EQUILIBRIUM – 2
CALCULATING CONCENTRATIONS AT EQUILIBRIUM

Dr. Sapna Gupta

CALCULATING CONCENTRATIONS

- Concentrations of chemicals can be calculated.
- Use the ICE method – where concentrations of:
- Initial
- Change and at
- Equilibrium are calculated

EXAMPLE: CALCULATING CONC.

When heated PCl_5, phosphorus pentachloride, forms PCl_3 and Cl_2 as follows:

$$PCl_5(g) \rightleftharpoons PCl_3(g) + Cl_2(g)$$

When 1.00 mol PCl_5 in a 1.00-L container is allowed to come to equilibrium at a given temperature, the mixture is found to contain 0.135 mol PCl_3. What is the molar composition of the mixture?

Solution:

	$PCl_5(g)$ $\rightleftharpoons$	$PCl_3(g)$ +	$Cl_2(g)$
Initial	1.00 mol	0	0
Change	$-x$	$+x$	$+x$
Equilibrium	$1.00 - x$	x	x

We were told that the equilibrium amount of PCl_3 is 0.135 mol.

That means x = 0.135 mol.

Moles PCl_5 = 1.00 – 0.135 = 0.87 mol

Moles PCl_3 = 0.135 mol

Moles Cl_2 = 0.135 mol

USING THE ICE METHOD

Hydrogen iodide decomposes to hydrogen gas and iodine gas.

$$2HI(g) \rightleftharpoons H_2(g) + I_2(g) \quad K_c = 0.016 \text{ at } 800\text{ K}$$

If 0.50 mol HI is placed in a 5.0-L flask, what will be the composition of the equilibrium mixture in molarities?

Solution:

$$[HI]_0 = \frac{0.50\text{ mol}}{5.0\text{ L}} = 0.10\ M$$

	$2HI(g)$	$H_2(g)$ +	$I_2(g)$
Initial	0.10 M	0	0
Change	$-2x$	$+x$	$+x$
Equilibrium	$0.10 - 2x$	x	x

The K_c expression is, $K_c = \dfrac{[H_2][I_2]}{[HI]^2}$

$$0.016 = \frac{[x][x]}{[0.10 - 2x]^2} = \frac{x^2}{(0.10 - 2x)^2}$$

USING THE ICE METHOD… CONTD…

Because the right side of the equation is a perfect square, we can take the square root of both sides. *(From previous slide)*

$$\sqrt{0.016} = \sqrt{\frac{x^2}{(0.10-2x)^2}}$$

$$0.016 = \frac{[x][x]}{[0.10-2x]^2} = \frac{x^2}{(0.10-2x)^2}$$

$$0.126 = \frac{x}{(0.10-2x)}$$

Solving:

$$0.126(0.10 - 2x) = x$$

$$0.0126 - 0.252x = x$$

$$0.0126 = 1.252x$$

$$x = 0.010\ M$$

Substituting:

$$[H_2] = [I_2] = x = 0.010\,M$$

$$[HI] = 0.10 - 2x = 0.10 - 0.020 = 0.08\,M$$

WHEN K_c EXPRESSION IS NOT SQUARE ROOT

When the K_c expression is not a perfect square, the equation must be rearranged to fit the quadratic format:

$$ax^2 + bx + c = 0$$

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

EXAMPLE: 1

N_2O_4 decomposes to NO_2. The equilibrium reaction in the gas phase is

$$N_2O_4(g) \rightleftharpoons 2NO_2(g) \quad \text{At } 100°\text{C, } K_c = 0.36.$$

If a 1.00-L flask initially contains 0.100 *M* N_2O_4, what will be the equilibrium concentration of NO_2?

Solution:

	$N_2O_4(g)$	$2NO_2(g)$
Initial	0.100 *M*	0
Change	$-x$	$+2x$
Equilibrium	$0.100 - x$	$2x$

The K_c expression is, $K_c = \dfrac{[NO_2]^2}{[N_2O_4]}$

$$0.36 = \frac{[2x]^2}{[0.100 - x]} = \frac{4x^2}{(0.100 - x)}$$

continued on next slide…

CONTD….

Substitute: $$0.36 = \frac{[2x]^2}{[0.100 - x]} = \frac{4x^2}{(0.100 - x)}$$

Rearrange: (by cross multiplication) $$4x^2 + 0.36x - 0.036 = 0$$

$$ax^2 + bx + c = 0$$

$$a = 4 \qquad b = 0.36 \qquad c = -0.036$$

Substitute:

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

$$x = \frac{-0.36 \pm \sqrt{(0.36)^2 - 4(4)(-0.036)}}{2(4)}$$

Solve:

$$x = \frac{-0.36 \pm \sqrt{0.7056}}{8}$$

$$x = -0.045 \pm 0.105$$

$$x = 0.06 \qquad x = \cancel{-0.15}$$

Substitute to find the equilibrium concentration of NO_2:

$$[NO_2] = 2x = 2(0.06) = 0.12\,M$$

EXAMPLE: 2

Given: $H_2(g) + F_2(g) \rightleftharpoons 2HF(g)$; $K_c = 1.15 \times 10^2$

3.000 mol of each species is put in a 1.500-L vessel. What is the equilibrium concentration of each species?

Solution:

Calculate initial conc. : $[H_2]_0 = [F_2]_0 = [HF]_0 = \dfrac{3.000 \text{ mol}}{1.500 \text{ L}} = 2.000\ M$

	$H_2(g)$ +	$F_2(g)$ ⇌	$2HF(g)$
Initial	2.000 *M*	2.000 *M*	2.000 *M*
Change	$-x$	$-x$	$+2x$
Equilibrium	$2.000 - x$	$2.000 - x$	$2.000 + 2x$

$$K_c = \frac{[HF]^2}{[H_2][F_2]}$$

$$1.15 \times 10^2 = \frac{[2.000 + 2x]^2}{[2.000 - x]^2}$$

CONTD.....

- Contd….

$$\sqrt{1.15\times10^{2}} = \sqrt{\frac{[2.000+2x]^{2}}{[2.000-x]^{2}}}$$

$$10.72 = \frac{[2.000+2x]}{[2.000-x]}$$

$$10.72(2.000-x) = (2.000+2x)$$

$$21.44-10.72x = 2.000+2x$$

$$19.44 = 12.72x$$

$$x = \frac{19.44}{12.72} = 1.528\,M$$

- Now compute the equilibrium concentrations:

$$[H_2] = [F_2] = 2.000 - x = 2.000 - 1.528 = 0.47\,M$$

$$[HF] = 2.000 + 2x = 2.000 + 3.06 = 5.06\,M$$

- You can do a cross – check:

$$K_c = \frac{[HF]^{2}}{[H_2][F_2]} = \frac{(5.06)^{2}}{(0.47)^{2}} = 1.16\times10^{2}$$

KEY CONCEPTS

- Calculate concentrations at equilibrium
- Be able to use the quadratic equation.