Solubility enhancement of PCDD/F in the presence of dissolved humic matter

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Abstract

From previous studies, we, the authors collected and arranged the octanol-water partition coefficients (K_{ow}), water solubility (S_0), and dissolved humic matter (DHM)-water partition coefficients (K_{oc}) for 95 organic compounds, and presented the correlations between each physical property. The K_{oc} and K_{ow} of dioxins estimated were significantly increased while S_0 was decreased on increasing the chlorine number. In the presence of DHM, solubility enhancement (S_w/S_0, S_w is the actual solubility in the presence of DHM) in highly chlorinated PCDD/F such as HpCDDs and OCDD is higher than that in low chlorinated ones. It means that dioxins abundant wastes (fly ash) should not be codisposed with organic abundant wastes (sewage sludge, food waste or bottom ash, etc.) to minimize the leachability of dioxins. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: K_{ow}; K_{oc}; Dissolved humic matter (DHM); Leachability; Solubility enhancement

1. Introduction

Many researches have shown that leachability of PCDD/F was different depending on its chlorination degree. Carsch et al. [1] found that only highly chlorinated polychlorinated dibenzo-*p*-dioxins and polychlorinated dibenzofurans (PCDD/F, dioxins) leached by stirring 1 kg of fly ash with 10 l of distilled water for 2 weeks. Fischer et al. [2] asserted that only highly chlorinated congeners were detected in the solution obtained from leaching experiments following the method of the German DIN38414 test. Schramm et al. [3] suggested that leaching experiments with fly ash and soil by fire-extinguishing water resulted in significant amounts of PCDD/F, especially highly chlorinated congeners

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in the leachate. Besides, they [4] conducted another research measuring the leachability of PCDD/F in soil and fly ash column eluted with pure water and linear alkylbenzene sulfonate (LAS) water. From their results, the leachability was increased significantly by using LAS water. The concentration of PCDD/F in the leachate as well as the relative leaching ratio (calculated by the PCDD/F content in fly ash) increased with increasing chlorination degree and decreasing water solubility. According to the main element analysis to investigate the effect factors for the vertical mobility of PCDD/F in incineration residue landfill, Ohsako et al. [5] found that the PCDD/F, especially highly chlorinated compounds had moved downward in the region of high pH. In the leaching test depending on dissolved humic matter (DHM) concentration and pH of Lee et al. [6], the leachability of PCDD/F increased with increasing DHM concentration in overall pH. Especially, the increase of leachability is remarkable in congeners of highly chlorinated compounds.

The results of leachability mentioned above were in contrast to those of water solubility, i.e. although the solubility of highly chlorinated congeners was low, they were leached more easily than the low chlorinated tetra- and penta-congeners.

The objective of this study is to estimate the K_{oc} of PCDD/F, especially 17 kinds of 2,3,7,8-substituted isomers, and to show the leachability depending on the chlorination degree in the presence of DHM using the K_{oc}. To estimate K_{oc} for PCDD/F statistical method was adopted. The physical properties of hydrophobic organic pollutants (HOPs) such as octanol-water distribution coefficients (K_{ow}), solubility (S_0), and distribution coefficients to DHM (K_{oc}) were referred from many previous researches. By the results of correlation analysis, the physical properties of dioxins were estimated, and the distribution patterns and leachability of dioxins isomers were evaluated.

2. Solubility (S_w) of HOPs in the presence of DHM

The hydrophobic binding between HOPs and organic matter is explained by the distribution theory, and so the competition reaction with the other chemicals could be ignored. Kile and Chiou [7] suggested the distribution theory, and explained a lot of phenomena in nature. From this theory, it could be thought that the solubility of HOPs is in proportion to the concentration of DHM in water. As a result, the solubility of HOPs can be modified as Eq. (1) in the presence of DHM, i.e. actual solubility, S_w,

$$S_w = S_0 + [DHM]\, C_0 \tag{1}$$

From the relation of C_0 and S_0, K_P of distribution coefficient between DHM and pure water is

$$K_P = \frac{C_0}{S_0} \tag{2}$$

From Eqs. (1) and (2),

$$S_w = S_0\, (1 + [DHM]\, K_P) \tag{3}$$

The parameter [DHM] and K_P in Eq. (1) can be rewritten by the parameters based on the organic carbon of DHM.

