7.4 Predicting the Direction of a Reaction

Effect of a Change in Conc. of an Equilibrium System

- If a system in equilibrium is disturbed, the system will tend to react so as to establish a new equilibrium.
- Le Châtelier's Principle states that when a stress is applied to a system at equilibrium, the system readjusts so as to relieve or offset the stress.
- An external stress to an equilibrium could be any one or more of the following:
  - a) Change in [reactant]
  - b) Change in [product]
  - c) Change in temperature
  - d) Change in pressure } only for gases
  - e) Change in volume }

- E.g. $H_{2(g)} + I_{2(g)} \leftrightarrow 2HI_{(g)}$

Change (Stress)	**Response**	**Result**
↑ $[H_2]$	shift → to decrease $[H_2]$	↑ [HI]
↑ $[I_2]$	shift → to decrease $[I_2]$	↑ [HI]
↓$[H_2]$ or ↓$[I_2]$	shift ← to decrease [HI]	↑ $[H_2]$ + ↑ $[I_2]$
↑ [HI]	shift ← to decrease [HI]	↑ $[H_2]$ + ↑ $[I_2]$
↓ [HI]	shift → to decrease $[H_2]$ & $[I_2]$	↑ [HI]

Effect of a Change in Volume or Pressure

- When the volume of a gaseous reaction that has an unequal number of gases on each side of the equation is decreased, the equilibrium will shift so as to reduce the number of gas molecules.

- E.g. $N_{2(g)} + 3H_{2(g)} \leftrightarrow 2NH_{3(g)}$ $\Delta H = -92$ kJ

Change (Stress)	**Response**	**Result**
↑ pressure = ↓ volume	shift → to decrease # of gas molecules	↑ $[NH_3]$
↓ pressure = ↑volume	shift ← to increase # of gas molecules	↑ $[N_2]$ + ↑ $[H_2]$

- E.g. $H_{2(g)} + I_{2(g)} \leftrightarrow 2HI_{(g)}$
  Changing the pressure in this reaction will not change equilibrium since there is an equal number of reactant and product molecules.

Effect of a Change in Temperature

- Increasing the temperature shifts the reaction in the direction that produces an endothermic change, while decreasing the temperature shifts the reaction in a direction that produces an exothermic change.
- E.g. $N_{2(g)} + 3H_{2(g)} \leftrightarrow 2NH_{3(g)}$ $\Delta H = -92$ kJ

Change (Stress)	**Response**	**Result**
↑ temperature	shift ← decomposition of NH_3 to absorb heat to compensate (favours endothermic reaction)	↑ $[N_2]$ + ↑ $[H_2]$
↓ temperature	shift → formation of NH_3 to generate heat to compensate (favours exothermic reaction)	↑ $[NH_3]$

- Increasing the temperature increases both the forward and reverse reaction. However, an endothermic reaction is affected by greater extent than an exothermic reaction.

Effect of Catalysts

- Catalysts cause reactions to reach equilibrium faster, but they do not alter the amounts of components at equilibrium.
- A catalyst speeds up the forward and reverse reaction to the same degree. It only allows the system to reach equilibrium faster.

Common Ion Effect

- The effect of a common ion is similar to the addition of reactant or product.
- E.g. $AgI_{(aq)} + NaCl_{(aq)} \leftrightarrow AgCl_{(s)} + NaI_{(aq)}$, the addition of $Cl^-_{(aq)}$ will shift the equilibrium to the right since it will increase the common ion on the reactant side and in an attempt to reduce the concentration of the common ion, more precipitate if formed.

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 concentrations instead of equilibrium concentrations.
- If $Q < K_{eq}$, products will be formed (reaction goes to the right)
- If $Q > K_{eq}$, reactants will be formed (reaction goes to the left)
- If $Q = K_{eq}$, 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 448ºC, will a reaction occur? If so, which reaction takes place? At 448ºC, $K_e = 50$.

$H_2 + I_2 \leftrightarrow 2HI$

$$K_{eq} = \frac{[HI]^2}{[H_2][I_2]} = 50$$

$$Q = \frac{[HI]^2}{[H_2][I_2]} = \frac{[3.0]^2}{[2.0][1.5]} = \frac{9.0}{3.0} = 3.0$$

$K_{eq} > Q$, $\therefore$ the reaction goes to the right and HI is formed

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: $[SO_2] = 4.0$ mol/L; $[SO_3] = 3.0$ mol/L; $[NO_2] = 0.50$ mol/L; and $[NO] = 2.0$ 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.

$SO_{2(g)} + NO_{2(g)} \leftrightarrow SO_{3(g)} + NO_{(g)}$

$$K_{eq} = \frac{[SO_3][NO]}{[SO_2][NO_2]} = \frac{(3.0)(2.0)}{(4.0)(0.50)} = 3.0$$

		$SO_{2(g)}$	+	$NO_{2(g)}$	$\leftrightarrow$	$SO_{3(g)}$	+	$NO_{(g)}$
(I)	1st equilibrium	4.0		0.50		3.0		2.0
(C)	change	–x		1.5–x		+x		+x
(E)	2nd equilibrium	(4.0 –x)		(0.50+1.5–x)		(3.0+x)		(2.0+x)

$$K_{eq} = \frac{[SO_3][NO]}{[SO_2][NO_2]} = \frac{(3.0+x)(2.0+x)}{(4.0-x)(0.50+1.5-x)} = 3.0$$

$2.0x^2 - 23x + 18 = 0$ where $x = 0.85$ (discard 10.7)

$SO_{2(g)}$ = 4.0 – 0.85 = 3.15 mol/L
$NO_{2(g)}$ = 2.0 – 0.85 = 1.15 mol/L
$SO_{3(g)}$ = 3.0 + 0.85 = 3.85 mol/L
$NO_{(g)}$ = 2.0 + 0.85 = 2.85 mol/L

The Haber Process: Ammonia for Food and Bombs

- The Haber process is a practical industrial application of Le Châtelier's Principle.
- The process synthesizes ammonia from elemental hydrogen and nitrogen for use in agriculture.
- Originally for the production of bombs during WWII, but, it won Haber a Nobel Prize because the process created ammonia that could be used as fertilizer to increase crop yields.

Homework

- Read 7.4
- All Practice Questions
- All Section Review Questions
- Start working on review for test.