Chemical Equilibrium

Chemical equilibrium is reached when the **RATE** of the forward reaction equals the **RATE** of the reverse reaction. *Note*: This does **NOT** mean that the quantities of reactants and products are equal. At equilibrium we can determine the equilibrium constant, K_c.

For the general reaction:

$$aA + bB \rightleftharpoons cC + dD$$

The equilibrium constant can be expressed as:

$$K_c = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

Uppercase letters represent the various compounds in any reaction and the lowercase letters represent the coefficients for each compound.

For example:

i. $H_2O_{(g)} + CH_{4(g)} \rightleftharpoons CO_{(g)} + 3H_{2(g)}$

$$K_c = \frac{[CO][H_2]^3}{[H_2O][CH_4]}$$

ii. $N_{2(g)} + 3H_{2(g)} \rightleftharpoons 2NH_{3(g)}$

$$K_c = \frac{[NH_3]^2}{[N_2][H_2]^3}$$

To determine K_c, substitute in the concentrations of each compound at equilibrium.
For example, using $N_{2(g)} + 3H_{2(g)} \rightleftharpoons 2NH_{3(g)}$ at 500 K

$[N_2] = 3.0 \times 10^{-2}$ M
$[H_2] = 3.7 \times 10^{-2}$ M
$[NH_3] = 1.6 \times 10^{-2}$ M

$$K_c = \frac{[NH_3]^2}{[N_2][H_2]^3} = \frac{(1.6 \times 10^{-2})^2}{(3.0 \times 10^{-2})(3.7 \times 10^{-2})^3} = \frac{2.56 \times 10^{-4}}{1.52 \times 10^{-6}} = 1.68 \times 10^2$$

$\mathbf{K_c = 1.7 \times 10^2}$

Note: I carry one more digit than the correct number of significant figures until the end to prevent rounding errors – ask your professor how they would like calculations to be done.
You can also calculate the concentration of one compound if you know the concentrations of the others and K_c.

For example, using the same reaction as above but different concentrations of reactants:

$[N_2] = 6.0 \times 10^{-2}$ M
$[H_2] = 5.6 \times 10^{-2}$ M
$K_c = 1.7 \times 10^{2}$

From this we can determine the concentration of NH_3 at equilibrium.

$$K_c = \frac{[NH_3]^2}{[N_2][H_2]^3} = \frac{(x)^2}{(6.0 \times 10^{-2})(5.6 \times 10^{-2})^3} = 1.7 \times 10^2$$

$$1.7 \times 10^2 = \frac{x^2}{1.05 \times 10^{-5}} \Rightarrow x^2 = 1.79 \times 10^{-3} \Rightarrow x = 4.23 \times 10^{-2}$$

$[NH_3] = 4.2 \times 10^{-2}$ M

To determine if a reaction is at equilibrium, you use a term called Q_c. It is calculated in the same way as the K_c only using the current concentrations of the compounds. At equilibrium the Q_c equals the K_c. When Q_c is larger than K_c the reaction has too many products and the reaction will move to the left to reach equilibrium. When Q_c is smaller than the K_c the reaction has too many reactants and will move to the right to reach equilibrium.

For the reaction $N_{2(g)} + 3H_{2(g)} \rightleftharpoons 2NH_{3(g)}$

$Kc = 1.7 \times 10^{2}$ at 500 K
$[N_2] = 2.0 \times 10^{-2}$ M
$[H_2] = 3.5 \times 10^{-2}$ M
$[NH_3] = 2.0 \times 10^{-2}$ M

Is the reaction at equilibrium, if not in which direction will the reaction proceed?

$$Q_c = \frac{[NH_3]^2}{[N_2][H_2]^3} = \frac{(2.0 \times 10^{-2})^2}{(2.0 \times 10^{-2})(3.5 \times 10^{-2})^3} = \frac{4.00 \times 10^{-4}}{8.58 \times 10^{-7}} = 4.66 \times 10^2$$

$Q_c = 4.7 \times 10^2$ $K_c = 1.7 \times 10^2$

Q_c is larger than K_c, therefore the reaction will move to the left (making more reactants).

Steps to solve equilibrium problems:

1. Write out the balanced equation for a reaction.

2. List any pertinent information given to you in the problem. Also define what it is that you need to find. You may need to convert some information given to you in the problem into another form to be able to utilize it in the problem. For example you may need to convert moles into molarity or pH into H^+ concentration.

3. If any concentrations are changing, under the equation make a table listing the Initial concentration, the Change in concentration and the Equilibrium concentration (an ICE table). Define x as one of the unknown concentrations.

   You can check your answer by substituting the information back into the equilibrium equation and solving for the equilibrium constant.

4. Use the pertinent information from the ICE table (and x) and finish the problem.

Tip: In general you will either be given K_c and the initial concentrations and asked to find the equilibrium concentrations or you will be given enough information about the some of the initial and equilibrium concentrations to find K_c and the other equilibrium concentrations.

