Rafa Muñoa
Lizardi Institutua
Zarautz

Chemical Equilibrium: Exercises

1. At 670 °C, a 1 L-flask contains a mixture of gases at equilibrium: 0.003 mol hydrogen, 0.003 mol iodine and 0.024 mol of hydrogen iodide. The reaction is:

$$H_2\,(g) + I_2(g) \rightleftarrows 2\,HI\,(g)$$

Determine:
a) The values of Kc and Kp
b) The total pressure and the partial pressures at equilibrium in the previous conditions

The values of Kp and Kc are equal: $Kp = Kc * (RT)^{\Delta n} \xrightarrow{\Delta n = 0} Kp = Kc$

At equilibrium we have:

$$H_2\,(g) + I_2(g) \rightleftarrows 2\,HI\,(g)$$

	H_2	I_2	HI
# of moles	0.003	0.003	0.024
conc.	0.003 M	0.003 M	0.024 M

$$Kp = Kc = \frac{[HI]^2}{[H_2]\,[I_2]} = \frac{(0.024)^2}{(0.003)^2} = 64$$

The total pressure is:

$$P_{tot} = C_{tot} * R * T = 0.03\text{ M} * 0.082\,\frac{\text{atm.L}}{\text{K.mol}} * (670 + 273\,)\text{ K} = 2.32\text{ atm}$$

The partial pressures are:

$$P_{H_2} = P_{I_2} = 0.003\text{ M} * 0.082\,\frac{\text{atm.L}}{\text{K.mol}} * (670 + 273\,)\text{ K} = 0.232\text{ atm}$$

$$P_{HI} = 0.024\text{ M} * 0.082\,\frac{\text{atm.L}}{\text{K.mol}} * (670 + 273\,)\text{ K} = 1.856\text{ atm}$$

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2. The equilibrium constant for this process $I_2(g) \rightleftarrows 2\,I\,(g)$

At 1000 K is $Kc=3.76*10^{-5}$. If a 2 L-flask that contains $5*10^{-3}$ moles of I is charged with 1 mol of I_2, determine the concentrations of both components at equilibrium

First, we have to compare K and Q in order to know the direction of the reaction:

$$Kc = \frac{[I]^2}{[I_2]} = 3.76*10^{-5} \quad Q = \frac{[I]^2}{[I_2]} = \frac{(2.5*10^{-3}\ M)^2}{0.5\ M} = 1.25*10^{-5} \quad Q < Kc$$

Therefore, the reaction goes to the right

The value of "x" is:

$$I_2(g) \rightleftarrows 2\,I\,(g)$$

	$I_2(g)$	$2\,I\,(g)$
n initial	1	0.005
n change	-x	2x
n equil.	1-x	0.005+2x
[ ] equil.	(1-x)/2	(0.005+2x)/2

$$Kc = \frac{[I]^2}{[I_2]} = 3.76*10^{-5} = \frac{(0.005 + 2x)^2}{2\,(1-x)}$$

$$7.52*10^{-5} - 7.52*10^{-5}\ x = 4\ x^2 + 0.02\ x + 2.5*10^{-5}$$

Approximation: $0.02\ x + 7.52*10^{-5}\ x \simeq 0.02\ x$

$$4\ x^2 + 0.02\ x - 5.02*10^{-5} = 0$$

$$x = \frac{-0.02 \pm \sqrt{(0.02)^2 + 8.032*10^{-4}}}{8} \rightarrow x = 1.84*10^{-3}$$

The concentrations at equilibrium are:

$$[I] = \frac{0.005 + 2x}{2} = 4.34*10^{-3}\ M;\ [I_2] = \frac{1 - x}{2} = 0.499\ M$$

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3. A 5 L-container is charged with 2 moles of PCl_5 (g) and 1 mole of PCl_3 (g). The mixture is heated at 250 °C and this equilibrium is reached:

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

The equilibrium constant at that temperature is Kc = 0.042. Determine:
a) The concentration of Cl_2 at equilibrium. b) The value of Kp at that temperature
c) The dissociation percent of PCl_5

At equilibrium we have:

