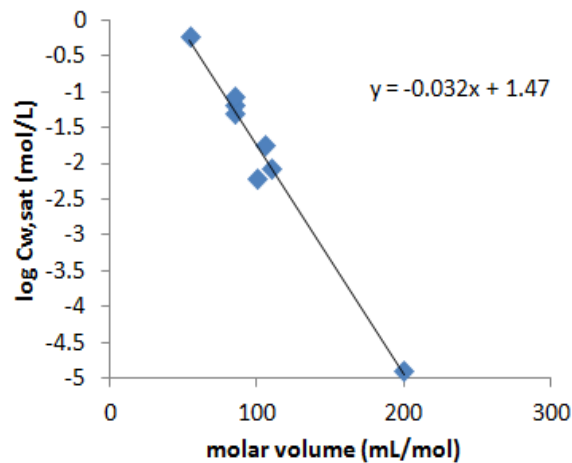


Partitioning part 1 - Solutions

1. Aqueous solubility of chlorinated alkanes

Recall from the notes that within a class of compounds (here: chlorinated alkanes), there is a linear relationship between $\log C_w^{\text{sat}}$ and the molar volume. Plot the data from the table as follows:



We can thus establish the relationship: $\log C_w^{\text{sat}} = -0.032 * (\text{molar volume}) + 1.47$

For dichloromethane we find: $\log C_w^{\text{sat}} = -0.594$; $C_w^{\text{sat}} = 0.25 \text{ mol/L}$.

Now we can determine the K_{ow} using the general relationship between K_{ow} and C_w^{sat} :

$$\log K_{i,ow} = (-\log C_{i,w}^{\text{sat}} + 3.70 + \log MW_i) / 1.08.$$

In this relationship, C_w^{sat} must be in units of ppm, whereby 1 ppm = 1 mg/L. So

$$C_w^{\text{sat}} = (0.25 \text{ mol/L}) * (85 \text{ g/mol}) = 21.25 \text{ g/L} = 21250 \text{ ppm}.$$

$$K_{i,ow} = (-\log (21250) + 3.70 + \log(85)) / 1.08 = 1.20; K_{ow} = 15.85$$

2. Benzene in groundwater

First calculate $K_{\text{benzene, aw}}$ at 5°C. This can be done using the relationship $\ln \frac{K_{12}(T_2)}{K_{12}(T_1)} = \frac{\Delta_{12}H}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$

Or, more simply, from table 3.5 given in the notes, we know that – given a $\Delta_{12}H$ of 20 kJ/mol – K_{12} decreases by a factor of 1.33 for every 10°C decrease in temperature. So:

$$K_{\text{benzene, aw}}(5^\circ\text{C}) = K_{\text{benzene, aw}}(25^\circ\text{C}) / (1.33)^2 = 0.12 = C_{\text{benzene, air}} / C_{\text{benzene, water}}$$

Since we know both $K_{\text{benzene, aw}}$ and $C_{\text{benzene, water}}$, we can calculate the concentration of benzene in air:

$$C_{\text{benzene, air}} = K_{\text{benzene, aw}} * 100 \text{ } \mu\text{g/L} = 12 \text{ } \mu\text{g/L}$$

We have 900 mL of air in the bottle, so the total mass of benzene in air is:

$$0.9 \text{ L} * 12 \text{ } \mu\text{g/L} = 10.8 \text{ } \mu\text{g}$$

The mass of benzene in 100 mL water is:

Partitioning part 1 - Solutions

$$0.1 \text{ L} * 100 \text{ } \mu\text{g/L} = 10 \text{ } \mu\text{g}$$

So total mass of benzene in the bottle is:

$$10.8 \text{ } \mu\text{g} + 10 \text{ } \mu\text{g} = 20.8 \text{ } \mu\text{g}$$

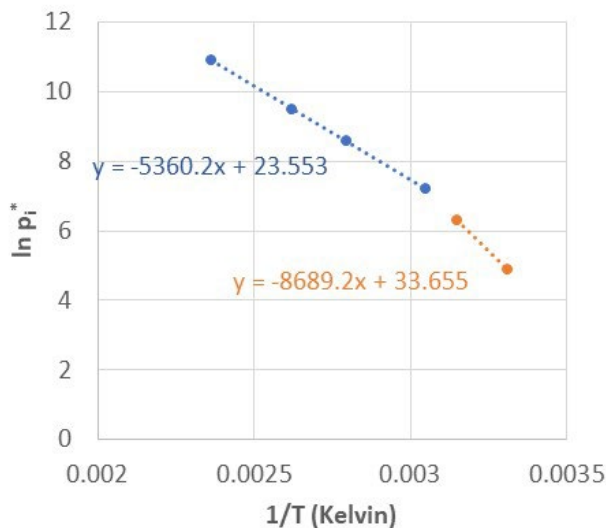
Considering that all this benzene originally came from 100 mL of groundwater, the concentration of benzene in the original groundwater was $20.8 \text{ } \mu\text{g} / 100\text{mL} = 208 \text{ } \mu\text{g/L}$.

3. Disinfectant in air

Recall the relationship between partitioning constants and temperature:

$$\ln K_{12} = -\frac{\Delta_{12}G}{RT} + \ln(\text{constant})$$

Plot $\ln p_i^*$ vs. $1/T$ (in Kelvin) to find p_i^* (separately for $T > T_m$, where 1,4-DCB is a **liquid** and $T < T_m$, where it is a **solid**). We find:



Inserting for $T = 20 \text{ } ^\circ\text{C}$, we obtain: $\ln p_i^* = -8689.2 * (1/293) + 33.655 = 3.99$; $p_i^* = 54.5 \text{ Pa}$

Inserting for $T = 60 \text{ } ^\circ\text{C}$, we obtain: $\ln p_i^* = -5360.2 * (1/333) + 23.553 = 7.46$; $p_i^* = 1730.7 \text{ Pa}$