$$S_w = S_0 (1 + [DHMoc]K_{oc}) \tag{4}$$

where, C_0 is mass of solute distributed to unit mass of DHM, S_w is the actual solubility in the presence of DHM, S_0 is the pure solubility in the absence of DHM, K_P is the distribution coefficient of HOPs between DHM and water, K_{oc} is the distribution coefficient based on the organic carbon of DHM and [DHMoc] is the DHM concentration ([DHM]) based on organic carbon in water. From above equation, it could be thought that the solubility of HOPs is in proportion to the concentration of DHM in water, and its K_{oc}. While studies on K_{oc} of HOPs, more particularly of PAHs, have been done by many researchers, the K_{oc} on PCDD/F is not enough to explain its environmental behavior. Some studies for PCDD/F have been conducted by Lodge and Cooke [8], Jackson et al. [9], Marple et al. [10], Puri et al. [11], and Walter et al. [12], however, the studies have shown results of mainly 2,3,7,8-TCDD which is known as a most toxic isomer.

And, as suggested by Shinozuka [13], the sudden increase of solubility by critical micelle concentration (CMC) of DHM is very rare because the CMC of DHM is above 0.1% that is too high to reach the level in environment. In this study, the concentration of DHM satisfying the Eqs. (1)–(4) is below the CMC.

3. Data analysis

Solubility enhancement method, fluorescence quenching technique, equilibrium dialysis method, reverse phase separation method and complexation–flocculation method are used to measure the distribution coefficients between DHM and organic chemicals. Distribution coefficient may have different value depending on measurement methods and sources of DHM. Statistical analysis for K_{oc}, K_{ow} and S_0 was conducted to find out the correlation between the parameters of 95 HOPs. Some of raw data were modified to get K_{oc} values from K_p and organic carbon contents. The kinds and sources of 95 data are shown in Appendix A. The water solubility of compounds in Appendix A is below 10^{-1} M. For that reason, HOPs in this study mean the solutes under 10^{-1} M of water solubility.

4. Discussion

4.1. The relationships of K_{oc}, K_{ow}, and S_0

4.1.1. The correlation of K_{ow} with K_{oc}
Many researchers have studied the distribution of HOPs to DHM and the effect of DHM on the increase of HOPs solubility. Generally, the correlation of K_{ow} with K_{oc} is positively linear, and it is well known that it provides an accurate method of estimating the K_{oc} with K_{ow} [14–16]. Fig. 1 shows the correlation of K_{ow} with K_{oc} of 56 HOPs with 95%
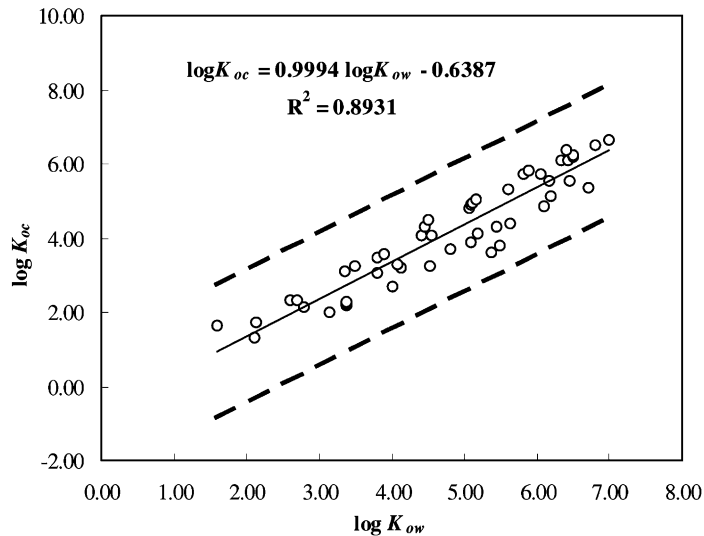
Fig. 1. Correlation plots of $\log K_{oc}$ and $\log K_{ow}$ ($n = 56$).

