

1. Show that  $x_{tol} = 0.11$  in the gasoline.

Suppose we consider 1 L of gasoline.

$$\text{Mass of gasoline} = (1 \text{ L})(950 \text{ g/L}) = 950 \text{ g.}$$

$$\text{Moles of gasoline} = 950 \text{ g gasoline} * \frac{1 \text{ mol gasoline}}{51 \text{ g gasoline}} = 18.63 \text{ mol}$$

$$\text{Mass of toluene} = (950 \text{ g gasoline})(0.20) = 190 \text{ g toluene}$$

$$\text{Moles of toluene} = 190 \text{ g toluene} * \frac{1 \text{ mol toluene}}{92.14 \text{ g toluene}} = 2.062 \text{ mol}$$

$$X = \frac{2.062 \text{ mol toluene}}{18.63 \text{ mol gasoline}} = 0.11 \quad \checkmark$$

2. Estimate  $x^{sl}$  from  $C^{sl}$

$$\text{Given } C^{sl} = \frac{530 \text{ mg toluene}}{1 \text{ L water}}$$

$$X^{sl} = \frac{530 \text{ mg toluene}}{1 \text{ L water}} * \frac{1 \text{ g toluene}}{1000 \text{ mg tol}} * \frac{1 \text{ mol tol}}{92.14 \text{ g tol}} * \frac{1 \text{ L water}}{998 \text{ g water}} * \frac{18.01 \text{ g water}}{1 \text{ mol water}} = \boxed{1.0 \times 10^{-4}}$$

3. Estimate/calculate  $x^{a2}$

$$\text{Equilibrium between phases: } f_{tol}^{gas} = f_{tol}^{a2}$$

Gasoline is ideal liquid, water is not.

$$X_{tol}^{gas} p^{sat} = X_{tol}^{a2} \alpha p^{sat}$$

Notice  $p^{sat}$  drops out of equation.

$$\text{Also notice } X^{sl} < 10^{-3} \text{ so } \alpha = \alpha^{\infty} = \frac{1}{X^{sl}} !$$

$$X_{tol}^{gas} = X_{tol}^{a2} \cdot \frac{1}{X^{sl}} \Rightarrow X_{tol}^{a2} = (X_{tol}^{gas})(X^{sl})$$

$$X_{tol}^{a2} = (0.11)(1.0 \times 10^{-4}) = \boxed{1.1 \times 10^{-5}}$$

4. Estimate/calculate  $C_{tol}^{aq}$

We just derived  $X_{tol}^{aq} = (X_{tol}^{gas})(X^{sl})$  in problem 3

But this is the same as  $C_{tol}^{aq} = (X_{tol}^{gas})(C^{sl})$

$$\text{Thus } \frac{C_{tol}^{aq}}{C^{sl}} = X_{tol}^{gas} = 0.11 !!$$

$$C_{tol}^{aq} = (0.11)(530 \text{ mg/L}) = \boxed{58 \text{ mg/L}} \quad \dots \text{ OK if you said } 58.3 \frac{\text{mg}}{\text{L}}$$

5. Estimate/calculate conc. of toluene in the sediment

$$q = K_d C_{tol}^{aq}$$

$K_d = f_{oc} K_{oc}$  ... so we need  $K_{oc}$

Assume  $\log_{10}(K_{oc}) \approx \log_{10}(K_{ow}) - 0.21$  from Karickhoff

$$\Rightarrow \log_{10}(K_{oc}) = 2.73 - 0.21 = 2.52$$

$$K_{oc} = 331 \text{ L/kg} = 331 \frac{\text{L water}}{\text{kg organic matter}}$$

$$K_d = f_{oc} K_{oc} = \left(0.10 \frac{\text{kg organic matter}}{\text{kg sediment}}\right) \left(331 \frac{\text{L water}}{\text{kg organic matter}}\right) \\ = 33.1 \text{ L water / kg sediment}$$

$$q = \left(33.1 \frac{\text{L water}}{\text{kg sediment}}\right) \left(58.3 \frac{\text{mg toluene}}{\text{L water}}\right) = \boxed{1930 \frac{\text{mg toluene}}{\text{kg sediment}}}$$

6. Express conc. of toluene in the sediment as  $\text{mg/L}$ .

$$q_{\text{tol}}^{\text{sed}} = 1930 \frac{\text{mg toluene}}{\text{kg sediment}} \times \frac{1500 \text{ kg sediment}}{\text{m}^3 \text{ sediment}} \times \frac{1 \text{ m}^3}{1000 \text{ L}}$$
$$= 2900 \text{ mg/L}$$

$$q_{\text{tol}}^{\text{sed}} = 2900 \frac{\text{mg}}{\text{L}}, \quad C_{\text{tol}}^{\text{aq}} = 58 \frac{\text{mg}}{\text{L}}$$

