

There are 2 questions worth a total of 17 marks. Only non-programmable scientific calculators without text or graphics storage are permitted. Show all work.

Name: \_\_\_\_\_ Student ID: \_\_\_\_\_

- 1) Given the information provided below, indicate which Log  $K_{OW}$  values (3.15 and 4.88) and which boiling points (136°C and 404°) would be expected for each compound and explain why. (3 marks)  
For a bonus mark match the chemical formulas ( $C_{16}H_{10}$  and  $C_8H_{10}$ ) and explain your answers.

	Pyrene	Ethyl benzene
Water solubility (mg/L)	0.148	152
Henry's Law constant ( $\text{atm}\cdot\text{m}^3/\text{mol}$ )	$1.87 \times 10^{-5}$	$5.43 \times 10^{-3}$
Log $K_{OW}$	4.88	3.15
Boiling points (°C)	404	136
Chemical formula	$C_{16}H_{10}$	$C_8H_{10}$

Ethyl benzene has high Henry's law constant and is more volatile, enters the atmosphere more easily and would therefore have a lower boiling point.

Ethyl benzene has a higher water solubility and greater preference for the aqueous phase and would have a lower log  $K_{OW}$ .

Smaller molecular weight compounds are more easily mixed between different phases and are usually more volatile.

- 2) A landfill will be sited on a naturally occurring clay layer that is 3 m thick. The maximum allowable head of leachate that can collect on top of the clay is 30 cm. The self diffusion coefficient for the clay is  $10.2 \times 10^{-10} \text{ m}^2/\text{s}$ , the hydraulic conductivity of the clay is  $1 \times 10^{-10} \text{ m/s}$  and the tortuosity is 0.6. The clay has a porosity of 50%, an average particle size is 0.003 mm, a dry density of  $1.7 \text{ g/cm}^3$ , a specific surface area of  $40 \text{ m}^2/\text{g}$  and contains 1.2% organic carbon. Some of the landfill leachate contains Carbofuran that has a Log  $K_{OW}$  of 1.62 and belongs to the insecticide and herbicide group for which the regression formula is:  $\log K_{OC} = 1.029 \log K_{OW} - 0.18$ .
- Find the Peclet number for these conditions and indicate the type of transport predicted. (4 marks)
  - If the leachate migrating through the clay layer is controlled by diffusion and there is no retardation, when will the concentration ratio,  $C/C_0$  equal 0.1? No interpolation from table is required. (4 marks)
  - What is the retardation factor for the Carbofuran component of the leachate? (6 marks)

2)

$$L = 3 \text{ m}$$

$$h = 0.3 \text{ m}$$

$$D_0 = 10.2 \times 10^{-10} \text{ m}^2/\text{s}$$

$$K = 1 \times 10^{-10} \text{ m/s}$$

$$\tau = 0.6$$

$$n = 0.50$$

$$d = 0.003 \text{ mm}$$

$$\rho_d = 1.7 \text{ g/cm}^3$$

$$\text{SSA} = 40 \text{ m}^2/\text{g}$$

$$1.2\% \text{ organic carbon} = f_{oc}$$

Carbofuran

$$\log K_{oc} = 1.62$$

$$\log K_{oc} = 1.029 \log K_{ow} - 0.18$$

g)

$$Pe = \frac{V_s d}{D_0} \quad D^* = \tau D_0 \quad V_s = \frac{K_i}{n}$$

$$i = \frac{0.3 + 3.0}{3.0} = 1.1$$

$$\frac{0.3 \text{ m}}{3 \text{ m}}$$

$$V_s = \frac{K_i}{n} = 1 \times 10^{-10} \frac{\text{m}}{\text{s}} \times \frac{1.1}{0.5} = 2.2 \times 10^{-10} \frac{\text{m}}{\text{s}}$$

$$Pe = 2.2 \times 10^{-10} \frac{\text{m}}{\text{s}} \times \frac{3 \times 10^{-6} \text{ m}}{10.2 \times 10^{-10} \text{ m}^2} = 6.47 \times 10^{-7} \ll 0.01$$

Therefore diffusion controls transport

b)

$$R = 1$$

$$\frac{C}{C_0} = 0.1 = \exp\left(-\frac{x}{2\sqrt{D^*t}}\right)$$

$$D^* = D_0 \tau = 10.2 \times 10^{-10} \frac{\text{m}^2}{\text{s}} \times 0.6 = 6.12 \times 10^{-10} \frac{\text{m}^2}{\text{s}}$$

convert to years:  $6.12 \times 10^{-10} \frac{\text{m}^2}{\text{s}} \times 60 \times 60 \times 24 \times 365 \frac{\text{s}}{\text{yr}}$

$$= 0.0193 \frac{\text{m}^2}{\text{yr}}$$

$$0.1 = \text{erfc}(\beta) \quad \therefore \beta = 1.16$$

$$\frac{3M}{2\sqrt{0.0193 \frac{\text{m}^2}{\text{y}} \sqrt{t}}} = 1.16$$

$$(\sqrt{t})^2 = \left(\frac{10.8}{1.16}\right)^2 = (9.31)^2 = 86.6 \text{ years.}$$

$$c) \quad R = 1 + \frac{p_d k_d}{n} \quad f_{oc}^* = \frac{SSA}{200 (K_{ar})^{0.84}}$$

$$k_d = K_{oc} \times f_{oc}$$

$$\begin{aligned} \log K_{oc} &= 1.029 \log K_{ar} - 0.18 \\ &= 1.029 \times 1.62 - 0.18 \\ &= 1.487 \end{aligned}$$

$$\begin{aligned} K_{oc} &= 30.69 \\ K_{ar} &= 41.69 \end{aligned}$$

$$f_{oc}^* = \frac{40}{200 (41.69)^{0.84}} = 8.71 \times 10^{-3} = 0.00871 < 0.012$$

so regression eq. valid.

$$k_d = K_{oc} \times f_{oc} = 30.69 \times 0.012 = 0.368$$

$$R = 1 + \frac{1.7 \times 0.368}{0.5} = 2.25$$

2:38.