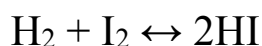


7.5 Quantitative Changes in Equilibrium Systems

What is Q?

- Q is the reaction quotient.
- It is a mathematical application of Le Châtelier's Principle
- Use the equilibrium constant expression. But, use initial or given concentrations instead of equilibrium concentrations.
- Solve using equilibrium equation
- Compare Q value to actual equilibrium value K_e
 - If $Q < K_e$, products will be formed (reaction goes to the right)
 - If $Q > K_e$, reactants will be formed (reaction goes to the left)
 - If $Q = K_e$, there will not be a change in concentration
- E.g. When 3.0 mol of HI, 2.0 mol of H_2 and 1.5 mol of I_2 are placed in a 1.0 L container at 448°C , ~~will a reaction occur? If so~~, which reaction takes place? At 448°C , $K_e = 50$.



$$K_e = \frac{[HI]^2}{[H_2][I_2]} = 50 \quad \text{vs} \quad Q = \frac{[HI]^2}{[H_2][I_2]} = \frac{[3.0]^2}{[2.0][1.5]} = \frac{9.0}{3.0} = 3.0$$

$K_e > Q$, 滯 the reaction goes to the right and HI is formed

How to solve an equilibrium problem.

- a. Write the equilibrium reaction equation.
- b. Write the equilibrium constant expression.
- c. Identify the problem type.

Type 1: equilibrium [reactant(s)] and [product(s)] are given, find the value of K_e .

Type 2: K_e given; find the values of [reactant(s)] and [product(s)] at equilibrium.

- d. Solve.

Solving a Type 1 Problem

- Input concentrations of solutes or gases (or partial pressure of gases) into K_e expression and calculate K_e .
- Units of all equilibrium species must be the same (usually mol/L)

Solving a Type 2 Problem

- Range from simple to difficult.
- If only one concentration missing, substitute and solve.
- If presented with unknown concentrations use ICE method. (Initial, Change, Equilibrium).
 - a. Input the algebraic representations for [reactant(s)] and [product(s)] into K_e expression and solve to given value of K_e .
 - b. Isolate for “x” in simple cases and re-substitute “x” into algebraic expressions for [reactant(s)] and [product(s)] to determine exact values.

E.g. For the reaction: $\text{NH}_4\text{Cl}_{(s)} \leftrightarrow \text{NH}_{3(g)} + \text{HCl}_{(g)}$

K_e is found to be 6.0×10^{-9} . What is the concentration of the products at equilibrium?

∴ $K_e = [\text{NH}_3][\text{HCl}] = 6.0 \times 10^{-9}$

Use your ICE Tables

	NH_4Cl	\leftrightarrow	$[\text{NH}_3]$	$[\text{HCl}]$
initial	some amount		0	0
change			+x	+x
equilibrium			x	x

$$K_e = [\text{NH}_3][\text{HCl}]$$

$$6.0 \times 10^{-9} = (x)(x)$$

$$x = 7.7 \times 10^{-5}$$

∴ for the above reaction with the given K_e value the concentrations of the products would each be $7.7 \times 10^{-5} \text{ mol/L}$

- If both the numerator and denominator in the K_e expression are squares, solve by taking the root of both sides and isolate for “x”. See example on p. 467.
- If only the numerator or the denominator in the K_e expression is a square (the other is not) solve by approximation or the quadratic equation. See example on p. 469 and p. 476.

