AME 60636
Prof. J. M. Powers
Homework 6
Due: Wednesday, 2 March 2022

1. Consider the reaction mechanism for the combustion of H_2 with O_2 as given by Powers and Paolucci[1] in their Table 1. This is available in the `documents` section of the course web page. Consider combustion in a fixed volume which is a cube whose side is of length 200 mm. The gas has initial mole fractions of $y_{H_2} = 0.2$, $y_{O_2} = 0.1$, $y_{N_2} = 0.7$, and an initial pressure and temperature of 0.1 MPa and 1000 K. Take N_2 to be an inert diluent.

   For adiabatic, isochoric combustion, determine the variation of all species concentrations, temperature, and pressure, as functions of time; give computer-generated plots on logarithmic scales. Plot all species concentrations on a single plot. Plot the relative error in mixture specific internal energy $\frac{e(t)-e(0)}{e(0)}$, and the relative error in moles for each atom versus time.

2. Repeat the previous problem if there is lumped heat transfer from the volume to the surroundings. Take the heat transfer coefficient to be $\mathsf{h} = 10$ W/m^2/K and the far field temperature to be 300 K. Perform your calculations until the temperature reaches the far field temperature.

3. Return to adiabatic conditions, $\mathsf{h} = 0$, and exercise your code for a variety of initial temperatures, $T(0) \in [500\text{ K}, 2000\text{ K}]$ and plot the so-called ignition delay time τ_i as a function of initial temperature. Use a log-log scale for your plot. The ignition delay is the time where a so-called thermal explosion event occurs, often defined as the time where an inflection point in $T(t)$ occurs, i.e. the time when $d^2T/dt^2 = 0$.

[1] Powers, J. M., and Paolucci, S., 2005, "Accurate Spatial Resolution Estimates for Reactive Supersonic Flow with Detailed Chemistry," *AIAA Journal*, Vol. 43, No. 5, pp. 1088-1099.