AME 60636
Prof. J. M. Powers
Homework 5
Due: Wednesday, 16 February 2022

1. Use `chemkin` to plot on a single graph $\overline{c}_{P,i}(T)$ 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 $\overline{c}_{P,i}(T)/\overline{R}$ for the same range of temperature. Give a physical interpretation of your results.

2. Use `chemkin` to plot on a single graph $\overline{h}_i(T)$ 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 $\overline{h}_i$. 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 mass fractions $Y_O = 0.25$, $Y_{O_2} = 0.25$, $Y_{O_3} = 0.5$, $T = 3000$ 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` (or equivalent) code to integrate the full equations from the initial state to the equilibrium state. Include a copy of your codes 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 $\overline{\rho}_O$ versus $\overline{\rho}_{O_3}$.

   (h) Plot $P(t)$.