CHEMICAL EQUILIBRIUM *(ICE METHOD)*

Introduction

- Chemical equilibrium occurs when opposing reactions are proceeding at equal rates.
- The rate at which the products are formed from the reactants equals the rate at which the reactants are formed from the products.
- As a result, concentrations cease to change, making the reaction appear to be stopped. How fast a reaction reaches this equilibrium state is a matter of kinetics.
- An ***equilibrium state*** results when a reaction is ***reversible***

$$aA + bB \underset{k_r}{\overset{k_f}{\rightleftharpoons}} cC + dD$$

At equilibrium the concentrations of reactants and products is still changing, however, ***the rate of the forward reaction (k_f) is equal to the rate of the reverse reaction (k_r)*** in what is described as a ***dynamic equilibrium*** such that no change in their concentrations is observed. Thus, for equilibrium to occur, neither reactants nor products can escape from the system.

- The ***law of mass action*** states the ratio of forward and reverse processes is described by the ***equilibrium constant K_C*** which can be calculated using a knowledge of the equilibrium concentrations of reactants and products.

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

The equilibrium constant expression depends only on the stoichiometry of the reaction, not on the mechanism.

Objectives and Success Criteria

- Mastering the application of the ICE table methodology to equilibrium problems.
- Accurate solutions to problems involving reactant and product concentrations and equilibrium constants.

Prerequisites

- Stoichiometry
- Kinetics

MODEL 1: The ICE Table

A worked example:
Initially 1.50 moles of N_2(g) and 3.50 moles of H_2(g) were added to a 1 L container at 700 °C. As a result of the reaction

$$N_2(g) \quad + \quad 3H_2(g) \quad \rightleftharpoons \quad 2NH_3$$

the equilibrium concentration of NH_3(g) became 0.540 M. What is the value of the equilibrium constant for this reaction at the given temperature of 700 °C.

	$N_2(g)$	+ $3H_2(g)$	$\rightleftharpoons$ $2NH_3$
I. Write the **I**nitial concentrations of reactants and products:	1.50 mol L^{-1}	3.50 mol L^{-1}	0 mol L^{-1}
C. Write the **C**hange in concentration due to reaction using the given reaction stoichiometric coefficients:	–x	–3x	+2x
E. Write the reactant and product concentrations at **E**quilibrium.	1.50 mol L^{-1} –x	3.50 mol L^{-1} –3x	+2x mol L^{-1}

We are now set to solve for the equilibrium constant K_C using the *equilibrium equation*:

$$K_C = \frac{[NH_3]^2}{[N_2][H_2]^3} \qquad \textit{eqn. 1}$$

where the reactant and product concentrations should be expressed at equilibrium. The problem tells us that the equilibrium concentration of NH_3 is 0.540 M, thus we can solve for the unknown 'x'

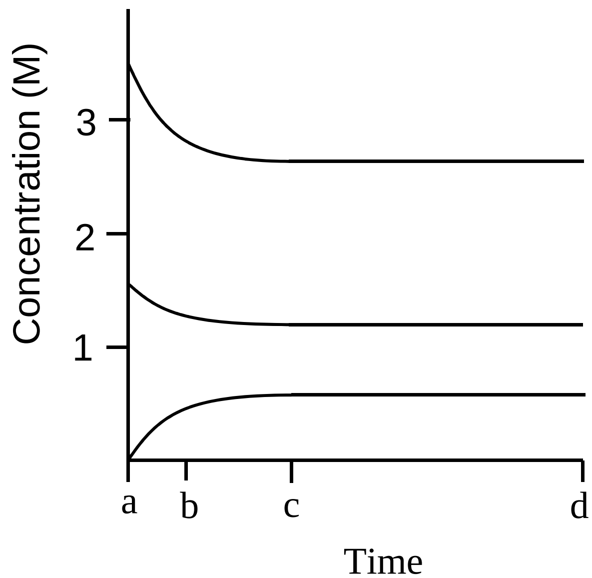
$$[NH_3]_{eq} = +2x = 0.540 \text{ M}$$
$$x = 0.270 \text{ M}$$

we can now solve for K_C

$$K_C = \frac{(0.540 \text{ M})^2}{(1.50 \text{ M} - x)(3.50 \text{ M} - 3x)^3} = \frac{(0.540 \text{ M})^2}{(1.23 \text{ M})(2.69 \text{ M})^3} = 0.0122$$

Key Questions

(i) In the above reaction we can monitor the change in concentration of reactants over time (just as we discussed when dealing with kinetics) and we can plot the data as follows:



Using the worked example from Model 1 label each data plot as either $[H_2]$, $[N_2]$ or $[NH_3]$.

Why does one data plot show an initial positive slope whereas the other two data plots show initial negative slopes?

Why does the uppermost plot have a steeper initial slope than the middle plot.

At which time a, b, c or d is an equilibrium state reached?

(ii) The equilibrium constant for this reaction was calculated as shown below. What is K_c for the reverse reaction?

$$K_c = \frac{[NH_3]^2}{[N_2][H_2]^3} = 0.0122$$

EXERCISES

1. Initially, 1.0 mol of NO(g) and 1 mol of Cl_2(g) were added to a 1 L container. As a result of the reaction

$$2NO(g) + Cl_2(g) \rightleftharpoons 2NOCl(g)$$

the equilibrium concentration of NOCl(g) became 0.96 M. Using the RICE table methodology determine the value of the equilibrium constant K_C for this reaction.

I. Write the **I**nitial concentrations of reactants and products:

C. Write the **C**hange in concentration due to reaction using the given reaction stoichiometric coefficients:

E. Write the reactant and product concentrations at **E**quilibrium.

Solve for K_C :

Answer: $K_C = 1.11 \times 10^3$

PROBLEMS

1. If a 10.00 L flask at 500 K is filled with a 0.30 mole of hydrogen and 0.30 mole of iodine, what are the equilibrium concentrations of the three gases?

   The equilibrium constant K_C = 45.0. The relevant reaction is

$$H_2(g) \quad + \quad I_2(g) \quad \rightleftharpoons \quad 2HI(g)$$

Answer: $[H_2] = [I_2] = 0.0069$ M; $[HI] = 0.0462$ M

2. Nitrogen dioxide is introduced into a flask at a pressure of one atmosphere (1.00 atm). After some time it dimerizes to produce N_2O_4.

    a) What is the equilibrium partial pressure of N_2O_4 at a temperature where the equilibrium constant for dimerization is $K_C = 3.33$?

    Answer: $P\,(N_2O_4) = 0.32$ atm

    b) Calculate the total pressure in the flask.

    Answer: $P_{\text{Total}} = 0.68$ atm

    c) Explain why the total pressure is more than, less than, or still equal to the initial pressure (1.00 atm).

3. Gaseous carbon dioxide is partially decomposed according to the following equation.

$$2CO_2(g) \rightleftharpoons 2CO(g) + O_2(g)$$

An initial pressure of 1.00 atm of CO_2 is placed in a closed container at 2500 K, and 2.1 % of the molecules decompose. Determine the equilibrium constant K_p at this temperature.

Answer: $K_p = 4.83 \times 10^{-6}$