

19-7

tetrachloroethene  $C_2Cl_4$

1,4-dichlorobenzene  $C_6H_4Cl_2$

The average depth  $h = 0.4m$  mean flowing velocity  $\bar{u}_7 = 0.67 m/s$

According to equation 19-2

$$\frac{1}{V_{ia}} = \frac{1}{V_{iw}} + \frac{1}{V_{ia} K_{iaw}}$$

$$V_{ia} = 1.52 \times \bar{V}_i^{-0.67} \quad (19-21) \quad \bar{V}_i(C_2Cl_4) = 116.5 \frac{cm^3}{mol} \quad (\text{Table 7-2})$$

$$= 1.52 \times (116.5)^{-0.67} = 0.06 \text{ cm}^2/s$$

$$V_{ia} = \left( \frac{D_{ia}}{D_{H_2O,a}} \right)^{2/3} V_{H_2O,a} \quad (D_{H_2O,a} = 0.26 \text{ cm}^2/s, V_{H_2O,a} = 0.15 \text{ cm/s})$$

From textbook.

$$= \left( \frac{0.06}{0.26} \right)^{2/3} \times 0.15 = 0.06 \text{ cm}^2/s$$

Using Small-Eddy and Small Roughness Model

$$V_{iw} = 0.17 (Sc_{iw})^{-1/2} \cdot \left( \frac{V_w \times (\bar{u}_7 / \alpha)^3}{h} \right)^{1/4}$$

where  $h$  is total water depth  $h = 4m$

$\alpha$  is a nondimensional factor then  $\alpha = 15$   $\bar{u}_7 = 0.67 m/s$

$$V_w = 1.004 \times 10^{-6} \text{ m}^2/s \quad (T = 293K)$$

$$V_{iw} = 6.57 \times 10^{-4} \cdot Sc_{iw}^{-1/2}$$

Given the table of  $C_2Cl_4$

|        |        |               |
|--------|--------|---------------|
| 0 m    | 0 s    | 690 $\mu g/L$ |
| 600 m  | 900 s  | 585 $\mu g/L$ |
| 1200 m | 1800 s | 505 $\mu g/L$ |
| 2400 m | 3600 s | 565 $\mu g/L$ |

$\bar{V}_{iw}$

$$6.3 \times 10^{-6} \text{ cm}^2/s \quad \frac{dc}{dt} = D_w \frac{dc}{dx^2}$$

\* detailed calculation by python.

$$\therefore \bar{D}_{iw} = 6.3 \times 10^{-6} \text{ cm}^2/\text{s} \quad \bar{S}_{ciw} = \frac{V_w}{\bar{D}_{iw}} = 1593.7$$

According to the Appendix C  $K_{iaw} = 10^{2.08}$

$$\therefore \frac{1}{V_{iaw}} = \frac{1}{V_{iw}} + \frac{1}{V_{ia} \cdot K_{iaw}}$$

the  $V_{iw}$  equation mentioned before.

$$\bar{V}_{iw} = 6.57 \times 10^{-4} \times (\bar{S}_{ciw})^{-1/2} = 1.65 \times 10^{-5} \text{ cm/s}$$

$$\frac{1}{V_{iaw}} = \frac{1}{V_{iw}} + \frac{1}{V_{ia} \cdot K_{iaw}} \Rightarrow V_{iaw} = 0.072 \text{ cm/s}$$

(2) In the same way. for 1,4-dichlorobenzene

$$\bar{V}_i = 174.8 \frac{\text{cm}^3}{\text{mol}}$$

$$D_{ia} = 1.52 \times \bar{V}_i^{-0.67} = 0.05 \text{ cm}^2/\text{s}$$

$$V_{ia} = \left( \frac{D_{ia}}{D_{H_2Oa}} \right)^{2/3} \cdot V_{H_2Oa} = 0.05 \text{ cm/s}$$

