

AME 598t
Prof. J. M. Powers
Homework 5
Due: Friday, 24 February 2005

1. Use chemkin to plot on a single graph $\bar{c}_p(T)$ for O , O_2 , O_3 , N , N_2 , CH_4 , Ar , and He for $298\text{ K} < T < 5000\text{ K}$. Use the units of erg/mol/K for \bar{c}_p . Clearly label your plot. Produce a second related plot which gives $\bar{c}_p(T)/\mathcal{R}$ for the same range of temperature. Give a physical interpretation of your results.
2. Use chemkin to plot on a single graph $\bar{h}(T)$ for O , O_2 , O_3 , N , N_2 , CH_4 , Ar , and He for $298\text{ K} < T < 5000\text{ K}$. Use the units of erg/mol for \bar{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 $t = 0\text{ s}$, we have $Y_O = 0.25$, $Y_{O_2} = 0.25$, $Y_{O_3} = 0.5$, $T = 3000\text{ K}$, and $p = 100\text{ kPa}$. 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 `dlode` 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 $p(t)$.