Calculating K_{eq}

Calculating Keq

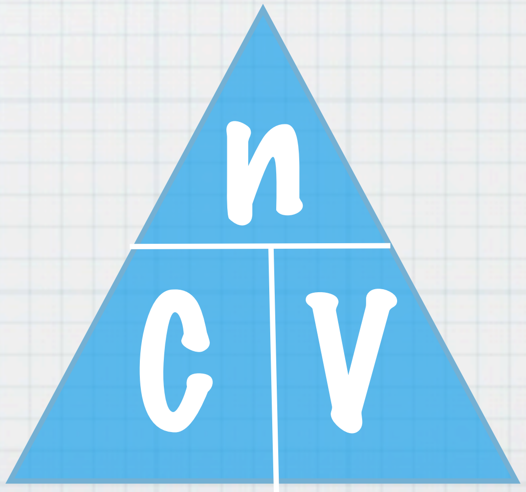
* Depending on the nature of the reaction and the quantitative information that is available, there are several ways to calculate K_{eq}
  * Using Concentration
  * Using Partial Pressure
  * Using ICE Tables

Using Molar Concentration

* Remember:

$$K_{eq} = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

* So if we can determine molar concentrations we can determine K_{eq}



Example

* A 5.0 L flask contains N_2, chlorine, Cl_2, and nitrogen trichloride, NCl_3. The reaction at equilibrium can be represented as:
    * $N_{2(g)} + 3Cl_{2(g)} \rightleftharpoons 2NCl_{3(g)}$
* When the system is analyzed, it contains 0.0070 mol of N_2, 0.0022mol of Cl_2, and 0.95 mol of NCl_3. Calculate the equilibrium constant for the reaction.

Solution

* First calculate the concentration of each product and reactant:

$$[N_2] = \frac{n}{V} = \frac{0.0070 \text{ mol}}{5L} = 1.4 \times 10^{-3} \text{ mol/L}$$

$$[Cl_2] = \frac{n}{V} = \frac{0.0022 \text{ mol}}{5L} = 4.4 \times 10^{-4} \text{ mol/L}$$

$$[NCl_3] = \frac{n}{V} = \frac{0.95 \text{ mol}}{5L} = 1.9 \times 10^{-1} \text{ mol/L}$$

Solution

* Now write the equilibrium constant expression for the reaction

$$K_{eq} = \frac{[NCl_3]^2}{[N_2][Cl_2]^3}$$

Solution

* Now substitute and solve

$$K_{eq} = \frac{[1.9 \times 10^{-1}]^2}{[1.4 \times 10^{-3}][4.4 \times 10^{-4}]^3}$$

$$K_{eq} = 3.0 \times 10^{11}$$

Example

* N_2 and H_2 are mixed in a 3500 mL flask. The reaction can be represented below.
  * $N_2 + 3H_2 \rightleftharpoons 2NH_3$
* At equilibrium 0.25 mol of NH_3 and 0.080 mol of H_2 were recorded. If the equilibrium constant for the reaction is $K_{eq}=5.81 \times 10^5$, what amount of nitrogen gas is present?

Solution

* First calculate the concentration of each product and reactant:

$$[NH_3] = \frac{n}{V} = \frac{0.25\ mol}{3.5L} = 7.143 \times 10^{-2}\ mol/L$$

$$[H_2] = \frac{n}{V} = \frac{0.080\ mol}{3.5L} = 2.286 \times 10^{-2}\ mol/L$$

$$[NCl_3] = \frac{n}{V} = \frac{0.95\ mol}{5L} = 1.9 \times 10^{-1}\ mol/L$$

Solution

* Now write the equilibrium constant expression for the reaction

$$K_{eq} = \frac{[NH_3]^2}{[H_2]^3[N_2]}$$

Solution

* Now substitute and solve

$$[N_2] = \frac{[NH_3]^2}{[H_2]^3[K_{eq}]}$$

$$[N_2] = \frac{(0.07143\ mol/L)^2}{(0.02286\ mol/L)^3(5.81 \times 10^5)}$$

$$[N_2] = 7.4 \times 10^{-4}\ mol/L$$

Solution

* Now calculate the number of moles

$n = C \times V$

$n = (7.3512 \times 10^{-4} \text{ mol/L})(3.5 \text{ L})$

$n = 2.6 \times 10^{-3} \text{ mol}$

Using Partial Pressure

* Remember:

$$PV=nRT$$

* If we rearrange:

$$\frac{P}{RT} = \frac{n}{V}$$

Since R and T are constant, we can use P in place of concentration

Example

* The following reaction shows the production of $CH_3Cl_{(g)}$
    * $CH_{4(g)} + Cl_{2(g)} \rightleftharpoons CH_3Cl_{(g)} + HCl_{(g)}$
* At 1500 K the mixture contains P_{CH4}=0.13 atm, P_{CH3Cl}= 0.24 atm, and P_{HCl}=0.47 atm. What is K_{eq}?

Solution

* Find the K_p expression

$$K_p = \frac{P_{CH3Cl}P_{HCl}}{P_{CH4}P_{Cl2}}$$

Solution

* Now substitute and solve

$$K_p = \frac{(0.24)(0.47)}{(0.13)(0.035)} = 24.79$$

Using ICE Tables

Initial			
Change			
Equilibrium			

Example

* A 2.0L flask has 0.200 mol of HI. HI then decomposes to $H_{2(g)}$ and $I_{2(g)}$ until it reaches equilibrium. At equilibrium the concentration of HI is 0.078 mol/L. What is K_{eq}?

