Quantitative equilibrium calculations

Fundamentals

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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: $K_{i \text{ ethylacetate / water}} = 10^{2.60}$ [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 <u>here</u> and use the inverse of the given partition constant:

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

 $0.99 = \frac{1}{\left(1 + K_{i \ WS} [L_{S} / L_{W}] \frac{V_{W} [L_{W}]}{V_{S} [L_{S}]}\right)}$

$$0.99\left(1+K_{j|WS}[L_S/L_W]\frac{V_W[L_W]}{V_S[L_S]}\right)=1$$

 $0.99 \left(V_{S}[L_{S}] + K_{i w s}[L_{S} / L_{w}] V_{w}[L_{w}] \right) = V_{S}[L_{S}]$

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

