Some Math Tips: CHEMICAL EQUILIBRIA Chem 160-Jasperse Ch. 14

1. $(a + b)^2 = a^2 + 2ab + b^2$

example: $(0.24 - x)^2 = 0.0576 - 0.48x + x^2 = x^2 - 0.48x + 0.0576$

example: $(3.2e-5 - x)^2 = 1.02e-9 - 6.4e-5x + x^2 = x^2 - 6.4e-5x + 1.02e-9$

2. Quadratic Equation: $ax^2 + bx + c = 0$

$$= \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

example: $x^2 - 1.48x + 0.0576 = 0$ x = 1.44 or 0.04

example: $x^2 - .60 x + 0.025 = 0$ x = 0.43 or 0.17

Note 1: Quadratics are a bother to solve. Avoid them if possible. Often the "simplifying assumption" (see #4) can enable you to avoid quadratic solutions.

Note 2: Quadratics can often give 2 answers, but one will frequently be nonsense.

3. "SIMPLIFYING ASSUMPTION": If m>>x, then m - x = m (approximately)

examples: 0.14 - 3.6e - 5 = 0.14

1.23e-3 - 1.0e-6 = 1.23e-3

х

Use: for many equations in which K is small, "x" will also be relatively small. In these circumstances, the degree to which the starting materials react ("x") will be relatively insignificant, and we can assume the equilibrium concentration of the reactants will not differ significantly from their initial concentration.

- THE SIMPLIFYING ASSUMPTION WILL OFTEN MAKE THE USE OF THE OUADRATIC EQUATION UNNEEDED
- Guide: If "x" is >5% of "m", then the simplifying assumption is not appropriate.
- 4. The "Square Root" Simplification: If both numerator and denominator have "squares", it is convenient to take the square root of both sides to simplify

examples: $0.10 = x^2/(0.050 - x)^2$ Take square root of both sides: 0.316 = x/(0.050 - x)Rearrange: 0.0158 - 0.316x = xSolve for "x": x = 0.0125. $m = x^n$ To solve for x, when "m" and "n" are known: a. enter "m"

b. hit $x^{1/y}$ or $\sqrt[4]{x}$ button (depending on your calculator)

c. enter "n"

example:

$25 = x^3$	x = 2.92	
$1.48e-6 = x^3$	x = 0.0114	
$2.14e-13 = x^4$	x = 6.80e-4	

Using the "ICE" Method to Calculate K, Given Initial Concentrations and One Final Concentration

- 1. Write balanced equation, and expression for K_c
- 2. Make an "ICE" table, and enter the knowns
 - a. <u>I</u>nitial
 - b. Change
 - c. Equilibrium
- 3. Find the Change for the chemical whose final concentration is known
- 4. Use stoichiometric relationship to determine the change in concentrations for the others
- 5. From the initial concentrations and the deduced changes, determine all equilibrium concentrations
- 6. With all equilibrium concentrations now known, plug into the K_c expression and solve for K
- 7. Check: Does Answer Make Any Sense?
- Note: equilibrium concentrations must be in Molarity, moles/liter. If information is given in grams or moles plus solvent volume, you will need to convert into molarity.

Using the "ICE" Method to Calculate Equilibrium Concentrations, Given Only Initial Concentrations and K_c

- 1. Write balanced equation, and expression for K_c
- 2. Make an "ICE" table, and enter the known initial concentrations
 - a. <u>I</u>nitial
 - b. Change
 - c. Equilibrium
- 3. Use "x" to define the change of one substances. Use stoichiometric relationships to determine the changes in the concentrations for the others, in terms of "x".
- 4. Calculate the equilibrium concentrations of all chemicals in terms of initial concentrations and "x", and enter them in the table.
 - If K is small so that "x" is likely to be small, the simplifying assumption that $[A]_{initial} "x" = [A]_{initial}$ is often justified, and can greatly simplify the math.
- 5. Solve for "x" (This is the hard part!)
- 6. Once "x" is known, solve for the actual equilibrium concentrations
- 7. Check: Does Answer Make Any Sense? If you made the "simplifying assumption", was it justified?

14-12

Solution with + Without Simplifying Assumption Kc=2.0 x10 \$ À ⇒ 28 + C $\frac{\text{with}}{C} \pm 0.20$ 0 2x Х E .20-x 2X X E* 0.20 X Х So $K = 2.0 \times 10^{-8} = \frac{(2x)^2}{(3.20)} \times \frac{(4x)^3}{.20}$ Easer $0.4 \times 10^8 = 4 \times 3$ $x^{3} = 1.0 x 10^{-9}$ $x = 1.0 x 10^{-3}$ Without (Using , 20-x for IA3 at eq.) $K = 2.0 \times (C^{-F} = (2 \times)^{2} \times)^{2}$ so $2.0 \times 10^8 (0.20 - x) = 4 \times 3$ $40 \times 10^{-9} - 20 \times 10^{-8} \times = 4 \times 3$ SO 4x3 + 2.0×108x - 4.0×109=0 50 Not Easy !!

LeChatelier's Principle: Summary

A change in any of the factors that determine the equilibrium conditions of a system will cause the system to change in such a manner as to reduce or counteract the effect of the change.

Factors		Change	Consider	Direction to reach Equilibrium
1. Concentration	Î	Reactant		Forward
	t	Product		Reverse
2. Temperature	t	Т	∆H>0	Forward - K increases
•			∆H<0	Reverse - K decreases
3. Volume	t	V (P decreases)	$\Delta n_{gas} > 0$	Forward
			$\Delta n_{gas} = 0$	No effect
			$\Delta n_{gas} < 0$	Reverse

If you reverse any of the Changes above, the Direction to reach Equilibrium reverses.