1.725 Fate + Transport

Problem Set # 1

Solutions

1-1, 6, 8, 19, 22

1. a) $\frac{1.5\,g\,SO_4^{2-}}{L} \times \frac{mol}{96\,g\,SO_4^{2-}} \times \frac{32\,g\,S}{mol} = \boxed{0.5\,g/L}$

b) $\frac{1.5\,g\,SO_4^{2-}}{L} \times \frac{mol}{96\,g\,SO_4^{2-}} = \boxed{0.016\,mol/L}$

c) # of charge units = # of equivalents (per mole)

$N = equiv/L$

$(M = mol/L)$

$\frac{0.016\,mol}{L} \times \frac{2\,equiv}{mol} = \boxed{0.031\,N}$

d) $\frac{1.5\,g\,SO_4^{2-}}{L} \times \frac{1000\,mg}{g} = 1500\,mg/L = \boxed{1500\,ppm}$

In dilute aqueous solutions, mg/L = ppm.

for example.

$$\underset{\substack{\uparrow\\ \text{definition}\\ \text{of ppm}}}{\frac{1\,\cancel{g\,SO_4^{2-}}}{10^6\,\cancel{g\,water}}} \times \underset{\substack{\uparrow\\ \text{density}\\ \text{of water}}}{\frac{1\,\cancel{g\,water}}{1\,\cancel{mL\,water}}} \times \frac{1000\,mg\,SO_4^{2-}}{1\,\cancel{g\,SO_4^{2-}}} \times \frac{1000\,\cancel{mL\,water}}{1\,L\,water} = \frac{mg\,SO_4^{2-}}{L\,water}$$

6. a) advection

$J = C \cdot V$

$$= \frac{10\,mg}{L} \times \frac{2\,cm}{hr} \times \underset{\substack{\uparrow\\ 1\,L = 1000\,mL\\ mL = cm^3}}{\frac{L}{1000\,cm^3}} = \boxed{0.02\,\frac{mg}{cm^2 \cdot hr}}$$

b) Fickian transport

$J = D \frac{dc}{dx}$

$= 10^{-5} \frac{cm^2}{sec} \times \frac{30 g/L}{10 cm} \times \frac{L}{1000 cm^3} = \boxed{3 \times 10^{-8} \frac{g}{cm^2 \cdot s}}$

c) advection

$J = C \cdot V$

$= \frac{0.05 g}{L} \times \frac{30 cm}{sec} \times \frac{L}{1000 cm^3} = \boxed{0.0015 \frac{g}{cm^2 \cdot s}}$

8. call citric acid HA (standard notation for any acid; A^- is the conjugate base)

unknown species: HA, A^-, H^+, OH^-

constraints: K_a, K_w, electroneutrality, conservation of mass

more specifically,

① $[H^+][OH^-] = 10^{-14}$

② $HA \rightleftharpoons H^+ + A^-$ $\quad \frac{[H^+][A^-]}{[HA]} = 8.4 \times 10^{-4}$

③ $[H^+] = [OH^-] + [A^-]$

④ $[HA] + [A^-] = 0.1$ mol/L

We have 4 equations and 4 unknowns, so the system can be solved. This can be done either through "brute force", or by making simplifying assumptions.

Here is one approach:

1) acidic solution → assume $[OH^-]$ is small/negligible (10^2 smaller than anything else in the equation)

③ becomes $[H^+] = [A^-]$

2) assume very little of [HA] dissociates, so $[HA] >> [A^-]$

④ becomes $[HA] = 0.1$ mol/L

3) plug into ②

$$\frac{[H^+]^2}{0.1} = 8.4\times10^{-4} \qquad [H^+] = 9.2\times10^{-3}\ M$$

$$pH = -\log[H^+] = 2.04$$

4) check assumptions

from ①, $[OH^-] = \frac{10^{-14}}{[H^+]} = \frac{10^{-14}}{9.2\times10^{-3}} = 1.1\times10^{-12}$

so neglecting $[OH^-]$ is valid

$$\left.\begin{aligned}&[A^-] = [H^+] = 9.2\times10^{-3}\ M\\ &[HA] = 0.1 - [A] = 9.1\times10^{-2}\ M\end{aligned}\right\} \text{ not } 10^2 \text{ apart, so } [HA] \gg [A^-] \text{ } \underline{\text{not}} \text{ valid}$$

