ME 456
Prof. J. M. Powers
Homework 2
Due: Friday, 5 February 1999

1. Consider the system of equations

$$\frac{dx_1}{dt} = -x_1 + 4x_2 - 1, \qquad x_1(0) = 0,$$

$$\frac{dx_2}{dt} = -4x_1 - x_2 + 1, \qquad x_2(0) = 1.$$

Find the equilibrium points and analyze their stability. With hand calculations, find explicit expressions for $x_1(t)$ and $x_2(t)$. Give a computer generated plot of $x_1(t)$ and $x_2(t)$. Give a computer generated plot of the vectors in the $x_1 - x_2$ phase plane along with the solution trajectory. The matlab macro, pplane5, will be helpful in generating plots.

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

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

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

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

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

   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 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 $[O_2]$ versus t, $[N_2]$ versus t and $[N_2]$ versus $[O_2]$.
   - Plot $P(t)$.
   - Using the thermochemical calculator (http://adam.caltech.edu/tcc) to estimate the enthalpies at the end states, calculate the total heat transfer in kJ in the process.