

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 448°C, which direction does the reaction go to reach equilibrium? $K_e = 50$.

$$\begin{array}{ccc} H_2 + I_2 \leftrightarrow 2HI & & \\ K_e = \frac{[HI]^2}{[H_2][I_2]} = 50 & \text{vs} & Q = \frac{[HI]^2}{[H_2][I_2]} = \frac{[3.0]^2}{[2.0][1.5]} = \frac{9.0}{3.0} = 3.0 \end{array}$$

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

Scenario #2 – Equilibrium constant calculation

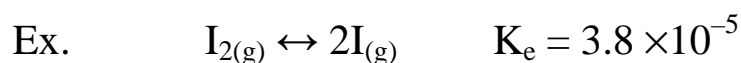
- a) Write the balanced equation.
- b) Write the equilibrium expression.
- c) Input concentrations of solutes or gases (or partial pressure of gases) into K_e expression and calculate K_e .
- d) Units of all equilibrium species must be the same (usually mol/L)
- e) Page 443

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 or the quadratic equation. See example on p. 469 and p. 476.



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

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

	$\text{I}_{2(\text{g})}$	\leftrightarrow	$2\text{I}_{(\text{g})}$
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: $\frac{0.200}{3.8 \times 10^{-5}} = 5260$, 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

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

$$4x^2 + 3.8 \times 10^{-5}x - 7.6 \times 10^{-6} = 0 \quad \text{substitute into:} \quad x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$
$$x = 1.38 \times 10^{-3}$$

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

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

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

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

Ex. 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?

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

Use your ICE Tables

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

$$K_e = [\text{NH}_3][\text{HCl}] = 6.0 \times 10^{-9} = (x)(x)$$
$$x = 7.7 \times 10^{-5}$$

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

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

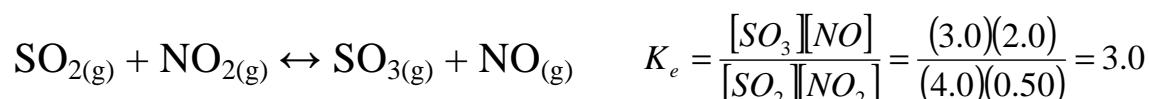
- When a system in equilibrium is disturbed, the equilibrium position will shift.
- Calculate K from equilibrium values
- Change will determine what direction the equilibrium will shift
- Solve for “x”

Ex. Analysis of an equilibrium mixture is shown to be:

$[\text{SO}_2] = 4.0 \text{ mol/L}$; $[\text{SO}_3] = 3.0 \text{ mol/L}$;

$[\text{NO}_2] = 0.50 \text{ mol/L}$; and $[\text{NO}] = 2.0 \text{ mol/L}$.

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?



	$\text{SO}_{2(g)}$	+	$\text{NO}_{2(g)}$	\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)

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

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

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

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

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

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

Homework

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