And use small-Zddy and small Roughness model

$$V_{iw} = 0.17 \cdot (\bar{S}_{ciw})^{-1/2} \cdot \left( \frac{V_w \cdot (\bar{u}_{\tau/\alpha})^3}{\eta} \right)^{1/4}$$

$$= 3.6970 \times 10^{-4} \times (\bar{S}_{ciw})^{-1/2}$$

Given the table of  $\text{C}_6\text{H}_4\text{Cl}_2$   $\bar{D}_{iw}$

|        |        |                     |  |
|--------|--------|---------------------|--|
| 0 m    | 0 s    | 234 $\mu\text{g/L}$ | $4.8 \times 10^{-6} \text{ cm}^2/\text{s}$ |
| 600 m  | 900 s  | 201 $\mu\text{g/L}$ |  |
| 1200 m | 1800 s | 180 $\mu\text{g/L}$ |  |
| 2400 m | 3600 s | 130 $\mu\text{g/L}$ |  |



$$\bar{D}_{iw} = 4.8 \times 10^{-6} \text{ cm}^2/\text{s}$$

$$\bar{S}_{ciw} = \frac{V_w}{\bar{D}_{iw}} = 2100$$

$$\text{Then } \bar{V}_{iw} = 3.6970 \times 10^{-4} \times (\bar{S}_{ciw})^{-1/2} = 1.43 \times 10^{-5} \text{ cm/s}$$

$$\text{Therefore } \frac{1}{V_{iaw}} = \frac{1}{V_{iw}} + \frac{1}{V_{ia} K_{iaw}}$$

$$\text{According to the Appendix-C } K_{iaw} = 10^{-11.04}$$

$$\frac{1}{V_{iaw}} = \frac{1}{1.43 \times 10^{-5}} + \frac{1}{0.05 \times 10^{-11.04}}$$

$$V_{iaw} = 0.0046 \text{ cm/s}$$



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According to the Kow equation

$$\frac{1}{V_{iaw}} = \frac{1}{V_{iw}} + \frac{1}{V_{ia} K_{iaw}}$$

when value of  $K_{iaw}$  increase the term of  $\frac{1}{V_{ia} K_{iaw}}$  decline

Therefore,  $\frac{1}{V_{ia} K_{iaw}}$  close to 0 with a larger  $K_{iaw}$  value.

Then  $V_{iaw} \approx \frac{1}{V_{iw}}$  (At constant). As we can seen from this figure.  $V_{iaw}$  nearly doesn't change when  $K_{iaw}$  is relatively large. On the other hand, when  $K_{iaw}$  is relatively small, the term of  $\frac{1}{V_{ia} K_{iaw}}$  cannot be ignored. Therefore,  $V_{iaw}$  increase with the increase in  $K_{iaw}$ .

For different value of  $U_{10}$ . According to the equation.

$$V_{iw} = (9 \times 10^{-4} + 7.2 \times 10^6 \cdot U_{10}) \times \left( \frac{Sc_{iw}}{660} \right)^{-1/2}$$

When  $U_{10}$  increase,  $V_{iw}$  will increase too. In Addition

$K_{iaw}$  is relatively large.  $\frac{1}{V_{iaw}} \approx \frac{1}{V_{iw}}$ . Therefore,  $\frac{1}{V_{iaw}} (U_{10}=20 \text{ m/s})$  is larger than  $\frac{1}{V_{iaw}} (U_{10}=10 \text{ m/s})$  due to  $\frac{1}{V_{iw}} (U_{10}=20 \text{ m/s})$  is higher than  $\frac{1}{V_{iw}} (U_{10}=10 \text{ m/s})$ . And this figure can valid this assumption.



3. (a) trichloroethene (TCE)  $\text{C}_2\text{HCl}_3$ .

$$\bar{U}_f = 0.27 \text{ m/s} \quad h = 2 \text{ m.}$$

I assume it's water-control in this situation.

$$\text{Then } \frac{1}{V_{iaw}} = \frac{1}{V_{iw}}$$

$$\text{Then } \bar{V}_i = 104.3 \frac{\text{cm}^3}{\text{mol}} \quad (\text{box 7.2 from textbook})$$

$$D_{iw} = \frac{13.26 \times 10^{-5}}{\eta^{1.14} \bar{V}_i^{-0.57}} = 5.39 \text{ cm}^2/\text{s} \quad (T = 293 \text{ K} \quad \eta = 1.002 \times 10^{-3} \frac{\text{kg}}{\text{m} \cdot \text{s}})$$

$$V_w = 1.004 \times 10^{-6} \text{ m}^2/\text{s.}$$

Then

$$S_{ciw} = \frac{V_w}{D_{iw}} = 186.5.$$

$$\therefore V_{iw} = 0.17 \times \left( \frac{V_w (\bar{U}_f / \alpha)^3}{h} \right)^{1/4} \times (S_{ciw})^{-1/2} \quad 19-23$$

where  $h = 2 \text{ m}$   $\alpha = 15$  in this situation.

