APPLICATION CHEMISTRY : ANALYTICAL CHEMISTRY

Partition Coefficient

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Partition Coefficient

- **Iodine** is **soluble in two immiscible solvents** (e.g. water and hexane), its **solubility is very unlikely to be the same** in both solvents.
- **One solvent will be better at dissolving it** than the other.
- When some iodine crystals are shaken with a mixture of hexane and water until no further change takes place, two layers allowed to separate
- The ratio of the concentrations of iodine in each layer is a constant,

Partition Coefficient

- This constant is the equilibrium constant for the change:

$$I_2(aq) \rightleftharpoons I_2(hexane)$$

$$K_c = [I_2(hexane)]/(I_2(aq)]$$

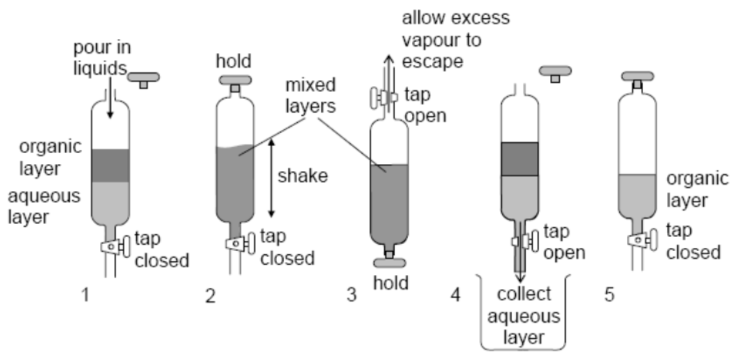

Figure 2.27 – solvent extraction

Partition Coefficient

- K_c refers to K_{pc}, **partition coefficient** of iodine between hexane and water.
- **Partition coefficient (K_{pc}):** the **ratio** of the **concentrations** of a **solute** in two different **immiscible solvent** when an equilibrium has been established
- Partition coefficients have **no units**.
- **Useful in working out how much solvent we need in order to extract a minimum amount of solute from one solvent into another**.

Example 1:
Question:
When 100 cm^3 of an aqueous solution containing 2.0g of the organic dye X was shaken with 20 cm^3 of hexane, it was found that 1.6g of the dye had been extracted into the hexane.
(i) Calculate the partition coefficient of X between hexane and water.
(ii) Calculate the minimum volume of hexane needed to reduce the amount of X in the aqueous layer to less than 0.1g.

Exercise 1

When 500 cm^3 of an aqueous solution containing 10 g of solute *X* were shaken with 50.0 cm^3 of an organic solvent, 2.0 g of solute were extracted by the organic solvent. Calculate the partition coefficient for solute *C* between water and the organic solvent.

Exercise 2

The partition coefficient for a non-polar solute X between ether (an organic solvent) and water is 5.0. In an experiment, 0.96 g of X is shaken with 30 cm^3 of the ether and 10 cm^3 of water. What mass of X dissolves in the ether?

Exercise 3

(a) A solute S is shaken with 100 cm^3 of water and 50 cm^3 of an organic solvent. The concentration of solute S in the water layer is 0.0080 mol dm^{-3} and in the organic solvent is 0.0010 mol dm^{-3}. Calculate the partition coefficient for solute S between the organic solvent and water.

(b) The aqueous layer was removed and shaken with an equal volume (100 cm^3) of pure organic solvent. What will be the concentration of solute S in the organic solvent at equilibrium?

Successive extractions

- Solvents are often expensive and flammable, and can also be polluting to the environment.
- Use the minimum amount of solvent that is needed to achieve the intended goal.
- The use of 20 cm^3 of hexane allowed 1.6g of the dye X to be extracted from its aqueous solution, i.e. (1.6/2.0) x 100 = **80%.**
- We can extract more than this if we use two separate 10 cm^3 portions of hexane,

Example 2:

1st extraction: Let us assume that *x* grams of X have been extracted by the first 10 cm^3. The equilibrium concentrations will therefore be:

2nd extraction: We now separate the 10 cm^3 of hexane solution of X from the aqueous layer, and add another 10 cm^3 of hexane and shake again. Let us assume that the second 10 cm^3 will extract *y* grams of X, the equilibrium concentrations will be:

Exercise 4

100 cm^3 of an aqueous solution contain 10 g of an organic nitrophenol. The partition coefficient of the nitrophenol between ether and water is 3.0 at room temperature. Calculate the mass of nitrophenol extracted by 100 cm^3 of ether

(a) in one extraction

(b) in two extractions, using 50 cm^3 of ether for each extraction

Exercise 5

100 cm^3 of an aqueous solution contain 10 g of an organic acid. The partition coefficient of the acid between ether and water is 0.54 at room temperature. Calculate the mass of acid extracted by 100 cm^3 of ether

(a) in one extraction

(b) in two extractions, using 50 cm^3 of ether for each extraction.

Successive extractions

- Similar calculations show that if we had split the 20 cm^3 of hexane into four 5 cm^3 portions, the amounts of X extracted at each stage would have been as follows:

- 1st extraction by 5 cm^3 : 1.00g
- 2nd extraction by 5 cm^3 : 0.50g
- 3rd extraction by 5 cm^3 : 0.25g
- 4th extraction by 5 cm^3 : 0.125g
- **total extracted = 1.875 g (94%)**

Successive extractions

- All these results are collected together in the following table:

extraction method	percentage extracted
1 x 20 cm^3 of hexane	80%
2 x 10 cm^3 of hexane	89%
4 x 5 cm^3 of hexane	94%

- However, it is impossible to extract **all** of a solute, no matter how many portions of solvent we use.

- It is never possible to move any equilibrium **completely** to one side or the other.

Successive extractions

- But, if the solvent is a volatile one, and if the solute is involatile and stable to heat, it is possible to 'automate' the process by using a continuous extraction apparatus.

- Solvent extraction is used to extract perfumes and pharmaceutical precursors from plants, and in the analysis of insecticide residues and other pollutants in drinking water supplies, blood and milk.

Successive extractions

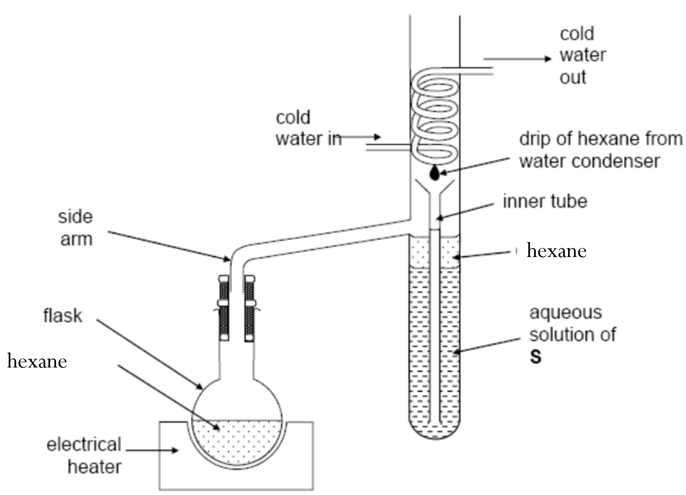

Figure 2.28 – continuous hexane extraction

- Hexane in flask is heated → vapour condenses at the condenser → collected via inner tube → bubbled through aqueous solution → extraction → hexane floats on the aqueous layer.
- As more and more hexane condenses, hexane extract overflows → return to flask.
- Process repeated – more and more S extracted from the aqueous layer into hexane layer in flask.