Example:

I The equilibrium constant for the reaction of hydrogen gas and iodine gas to form hydrogen iodide is 57.0 at 700 K. If 1.00 mole of each reactant is put into a 10.0 L reaction vessel at 700 K, what are the concentrations of each of the 3 gases at equilibrium? How many moles of each gas are present?

1. *Write out the balanced equation for a reaction.*

$$H_{2(g)} + I_{2(g)} \rightleftharpoons 2HI_{(g)}$$

2. *List any pertinent information given to you in the problem. Also define what it is that you need to find. You may need to convert some information given to you in the problem into another form to be able to utilize it in the problem. For example you may need to convert moles into molarity or pH into H^+ concentration.*

   Since we need to use molarity for the ICE table we need to convert moles to molarity.

$$\frac{1.00 \text{ moles } H_2 \text{ and } I_2}{10.0 \text{ L}} = 0.100 \text{ M } H_2 \text{ and } I_2$$

3. *If any concentrations are changing, under the equation make a table listing the Initial concentration, the Change in concentration and the Equilibrium concentration (an ICE table). Define x as one of the unknown concentrations.*

Since the concentrations will change, let x equal the change in the H_2 concentration.

	$H_{2(g)}$ +	$I_{2(g)}$ ⇌	$2HI_{(g)}$
Initial (M)	0.100	0.100	0
Change (M)	-x	-x	+2x
Equilibrium (M)	0.100 – x	0.100 – x	2x

$$K_c = \frac{[HI]^2}{[H_2][I_2]} \Rightarrow 57.0 = \frac{(2x)^2}{(0.100\text{-}x)(0.100\text{-}x)} \Rightarrow 57.0 = \frac{(2x)^2}{(0.100\text{-}x)^2}$$

Since this equation is a perfect square, take the square root of both sides of the equation.

$$7.550 = \frac{2x}{0.100 - x} \Rightarrow 7.550(0.100\text{-}x) = 2x \Rightarrow 0.7550 - 7.550x = 2x$$

$$0.7550 = 9.550x \Rightarrow x = 7.906 \times 10^{-2} \Rightarrow \mathbf{x = 7.91 \times 10^{-2}\ M}$$

Therefore at equilibrium:

$$\mathbf{[I_2] = [H_2] = 0.100 - 7.91 \times 10^{-2} = 2.09 \times 10^{-2}\ M}$$
$$\mathbf{[HI] = (2)(7.91 \times 10^{-2}\ M) = 0.158\ M}$$

Note: If you use the negative part of the square root (i.e. –7.55) you will get a number for x that is larger than your original concentration of H_2 and I_2. We don't include numbers that don't make sense in the context of the problem.

Check if the answer is correct so far:

$$K_c = \frac{[HI]^2}{[H_2][I_2]} \Rightarrow K_c = \frac{(0.158)^2}{(2.09 \times 10^{-2})(2.09 \times 10^{-2})} \Rightarrow \frac{2.496 \times 10^{-2}}{4.368 \times 10^{-4}} = 57.14$$

K_c = 57.1 **K_c (given) = 57.0**

The K_c's are close enough for our purposes, therefore the concentrations are correct.

4. *Use the pertinent information from the ICE table (and x) and finish the problem.*
To determine the number of moles at equilibrium we take the molarity and multiply by the liters in the container.

$(2.09 \times 10^{-2}$ M)(10.0 L) = **0.209 moles of H_2 and I_2**
(0.158 M)(10.0 L) = **1.58 moles of HI**

Problems:

1. Hydrogen gas is made commercially from methane by the following reaction:

$$H_2O_{(g)} + CH_{4(g)} \rightleftharpoons CO_{(g)} + 3H_{2(g)}$$

This reaction is carried out at 1400 K. At this temperature the K_c is 4.7. If the mixture contains 0.050 M H_2O, 0.030 M CH_4, 0.20 M CO and 0.30 M H_2, is it at equilibrium? If not, which way does the reaction go to reach equilibrium?

Solution

2. Acetic acid dissociates in water to produce acetate ion.

$$CH_3COOH_{(aq)} \rightleftharpoons H^+_{(aq)} + CH_3COO^-_{(aq)} \qquad K_c = 1.76 \times 10^{-5} \text{ at } 25^oC$$

You dilute 5.00 ml of 6.00 M acetic acid with 45.0 ml H_2O. What is the molarity of the acetate ion in the diluted solution?

Solution

3. At 450^{o}C ammonia gas decomposes into hydrogen and nitrogen gases. An experiment starts by placing 2.25 moles of ammonia in a 3.00 L container and heating it to 450^{o}C. At equilibrium there are 0.522 moles of ammonia. Based on this information determine the final concentration of each gas and the K_c of the reaction.