$$\therefore V_{iw} = 1.64 \times 10^{-5} \text{ m/s}$$

$$\text{Then } \frac{1}{V_{iaw}} = \frac{1}{V_{iw}} \Rightarrow V_{iaw} = 1.64 \times 10^{-5} \text{ m/s}$$

$$K_v = \frac{1}{h} \times V_{iaw} = 0.5 \text{ m}^{-1} \times 1.64 \times 10^{-5} \text{ m/s} = 8.2 \times 10^{-6} \text{ s}^{-1}$$

(b) According to  $K_{iaw} = 10^{-0.4} \Rightarrow 10^{-3} = K_{iaw}^{\text{critical}}$

Then it's water controlled.

$$\frac{1}{V_{iaw}} = \frac{1}{V_{iw}} + \frac{1}{V_{ia} \times K_{iaw}} \quad \text{Then the term of } \frac{1}{V_{ia} \times K_{iaw}} \text{ can be ignored due to large of } K_{iaw}.$$

$$\text{Then } R_{iw} = \frac{1}{V_{iw}} = 6.1 \times 10^4$$

$$V_{ia} = \left( \frac{D_{ia}}{D_{H_2O,a}} \right)^{2/3} \times V_{H_2O,a} \quad , \quad D_{ia} = 1.52 \times \bar{V}^{-0.67} \quad (17-21)$$



then

$$D_{ia} = 0.107 \text{ cm}^2/\text{s}$$

$$V_{ia} = \left( \frac{D_{ia}}{D_{H_2O,a}} \right)^{2/3} \times V_{H_2O,a} \quad \text{where } \begin{cases} V_{H_2O,a} = 0.15 \text{ cm}^3/\text{s} \\ D_{H_2O,a} = 0.16 \text{ cm}^2/\text{s} \end{cases}$$

$$= 0.06 \text{ cm}^3/\text{s}$$

$$\therefore K_{ia} = \frac{1}{V_{ia}} = \frac{1}{0.06} = 16.67 \frac{\text{s}}{\text{cm}^3}$$

$$\therefore f = \frac{K_{ia}}{K_{ia} + K_{iw}} = \frac{16.67}{16.67 + 6.1 \times 10^4} = 2.73 \times 10^{-4}$$

Then air phase can be ignored safely

$\therefore$  After revised.

$$\frac{1}{V_{iaw}} = \frac{1}{K_{iaw} V_{ia}} + \frac{1}{V_{iw}} = 0.02 \text{ cm}^3/\text{s}$$

(c) For chlorophenol  $\text{C}_6\text{H}_5\text{ClO}$   $K_{iaw} = 10^{-3.24}$

$$\bar{V}_i = 175.03 \frac{\text{cm}^3}{\text{mol}}$$

$$D_{ia} = 1.52 \times \bar{V}_i^{-0.67} = 0.05 \text{ cm}^2/\text{s}$$

$$V_{ia} = \left( \frac{D_{ia}}{D_{H_2O,a}} \right)^{2/3} \times V_{H_2O,a} = 0.05 \text{ cm}^3/\text{s}$$

$$D_{iw} = 1.52 \times 10^{-4} \times \bar{V}_i^{-0.64} = 5.58 \times 10^{-6} \text{ cm}^2/\text{s}$$

$$Sc_{iw} = \frac{V_w}{D_{iw}} = 180.0$$

$$\therefore V_{iw} = 0.17 \times \left( \frac{V_w \times (\bar{U}_F \times \alpha)^3}{h} \right)^{1/4} \times (Sc_{iw})^{1/2}$$
$$= 1.66 \times 10^{-5} \text{ cm}^3/\text{s}$$



$$\frac{1}{V_{iaw}} = \frac{1}{V_{iw}} + \frac{1}{V_{iaw} \cdot K_{iaw}} \Rightarrow V_{iaw} = 2.88 \times 10^{-5} \text{ cm/s}$$

Then  $K_{iaw} = 10^{-3.24} \approx 10^{-3} = K_{iaw}^{\text{critical}}$

then liquid-phase resistance cannot be ignored safely

(d) the river bottom is fine-grained sand

then  $\alpha = 20$  due to this situation.

$$\therefore V_{iw} = 0.17 \times \left( \frac{V_w \times (\bar{u}_b/\alpha)^3}{n} \right)^{1/4} \times (S_{ciw})^{-1/2}$$

$$= 1.34 \times 10^{-5} \text{ cm/s}$$

$$\therefore \frac{1}{V_{iaw}} = \frac{1}{V_{iw}} + \frac{1}{V_{iw} \cdot K_{iaw}}$$

$$V_{iaw} = 0.04 \text{ cm/s}$$

the  $v_{iaw}$  nearly change because of  $K_{iaw}$  is very large.  
then still a air-contrast.



