7.5 Quantitative Changes in Equilibrium Systems

Goal: Develop strategies to solve various equilibrium scenarios

Scenario #1 – Direction of reaction – What is Q?

- Q is the reaction quotient.
- It is a mathematical application of Le Châtelier's Principle
- Use the equilibrium constant expression
- Use initial or given concentrations instead of equilibrium concentrations.
- Solve using equilibrium expression – calculate a Q value
- Compare Q value to actual equilibrium value K_e
  - If $Q < K_e$, products will be formed (reaction goes forward)
  - If $Q > K_e$, reactants will be formed (reaction goes in reverse)
  - If $Q = K_e$, there will not be a change in concentration

- Ex. 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, which direction does the reaction go to reach equilibrium? $K_e = 50$.

$$H_2 + I_2 \leftrightarrow 2HI$$

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

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

Scenario #2 – Equilibrium constant calculation

a) Write the balanced equation.
b) Write the equilibrium expression.
c) Input concentrations of solutes or gases (or partial pressure of gases) into K_e expression and calculate K_e.
d) Units of all equilibrium species must be the same (usually mol/L)
e) Page 443

Scenario #3 – One unknown concentration at Equilibrium

a) Write the balanced equation.
b) Write the equilibrium expression.
c) Input concentrations
d) Solve for missing value
e) Page 466

Scenario #4 – Unknown Concentrations at Equilibrium

- Range from simple to difficult.
  - Given initial concentrations
  - Calculate Q
  - Use ICE table
  - Solve for "x"

- 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 <u>**or**</u> the quadratic equation. See example on p. 469 and p. 476.

Ex. $I_{2(g)} \leftrightarrow 2I_{(g)}$ $K_e = 3.8 \times 10^{-5}$

What are the concentrations at equilibrium if the initial concentration of I_2 is 0.200 mol/L?

$$K_e = \frac{[I]^2}{[I_2]} = 3.8 \times 10^{-5}$$

	$I_{2(g)}$	$\leftrightarrow$	$2I_{(g)}$
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: $\dfrac{0.200}{3.8 \times 10^{-5}} = 5260$ *, since it is greater than 100 you can use the approximation 0.200 ≈ (0.200 – x)*

- What does this mean? The concentration of the product is very small compared to the reactant. Very little "I" produced.
- Solve: $3.8 \times 10^{-5} = \dfrac{(2x)^2}{(0.200)}$

x = 1.38×10^{-3}

$[I_2]$ = 0.200 – x = 0.200 – 1.38×10^{-3} = 0.198 mol/L

[I] = 2x = 2(1.38×10^{-3}) = 0.003 mol/L

Option 2: quadratic equation

$$3.8\times10^{-5} = \frac{(2x)^2}{(0.200 - x)}$$

$4x^2 + 3.8\times10^{-5}x - 7.6\times10^{-6} = 0$ substitute into: $x = \dfrac{-b \pm \sqrt{b^2 - 4ac}}{2a}$

$x = 1.38\times10^{-3}$

$[I_2] = 0.200 - x = 0.200 - 1.38\times10^{-3} = 0.198$ mol/L

$[I] = 2x = 2(1.38\times10^{-3}) = 0.003$ mol/L

Scenario #5 – K is provided but No concentration values are

- Most intimidating
- One of the susbstances is a solid or liquid
- ICE table helps make the connection between "x" and K value

Ex. For the reaction: $NH_4Cl_{(s)} \leftrightarrow NH_{3(g)} + HCl_{(g)}$

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

Use your ICE Tables

$\therefore K_e = [NH_3][HCl] = 6.0\times10^{-9}$

	NH_4Cl	→	$[NH_3]$	$[HCl]$
initial	some amount		0	0
change			+x	+x
equilibrium			x	x

$K_e = [NH_3][HCl] = 6.0\times10^{-9} = (x)(x)$

$x = 7.7\times10^{-5}$

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

Scenario #6 – A system in equilibrium is stressed – Quantitative Analysis of Le Châtelier's Principle

- When a system in equilibrium is disturbed, the equilibrium position will shift.
- Calculate K from equilibrium values
- Change will determine what direction the equilibrium will shift
- Solve for "x"

Ex. 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?

$SO_{2(g)} + NO_{2(g)} \leftrightarrow SO_{3(g)} + NO_{(g)}$ $\quad K_e = \frac{[SO_3][NO]}{[SO_2][NO_2]} = \frac{(3.0)(2.0)}{(4.0)(0.50)} = 3.0$

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

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

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

Homework

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