AME 60636
Prof. J. M. Powers
Homework 3
Due: Monday, 11 September 2006

1. Write a description of less than one page of the Zel'dovich mechanism of NO_x production. Use the LaTeX text formatter to generate your output. Include appropriate formatted equations and appropriate references. Your text is a starting point.

2. Consider a system which is a part of the Zel'dovich mechanism for formation NO:

   (a) $N + NO \leftrightharpoons N_2 + O, \qquad a_1 = 1.207 \times 10^{13} \; \frac{cm^3}{mol\ s} \qquad \beta_1 = 0, \qquad T_{a1} = 0\ K$

   (b) $N + O_2 \leftrightharpoons NO + O, \qquad a_2 = 5.839 \times 10^{9} \; \frac{cm^3}{mol\ s\ K^{1.01}} \qquad \beta_2 = 1.01, \qquad T_{a2} = 3120\ K.$

   Take the system to be isothermal with $T = 6000\ K$ and isobaric with $P = 10^6\ dyne/cm^2$. At $t = 0\ s$, we have $n_N = 10^{-6}\ mol$, $n_{NO} = 10^{-6}\ mol/cm^3$, $n_{N_2} = 10^{-6}\ mol$, $n_O = 10^{-6}\ mol$, $n_{O_2} = 10^{-6}\ mol$.

   - 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 $\overline{\rho}_{NO}$ and $\overline{\rho}_N$.
   - 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 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 $\overline{\rho}_N$ versus $\overline{\rho}_{NO}$.
   - Plot $P(t)$.
   - Using the thermodynamic tables to estimate the enthalpies at the end states, calculate the total heat transfer in kJ in the process. Compare these predictions to those in which the gases are estimated to be calorically perfect.