

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

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  $298 K < T < 5000 K$ . 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  $298 K < T < 5000 K$ . 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  $t = 0 s$ , 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 dsode 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  $p(t)$ .