Environmental Chemistry, Homework set

Partitioning – part 1

1. Aqueous solubility of chlorinated alkanes

Estimate the aqueous solubility (C_w^{sat}) and the K_{ow} of dichloromethane at 25°C using a molar volume of 64.5 mL/mol as a measure of its size.

Compound	Molar volume	log C _w ^{sat}
	(mL/mol)	(mol/L)
Chloromethane	54.5	-0.22
1,1-dichloroethane	84.8	-1.3
Trichloromethane	85	-1.19
Tetrachloromethane	100	-2.2
1,2-dichloroethane	85	-1.07
1,1,1-trichloroethane	110	-2.07
1,1,2,2-tetrachloroethane	105.8	-1.74
Hexachlorocyclohexane	200	-4.9

Dichloromethane MW = 85 g/mol

2. Benzene in groundwater

You take a 100 mL sample of groundwater from a contaminated site near a leaking fuel station. You store the sample in a tightly sealed 1L bottle in the refrigerator at 5°C. After two days you analyze the benzene concentration in the water, and you find that it is 100 μ g/L. What was the original benzene concentration in the ground water?

You are given the following data:

 $K_{benzene, aw} = 0.21 at 25^{\circ}C$

 $\Delta_{\text{benzene, aw}}$ H= 20 kJ/mol

3. Disinfectant in the air

Pure 1,4-dichlorobenzene (1,4-DCB) is used as a disinfectant and air freshener in some public toilets. You are asked to evaluate whether 1,4-DCB present in the air may pose a problem to personnel that work in toilet facilities. In this context, you are interested in the maximum pressure of 1,4-DCB that could be present in the toilet air. You are given the following data.

 $T_m = 53.1$ °C (melting point)

 $T_b = 174.0 \, ^{\circ}\text{C} \text{ (boiling point)}$

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Measured vapor pressures at various temperatures:

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p_i^*(29.1 \text{ °C}) = 133.3 \text{ Pa}
p_i^*(44.4 \text{ °C}) = 533.3 \text{ Pa}
p_i^*(54.8 \text{ °C}) = 1333.2 \text{ Pa}
p_i^*(84.8 \text{ °C}) = 5332.8 \text{ Pa}
p_i^*(108.4 \text{ °C}) = 13'332 \text{ Pa}
p_i^*(150.2 \text{ °C}) = 53'328 \text{ Pa}
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- (a) What is the maximum possible 1,4-DCB air concentration that would occur in the public toilet at 20 °C?
- (b) Assume the toilet is located in an uncooled building in the south of Spain. What is the maximum possible 1,4-DCB air concentration that would occur in the public toilet at 60 °C?