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

	PCl_5	PCl_3	Cl_2
n initial	2	1	0
n change	-x	x	x
n equil	2-x	1+x	x
[ ] equil	(2-x)/5	(1+x)/5	x/5

$$Kc = \frac{[PCl_3]\,[Cl_2]}{[PCl_5]} = 0.042 = \frac{(1+x)\,x}{5\,(2-x)}$$

From this expression we can calculate x:

$$x^2 + 1.21\,x - 0.42 = 0$$

$$x = \frac{-1.21 \pm \sqrt{1.4641 + 1.68}}{2} \rightarrow x = 0.282$$

a) The concentration of Cl_2 is: $[Cl_2] = x/5 = 5.64*10^{-2}\ M$

b) The value of Kp: $Kp = Kc\,(RT) = 0.042 * 0.082 * (250+273) = 1.80$

c) The dissociation percent: $\alpha = \frac{x}{2} = 0.141 = 14.1\ \%$

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Chemical Equilibrium: Exercises

4. A 5 L-container is charged with 0.92 moles of N_2 and 0.51 moles of O_2. The mixture is heated at 2200 K and the following equilibrium is reached:

If 1.09 % of the initial nitrogen reacts, determine:
a) The concentrations of all components at equilibrium
b) The values of Kc and Kp

$$N_2\,(g) + O_2(g) \rightleftarrows 2\,NO\,(g)$$

	N_2	O_2	NO
n initial	0.92	0.51	0
n change	-x	-x	2x
n equil	0.92-x	0.51- x	2x
[ ] equil	(0.92-x)/5	(0.51- x)/5	2x/5

where $x = 0.92\,\alpha = 0.92\,\frac{1.09}{100} \simeq 0.01$

a) The concentrations at equilibrium

$$[NO] = \frac{2x}{5} = 0.004\ M$$

$$[N_2] = \frac{0.92 - x}{5} = 0.182\ M$$

$$[O_2] = \frac{0.51 - x}{5} = 0.10\ M$$

b) The values of Kc and Kp

$$Kp = Kc = \frac{[NO]^2}{[N_2]\,[O_2]} = \frac{(0.004)^2}{(0.182)\,(0.10)} = 8.79{*}10^{-4}$$

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Zarautz

Chemical Equilibrium: Exercises

5. The synthesis of methanol is based on this equilibrium

$$CO\,(g) + 2\,H_2(g) \rightleftarrows CH_3OH\,(g)$$

In a 1 L-flask we have initially 2 moles of CO and 2 moles of hydrogen and the mixture is heated to 600 K. At equilibrium 0.8 moles of methanol are formed. Determine:

a) The number of moles of each component at equilibrium b) The value of Kp at 600 K
c) The effect produced when the equilibrium is disturbed by increasing the volume of the container

b) The value of Kp

$$CO\,(g) + 2\,H_2(g) \rightleftarrows CH_3OH\,(g)$$

	CO	H_2	CH_3OH
n initial	2	2	0
n change	-x	-2x	x
n equil	2-x=1.2	2-2x=0.4	x = 0.8
[ ] equil	1.2 M	0.4 M	0.8 M

$$Kc = \frac{[CH_3OH]}{[CO]\,[H_2]^2} = \frac{0.8}{1.2 * (0.4)^2} = 4.17$$

$$Kp = \frac{Kc}{(RT)^2} = \frac{4.17}{(0.082 * 600)^2} = 1.72 * 10^{-3}$$

c) The effect

volume ↑ → total pressure ↓ → system reacts increasing pressure → # of moles ↑ → to the left more reactants

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Chemical Equilibrium: Exercises

6. At 400 °C ammonia is 40 % dissociated in nitrogen and hydrogen when the pressure of the mixture is 710 mm Hg. Determine:

$$2\,NH_3(g) \rightleftarrows N_2\,(g) + 3\,H_2\,(g)$$

a) The partial pressures of each component when we start with 4 moles of ammonia
b) The value of Kp

a) The partial pressures:

$$2\,NH_3(g) \rightleftarrows N_2\,(g) + 3\,H_2\,(g)$$

	NH_3	N_2	H_2
n initial	4	0	0
n change	$-n\alpha = -1.6$	0.8	2.4
n equil	2.4	0.8	2.4

n = 2.4 mol + 0.8 mol + 2.4 mol = 5.6 mol

$$P_{NH_3} = P_{H_2} = \frac{2.4\ \text{mol}}{5.6\ \text{mol}} * 710\ \text{mm Hg} = 304.3\ \text{mm Hg}$$

$$P_{N_2} = \frac{0.8\ \text{mol}}{5.6\ \text{mol}} * 710\ \text{mm Hg} = 101.4\ \text{mm Hg}$$

b) Kp:

