

AME 598t
Prof. J. M. Powers
Homework 6
Due: Thursday, 17 March 2005

1. Consider a 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 on the links 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 $X_{H_2} = 0.3$, $X_{O_2} = 0.15$, $X_{N_2} = 0.55$, and an initial pressure and temperature of 1 MPa and 1000 K. Take N_2 to be an inert diluent.
 - (a) For adiabatic, isochoric combustion, determine the variation of all species concentrations, temperature, pressure, and time scales of reaction as functions of time; give computer-generated plots on logarithmic scales. Plot all species concentrations on a single plot. Plot all time scales on a single plot. Plot the relative error in energy $\frac{u(t)-u(0)}{u(0)}$, and the relative error in moles for each atom versus time.
 - (b) Repeat the previous problem if there is lumped heat transfer from the volume to the surroundings. Take the heat transfer coefficient to be $\hat{h} = 10 \text{ W/m}^2/\text{K}$ and the far field temperature to be 300 K. Perform your calculations until the temperature reaches the far field temperature.

¹Powers, J. M., and Paolucci, S., 2005, "Accurate Spatial Resolution Estimates for Reactive Supersonic Flow with Detailed Chemistry," *AIAA Journal*, to appear.