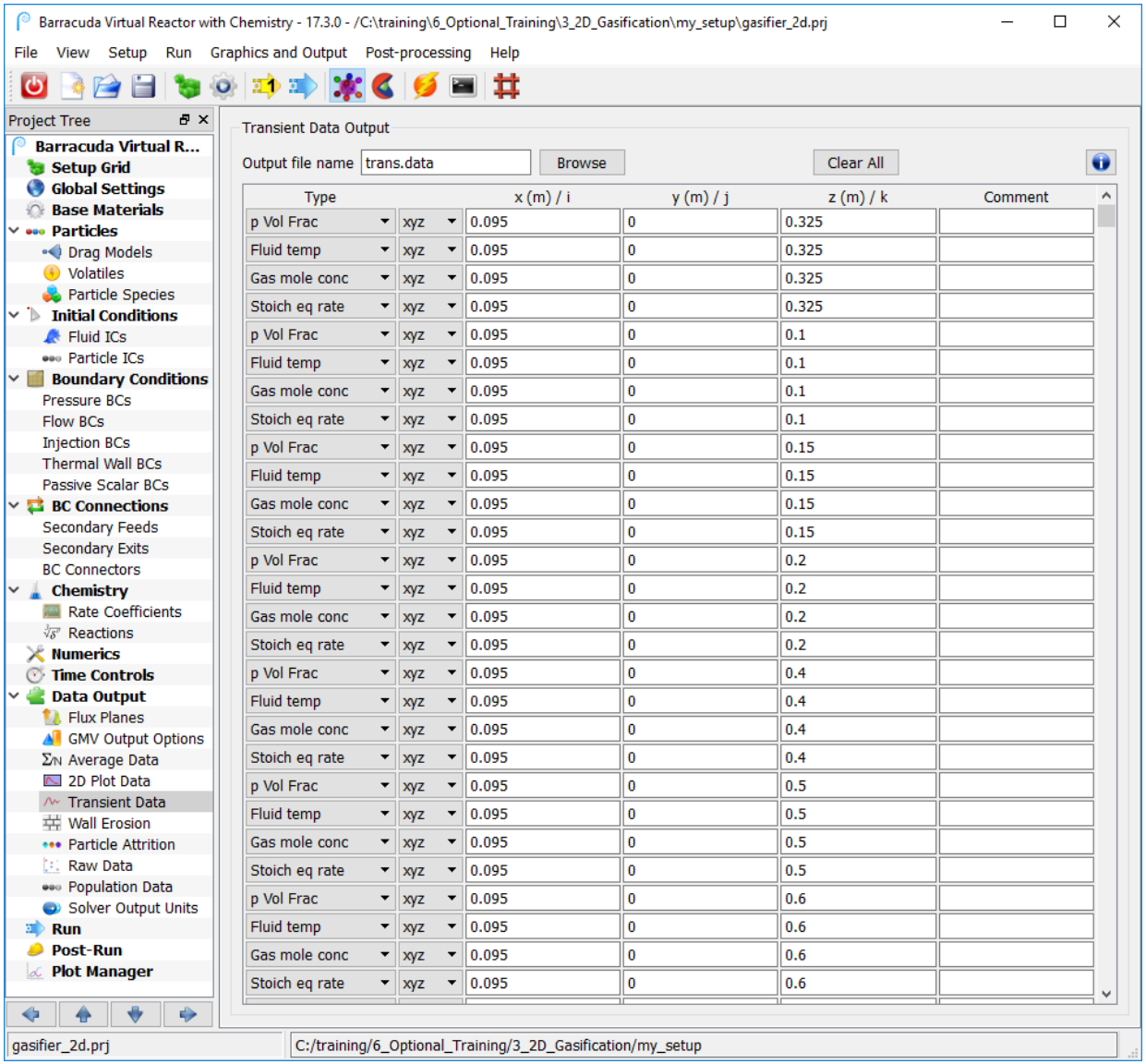
Select GMV Output Options



Map particle temperature to the grid

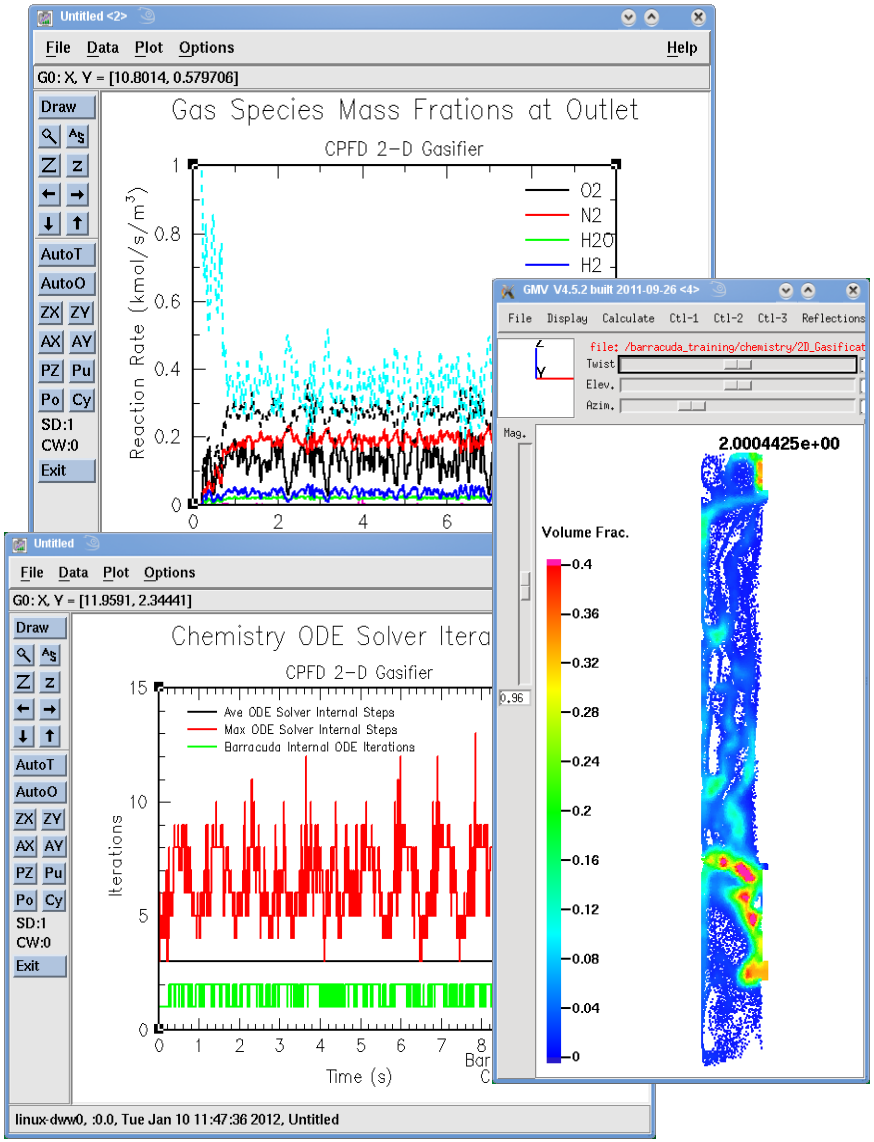
Select Transient Data Points

- 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



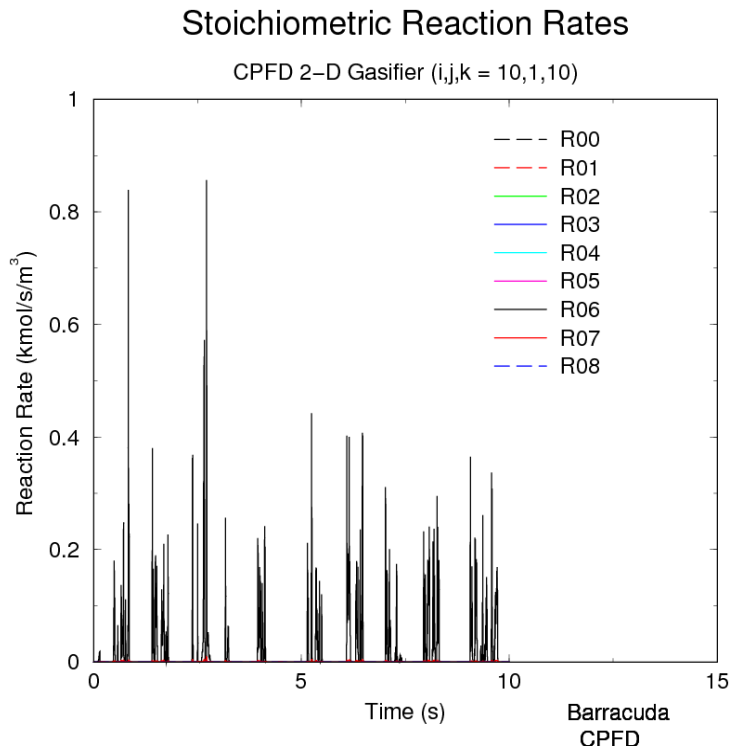
Start and Monitor the Simulation

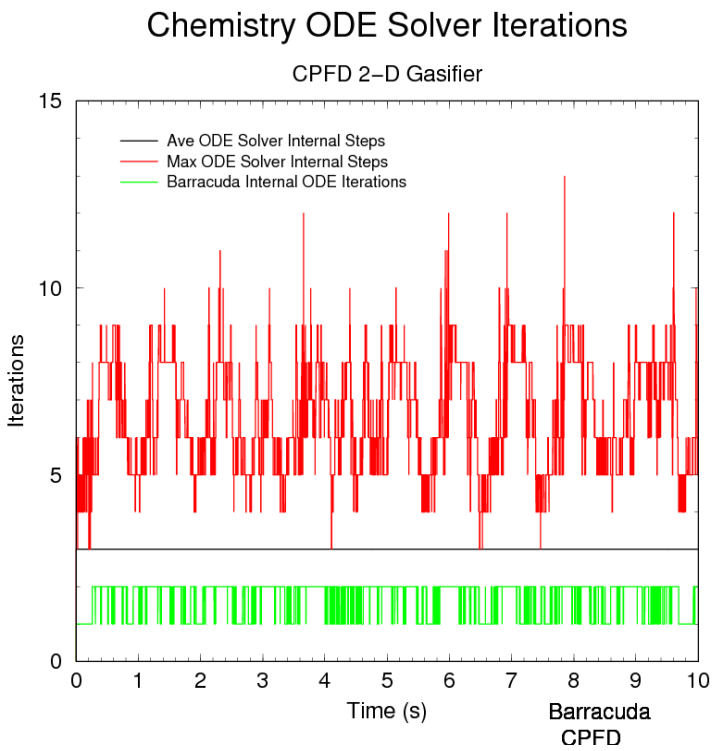
