AME 60636
Prof. J. M. Powers
Homework 7
Due: Wednesday, 16 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 volume which is initially 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, *isobaric* 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 enthalpy $(h(t) - h(0))/h(0)$, mixture pressure $(P(t) - P(0))/P(0)$, and the relative error in moles for each atom versus time. Use `dlsode` for time integration, which likely requires the `ifort` compiler.

2. Consider a stoichiometric mixture of CH_4 and O_2. Initially, the mixture is at 3000 K and 100 kPa. The mixture comes to equilibrium in an isothermal, isobaric fashion. Using the method of Lagrange multipliers and Gibbs free energy minimization, find the equilibrium concentrations if the allowable species are CO_2, H_2O, O_2, and CH_4. Repeat the calculation if CO, O, H, OH is additionally allowed along with the original major species.

[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.