CHEN 1703 - HOMEWORK 5

Submit your solutions via the course web site. Be sure to include your name and UNID in your m-file. Submit each solution seperately. Also be sure to document your solutions well.

Problem 1 (10 pts)

Consider a chemical reaction where species A decomposes to form B and C,

$$A \xrightarrow{k} B + C$$

As you will learn in your kinetics class, there are a few possible ways that this reaction may proceed. From these, we obtain the following equations for the concentration of A, c_A as a function of time:

$$c_A = c_A^0 \exp(-kt) \qquad \text{First order reaction} \tag{1}$$

$$c_A = \frac{c_A^0}{1 + ktc_A^0} \qquad \text{Second order reaction} \tag{2}$$

If we take the natural log of (1) then we find

$$\ln c_A = \ln c_a^0 - kt.$$

Therefore, if we plot $\ln c_A$ as a function of t then we should obtain a straight line if the reaction is first order. Similarly, if we rearrange (2) we find

$$\frac{1}{c_A} = \frac{1}{c_A^0} + kt.$$

Therefore, if we plot $\frac{1}{c_A}$ as a function of t then we should obtain a straight line if the reaction is second order.

From the data shown in Table 1, make plots of $\frac{1}{c_A}$ versus t and $\ln c_A$ versus t, and plot these on the same figure. Use them to conclude whether the reaction is first or second order. Be sure to label your plot axes.

You may use either MATLAB or Excel to solve this problem. In either case, you must clearly indicate whether the reaction is first or der or second order.

t (s)	0	0.43	0.86	1.29	1.71	2.14	2.57	3.00
c_A $\left(\frac{\text{mol}}{\text{cm}^3}\right)$	0.96	0.64	0.40	0.27	0.18	0.12	0.07	0.049

Table 1: The concentration of species A as a function of time.

Problem 2 (10 pts)

The ideal gas law can be written as

$$\rho = \frac{pW}{RT},$$

where ρ is the density of the gas, W is its molecular weight, $R = 0.0820574587 \, \frac{\mathrm{L \cdot atm}}{\mathrm{mol \cdot K}}$ is the gas constant, and T is the temperature.

Plot the density of Hydrogen (H_2), Nitrogen (N_2), Argon (Ar), and Chlorine (Cl_2) as functions of temperature at pressures of 1, 5, and 10 atm. Your plot should look like the one shown in Figure 1. You must use loops to accomplish this. An algorithm might look like:

```
Define a vector of molecular weights
Define a vector of species names
Define the temperature points
for each species
  calculate the density at all temperatures for p=1 atm.
  calculate the density at all temperatures for p=5 atm.
  calculate the density at all temperatures for p=10 atm.
  select the appropriate sub-plot
  plot the density vs. temperature for each pressure
  create axis labes and legend
end
```

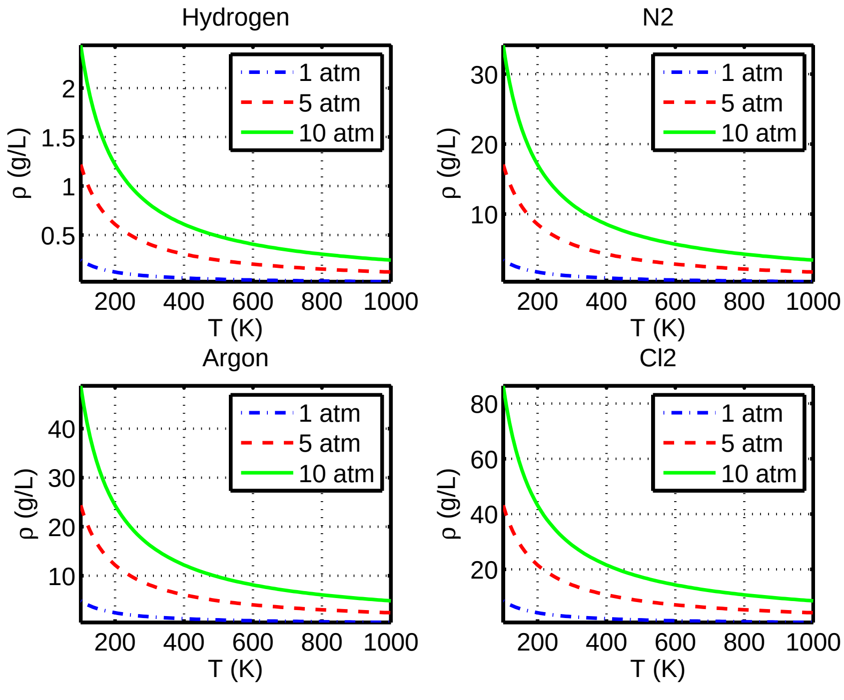

Figure 1: Your plot for Problem 2 should look like this.

Problem 3 (10 pts)

The *heat capacity* of a material indicates how much heat (thermal energy) the material must absorb to change its temperature. It is often fit to a polynomial form such as

$$C_p = a + bT + cT^2 + dT^3, \quad (3)$$
$$C_p = a + bT + cT^{-2}. \quad (4)$$

Table 2 shows the coefficients for several chemical compounds, along with the equation that should be used to calculate C_p. For example, to determine C_p for steam we use (3):

$$C_p = (33.46) + \left(6.88 \times 10^{-3}\right) T + \left(7.604 \times 10^{-6}\right) T^2 + \left(-3.593 \times 10^{-9}\right) T^3,$$

and the units for temperature would be $^\circ C$. The units of C_p would be $\frac{\text{J}}{\text{mol}\cdot{}^\circ\text{C}}$. Similarly, for $CaCO_3$, we use (4):

$$C_p = (82.34) + (4.975 \times 10^{-2})T - (1.287 \times 10^6)T^{-2},$$

and the units for temperature would be K and the units for C_p would be $\frac{\text{J}}{\text{mol}\cdot\text{K}}$.

Compound	Eqn.	T Unit	a	b	c	d	T Range (units of T)
Hydrogen (H_2)	(3)	Celsius	28.84	7.65×10^{-5}	3.288×10^{-6}	-8.698×10^{-10}	0-1500
Calcium Carbonate ($CaCO_3$)	(4)	Kelvin	82.34	4.975×10^{-2}	-1.287×10^{6}	-	273-1033
Steam (H_2O)	(3)	Celsius	33.46	6.88×10^{-3}	7.604×10^{-6}	-3.593×10^{-9}	0-1500
Copper (Cu)	(3)	Kelvin	22.76	6.117×10^{-3}	0	0	273-1357
Propane (C_3H_8)	(3)	Celsius	68.032	0.2259	-1.311×10^{-4}	3.171×10^{-8}	0-1200

Table 2: Heat capacity data for several compounds. Units for C_p are $\frac{\text{J}}{\text{mol}\cdot\text{K}}$ or $\frac{\text{J}}{\text{mol}\cdot\text{C}}$, depending on the unit of temperature indicated in the table. Data are from *Elementary Principles of Chemical Processes*, Felder & Rousseau, 2nd edition, (1986).

Write a MATLAB script to have the user select the compound and then plot C_p as a function of T over the valid temperature range for that compound. Be sure to label the axes appropriately.

You may want to start with the file posted on the class web site.