Much higher concentration in the sediment.

$$\text{Mass in water} = V^{\text{water}} C_{\text{tol}}^{\text{aq}} = (5 \times 10^5 \text{ m}^3) \left(1000 \frac{\text{L}}{\text{m}^3}\right) \left(58.3 \frac{\text{mg}}{\text{L}}\right) \left(\frac{1 \text{ kg}}{10^6 \text{ mg}}\right)$$
$$= 29,150 \text{ kg in the water}$$

$$\text{Mass in sediment} = V^{\text{sed}} q_{\text{tol}}^{\text{sed}} = (1.5 \times 10^3 \text{ m}^3) \left(1000 \frac{\text{L}}{\text{m}^3}\right) \left(2900 \frac{\text{mg}}{\text{L}}\right) \left(\frac{1 \text{ kg}}{10^6 \text{ mg}}\right)$$
$$= 4,350 \text{ kg in the sediment}$$

Higher mass of toluene in the water.

How do these make sense?

Toluene is moderately hydrophobic ...  $\log(K_{ow}) = 2.73$

So its concentration in organic phases will be much higher than its concentration in water.

But the volume of water is much higher than the volume of sediment. -- thus the mass of toluene in the water is about 6 or 7 times higher than the mass of toluene in the sediment.

7. Flux from water into sediment

Because  $q_{tol}^{sed} < K_d C_{tol}^{aq}$ , we know the mass must be moving from the water to the sediment.

Thus the flux is positive based on the problem statement.

$$N = K_L [C_{tol}^{aq} - C^*]$$

$$N = \text{toluene mass flux, } \frac{\text{mass toluene}}{\text{area} \cdot \text{time}}$$

$K_L$  = overall mass-transfer coefficient

$C_{tol}^{aq}$  = concentration of toluene in the water

$C^*$  = hypothetical aqueous concentration that would be in equilibrium with the sediment

$$= q_{tol}^{sed} / K_d$$

$$N = K_L \left[ C_{tol}^{aq} - \frac{q_{tol}^{sed}}{K_d} \right]$$

From the values given,

$$A \times N = (15,000 \text{ m}^2) (1.0 \times 10^{-6} \frac{\text{m}}{\text{s}}) \left[ 58.4 \frac{\text{mg}}{\text{L}} - \frac{579 \text{ mg/kg}}{33.1 \text{ L/kg}} \right] \left( \frac{1000 \text{ L}}{1 \text{ m}^3} \right)$$

$$= 613.6 \frac{\text{mg toluene}}{\text{s}} \times \frac{86400 \text{ s}}{1 \text{ d}} \times \frac{1 \text{ kg}}{10^6 \text{ mg}}$$

$$= 53 \text{ kg/d moving from water to sediment.}$$

8. Partial pressure and concentration in the air

$$\hat{f}_{\text{tol}}^{\text{air}} = \hat{f}_{\text{tol}}^{\text{gas}}$$

$$y_i P = X_{\text{tol}} P^{\text{sat}} = (0.11)(37.6 \times 10^{-3} \text{ atm})$$

$$P_{\text{tol}} = \boxed{4.1 \times 10^{-3} \text{ atm} = 420 \text{ Pa}}$$

$$\frac{n}{V} = \frac{P}{RT} = \frac{419 \text{ Pa}}{(8.314 \text{ Pa} \cdot \text{m}^3 / \text{mol} \cdot \text{K})(298.15 \text{ K})} = 0.169 \frac{\text{mol}}{\text{m}^3}$$

$$C_{\text{tol}}^{\text{air}} = \left(0.169 \frac{\text{mol}}{\text{m}^3}\right) \left(92.14 \frac{\text{g}}{\text{mol}}\right) \left(\frac{1000 \text{ mg}}{1 \text{ g}}\right) = \boxed{15,600 \text{ mg}/\text{m}^3}$$

9. Estimate  $H_{cc}$

From questions 4 and 8:

$$H_{cc} = \frac{15,578 \text{ mg}/\text{m}^3}{58.3 \text{ mg}/\text{L}} \times \frac{1 \text{ m}^3}{1000 \text{ L}} = 0.2672 \approx \boxed{0.27}$$

From given value of  $H_{cc}$

$$H_{cc} = \frac{6.6 \times 10^{-3} \text{ atm} \cdot \text{m}^3 / \text{mol}}{\left(8.206 \times 10^{-5} \frac{\text{atm} \cdot \text{m}^3}{\text{mol} \cdot \text{K}}\right) (298.15 \text{ K})} = 0.2698 \approx \boxed{0.27}$$

They agree to two significant digits! Good news.  
This probably means I did everything correctly.