The partial pressures in atm

$$P_{NH_3} = P_{H_2} = 304.3\ \text{mm Hg}\ \frac{1\ \text{atm}}{760\ \text{mm Hg}} = 0.4\ \text{atm}$$

$$P_{N_2} = 101.4\ \text{mm Hg}\ \frac{1\ \text{atm}}{760\ \text{mm Hg}} = 0.133\ \text{atm}$$

$$Kp = \frac{P_{N_2} * P_{H_2}{}^3}{P_{NH_3}{}^2} = \frac{0.133 * (0.4)^3}{(0.4)^2} = 0.0532$$

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Zarautz

Chemical Equilibrium: Exercises

7. A 400 mL-flask is charged with 2.032 g of iodine and 1.28 g of bromine. The mixture is heated at 150 °C and the following equilibrium is reached:

$$I_2\ (g) + Br_2(g) \rightleftarrows 2\ IBr\ (g)$$

Determine:
a) The molar concentrations of each component and the total pressure
b) The value of Kp at this temperature

Kc (at 150 °C) = 280; R = 0.082 atm.L/K.mol; Atomic weights: Br=79.9 I=126.9

The initial amounts in moles:

$$n(I_2) = 2.032\ g\ \frac{1\ mol}{253.8\ g} = 0.008\ mol$$

$$n(Br_2) = 1.28\ g\ \frac{1\ mol}{159.8\ g} = 0.008\ mol$$

$$I_2\ (g) + Br_2(g) \rightleftarrows 2\ IBr\ (g)$$

	I_2	Br_2	IBr
n initial	0.008	0.008	0
n change	-x	-x	2x
n equil	0.008-x	0.008-x	2x
[ ] equil	(0.008-x)/0.4	(0.008-x)/0.4	2x/0.4

a) The molar concentrations ant total pressure:

$$Kc = 280 = \frac{(2x)^2}{(0.008-x)^2} \rightarrow 16.73 = \frac{2x}{0.008-x}$$

$$x = \frac{0.1338}{18.73} = 0.0071 \rightarrow [I_2] = [Br_2] = 2.25*10^{-3}\ M$$

$$[IBr] = 3.55*10^{-2}\ M$$

$$P = cRT = 0.04 * 0.082 * (150+273) = 1.387\ atm$$

b) Kp

$$Kp = Kc * (RT)^{\Delta n} \xrightarrow{\Delta n = 0} Kp = Kc = 280$$

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Zarautz

Chemical Equilibrium: Exercises

8. A 0.4 L-flask is charged with 1 mole of N_2 and 3 moles of H_2 at 780 K. When the following equilibrium is reached $N_2\,(g) + 3\,H_2(g) \rightleftarrows 2\,NH_3\,(g)$

the mixture has a 28 % of ammonia (in moles). Determine:
a) The number of moles of each component in equilibrium b) The total pressure at equilibrium c) The value of Kp

$$N_2\,(g) + 3\,H_2(g) \rightleftarrows 2\,NH_3\,(g)$$

	N_2	H_2	NH_3
n initial	1	3	0
n change	-x	-3x	2x
n equil	1-x	3-3x	2x
[ ] equil	(1-x)/0.4	(3-3x)/0.4	2x/0.4

The value of x:

$$n_{tot} = (1-x) + (3-3x) + 2x = 4 - 2x$$

$$2x = 0.28\,(4 - 2x) \rightarrow x = \frac{1.12}{2.56} = 0.4375$$

a) The number of moles of each component in equilibrium:

$n(N_2) = 1-x = 0.5625$ mol
$n(H_2) = 3-3x = 1.6875$ mol
$n(NH_3) = 2x = 0.875$ mol

b) The total pressure at equilibrium:

$$P_{tot} = \frac{n_{tot} * R * T}{V} = \frac{3.125 \text{ mol} * 0.082 \text{ atm.L/K.mol} * 780 \text{ K}}{0.4 \text{ L}}$$

P_{tot} = 500 atm

c) The value of Kp:

$$P(N_2) = \frac{0.5625}{3.125} * 500 \text{ atm} = 90 \text{ atm}$$

$$P(H_2) = \frac{1.6875}{3.125} * 500 \text{ atm} = 270 \text{ atm}$$

$$P(NH_3) = \frac{0.875}{3.125} * 500 \text{ atm} = 140 \text{ atm}$$

$$Kp = \frac{P(NH_3)^2}{P(N_2) * P(H_2)^3} = 1.1*10^{-5}$$

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Zarautz

Chemical Equilibrium: Exercises

9. Chlorine reacts with phosphorus trichloride to yield phosphorus pentachloride, according to this equation:

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

In a 2 L-vessel, at a given temperature, there is a gas mixture in equilibrium that contains 132 g of PCl_3, 56.8 g of Cl_2 and 10.4 g of PCl_5.

a) Determine Kc at that temperature
b) Explain if Kp can be calculated with the data available in this exercise
c) Determine the composition at equilibrium (concentrations) if the volume is halved.