- Save your project file and start the Barracuda simulation
- How do you know if the simulation is running correctly, i.e. that flow BCs were defined as you intended, that chemistry is occurring, etc.?
- Barracuda outputs several useful text files with data about the simulation
    - For mass flow rates 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

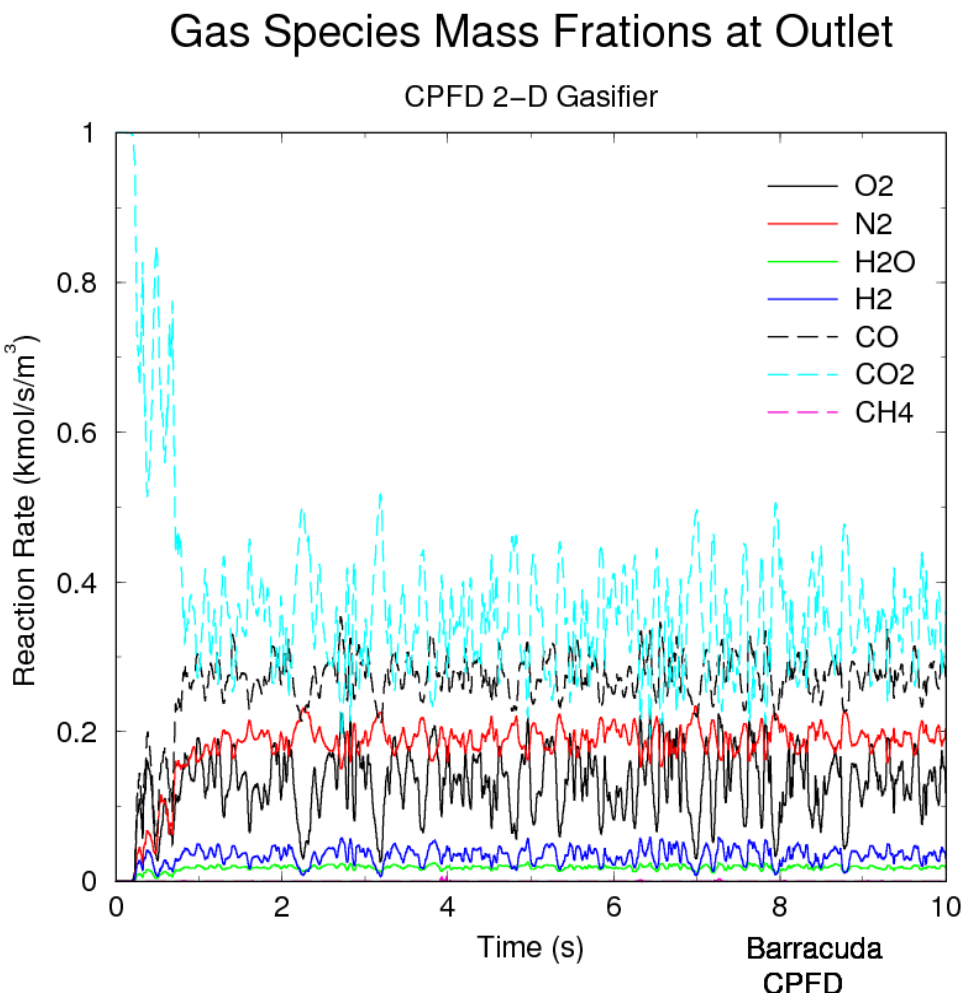
- The plots below show information about the performance of chemical reactions
  - On the left, the stoichiometric reaction rates are shown for the 9 reactions. This data is contained in trans.data files. R06 and R07 seem to dominate the system
  - On the right, information from history.log is plotted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





