Study Guide Test 1

In order to do well on the next test, you should be able to do the following:

1. Define stoichiometry and be able to apply the concept to balance stoichiometric equations.

2. Define limiting and excess reactant, fractional conversion and the extent of reaction.

3. Be able to determine limiting and excess reactants and conversion parameters.

4. Be able to write component mass balance equations for systems that include reactions.

5. Explain in your own words that the terms *elementary reactions*, *non-elementary reactions*, *rate equation*, *rate constant, reaction order, reaction dependence on temperature (Arrhenius' Law)*, *collision theory vs. transition theory.*

6. Be able to derive the relationship between rates of reaction of all reaction species and their stoichiometry coefficients.

7. Be able to derive relationship between time and concentration or conversion (C vs. t, X vs. t) for different types of reaction rate models (ie. zero order, 1^{st} order, 2^{nd} order, 3^{rd} order, n^{th} order).

8. Be able to develop reaction rate models from reaction mechanisms and apply necessary assumption (ie. regarding transition species behavior $dx/dt = 0$) to see if rate equations fit observed behavior (see examples 2.1 and 2.2 in text).

9. Be able to derive M-M rate equation for an enzymatic reaction as well as its integration form for obtaining the relationship between concentration and time.

Practice problems:

Problem 1
For a zero order reaction, what are the dimensions/units of the rate constant, k?

Problem 2
Calculate the time needed to react 75% of reactant (A -> B), assuming an initial concentration of Co for:

a. a first order reaction, $k = 7.31 \times 10^{-2}$ min^{-1}
b. a second order reaction, $k = 5.71 \times 10^{-4}$ L/mol-min

Problem 3:

2nd order, bimolecular elementary reaction
A + B -> products

with corresponding rate equation

$$-r_A = -\frac{dC_A}{dt} = -\frac{dC_B}{dt} = kC_AC_B \qquad \textbf{(13}\textbf{\textit{b}}\textbf{)}$$

[initial concentrations C_{A0}, C_{B0} at t = 0]

which on separation and formal integration becomes

$$\int_0^{X_A} \frac{dX_A}{(1 - X_A)(M - X_A)} = C_{A0}k \int_0^t dt$$

After breakdown into partial fractions, integration, and rearrangement, the final result in a number of different forms is

$$\boxed{\begin{aligned} \ln\frac{1 - X_B}{1 - X_A} &= \ln\frac{M - X_A}{M(1 - X_A)} = \ln\frac{C_BC_{A0}}{C_{B0}C_A} = \ln\frac{C_B}{MC_A} \\ &= C_{A0}(M - 1)kt = (C_{B0} - C_{A0})kt, \qquad M \neq 1 \end{aligned}} \qquad \textbf{(14)}$$

note that this is only valid for $C_{A0} \neq C_{B0}$

What if $C_{A0} = C_{B0}$?