EQUILIBRIUM CALCULATIONS

- We're often interested in figuring out what happens at equilibrium BEFORE we do an experiment!

- What's the problem? Initially, we know only ... INITIAL concentrations. Since these are NOT equilibrium concentrations, we cannot simply plug them into an equilibrium expression and solve.

So how do we find out what the concentrations are at equilibrium if we initially know NONE of them?

- To solve an equilibrium problem, write out the equilibrium constant expression. Then, try to RELATE ALL THE EQUILIBRIUM CONCENTRATIONS TO ONE ANOTHER using the chemical equation.

- It helps to assign a variable based on one of the substances in the reaction, then write the concentrations of the other substances based on that variable. How to do this? Take a look at the following examples...

AgCl: 107.9 + 35.45 = 143.35 g/mol

EXAMPLE: Calculate the grams per liter of silver(I) chloride (AgCl) in a solution that is at equilibrium with solid AgCl.

$$AgCl(s) \rightleftharpoons Ag^+(aq) + Cl^-(aq) \; ; \; K_c = 1.8 \times 10^{-10}$$

Start by writing an expression for Kc: $K_c = [Ag^+][Cl^-] = 1.8 \times 10^{-10}$

The problem is that the Kc expression has two variables - (Ag+) and (Cl-). Let's try to relate them.

Species	[Initial]	Δ	[Equilibrium]
Ag^+	0	+ X	0+x = X
Cl^-	0	+ X	0+x = X

* Let "x" equal the change in Ag+ concentration.

Plug (Equilibrium) expressions back into the equation we wrote for Kc ...

$$(x)(x) = 1.8 \times 10^{-10}$$

$$x^2 = 1.8 \times 10^{-10}$$

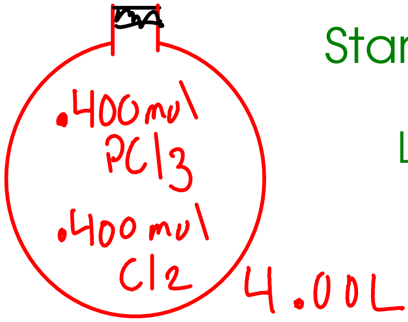
$$x = 1.341640786 \times 10^{-5}\ M = [Ag^+] = [AgCl]_{dissolved}$$

The dissolved AgCl concentration just equals the dissolved Ag+ concentration, but we need to change units from mol/L to g/L.

$$\frac{1.341640786 \times 10^{-5}\ mol\ AgCl}{L} \times \frac{143.35\ g\ AgCl}{mol\ AgCl} = \boxed{0.0019\ g\ AgCl/L}$$

$$PCl_3(g) + Cl_2(g) \rightleftharpoons PCl_5(g) \quad K_c = 49$$

If you add 0.400 moles of each reactant to a 4.00 L reaction vessel, what is the concentration of each species in the equilibrium mixture?



Initial conditions

Start by writing the expression for Kc: $K_c = \frac{[PCl_5]}{[PCl_3][Cl_2]} = 49$

Let's make a chart to try to combine these into one variable:

Species	[Initial]	Δ	[Equilibrium]
PCl_5	0	+x	x
PCl_3	$\frac{0.400 mol}{4.00 L} = 0.100$	−x	0.100 − x
Cl_2	$\frac{0.400 mol}{4.00 L} = 0.100$	−x	0.100 − x

Let "x" equal the change in phosphorus pentachloride concentration

Plug the (Equilibrium) expressions back into our Kc equation:

$$\frac{(x)}{(0.100 - x)(0.100 - x)} = 49$$

We'll need to solve for "x" to continue!

$$\frac{(x)}{(0.100-x)(0.100-x)} = 49$$

$$x = 49(0.100-x)^2$$

$$(a-b)^2 = a^2 - 2ab + b^2$$

$$x = 49(0.0100 - 0.200x + x^2)$$

$$x = 0.49 - 9.8x + 49x^2$$

$$0 = \underbrace{49x^2}_{a} \underbrace{-10.8x}_{b} + \underbrace{0.49}_{c}$$

$$x = \frac{+10.8 \pm \sqrt{(-10.8)^2 - 4(49)(0.49)}}{2(49)} = \frac{10.8 \pm \sqrt{20.6}}{98}$$

$$x = 0.157 \text{ or } 0.0639$$

The QUADRATIC EQUATION:

$$ax^2 + bx + c = 0$$

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

Each quadratic has two solutions (see the +/- part of the equation), but only one of them will be the correct chemical solution.

The quadratic equation has two possible solutions, but the chemical problem only has one. How do we tell which of these values for "x" is the correct one for the chemistry?

$x = 0.157$ or 0.0639

To figure out the correct solution, look at the concentrations that would result when you plug "x" back into our chart. 0.157 is an impossible answer, since it gives us negative concentrations for phosphorus trichloride and chlorine.

Species	[Equilibrium]
PCl_5	x
PCl_3	0.100 − x
Cl_2	0.100 − x

Plug x=0.0639 into the chart to find the concentrations:

$[PCl_5] = x = 0.0639\ M\ PCl_5$

$[PCl_3] = 0.100 - x = 0.0361\ M\ PCl_3$

$[Cl_2] = 0.100 - x = 0.0361\ M\ Cl_2$

Notice that the concentration of the phosphorus pentachloride is larger than the reactant concentrations. That's consistent with Kc = 49 (larger than 1).

An 8.00 L reaction vessel at 3900C is charged with 0.850 mol of nitrogen and oxygen gases. Find the concentration of all species at equilibrium.

$$N_2(g) + O_2(g) \rightleftharpoons 2NO(g) \quad K_c = 0.0123$$

$$K_c = \frac{[NO]^2}{[N_2][O_2]} = 0.0123$$

Write expression for Kc...

Species	[Initial]	Δ	[Equilibrium]
N_2	$\frac{0.850\text{ mol}}{8.00\text{ L}} = 0.10625$	$-x$	$0.10625 - x$
O_2	$\frac{0.850\text{ mol}}{8.00\text{ L}} = 0.10625$	$-x$	$0.10625 - x$
NO	0	$+2x$	$2x$

Let "x" equal the change in nitrogen gas concentration

$$\frac{(2x)^2}{(0.10625 - x)(0.10625 - x)} = 0.0123$$

We'll need to solve for "x" to continue...