Equilibrium Calculations

Example:

At 227°C, the equilibrium constant for the reaction

$2NO(g) + O_2(g) \Leftrightarrow 2NO_2(g)$ is $6.9x10^5$.

If at equilibrium there is $1.0x10^{-3}$M O_2 and $5.0x\ 10^{-2}$M NO_2, what is the concentration of NO?

$$K_c = \frac{[NO_2]^2}{[NO]^2[O_2]}$$

$$[NO]^2 = \frac{[NO_2]^2}{K_c[O_2]}$$

$$[NO] = \sqrt{\frac{[NO_2]^2}{K_c[O_2]}} = \sqrt{\frac{(5.0x10^{-2})^2}{(6.9x10^5)(1.0x10^{-3})}}$$

$[NO] = \pm 1.9x10^{-3}M$ correct value is $+1.9x10^{-3}M$

Check

$$K_c = \frac{[NO_2]^2}{[NO]^2[O_2]} = \frac{(5.0x10^{-2})^2}{(1.9x10^{-3})^2(1.0x10^{-3})} = 6.9x10^5$$

USING "ICE" CHARTS

Example 1:
At 715K, the equilibrium constant for the reaction
$H_2(g) + I_2(g) \Leftrightarrow 2HI(g)$ is 55.0. If 2.00mol H_2 and 2.00mol I_2 are allowed to react in a 20.0L vessel, what are the equilibrium concentrations of all species?
The initial concentrations of H_2 and I_2 are:

$$[H_2]_0 = [I_2]_0 = \frac{2.00\text{mol}}{20.0\text{L}} = 0.100\text{M}$$

	$H_2(g)$	+	$I_2(g)$	$\Leftrightarrow$	$2HI(g)$
I	0.100		0.100		0
C	–x		–x		+2x
E	0.100 – x		0.100 – x		2x

$$K_c = 55.0 = \frac{[HI]^2}{[H_2][I_2]} = \frac{(2x)^2}{(0.100-x)(0.100-x)}$$

$$55.0 = \frac{(2x)^2}{(0.100-x)^2}$$ Perfect square

$$\sqrt{55.0} = \sqrt{\frac{(2x)^2}{(0.100-x)^2}}$$

$$\pm 7.42 = \frac{2x}{0.100-x}$$ Solve for each root.

$$+7.42(0.100-x) = 2x$$
$$0.742 - 7.42x = 2x$$
$$0.742 = 9.42x$$
$$x = \frac{0.742}{9.55} = 0.0788\text{M}$$

$$-7.42(0.100-x) = 2x$$
$$-0.742 + 7.42x = 2x$$
$$-0.742 = -5.42x$$
$$x = \frac{-0.742}{-5.42} = 0.137\text{M}$$

The correct root is 0.0788M since 0.137M >0.100M, the initial concentration.

$[H_2] = [I_2] = 0.100 - x = 0.100M - 0.0788M = 0.021M$
$[HI] = 2x = 2(0.0788M) = 0.158M$
Check

$$K_c = \frac{[HI]^2}{[H_2][I_2]} = \frac{(0.158)^2}{(0.021)(0.021)} = 55.3$$

Example 2:
Vinegar, which contains acetic acid, is a weak acid; thus, it only partially ionizes in water.

$$CH_3COOH(aq) \Leftrightarrow H^+(aq) + CH_3COO^-(aq)$$

What is the value of K_c if the extent of ionization in 1.0M CH_3COOH solution is 0.42%.

$$\%\ \text{Ionization} = \frac{\text{amount reacted}}{\text{initial amount}} = \frac{x}{[CH_3COOH]_0}$$

$$x = \%\ \text{Ionization x } [CH_3COOH]_0 = 0.0042 \text{ x } 1.0M = 0.0042M$$

	$CH_3COOH(aq)$ ⇔	$H^+(aq)$	+	$CH_3COO^-(aq)$
I	1.0	0		0
C	–x	+x		+x
E	1.0 – x	x		x= 0.0042

$$K_c = \frac{[H^+][CH_3COO^-]}{[CH_3COOH]} = \frac{(x)(x)}{(1.0 - x)} = \frac{(0.0042)(0.0042)}{(1.0 - 0.0042)}$$

$$K_c = 1.8x10^{-5}$$

Example 3:

For the reaction $H_2(g) + I_2(g) \Leftrightarrow 2HI(g)$, if the initial concentration of $H_2(g)$ is 0.100M and that of $I_2(g)$ is 0.200M, what are the equilibrium concentrations of all species?

At 715K the $K_c = 55.0$.

	$H_2(g)$	+	$I_2(g)$	$\Leftrightarrow$	$2HI(g)$
I	0.100		0.200		0
C	–x		–x		+2x
E	0.100 – x		0.200 – x		2x

$$K_c = 55.0 = \frac{[HI]^2}{[H_2][I_2]} = \frac{(2x)^2}{(0.100 - x)(0.200 - x)}$$

Since this is NOT a perfect square, the **quadratic formula** must be used to solve for x. First step is to get relationship in correct form of $ax^2 + bx + c = 0$.

$55.0\,(0.100–x)(0.200–x) = 4x^2$

$55.0\,(0.0200–0.300x+x^2) = 4x^2$

$1.10 - 16.5x + 55.0x^2 = 4x^2$

$51.0x^2 - 16.5x + 1.10 = 0$

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

$$x = \frac{-(-16.5) \pm \sqrt{(-16.5)^2 - 4(51.0)(1.10)}}{2(51.0)} = \frac{16.5 \pm 6.92}{102}$$

Roots are x = 0.230M and 0.0939M. The first root is ignored because 0.230M > 0.100M initial concentration.

$[H_2] = 0.100 - x = 0.100\ M - 0.0939M = 0.006M$
$[I_2] = 0.200 - x = 0.200\ M - 0.0939M = 0.106M$
$[HI] = 2x = 2(0.0939M) = 0.188M$

Check

$$K_c = \frac{[HI]^2}{[H_2][I_2]} = \frac{(0.188)^2}{(0.006)(0.106)} = 55.6$$

Off slightly because only one sig. Fig. for H_2 concentration.

Another way to solve is to find the roots using calculator.

$$K_c = \frac{[HI]^2}{[H_2][I_2]}$$

$$55.0 = \frac{(2x)^2}{(0.100 - x)(0.200 - x)}$$

$$0 = \frac{4x^2}{(0.100 - x)(0.200 - x)} - 55.0$$

Make sure Y = screen is clear and Plots are off.
Plug into Y = screen.

$$Y1 = \frac{4x^2}{(0.100 - x)(0.200 - x)} - 55.0$$

$$Y2 = 0$$

Set window for Xmin, Xmax, Ymin, and Ymax.
Xmin = 0 and Xmax = 0.100. Why?

Ymin should be negative value and Ymax positive. For example Ymin = –5 and Ymax = 5.

Solving for intersection yields x = 0.0939M.