Presentation Assignment

(d)Yes, it dose. According to the result from summary. It shows a difference in concentration of compound in the different solid compartments. In my opinion, according to the concentration equation, this parameter is not only controlled by mole mass but also by volume. Although, some phase has a few mass fraction, smaller volume also makes concentration larger in some striation. For example, biomass with $3.5m^3$ volume total, which is pretty small compared to the other phases.

(e)In terms of different properties and structure of these compounds, it shows a great difference K_{iaw} and K_{iow}, which dominate the mass distribution result.As we can seen the result from summary, these compound shows big difference mass fraction in the different phase due to its compound structure and inter-molecule forces. According to the distribution of mass of the carious compounds. Chloroform and Tetrachloroethene is the most strongly into the air. Dimethyl phthalate is the most strongly into the water and Benzene, 1-Bromo-3-(4-Bromophenoxy), Arachlor and 2,3,7,8-Tetrachlorodibenzo-p-dioxin is the most strongly into the sediment. First, higher K_{iaw} value means vapor pressure of the compound is higher, such as Color form and Tetrachloroethene. it has relatively low bolting point, causing less hydrophilic. On the other hand, Dimethyl phthalate could form Hind with water and has a very high boiling, casing a very low K_{iaw} so that it's more hydrophilic compared to other compounds. Lastly, these compound which likes sediment phase has a higher K_{iow}, in this situation.

(f) As we known, the distribution condition will be affected by the change of K_{iaw} and K_{iow} greatly. According to the equation, $K_{iaw}(T_1) = K_{iaw}(T_0) \times e^{\frac{-\triangle_{aw} H_i}{R}[\frac{1}{T1}-\frac{1}{T_0}]}$ and $K_{iow}(T_1) = K_{iow}(T_0) \times e^{\frac{-\triangle_{ow} H_i}{R}[\frac{1}{T1}-\frac{1}{T_0}]}$, respectively.These two parameter are temperature dependance. Therefore, the mass fraction in air phase will change if temperature increases by $10C$. To be more quantitive, I assume the $\triangle_{aw} H_i = -25kj/mol$ of my compound, Dimethyl Phthalate. Then value K_{iaw} has changed up to $10^{-4.21}$ (compared to $10^{-4.35}$ before) by temperature increase. Plug new K_{iaw} and K_{iow} value into my model and make a table. As we can seen in this table, the fraction of air phase increase greatly by an increase of K_{iaw}. Because this compound is more likely to emit into atmosphere with a higher temperature environment (the concentration in air increase by 53.12%, which is a great increase). Inter-molecule forces dominate this process, which needs more energy to break H-bond to atmosphere. In this degree, a higher temperature provide extra energy for this process. Therefore, the concentration in air should go up, given a increase of K_{iaw}.

Input	(Increase Temperature by 10C and Concentration change is compared to 298K)					
	$K_{iaw} = 10^{-4.21}$	$K_{iow} = 10^{1.77}$			Dimethyl Phthalate	
	Volume	Density	f_{oc}	C change	Fraction %	Concentration mol/m^3
Air	2×10^9	1.19	N/A	.+53.12	11.22	5.61×10^{-9}
Water	9.5×10^5	1000	N/A	-4.79	86.795	9.14×10^{-5}
Soil	1.4×10^4	1500	0.02	-5.13	0.819	5.85×10^{-5}
Sediment	9.9×10^3	1500	0.04	-4.88	1.158	1.17×10^{-4}
Suspend matter	3.5×10	1500	0.04	-4.88	0.004	1.17×10^{-4}
Biomass	3.5×10^0	1000	0.2	-4.77	0.002	6.19×10^{-4}

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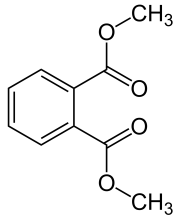
Appendix

$M_i = 194.2 g/mol$
$\rho_i = 1.19 g/cm^3$
$T_m = 5.5°C$
$T_b = 283.7°C$

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



* 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.