Solution

Solutions:

1. Hydrogen gas is made commercially from methane by the following reaction:

$$H_2O_{(g)} + CH_{4(g)} \rightleftharpoons CO_{(g)} + 3H_{2(g)}$$

This reaction is carried out at 1400 K. At this temperature the K_c is 4.7. If the mixture contains 0.050 M H_2O, 0.030 M CH_4, 0.20 M CO and 0.30 M H_2, is it at equilibrium? If not, which way does the reaction go to reach equilibrium?

$$H_2O_{(g)} + CH_{4(g)} \rightleftharpoons CO_{(g)} + 3H_{2(g)} \qquad K_c = 4.7$$

$[H_2O] = 0.050$ M
$[CH_4] = 0.030$ M
$[CO] = 0.20$ M
$[H_2] = 0.30$ M

$$Q_c = \frac{[CO][H_2]^3}{[H_2O][CH_4]} = \frac{(0.20)(0.30)^3}{(0.050)(0.030)} = \frac{5.40 \text{ x } 10^{-3}}{1.50 \text{ x } 10^{-3}} = 3.60$$

$Q_c = 3.6$ $\qquad$ $K_c = 4.7$

The reaction is not at equilibrium. Since K_c is larger than Q_c the reaction will move to the right making more products.

Return to Problems

2. Acetic acid dissociates in water to produce acetate ion.

$$CH_3COOH_{(aq)} \rightleftharpoons H^+_{(aq)} + CH_3COO^-_{(aq)} \qquad K_c = 1.76 \times 10^{-5} \text{ at } 25^oC$$

You dilute 5.00 ml of 6.00 M acetic acid with 45.0 ml H_2O. What is the molarity of the acetate ion in the diluted solution?

We have the balanced equation given to us in the problem. We need to calculate the initial concentration of acetic acid. Use the $M_1V_1 = M_2V_2$ formula.

$M_1 = 6.00$ M $\qquad M_2 = ?$

$V_1 = 5.00$ ml $\qquad V_2 = 45.0$ ml + 5.00 ml = 50.0 ml

(6.00 M)(5.00 ml) = (M_2)(50.0 ml)

$\Rightarrow$ $M_2 = 0.600$ M acetic acid is the initial concentration.

Since the concentrations will change let x equal the change in proton and acetate ion concentration.

	$CH_3COOH_{(aq)}$	$\rightleftharpoons$	$H^+_{(aq)}$	+	$CH_3COO^-_{(aq)}$
Initial	0.600		0		0
Change	-x		+x		+x
Equilibrium	0.600 - x		x		x

$$Kc = \frac{[H^+][CH_3COO^-]}{[CH_3COOH]} \Rightarrow 1.76 \times 10^{-5} = \frac{(x)(x)}{(0.600 - x)}$$

To determine if x will significantly alter the value for acetic acid, multiply the K_c by 100. If the resulting number is less than your original concentration x will not significantly alter the number so you can drop x out of that term.

$(1.76 \times 10^{-5})(100) = 1.76 \times 10^{-3}$

This is less than 0.600 so x can be dropped out of this term.

$$1.76 \times 10^{-5} = \frac{(x)(x)}{(0.600)} \Rightarrow (1.76 \times 10^{-5})(0.600) = x^2$$

$x^2 = 1.056 \times 10^{-5} \Rightarrow x = 3.25 \times 10^{-3}$

Since we defined x as the change in concentration of protons and acetate ions, the answer to this problem is that the final acetate ion concentration is 3.25×10^{-3} M.

Return to Problems

3. At 450°C ammonia gas decomposes into hydrogen and nitrogen gases. An experiment starts by placing 2.25 moles of ammonia in a 3.00 L container and heating it to 450°C. At equilibrium there are 0.522 moles of ammonia. Based on this information determine the final concentration of each gas and the K_c of the reaction.

The balanced equation is: $2NH_3 \rightleftharpoons N_2 + 3H_2$

Convert moles to molarity for the ICE table:

$$\frac{2.25 \text{ moles } NH_3}{3.00 \text{ L}} = 0.750 \text{ M } NH_3 \text{ initial concentration}$$

$$\frac{0.522 \text{ moles } NH_3}{3.00 \text{ L}} = 0.174 \text{ M } NH_3 \text{ final concentration}$$

We know from the problem that the concentrations will change so let x equal the change in N_2 concentration.

	$2NH_3$	$\rightleftharpoons$	N_2	+	$3H_2$
Initial	0.750		0		0
Change	-2x		+x		+3x
Equilibrium	0.174		x		3x

. $0.750 - 2x = 0.174 \Rightarrow 2x = 0.750 - 0.174 \Rightarrow x = 0.288$

Molarity of N_2 = x = **0.288 M N_2**

Molarity of H_2 = 3x = (3)(0.288) = **0.864 M H_2**

Molarity of NH_3 = 0.174 M NH_3

$$K_c = \frac{[N_2][H_2]^3}{[NH_3]^2} \Rightarrow K_c = \frac{(0.288)(0.864)^3}{(0.174)^2} = 6.14$$

K_c = 6.14

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