AME 598i
Prof. J. M. Powers
Homework 4
Due: Friday, 14 February 2003

1. Use chemkin to plot on a single graph $\overline{c}_p(T)$ for O, O_2, O_3, N, N_2, CH_4, Ar, and He for 298 $K < T <$ 5000 K. Use the units of $erg/mol/K$ for $\overline{c}_p$. Clearly label your plot. Produce a second related plot which gives $\overline{c}_p(T)/\Re$ for the same range of temperature. Give a physical interpretation of your results.

2. Use chemkin to plot on a single graph $\overline{h}(T)$ for O, O_2, O_3, N, N_2, CH_4, Ar, and He for 298 $K < T <$ 5000 K. Use the units of erg/mol for $\overline{h}$. Clearly label your plot. Give a physical interpretation of your results.

3. Consider the ozone reaction mechanism given by Powers, Singh, and Paolucci, 2002, *Journal of Chemical Physics*, Vol. 117, p. 1482-1496. At $t = 0$ s, we have $Y_O = 0.25$, $Y_{O_2} = 0.25$, $Y_{O_3} = 0.5$, $T = 3000$ K, and $p = 100$ kPa. Take the system to be isochoric and adiabatic.

   (a) Write a system of four ordinary differential equations in four unknowns to describe the evolution of each species concentration as well as temperature. Include appropriate initial conditions.

   (b) Find a physical equilibrium state.

   (c) Perform a local linear analysis around the physical equilibrium, and identify the time scales of reaction.

   (d) Write a Fortran 77 (or equivalent) code to integrate the full equations from the initial state to the equilibrium state. Include a copy of your codes (leaving out the dlsode subroutine) as an appendix to your solution. Use the chemkin software package to calculate reaction rates and thermodynamic properties.

   (e) Plot all species concentrations versus t.

   (f) Plot temperature versus t.

   (g) Plot the evolution of the time scales of the system as a function of time.

   (h) Plot $[O]$ versus $[O_3]$.

   (i) Plot $p(t)$.