4. PAH fluorene  $C_{17}H_{10}$

$$K_{iaw} = 10^{-2.39}$$

$$K_{iow} = 10^{4.32}$$

$$V_{sw} = f_s \frac{1-\phi}{\phi} = 1.52 \frac{kg}{L} \times \frac{1-0.37}{0.37} = 2.59 \frac{kg}{L}$$

$$D_{i,eff} = \frac{1}{V} D_{iw} \left( \frac{1}{1 + V_{sw} \cdot K_{id}} \right) \quad \text{where } K_{id} = 31.7 \frac{L}{kg}$$

I assume temperature is  $20^\circ C$  and there is non-sorbing

$$\bar{V} = 300.0 \frac{cm^3}{mol} \quad (\text{From table box 7.2})$$

$$D_{iw} = 1.52 \times 10^{-4} \times \bar{V} (1-0.64) = 3.95 \times 10^{-6} cm^2/s \quad 17.24a.$$

$$\therefore D_{i,eff} = \frac{1}{1.42} \times 3.95 \times 10^{-6} \times \left( \frac{1}{1 + 2.59 \times 31.7} \right)$$

$$= 2.43 \times 10^{-8} cm^2/s$$

(2) According to equation 17-9

$$C_2 = C_1 \operatorname{erfc} \left( \frac{x}{2(Dt)^{1/2}} \right)^{1/2} \Rightarrow \operatorname{erfc} \left( \frac{x}{2(Dt)^{1/2}} \right) = 0.1 = \frac{C_1}{C_2}$$

And use result of Appand A.2

$$\operatorname{erfc} \left( \frac{x}{2(Dt)^{1/2}} \right) = 0.1 \Rightarrow \frac{x}{2(Dt)^{1/2}} = 1.2$$

$$\therefore t = \frac{x^2}{2.4^2 \times D_{i,eff}} = \frac{0.01 cm^2}{2.4^2 \times 2.43 \times 10^{-8} cm^2/s} \approx 20.0h$$

(3) the constant is not constant.

When the fluorene concentration in sediment is depleting, it will take longer time to reach 10%  $C_0$  in  $x = 10cm$ .



(d) Sodium sand containing 0.3% organic carbon.

$$\therefore K_{id} = K_{iow} \times f_{oc} = 2.08 \times 10^4 \times 10^{-4.32} = 62.68 \frac{\text{L}}{\text{kg}}$$

$$D_{ieff} = \frac{1}{\tau^2} \times D_{iw} \times \frac{1}{1 + v_{sw} \times K_{id}} = 1.23 \times 10^{-8} \text{ cm}^2/\text{s}$$

In the same way

$$\text{erfc}\left(\frac{x}{2(D_{ieff} \cdot t)^{1/2}}\right) = 0.1 \Rightarrow \frac{x}{2(D_{ieff} \cdot t)^{1/2}} = 1.2 \quad (\text{Appendix A})$$

$$t = \frac{x^2}{2.4^2 \times 1.23 \times 10^{-8} \text{ cm}^2/\text{s}} = 1415 \text{ s} \approx 40 \text{ h}$$

(e) 0.4% organic carbon + 5% activated carbon → from an article.

$$K_d = f_{oc} \times K_{iow} + f_{ac} \times K_{iow}$$
$$= 62.68 + 0.05 \times 15 \times 10^3 = 137.7 \frac{\text{L}}{\text{kg}}$$

$$\therefore D_{ieff} = \frac{1}{\tau^2} \times D_{iw} \times \frac{1}{1 + v_{sw} \times K_d} = 5.64 \times 10^{-9} \text{ cm}^2/\text{s}$$

In the same way

$$\text{erfc}\left(\frac{x}{2(D_{ieff} \cdot t)^{1/2}}\right) = 0.1 \Rightarrow \frac{x}{2(D_{ieff} \cdot t)^{1/2}} = 1.2$$

$$\therefore t = \frac{x^2}{2.4^2 \times 5.64 \times 10^{-9} \text{ cm}^2/\text{s}} \approx 85 \text{ h}$$

(f) As the result, I think organic rich sands with activated can be an effective strategy. On the other hand the life-span of activated carbon and turbulence should be considered.