AME 598i
Prof. J. M. Powers
Homework 2
Due: Friday, 31 January 2003

1. Write a description of less than one page of the Zeldovich mechanism of NO_x production. Use the LaTeX text formatter to generate your output. Include appropriate formatted equations and appropriate references.

2. Consider a system which is a part of the Zeldovich mechanism for formation NO:

   (a) $O + N_2 \rightarrow NO + N$, $\quad k_1 = 1.8 \times 10^{14} \ \frac{cm^3}{mol \ s} \exp\left(\frac{-38370 \ K}{T}\right)$,

   (b) $NO + N \rightarrow O + N_2$, $\quad k_2 = 3.8 \times 10^{13} \ \frac{cm^3}{mol \ s} \exp\left(\frac{-425 \ K}{T}\right)$,

   (c) $N + O_2 \rightarrow NO + O$, $\quad k_3 = 1.8 \times 10^{10} \ \frac{cm^3}{mol \ s \ K} T \exp\left(\frac{-4680 \ K}{T}\right)$,

   (d) $NO + O \rightarrow N + O_2$, $\quad k_4 = 3.8 \times 10^{9} \ \frac{cm^3}{mol \ s \ K} T \exp\left(\frac{-20820 \ K}{T}\right)$,

   Take the system to be isothermal with $T = 1600 \ K$ and isochoric with $V = 1000 \ cm^3$. At $t = 0 \ s$, we have $N_N = 1 \ mol$, $N_{NO} = 2 \ mol$, $N_{N_2} = 3 \ mol$, $N_O = 4 \ mol$, $N_{O_2} = 5 \ mol$.

   - Write a system of five ordinary differential equations in five unknowns to describe the evolution of each species concentration. Include appropriate initial conditions.
   - Find conserved quantities and give the physical significance of each.
   - Reduce the system to two ordinary differential equations in two unknowns, where the unknowns are $[O_2]$ and $[N_2]$.
   - Find all equilibrium states, and identify which are physical.
   - Perform a local linear analysis around each physical equilibrium, and identify the time scales of reaction.
   - 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 code (leaving out the dlsode subroutine) as an appendix to your solution.
   - Plot all species concentrations versus t.
   - Plot $[N_2]$ versus $[O_2]$.
   - Plot $P(t)$.
   - Using the thermochemical calculator (http://blue.caltech.edu/tcc) to estimate the enthalpies at the end states, calculate the total heat transfer in kJ in the process.