Organic pollutants in water

For analyzing organic pollutants in water, the compounds may be pre-concentrated by extraction with an organic solvent. You have the job to determine the concentration of 1-naphthol in a contaminated groundwater by using gas chromatography.

You decide to extract 20 mL water samples with a convenient solvent: ethylacetate at 25°C: $K_{i\ ethylacetate\ /\ water} = 10^{2.60}$ [L water /L ethylacetate].

Now you wonder how much ethyl acetate you should use. Calculate the volume of ethylacetate that you need at minimum if you want to extract at least 99% of the total 1-naphthol from the water sample. Are you happy with this pre-concentration step? Somebody tells you that it would be much wiser to extract the sample twice with the goal to get each time 90% of the compound out of the water (which would also amount to an extraction efficiency of 99% in total), and then pool the two extracts.

Answer:

=> In a single extraction step you will need 5 ml of solvent to reach the desired extraction efficiency. A 99% preconcentration of a 20 mL water sample containing 1-naphtol by extraction with ethyl acetate requires at least 5 ml. For solving this problem the same approaches can be used as for the previous problem. Doing this calculation by hand you should start from here and use the inverse of the given partition constant:

- Excercises for an improved intuitive understanding
- Questions for recapitulation
- Good to know
- Minesweeper-problems

$$0.99 = \frac{1}{\left(1 + K_{i\,ws}[L_S / L_w]\frac{V_w[L_w]}{V_S[L_S]}\right)}$$

$$0.99\left(1 + K_{i\,ws}[L_S / L_w]\frac{V_w[L_w]}{V_S[L_S]}\right) = 1$$

$$0.99\left(V_S[L_S] + K_{i\,ws}[L_S / L_w]V_w[L_w]\right) = V_S[L_S]$$

$$0.99\ K_{i\,ws}[L_S / L_w]V_w[L_w] = V_S[L_S] - 0.99V_S[L_S]$$

$$V_S[L_S] = \frac{0.99\ K_{i\,ws}[L_S / L_w]V_w[L_w]}{0.01} = 0.00495[L_S]$$

A 2-fold 90% preconcentration of a 20 mL water sample containing 1-naphtol by extraction with ethyl acetate requires:

Same calculation as above but with 90% instead of 99% as the required extraction efficiency

Step 1: V_s = 0.45 mL

Step 2: V_s = 0.45 mL

V_{tot} = 2 * 0.45 mL = 0.9 mL