The molar masses and moles at equilibrium:

$$M(PCl_3) = 31 + (3 * 35.5) = 137.5\ g/mol$$

$$M(Cl_2) = 2 * 35.5 = 71\ g/mol$$

$$M(PCl_5) = 31 + (5 * 35.5) = 208.5\ g/mol$$

$$n(PCl_3) = \frac{132\ g}{137.5\ g/mol} = 0.96\ mol$$

$$n(Cl_2) = \frac{56.8\ g}{71\ g/mol} = 0.8\ mol$$

$$n(PCl_5) = \frac{10.4\ g}{208.5\ g/mol} = 0.05\ mol$$

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

	$PCl_3(g)$	$Cl_2(g)$	$PCl_5(g)$
n equil	0.96	0.8	0.05
[ ] equil	0.48 M	0.4 M	0.025 M

a) Kc $$Kc = \frac{[PCl_5]}{[PCl_3][Cl_2]} = \frac{0.025}{0.48 * 0.4} = 0.13$$

b) Kp cannot be calculated without the value of T or the total pressure

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Chemical Equilibrium: Exercises

9. Chlorine reacts with phosphorus trichloride to yield phosphorus pentachloride, according to this equation:

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In a 2 L-vessel, at a given temperature, there is a gas mixture in equilibrium that contains 132 g of PCl_3, 56.8 g of Cl_2 and 10.4 g of PCl_5.

a) Determine Kc at that temperature
b) Explain if Kp can be calculated with the data available in this exercise
c) Determine the composition at equilibrium (concentrations) if the volume is halved.

c) When volume is halved, the pressure increases and the reaction goes to the right (Le Châtelier)

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

	$PCl_3(g)$	$Cl_2\ (g)$	$PCl_5\ (g)$
n initial	0.96	0.8	0.05
n change	-x	-x	+x
n equil	0.96-x	0.8-x	0.05+x
[ ] equil	0.96-x	0.8-x	0.05+x

$$Kc = \frac{[PCl_5]}{[PCl_3][Cl_2]} = 0.13 = \frac{0.05 + x}{(0.96 - x) * (0.8 - x)} = \frac{0.05 + x}{x^2 - 1.76\,x + 0.768}$$

$$0.13\,x^2 - 1.229\,x + 0.05 = 0 \rightarrow x = \frac{1.229 \pm \sqrt{1.51 - 0.026}}{0.26} \rightarrow x = 0.042$$

$$n(PCl_3) = 0.96 - x = 0.918\ mol;\ n(Cl_2) = 0.758\ mol;\ n(PCl_5) = 0.092\ mol$$

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Zarautz

Chemical Equilibrium: Exercises

10. A 10 L-vessel is charged with 2 moles of PCl_5 at 162 °C. Determine
a) The concentrations of all components when the following equilibrium is reached:

$$PCl_5\,(g) \rightleftarrows PCl_3(g) + Cl_2\,(g)$$

b) The total pressure at equilibrium
Kc = 0.0454 (at 162 °C); R=0.082 atm.L/K.mol

a) The concentrations at equilibrium:

$$PCl_5\,(g) \rightleftarrows PCl_3(g) + Cl_2\,(g)$$

	PCl_5	PCl_3	Cl_2
n initial	2	0	0
n change	-x	x	x
n equil	2-x	x	x
[ ] equil	(2-x)/10	x/10	x/10

$$Kc = \frac{[PCl_3]\,[Cl_2]}{[PCl_5]} = \frac{x^2}{10\,(2-x)} = 0.0454$$

$$x^2 + 0.454\,x - 0.908 = 0$$

$$x = \frac{-0.454 \pm \sqrt{0.206 + 3.632}}{2} = 0.753$$

$[PCl_3] = [Cl_2] = 7.53*10^{-2}$ M

$[PCl_5] = 0.125$ M

b) The total pressure at equilibrium:

$$n_{tot} = 2 + x = 2.753 \text{ mol}$$

$$P_{tot} = \frac{n_{tot} * R * T}{V} = \frac{2.753 \text{ mol} * 0.082 \frac{\text{atm.L}}{\text{K.mol}} * (162+273)\text{ K}}{10 \text{ L}}$$

$$P_{tot} = 9.82 \text{ atm}$$