Sample preparation

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2) Purge and trap

Problem:

You got a two-liter water sample from which you intend to extract 1,2-dichloroethane (DCE) by a purge and trap procedure.

2a) How much air would you have to bubble through the water sample in order to extract at least 98% of DCE at 25°C?
The water/air partition constant is $K_{DCE\ water/air} = 4.2\ [L_{air}/L_{water}]$.

2b) Is it possible to use PU foam in order to trap at least 90% of the extracted DCE at 25°C?
Here is a hint: Since you don't know the exact shape of te breakthrough curve, you have to rely on some estimates: 90% extraction efficiency will be reached if the amount of PU is chosen such that half the retention volume of DCE on the foam is still larger than the air volume that is to be extracted. The porosity of the PU-foam typically is 0.98.

Help

for problem 2a): Use Equation 103 from the script.

for problem 2b): Use Table 19 from Box 11 in combination with Table 9 in Chapter V (script) in order to get the relevant partition constants. Furthermore, use equation 103 for R. Assume a density of 1kg/L for PU.

Answer:

2a) An air volume of 411 L is required.
Did you have a result of less than one liter? Why is this result not plausible?

$K_{DCE\ water/air} = 4.2\ [L_{air}/L_{water}]$ means that the equilibrium water concentration is 4.2 times larger than the equilibrium air concentration. Thus, 2 L of air would extract more than 50% of DCE out of the water (will definetely be higher than the water volume that is to be extracted). What did you do wrong? Note that Equation 103 in the script requires

$K_{air/water}$ while the constant given above is defined as $K_{water/air}$.

2b) In Table 19 (script) you find the following interaction descriptors for DCE:

Compound	**S_i**	**A_i**	**B_i**	**V_i**	**$L_{i\,16}$**	**E_i**
1,2-Dichloroethane	0.64	0.10	0.11	0.6352	2.573	0.416

With these you can calculate the partition constants $K_{PU/air}$ at various temperatures:

Temperature	**$K_{PU/air}$ [ml_{air}/g_{PU}]**
15 °C	2290
35 °C	891
65 °C	234
95 °C	95

From these data you can calculate $K_{PU/air}$ [ml_{air}/g_{PU}] at 25°C as 1430 (you can use the van't Hoff equation or use the average of the logarithmic values from 15 and 35°C).

For the calculation of the amount of PU needed, assume that PU has a density of ca. 1 g/ml. The porosity of 98% then means that 1 g of PU foam has a pore volume of 50 ml. The retention volume equals the retention factor times the pore volume of the sorbent phase. Hence, now you can calculate the retention factor of DCE on PU with Equation 103, Box 13 from Chapter XI in the script:

$R_i = V_R/V_{pore}$ $(=1 + K_{i\ stationary/mobile}\ \rho_b/\ \Theta)$

Porosity = 0.98 = $V_{pore}/V_{PUtotal}$ => $V_{pore} = V_{PUtotal} = 0.98\ (V_{PU}/0.02)$

$V_R = 822\ L_{air} = 0.98\ (V_{PU}/0.02) + K_{PU/air} * V_{PU} = V_{PU}(0.98/0.02 + K_{PU/air})$

Assuming a material density of 1 g/cm^3 for PU: V_{PU} (L) = M_{PU} (kg)

M_{PU} (kg) = 822 L_{air}/(49 [L_{air}/kg_{PU}] + 1438 [L_{air}/kg_{PU}]) = 0.552 kg_{PU}

The goal is to use so much PU that the retention volume is at least twice the volume of air that has to be extracted (here 411 L). Hence, 552 g of PU would be needed. This is a much too large amount of PU to allow a reasonable handling. You will have to look for another, better sorbent.

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