E.g. $\text{I}_{2(\text{g})} \leftrightarrow 2\text{I}_{(\text{g})}$ where $K_e = 3.8 \times 10^{-5}$

What are the concentrations at equilibrium if you initially start with 0.200 mol/L of I_2 ?

$$K_e = \frac{[\text{I}]^2}{[\text{I}_2]} = 3.8 \times 10^{-5}$$

	$[\text{I}_2]$	\leftrightarrow	$2[\text{I}]$
initial	0.200		0
change	-x		+2x
equilibrium	$0.200 - x$		2x

substitute:

$$3.8 \times 10^{-5} = \frac{(2x)^2}{(0.200 - x)}$$

Option 1: approximation

- Use approximation rule to see if it can be solved by approximation.
- If the concentration from which “x” is being subtracted from, or to which “x” is added, must be at least 100 times larger than the value of the given K_e .

check: $\frac{0.200}{3.8 \times 10^{-5}} = 5260$, since it is greater than 100 you can use the approximation $0.200 \approx (0.200 - x)$

- What does this mean? The concentration of the product is very small compared to the reactant. Very little I produced.

$$3.8 \times 10^{-5} = \frac{(2x)^2}{(0.200)}$$

Solve: $x = 1.38 \times 10^{-3}$
 $[\text{I}_2] = 0.200 - x = 0.200 - 1.38 \times 10^{-3} = 0.198 \text{ mol/L}$
 $[\text{I}] = 2x = 2(1.38 \times 10^{-3}) = 0.003 \text{ mol/L}$

Option 2: quadratic equation

$$3.8 \times 10^{-5} = \frac{(2x)^2}{(0.200 - x)}$$

$$4x^2 + 3.8 \times 10^{-5}x - 7.6 \times 10^{-6} = 0$$

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

$$x = 1.38 \times 10^{-3}$$

$$[I_2] = 0.200 - x = 0.200 - 1.38 \times 10^{-3} = 0.198 \text{ mol/L}$$

$$[I] = 2x = 2(1.38 \times 10^{-3}) = 0.003 \text{ mol/L}$$

Quantitative Aspects of Le Châtelier's Principle

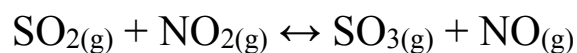
- When a system in equilibrium is disturbed, the equilibrium position will shift.

E.g. Analysis of an equilibrium mixture is shown to be:

$$[SO_2] = 4.0 \text{ mol/L}; [SO_3] = 3.0 \text{ mol/L};$$

$$[NO_2] = 0.50 \text{ mol/L}; \text{ and } [NO] = 2.0 \text{ mol/L}.$$

Using the reaction equation below, what is the new equilibrium concentrations when 1.5 mol of NO_2 is added to a litre of the mixture.



$$K_e = \frac{[\text{SO}_3][\text{NO}]}{[\text{SO}_2][\text{NO}_2]} = \frac{(3.0)(2.0)}{(4.0)(0.50)} = 3.0$$

	$\text{SO}_{2(g)}$	+	$\text{NO}_{2(g)}$	\leftrightarrow	$\text{SO}_{3(g)}$	+	$\text{NO}_{(g)}$
(I) 1 st equilibrium	4.0		0.50		3.0		2.0
(C) change	-x		1.5-x		+x		+x
(E) 2 nd equilibrium	(4.0 - x)		(0.50 + 1.5 - x)		(3.0 + x)		(2.0 + x)

$$K_e = \frac{[\text{SO}_3][\text{NO}]}{[\text{SO}_2][\text{NO}_2]} = \frac{(3.0 + x)(2.0 + x)}{(4.0 - x)(0.50 + 1.5 - x)} = 3.0$$

$$2.0x^2 - 23x + 18 = 0$$

where $x = 0.85$ (discard 10.7)

$$\text{SO}_{2(g)} = 4.0 - 0.85 = 3.15 \text{ mol/L}$$

$$\text{NO}_{2(g)} = 2.0 - 0.85 = 1.15 \text{ mol/L}$$

$$\text{SO}_{3(g)} = 3.0 + 0.85 = 3.85 \text{ mol/L}$$

$$\text{NO}_{(g)} = 2.0 + 0.85 = 2.85 \text{ mol/L}$$

Homework

- Practice 1,2,3,4,5,6,7,8,9,10 and Questions 1,2,3,4,5,6,7,8