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Presentation Assignment

Compound chosen: Dimethyl Phthalate

(1) Summary of Input and output

	Method one	Method two	Date in Appendix C
p_L^*	$10^{0.7}\ Pa$	$10^{-0.2} Pa$	$p_L^*(298K) = 10^{0.38}\ Pa$
$C_{i,w}^{sat}$	$10^{-0.81}\ mol/L$	$10^{-1.13}\ mol/L$	$C_{i,w}^{sat} = 10^{-1.66}\ mol/L$
K_{iaw}	$10^{-5.28}$	$10^{-4.89}$	$K_{iaw} = 10^{-4.35}$
K_{iow}	$10^{2.05}$	$10^{2.48}$	$K_{iocw} = 10^{1.53}$

* sources: physical values, such as melting point, boiling point is from KNOVEL website
* Estimation method: the parameters of pp-LFERS of this compound is from the article (Tunga Salthammer et al. 2019). And these parameters is used for p_L^*, K_{iaw} and K_{iocw}.
* Estimation method: Table 9.4, 10.4 in textbook and Table in Robort textbook has been used to estimate K_{iaw}, K_{iocw} and p_L^*, respectively.
* More detailed calculation process attached in the appendix in end of this page.

(2)According to the Tm and Tb, the compound should be liquid when temperature is 298K. Then Equation 8-17 should be rational in this situation. I find that it can estimate different parameters, such as p_L^*, K_{iaw} and K_{iocw} with pp-LFERs values. Hopefully, these values has been measured by Tunga Salthammer team at 2019. In some degree, the result should be reliable. On the other hand, it is a little harder to use bond-contribute table. Because this structure of this compound is quite complicated. As we can seen in the result, the error between bond-contribute estimate method is a little bit large in this situation. Therefore, I prefer to choose other methods in some large molar mass compound.

(3)

Input						
	K_{iaw}	K_{iocw}	$C_{i,w}^{sat}$	p_L^*		
	$K_{iaw} = 10^{-4.35}$	$K_{iocw} = 10^{1.53}$	$C_{i,w}^{sat} = 4248.6 g/m^3$	$p_L^* = 10^{0.38}\ Pa$		
	Volume	Density	f_{oc}	Molar Mol	Fraction %	Concentration mol/m^3
Air	2×10^9	1.19	N/A	67.4	6.74	3.37×10^{-9}
Water	9.5×10^5	1000	N/A	912.2	91.2	9.6×10^{-5}
Soil	1.4×10^4	1500	0.02	8.6	0.86	6.15×10^{-5}
Sediment	9.9×10^3	1500	0.04	1.2	1.21	1.23×10^{-4}
Suspend matter	3.5×10	1500	0.04	0.4	0.004	1.23×10^{-4}
Biomass	3.5×10^0	1000	0.2	0.2	0.002	6.5×10^{-4}

According to this result, This compound primarily reside in the water phase and air, because of its relative high solubility and large air volume, respective. Secondly, this result is basically fit my expectation. In terms of very low vapor presser and relatively high solubility, the mass fraction in water should be larger than Air. On the other hand, the concentration seemly depends on both the partition constant Kiow and phase volume as well. As we can seen in this table, the concentration of this compound in biomass phase is the highest due to very small volume, compared to other phase. At last, the solubility is a bit high due to forming H-bond when it into the water system.

Appendix (detailed calculation process)
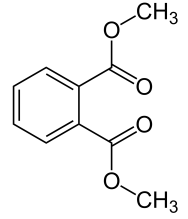
$M_i = 194.2 g/mol$
$\rho_i = 1.19 g/cm^3$
$T_m = 5.5°C$
$T_b = 283.7°C$

$p_L^*(298K) = 10^{0.38} \; bar$
$C_{i,w}^{sat} = 10^{-1.66} \; mol/L$
$K_{iaw} = 10^{-4.35}$
$K_{iocw} = 10^{1.53}$

L_i	V_i	S_i	A_i	B_i
6.75	1.71	1.26	0	0.90

Estimation Modeling chosen
(1) For vapor pressure
$p_L^*(T) = (1/2.303) \times K_F \times (4.4 + InT_b) \times [1.8 \times (T_b/T - 1) - 0.8 \times InT_b/T] = 10^{0.7} \; bar$
$logp_L^*(298K) = -0.89L_i - 0.44S_i^2 - 5.43A_iB_i + 6.51 = 10^{-0.2} \; bar$
(2) For water solubility
$logC_{i,w}^{sat} = -0.01 \times (T_m - 298K) - 1.25 \times logK_{iow} + 1.1 = -0.81$
$logC_{i,w}^{sat} = 4(Y - CH =) + 2(Y - COO-) + 2(X - COO-) + 2(X - CH_3)$
$= 4 \times 0.321 + 2 \times 0.706 - 2 \times 0.796 - 2 \times 1.117 = -1.13$
(3) For air-water partition
$logK_{iaw}(298K) = 2.55Vi - 0.48Li - 2.07Si - 3.67Ai - 4.87Bi + 0.59 = -5.28$
$logK_{iaw}(298K) = 6(C-H) + 6(C_{ar} - C_{ar}) + 4(C_{ar} - H) + 2(CO - O) + 2(C_{ar} - C) + 2(C - O)$
$= 6 \times 0.1197 - 6 \times 0.2638 + 4 \times 0.1543 - 2 \times 0.0714 - 2 \times 0.1619 - 2 \times 1.0855 = -4.89$
(4) For octanol-water partition
$logK_{iow}(298K) = \Sigma \; n_k f_k + \Sigma \; n_j f_j + 0.23$
$= (2 \times 0.55 - 2 \times 0.71 + 4 \times 0.38 - 2 \times 0.95) + (2 \times 1.26) + (0.23) = 2.05$
$logK_{iow} = 2.41Vi + 0.43Li - 1.41Si - 0.18Ai - 3.45Bi + 0.34 = 2.48$

According to the input from the question (1)

$$f_{i,phase} = \frac{M_{i,phase}}{\Sigma M_{i,phase}}$$

For air and water phase, it do not need to consider the oc fraction

$$M_{i,air} = K_{iaw} \times \rho_a \times V_a \times C_{i,w}^{eq}$$

$$M_{i,water} = V_w \times C_{iw}^{eq}$$

Except the air and water phase, others share the same mathematics models

$$M_{i,phase} = K_{iocw} \times f_{oc,phase} \times \rho_{soil} \times V_{soil} \times C_{iw}^{eq}$$

Then the distribution model is

$$f_{i,phase} = \frac{M_{i,phase}}{\Sigma M_{i,phase}} = \frac{M_{i,phase}}{M_{i,air} + M_{i,water} + M_{i,sed} + M_{i,soil} + M_{i,susp,} + Mi,bio}$$

$$= \frac{K_{iphasew} \times \rho_{phase} \times V_{phase} \times (f_{oc,phase})}{\Sigma K_{iphasew} \times \rho_{phase} \times V_{phase} \times (f_{oc,phase})}$$