AME 598T
Homework 2: Partial Solution
Due: Thursday, 3 February 2005, in class

Consider a problem of hydrogen dissociation and recombination:

$$H_2 + M \rightleftharpoons H + H + M.$$

1. Consider the approriate parameters for the reaction as found in the AIAA conference paper found in the documents section of the course home page. Take $T = 6000\ K$. Write a code in Fortran and Mathematica to calculate the concentrations as a function of time if initial concentrations are $[\hat{H}_2] = 0.001\ mol/cm^3$, $[\hat{H}] = 0.001\ mol/cm^3$. Give plots of concentration versus time and pressure versus time.

Solution

Several people had some unit problems here. Some intermediate values that you should have found were

$$E = 4.00014 \times 10^{12}\ \frac{erg}{mole}.$$
$$g^o_H = -7.26136 \times 10^{12}\ \frac{erg}{g},$$
$$g^o_{H_2} = -1.1754 \times 10^{13}\ \frac{erg}{g}.$$
$$\Delta G^o = -2.768 \times 10^{12}\ \frac{erg}{g}.$$
$$K^c = 0.0005225\ \frac{mol}{cm^3}.$$

Here the equilibrium values are

$$\lim_{t\to\infty} [H] = 0.000764261\ \frac{mole}{cm^3},$$
$$\lim_{t\to\infty} [H_2] = 0.00111787\ \frac{mole}{cm^3},$$
$$\lim_{t\to\infty} p = 9.389\ \frac{dyne}{cm^2}.$$

Equilibrium was reached in roughly $10^{-7}\ s$, and the time constant near equilibrium was

$$\tau = 1.64 \times 10^{-8}\ s.$$

2. For the same initial conditions, generate a plot of how the equilibrium concentrations of H and H_2 vary with temperature.

3. Give a plot of how the time scales found by linearization behave as temperature is varied over a wide range.

4. Using an appropriate text for guidance, give a derivation linking K^p to K^c.