Solution

* Fill out an ICE table. Write a chemical equation and add know values.

$$2HI_{(g)} \rightleftharpoons H_{2(g)} + I_{2(g)}$$

	$2HI_{(g)}$	$H_{2(g)}$	$I_{2(g)}$
Initial	[0.100 mol/L]	[0]	[0]
Change			
Equilibrium			

Solution

* Let x represent the change in concentration

$$2HI_{(g)} \rightleftharpoons H_{2(g)} + I_{2(g)}$$

	$2HI_{(g)}$	$H_{2(g)}$	$I_{2(g)}$
Initial	[0.100 mol/L]	[0]	[0]
Change	-2x	+x	+x
Equilibrium			

Solution

- Let x represent the change in concentration

$$2HI_{(g)} \rightleftharpoons H_{2(g)} + I_{2(g)}$$

	$2HI_{(g)}$	$H_{2(g)}$	$I_{2(g)}$
Initial	[0.100 mol/L]	[0]	[0]
Change	-2x	+x	+x
Equilibrium	0.100 - 2x	x	x

Solution

* Use your equilibrium concentration to determine x.

The equilibrium concentration of HI is 0.078 mol/L.

Therefore

0.100 mol/L - 2x = 0.078 mol/L
-2x= 0.078 - 0.100
x=0.011 mol/L

Solution

* Now we know the equilibrium concentrations of H_2 and I_2

$$2HI_{(g)} \rightleftharpoons H_{2(g)} + I_{2(g)}$$

	$2HI_{(g)}$	$H_{2(g)}$	$I_{2(g)}$
Initial	[0.100 mol/L]	[0]	[0]
Change	-2x	+x	+x
Equilibrium	0.100 - 2x	x	x

Solution

* Now we know the equilibrium concentrations of H_2 and I_2

$$2HI_{(g)} \rightleftharpoons H_{2(g)} + I_{2(g)}$$

	$2HI_{(g)}$	$H_{2(g)}$	$I_{2(g)}$
Initial	[0.100 mol/L]	[0]	[0]
Change	-2x	+x	+x
Equilibrium	0.078	0.011	0.011

Solution

* Now use the K_{eq} expression to solve

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

$$K_{eq} = \frac{(0.011)(0.011)}{(0.078)^2}$$

$$K_{eq} = 0.020$$

Example

* The equilibrium constant for the following reaction is found to be 0.83. If you start with 1.0 mol of $CO_{(g)}$ and 1.0 mol H_2O in a 5.0 L container, what concentration of each substance will be present in the container at equilibrium?
  * $CO_{(g)} + H_2O_{(g)} \rightleftharpoons H_{2(g)} + CO_{2(g)}$

Solution

* Calculate the initial concentration of each reactant in the container.

$$[CO] = \frac{n}{V} = \frac{1.0\ \text{mol}}{5.0\ \text{L}} = 0.20\ \text{mol/L}$$

$$[H_2O] = \frac{n}{V} = \frac{1.0\ \text{mol}}{5.0\ \text{L}} = 0.20\ \text{mol/L}$$

Solution

* Fill out an ICE table. Write a chemical equation and add know values.

$$CO_{(g)} + H_2O_{(g)} \rightleftharpoons H_{2(g)} + CO_{2(g)}$$

	$CO_{(g)}$	$H_2O_{(g)}$	$H_{2(g)}$	$CO_{2(g)}$
Initial	0.20	0.20	0	0
Change	-x	-x	+x	+x
Equilibrium	0.20 - x	0.20 -x	x	x

Solution

* Now use the K_{eq} expression to solve

$$K_{eq} = \frac{[H_2][CO_2]}{[CO][H_2O]}$$

$$0.83 = \frac{(x)(x)}{(0.20 - x)(0.20 - x)}$$

$$0.83 = \frac{(x)^2}{(0.20 - x)^2}$$

Solution

* Now use the K_{eq} expression to solve

$$K_{eq} = \frac{[H_2][CO_2]}{[CO][H_2O]}$$

$$0.83 = \frac{(x)(x)}{(0.20 - x)(0.20 - x)}$$

$$\sqrt{0.83} = \sqrt{\frac{(x)^2}{(0.20 - x)^2}} \rightarrow 0.9110 = \frac{(x)}{(0.20 - x)}$$

$$(0.9110)(0.20 - x) = x$$

$$1.1822 - 0.9110x = x$$

x=0.095

Solution

* Use the x value to determine final concentrations

$CO_{(g)} + H_2O_{(g)} \rightleftharpoons H_{2(g)} + CO_{2(g)}$

	$CO_{(g)}$	$H_2O_{(g)}$	$H_{2(g)}$	$CO_{2(g)}$
Initial	0.20	0.20	0	0
Change	-x	-x	+x	+x
Equilibrium	0.20 - x	0.20 -x	x	x

Solution

* Use the x value to determine final concentrations

$$CO_{(g)} + H_2O_{(g)} \rightleftharpoons H_{2(g)} + CO_{2(g)}$$

	$CO_{(g)}$	$H_2O_{(g)}$	$H_{2(g)}$	$CO_{2(g)}$
Initial	0.20	0.20	0	0
Change	-x	-x	+x	+x
Equilibrium	0.105	0.105	0.095	0.095

Homework

* pg 444 # 31, 32
* pg 447 # 41, 42
* pg 451 # 51-53