Without that simplification, ② becomes

$$\frac{[H^+]^2}{0.1-[H^+]} = 8.4\times10^{-4}$$

$$[H^+]^2 = 8.4\times10^{-5} - 8.4\times10^{-4}[H^+]$$

$$[H^+]^2 + 8.4\times10^{-4}[H^+] - 8.4\times10^{-5} = 0$$

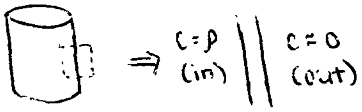
$$\frac{-b\pm\sqrt{b^2-4ac}}{2a} \Rightarrow \frac{-8.4\times10^{-4}\pm\sqrt{(8.4\times10^{-4})^2-4(1)(-8.4\times10^{-5})}}{2(1)}$$

$$[H^+] = 8.75\times10^{-3}\ M$$

$\boxed{pH = 2.06}$ (very close to our first answer!)

19. find flux density.

$$J = D\frac{dc}{dx}$$



$$= 10^{-10}\frac{cm^2}{sec} \times \frac{1.6\,g/cm^3}{0.1\,cm} = 1.6\times10^{-9}\frac{g}{cm^2\cdot sec}$$

flux = J × area

$$= 1.6\times10^{-9}\frac{g}{cm^2\cdot sec} \times 8\,cm^2 = \boxed{1.28\times10^{-8}\frac{g}{sec}}$$

b) Several possible conditions, including:

- The gas stream must move fast enough to remove the CCl_4, so that $c \approx 0$ just outside the tube.
- Temperature must be constant, so that D stays constant.
- The gas flow must be constant, so that the CCl_4 that diffuses out of the tube mixes with the same volume of gas at all times.

22. a) $J = c \cdot v$

$$= \frac{220 \times 10^{-6}\ \text{mol}}{\text{L}} \times \frac{10\ \text{cm}}{\text{sec}} \times \frac{35.45\ \text{g Cl}}{\text{mol Cl}} \times \frac{\text{L}}{1000\ \text{cm}^3} = \boxed{7.8 \times 10^{-5}\ \frac{\text{g}}{\text{cm}^2 \cdot \text{s}}}$$

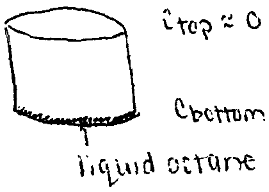
b) ppt = g/L

$$\frac{1\ \text{g Cl}}{1000\ \text{g water}} \times \frac{1\ \text{g}}{\text{cm}^3} \times \frac{1000\ \text{cm}^3}{\text{L}} = \frac{1\ \text{g Cl}}{1\ \text{L water}}$$

$$J = D\frac{dc}{dx}$$

$$= 10^{-5}\ \frac{\text{cm}^2}{\text{sec}} \times \frac{18\ \text{g/L}}{500\ \text{cm}} \times \frac{\text{L}}{1000\ \text{cm}^3} = \boxed{3.6 \times 10^{-10}\ \frac{\text{g}}{\text{cm}^2 \cdot \text{s}}}$$

c)



$c_{top} \approx 0$ (tank is open, so any octane vapor at the top will diffuse away)

C_{bottom} → determined by vapor pressure, since the air right above the octane layer is in equilibrium with the octane

for C_{bottom}:
$$\frac{n}{V} = \frac{P}{RT} = \frac{0.019\ \text{atm}}{0.08206\ \text{L atm/mol K}\ (298\ \text{K})} = 7.77 \times 10^{-4}\ \text{mol/L}$$

↑ assumption

$$7.77 \times 10^{-4}\ \frac{\text{mol}}{\text{L}} \times \frac{114\ \text{g}}{\text{mol}} = 0.089\ \text{g/L}$$

$$J = D\frac{dc}{dx} = \frac{0.2\ \text{cm}^2}{\text{sec}} \times \frac{0.089\ \text{g/L}}{400\ \text{cm}} \times \frac{\text{L}}{1000\ \text{cm}^3} = \boxed{4.4 \times 10^{-8}\ \frac{\text{g}}{\text{cm}^2 \cdot \text{s}}}$$

↑ standard value for D in air (p.18)