General Approach to Solving Chemical Equilibria Problems

The general form of a chemical reaction is: $aA + bB \Leftrightarrow cC + dD$

where A and B are reactants in the forward direction and C and D are products in the forward direction. The lower case letters are the stoichiometric coefficients for the balanced equation. The general form of the equilibrium constant equation is then

$$K_{eq} = [C]^c[D]^d/[A]^a[B]^b$$

Problems involving chemical equilibria can be placed into a matrix format with two kinds of concentrations identified: the initial or non-equilibrium concentration C_x and the equilibrium concentration $[X]$. (Note the bracket versus the capital C. It is the equilibrium concentrations, $[X]$, that are used to calculate K_{eq}.

	A	B	C	D
initial	C_A	C_B	C_C	C_D
change	C_A-[A]	C_A-[A]	[C]- C_C	[D] - C_D
equilibrium	[A]	[B]	[C]	[D]

There are a variety of equilibrium problems that can be solved using the construction above. In some cases the problems are solved directly, with one unknown per equation. Others problems require significant algebraic manipulation. All of them are easy if you can identify the type of information used and place it in the matrix.

Examples:
Model Equilibrium System As the chemical system for all the problems on this work sheet, we will use

$$2NH_3 \Leftrightarrow 3H_2 + N_2 \quad K_{eq} = 3.8 = [H_2]^3[N_2]/[NH_3]^2$$
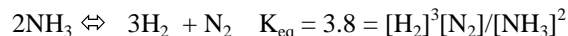
Problem 1.   Calculating K_{eq} from equilibrium concentrations.
In these problems it is necessary to identify all the bottom row equilibrium concentrations (the ones in [X]) so that K_{eq} is determined directly. For the ammonia equilibrium above, equilibrium concentrations are $[N_2]$ = .10 M, $[H_2]$ = .50 M, $[NH_3]$ =.057 M. What is K_{eq}? This is the easiest of problems because you are told what all the bottom row equilibria are.

	$2NH_3$	$3H_2$	N_2
initial			
change			
equilibrium	.057	.50	.10

$$K_{eq} = [.10]^1[.50]^3 /[.057]^2 = 3.8$$

Note that for constant temperaure, this value for K never changes. You will see it used in every example in the handout.

Problem 2. Using stoichiometry to complete the array.
A more complex type of problem provides some of the initial and some of the equilibria concentrations and you are asked to solve for the rest of the concentrations in the array. These problems are accomplished using stoichiometry and simple substitutions for unknowns.

Given K_{eq} = 3.8, $[N_2]$ = 0.3 M, $[H_2]$ = 0.2 M and C_{NH3} = 0.04 M. What is the initial concentration of C_{N2}?

	$2NH_3$	$3H_2$	N_2
initial	.04		?
change			
final		.2	.3

First find $[NH_3]$ at equilibrium from the K_{eq} expression: $3.8 = ((.2)^3(.3)/[NH_3]^2$ and $[NH_3]$]= .025 M.

Then use the stoichimetric relationships to back substitute throughout the matrix. Follow the steps shon.

	$2NH_3$	$3H_2$	N_2
initial	**.035**	.185 step 3	.295 step 3

change	-.01 step 1	+.015 step 2	+.005 step 2
final	.025	**.2**	**.3**

Problem 3. Problem solving using K_{eq} and initial concentrations.

The most realistic kind of equilibrium problem, the one you will use most often in Chapter 18 through 20, involves knowing the initial concentration of materials in the reaction, and the K_{eq}, obtained from a table. The equilibrium concentrations are then found through a series of algebraic substitutions. Note this problem represents what happens in real life. We can measure what we add to a reaction container, and we know K_{eq}

	A	B	C	D
initial	known	known	known	known
change				
final	unknown	unknown	unknown	unknown

This problem type is about the only kind you will work after Chapter 17. It is the most challenging and often requires solution of higher order polynomial equations.

Example. A quartic.

Your intial concentration of C_{NH3} is 0.1M. What is the equilibrium concentration of $[N_2]$? (Remember that $K_{eq} = 3.8$).

	$2NH_3$	$3H_2$	N_2
initial	.1	0	0
change			
final			x

To solve this problem you need to generate an algebraic solution for the equilibrium values all in terms of a single variable. So let x = the amount of $[N_2]$ at equilibrium. Then solve for the other unknowns using the stoichiometric relationship between the concentrations.

	$2NH_3$	$3H_2$	N_2
initial	**.1**	**0**	**0**
change	-2x	+3x	+x
final	.1-2x	3x	**x**

So the equilibrium equation in terms of the single variable x (which happens to be [N2] that we want to know) is
$$3.8 = (3x)^3(x)/(.1-2x)^2 = 27x^4/(.01-4x + 4x^2)$$

Yikes, a quartic. I will leave it to one of you to solve with your fancy calculators. This is why I don't write test questions. Don't worry, you'll never get one like this on a quiz or exam. Instead I will start giving you easier algebraic problems that are still solved the same way. Like this one from Chapter 18 on acids and bases.

Problem 4. [H+] in a weak monoprotic acid. What is the $[H^+]$ concentration for a 0.3M solution of acetic acid ($K_a=1.8 \times 10^{-5}$).

$$HC_2H_3O_2 \Leftrightarrow H^+ + C_2H_3O_2^- \qquad K_a=1.8 \times 10^{-5} = [H^+][C_2H_3O_2^-]/[HC_2H_3O_2]$$
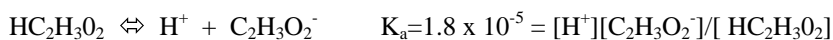
	$HC_2H_3O_2$	H^+	$C_2H_3O_2^-$
initial	**.3**	**0**	**0**
change			
final		**x**	

Solve in the same way, finding a single variable to substitute for equilibrium unknowns

	$HC_2H_3O_2$	H^+	$C_2H_3O_2^-$
initial	.3	0	0
change	-x	+x	+x
final	.3-x	x	x

So $K_a=1.8 \times 10^{-5} = (x)(x)/(.3-x) = x^2/(.3-x)$. A quadratic. Well I do know how to solve those using the quadratic formula.

x = [H$^+$] = 2.31 x 10^{-4}. The answer says that there is not much [H$^+$] in solution, which we would have guessed, because acetic acid is a weak acid.

Note that the way you solve an equilibrium for a weak acid in CH18 is exactly the same procedure you learned in Chapter 17. Don't lose sight of that fact as we start to get more and more complicated about things in later chapters. You can always set up an array and do the necessary substitutions for x, and solve for an unknown.