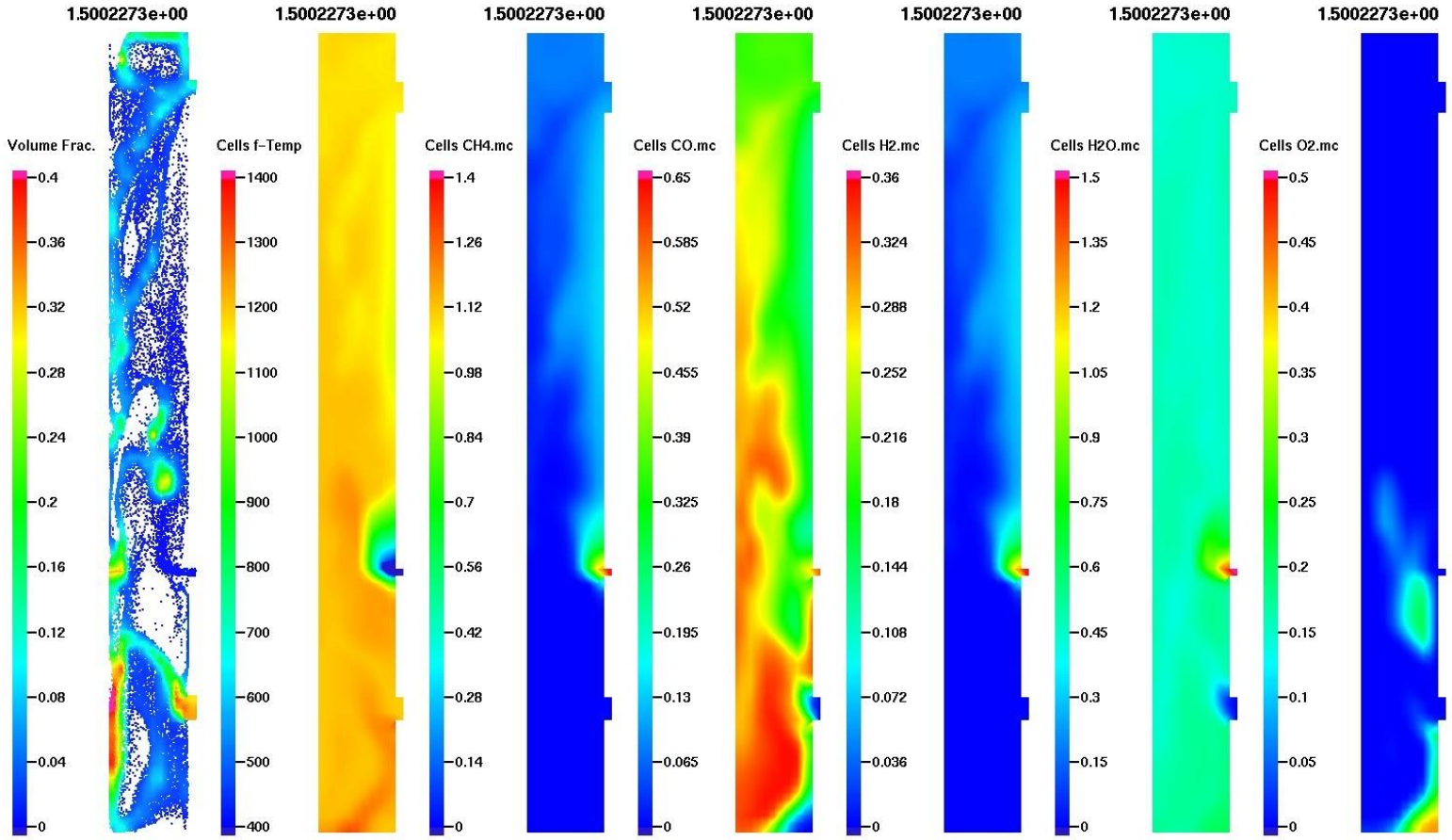
Gas Species Mass Fractions at Outlet

- 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



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