

① 3-5 $H = 5.5 \times 10^{-3} \frac{\text{atm m}^3}{\text{mol}}$ benzene = "A"

Convert to dimensionless: From units on H:

$p_A = H C_A \rightarrow$ convert to $y_A = H x_A$?

$y_A = H x_A$ identities: or $C_{A,G} = H C_{A,L}$?

$\frac{\text{mol A}}{\text{mol air}} - y_A = p_A / p$ — total pressure
 $\frac{\text{mol A}}{\text{mol H}_2\text{O}} - x_A = C_A / C$ — $\frac{\text{mol A} / \text{vol H}_2\text{O}}{\text{mol H}_2\text{O} / \text{vol H}_2\text{O}}$

$y_A p = H x_A C \Rightarrow y_A = \left(\frac{H C}{p} \right) x_A$

$\frac{H C}{p} = 5.5 \times 10^{-3} \frac{\text{atm m}^3}{\text{mol}} \frac{C}{p}$ — "dimensionless H"
 molar density of H₂O = 55,556 mol/m³
 1 atm

$= 5.5 \times 10^{-3} \frac{\text{atm m}^3}{\text{mol}} \frac{55,556 \text{ mol}}{\text{m}^3} \frac{1}{1 \text{ atm}}$

$= 305.6$

so $y_A = 305.6 x_A$

$C_{A,G} = H C_{A,L}$

$p_A = H C_{A,L}$

$p_A V = n_A R T$

$\frac{p_A}{R T} = \frac{H}{R T} C_{A,L}$

$\frac{n_A}{V} = C_{A,G} = \frac{p_A}{R T}$

$C_{A,G} = \left(\frac{H}{R T} \right) C_{A,L}$

$\frac{H}{R T} = \frac{5.5 \times 10^{-3} \text{ atm m}^3}{0.0821 \text{ L atm mol}^{-1} \text{ K}^{-1} \times 298 \text{ K}} \frac{\text{mol} \cdot \cancel{\text{K}}}{\cancel{\text{m}^3} \times 10^3 \cancel{\text{K}}}$ — "dimensionless H"
 $= 0.225$

so $C_{A,G} = 0.225 C_{A,L}$

(2)



b) $\text{MW} = 165.82$
 $\text{Sol} = 150 \text{ mg/L}$
 $\text{P}_{\text{vap}} = 60 \text{ mm Hg}$
 $H = \exp\left(12.5 - \frac{4920}{298}\right)$
 $= 0.018 \text{ atm} \cdot \text{m}^3/\text{mol}$
 $K_{\text{oc}} = 364 \text{ mL/g}$ mL H₂O/g O.C.
 $\log K_{\text{ow}} = 2.6$
 $\text{BCF} = 314/\text{Kg}$ L H₂O/Kg body wt

c) i) $p_A = \text{HCA}$

$$= 0.018 \frac{\text{atm} \cdot \text{m}^3}{\text{mol}} \cdot \frac{58 \text{ mg}}{\text{L}} \cdot \frac{\text{mol}}{165.82 \text{ g}}$$

$$\times \frac{10^3 \text{ L}}{\text{m}^3} \cdot \frac{\%}{10^5 \text{ mg}} = 6.34 \times 10^{-3} \text{ atm or } 4.8 \text{ mm Hg}$$

ii) $\frac{58}{150} \times 100 = 38.7\%$

iii) $K_{\text{ow}} = 10^{2.6} = 398 > 10 \Rightarrow$ prefers organic phase

iv) $f_{\text{oc}} = 0.12$ $K_p = K_{\text{oc}} f_{\text{oc}} = 364 \frac{\text{mL}}{\text{g}} \cdot 0.12 = 44.1 \frac{\text{mL}}{\text{g}}$

$$C_s = K_p C_w = 44.1 \frac{\text{mL H}_2\text{O}}{\text{g soil}} \cdot \frac{58 \text{ mg PCE}}{\text{L H}_2\text{O}} \cdot \frac{\text{L}}{10^3 \text{ mL}} \cdot \frac{10^3 \text{ g}}{\text{kg}}$$

$$= 2556 \frac{\text{mg PCE}}{\text{kg soil}} = 2556 \text{ ppm}$$

50 mL octanol
50 mL H₂O
0.2 g DDT

what is C_{oct} & C_w ?

$$\log K_{ow} = 6.19$$

$$K_{ow} = 1.55e6 = \frac{C_{oct}}{C_w} \Rightarrow C_{oct} = 1.55e6 C_w$$

$$\frac{\text{mg DDT}}{\text{L H}_2\text{O}} \quad \frac{\text{mg DDT}}{\text{L H}_2\text{O}}$$

Mass Balance on DDT:

$$\text{total mass}_{\text{DDT}} = \text{mass DDT in oct} + \text{mass DDT in H}_2\text{O}$$

$$0.2 \text{ g} = C_{oct} 50 \text{ mL oct} + C_w 50 \text{ mL H}_2\text{O}$$

$$0.2 \text{ g} = 1.55e6 C_w 50 \text{ mL oct} + C_w 50 \text{ mL H}_2\text{O}$$

$$= 7.744e7 C_w \text{ mL} \frac{\text{L}}{10^3 \text{ mL}} + 50 C_w \text{ mL} \frac{\text{L}}{10^3 \text{ mL}}$$

$$= 7.744e4 C_w (\text{L}) + 0.05 C_w (\text{L})$$

$$200 \text{ mg} = 7.744e4 C_w \frac{\text{mg DDT}}{\text{L H}_2\text{O}} (\text{L})$$

$$C_w = 0.0026 \text{ mg/L}$$

$$C_{oct} = 4003.1 \text{ mg/L}$$

— other way...

$$200 \text{ mg} = C_{oct} 50 \text{ mL oct} + 6.452e-7 C_{oct} 50 \text{ mL H}_2\text{O}$$

$$= 0.05 C_{oct}$$

$$C_{oct} = 4000 \text{ mg/L}$$

$$C_w = 0.0026 \text{ mg/L}$$

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1000 m³ Lake
1000 fish
1 g DDT

1 fish = 100 cm³, 5% lipids
What is C_{tissue} in fatty tissue?

$$BCF = 54000 \text{ L/kg} = \frac{C_{\text{tissue}} \text{ mg DDT/kg tissue}}{C_w \text{ mg DDT/L H}_2\text{O}}$$

Mass Balance on DDT

$$\text{total mass DDT} = \text{mass DDT in lake H}_2\text{O} + \text{mass DDT in fish fatty tissue}$$

$$1 \text{ g} = 1000 \text{ m}^3 C_w \frac{10^3 \text{ L}}{\text{m}^3} + (\cancel{1000 \text{ fish}}) \frac{100 \text{ cm}^3 \cancel{\text{fish}}}{\cancel{\text{fish}} \text{ cm}^3} C_{\text{tissue}} \times \frac{5 \text{ kg tissue}}{100 \text{ kg fish}} \frac{\text{kg}}{10^3 \text{ g}}$$

$$1000 \text{ mg} = 10^6 C_w \underset{\substack{\uparrow \\ \text{mg/L}}}{\text{L}} + 5 \underset{\substack{\uparrow \\ \text{kg}}}{\text{kg tissue}} (54000 C_w)$$

$$C_w = 0.000787 \text{ mg/L}$$

$$C_{\text{tissue}} = 42.5 \frac{\text{mg DDT}}{\text{kg fat tissue}}$$