Chem 155 Homework #4 Due at the start of class on MON. Feb. 6

Reading: Chapter 13

Chapter 12 Problems:

12.73---Compare this number to the energy cost required to recycle a corresponding quantity of Aluminum assuming the primary energy input for recycling is the melting of the Al (enthalpy of fusion of Al(s) is 10.7 kJ/mol) **12.76**

Math Skills Review Problems (review only, not to hand in-this section only!):

1) Evaluate the following integrals (see Appendix C for review if necessary):

a)
$$\int x^n dx \quad (n > 0)$$

b) $\int \frac{1}{x} dx$

2) Solve the following equation for x(t) by integration for the given initial conditions, showing all steps (see section 13.3 first if necessary):

a)
$$\frac{dx(t)}{dt} = -kx(t)$$
, given $x(0) = N_0$

b)
$$\frac{dx(t)}{dt} = kx(t)$$
, given $x(0) = N_0$

Chapter 13 Textbook Problems: (to be handed in)

13.8 13.16 13.22 13.26 13.27 13.36 13.47

Additional Problems (complete BOTH 1 and 2, only part of problem 1 is extra credit):

1) Approach to equilibrium

Consider a simple dissociation reaction:

 $AB \rightarrow A+B$ that proceeds with rate=k₁[AB] with k₁=0.1 s⁻¹

While the association $A + B \rightarrow AB$ proceeds with rate=k₂[A][B] and k₂=0.05 L mole⁻¹ s⁻¹

1A) What is the equilibrium constant for the reaction $AB \rightarrow A+B$?

1B)

i)Use excel to numerically integrate the rate equations and thus generate a plot of [AB] and [A] vs. time for the first 60 seconds of the reaction after a 1 mole/liter concentration of AB begins reacting. A starter worksheet is included on the discussion board.

ii) What is the concentration of [A] 17 seconds after a 1 mole/liter concentration of AB begins reacting?

If we want to find [AB] as a function of time for this reaction we can solve the following set of equations:

$$\frac{d[AB]}{dt} = -k_1[AB] + k_2[A][B]$$
$$\frac{d[A]}{dt} = \frac{d[B]}{dt} = k_1[AB] - k_2[A][B]$$

This is straightforward to do numerically in a fashion that can be adjusted. There are more efficient/accurate ways to perform the numeric integration of these equations than in the downloadable worksheet, but what we have is straightforward and sufficient for our needs. Basically, we calculate $k_1[AB]$, and $k_2[A][B]$ at each step, then multiply by some small time unit "dt" to calculate the change in concentration over that small interval, we then update the concentrations and continue.

1C) Part C is worth 5 points extra credit

What if the reaction was:

 $AB_2 \rightarrow A + 2B$

And the forward rate expression remained unchanged but the reverse reaction rate expression was $k_2[A][B]^2 = 0.5 L^2 \text{ mole}^{-2} \text{ s}^{-1}$ What is the equilibrium constant K? Modify the worksheet to generate a plot of [AB₂], [A], and [B] vs. time for the first 30 seconds of the reaction.

Problem 2 is NOT extra credit:

2) Download and read/skim the first half of the article by M. Levy and A. D. Ellington in PNAS Vol. 100, p 6416-6421 (2003). If you are on campus you will automatically be able to use the university subscription to the Proceedings of the National Academy of Sciences to download this article. From off-campus you can use the UW library proxy server (instructions are available at http://www.lib.washington.edu/help/connect.html).

Explain the steps that lead to "exponential growth" in the reaction? Which equations (reactions 1-6 in the paper) correspond to these steps? When will "exponential growth" of the reaction stop?