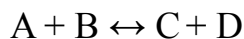


ICE Diagrams

Introduction

When a reversible reaction takes place a state of equilibrium will be reached where the concentrations remain the same. In this case the equilibrium constant can be used to set up an equation describing the state of the reaction. For example for the following reaction



will have an equilibrium equation like

$$k = \frac{[C][D]}{[A][B]}$$

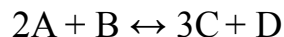
to be satisfied. The task now is to determine the concentrations at equilibrium given some initial or final condition. This is the purpose of the **ICE Diagram**.

The ICE Diagram

The trick is to set up the above equation remembering that any change in concentration must be consistent with the the chemical reaction that is the heart of the matter. The ICE Diagram is a table in which the columns represent the different molecules. The different rows are described below.

- First row for the Initial concentrations (I): Place the initial concentrations for each molecule on the first row.
- Second row for the Change in concentrations (C): Here create a variable designating the change in concentrations due to the reaction. Here we assume a net direction for the reaction and give the assumed reactants a negative sign and the product a positive sign. For example in the above reaction (assuming that the reaction flows from right to left) the change in concentration of A and B can be called $-x$ and the change in concentration for C and D is $+x$.

In the case that coefficients exists indicating that more than one of a particular molecule is involved, the change row must reflect this. Consider the following reaction:



We can let x represent the change in concentration of B or D.

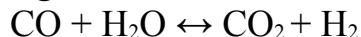
$$\Delta A = -2x, \Delta B = -x, \Delta C = +3x, \Delta D = +x$$

- Third row for the Equilibrium concentration (E): This is just the initial concentrations plus the change in concentrations.

You use the equilibrium concentrations in the equation involving the equilibrium constant

Example:

A mixture of 1.0 mole carbon dioxide and 1.0 mole carbon monoxide are contained in a 1 liter vessel. Later 2.0 moles of water vapor is then introduced into the vessel. The following reversible reaction takes place



This reaction has an equilibrium constant of 0.64. How many moles of the different molecules will be present after equilibrium is obtained?

Since there is initially no hydrogen gas in the vessel the reaction must begin going from the left to the right. So let the right side be the reactants and the left the product. So now consider the rows of the ICE table.

- Since the vessel has a volume of 1 L, the number of moles must equal the molarity. So the concentration of CO and CO₂ is 1.0 m, the H₂O is 2.0 m and the H₂ has zero molarity.
- Since all the coefficients are 1 the change is simple. Assuming that the left is the reactants.

$$\Delta\text{CO} = -x, \Delta\text{H}_2\text{O} = -x, \Delta\text{CO}_2 = +x, \Delta\text{H}_2 = +x$$

- The equilibrium is just the sum of the above.

So now put all this together into an ICE table.

	CO	H ₂ O	CO ₂	H ₂
I (initial)	1.0 M	2.0 M	1.0 M	∅
C (change)	-x	-x	+x	+x
E (Equilibrium)	1.0 - x	2.0 - x	1.0 + x	x

So now feed the last row into our equilibrium equation

$$k = \frac{[\text{CO}_2][\text{H}_2]}{[\text{CO}][\text{H}_2\text{O}]}$$

$$0.64 = \frac{(1.0+x)(x)}{(1.0-x)(2.0-x)}$$

Now to solve for the unknown variable. We can cross-multiply to eliminate the fractions then foil.

$$0.64(1.0-x)(2.0-x) = (1.0+x)(x)$$

$$1.28 - 1.92x + 0.64x^2 = x + x^2$$

Move all the variables to one side

$$0 = 0.36x^2 + 2.92x - 1.28$$

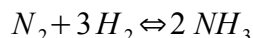
We can solve this using the quadratic equation, graphing etc. Our two solutions are $x = -8.5, 0.42$ m. The first solution cannot be physically realistic as it would mean that hydrogen would end up with a negative concentration. So the latter number must be the desired solution. Putting our value for x into the last row of our ICE table gives the final concentrations as well as the number of moles.

Molecule	Moles
CO	0.58
H ₂ O	1.58
CO ₂	1.42
H ₂	0.42

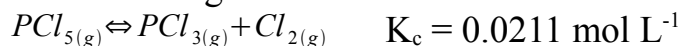
Note: It usually is not necessary to use the equilibrium equation if you are given the beginning conditions and some information as to the final condition.

Practice Questions: (Answers below).

1. 3.00 moles of N₂ gas and 1.00 mole of H₂ gas are combined in a 1 L reaction vessel. At equilibrium 0.663 moles of H₂ remain. What are the resulting concentrations?



2. Phosphorus pentachloride decomposes into Phosphorous trichloride and Chlorine gas. 0.500 moles of pure Phosphorus pentachloride is placed in a 2.00 L bottle. What are the resulting concentrations?



3. A mixture consists of 1.00 M Hydrofluoric acid 0.200 M Sodium Fluoride. What will be the concentration of F⁺? What will be the pH? $K_a = 7.2 \times 10^{-4} \text{ mol L}^{-1}$ for Hydrofluoric acid. (Hint: The NaF completely disassociates releasing all the F⁺)

Solutions

1. N_2 : 2.89 M H_2 : 0.663 M NH_3 : 0.225 M
2. PCl_5 : 0.187 M PCl_3 : 0.0628 M Cl_2 : 0.0628 M
3. F^+ : 0.203 M pH: 2.45

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