of confidence interval. As a result of regression analysis, the slope of the estimated equation is 0.9994; determination coefficient (R^2) 0.8931 and standard error (S.E.) 0.92. The deviations of data, however, were very large depending on the chemicals and researchers. Besides, the equations which estimated the K_{oc} with K_{ow} in the previous studies were various as showing in Fig. 2. In Fig. 2, lines "a–g" are the results of the others' studies and the heavy solid line "h" is the result of the present study. As shown in Fig. 2, the number of data used for line "h" was more numerous than that of lines "a–g", and the range of data is wider than that in lines "a–g". That is, line "h" is comprehensive in respect to the number and range of data used. Girvin and Scott [23] suggested the estimation equation of K_{oc} with the experimental data of PCBs isomers. Their data and K_{ocs} of PCBs estimated in this study are shown in Fig. 3. As shown in Fig. 3, the K_{oc} estimated by the equation of this study corresponded well with the K_{oc} estimated by Girvin and Scott.

4.1.2. The correlation of K_{oc} with S_0

Fig. 4 shows the relationship of K_{oc} and solubility (S_0) with 95% of confidence interval, and shows strongly the negative relationship between the K_{oc} and S_0 ($n = 49$, $R^2 = 0.8786$, S.E.=0.89). Because the relationships of K_{oc} and S_0 in some references used the different unit, those were converted to logarithm of mg/l and rewritten as Eq. (5) [21], Eq. (6) [16] and Eq. (7) [24]. Those results show strong relevance to the present study.

$$\log K_{oc} = -0.814 \log S_0 + 3.919 \ (R^2 = 0.993, \ n = 12) \ [21] \tag{5}$$

$$\log K_{oc} = -0.82 \log S_0 + 4.070 \ (R^2 = 1, \ n = 4) \ [16] \tag{6}$$

$$\log K_{oc} = -0.686 \log S_0 + 4.273 \ (R^2 = 0.933, \ n = 22) \ [24] \tag{7}$$
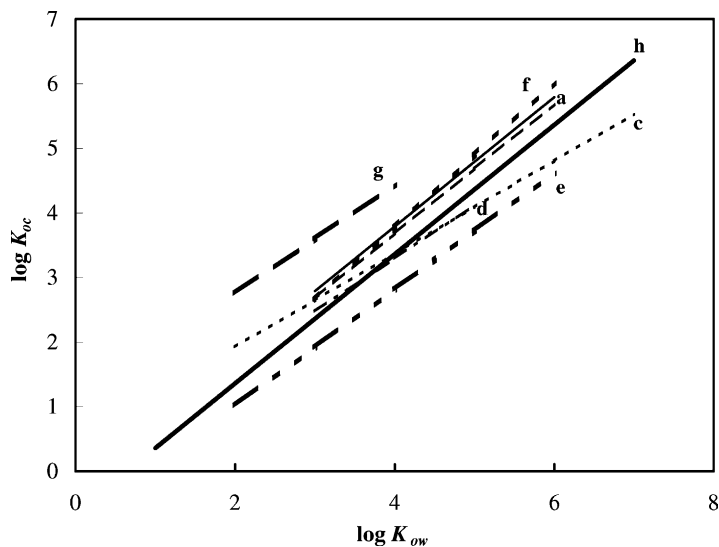
Fig. 2. Graphical representation of several models. (a) $\log K_{oc} = 1.00 \log K_{ow} - 0.21$ ($R^2 = 1$, $n = 1$) [17]; (b) $\log K_{oc} = 1.00 \log K_{ow} - 0.317$ ($R^2 = 0.980$, $n = 22$) [18]; (c) $\log K_{oc} = 0.72 \log K_{ow} + 0.49$ ($R^2 = 0.95$, $n = 13$) [19]; (d) $\log K_{oc} = 0.82 \log K_{ow} + 0.02$ ($R^2 = 0.98$, $n = 8$) [20]; (e) $\log K_{oc} = 0.90 \log K_{ow} - 0.079$ ($R^2 = 0.989$, $n = 12$) [21]; (f) $\log K_{oc} = 1.118 \log K_{ow} - 0.692$ ($R^2 = 0.831$, $n = 15$) [22]; (g) $\log K_{oc} = 0.840 \log K_{ow} + 1.08$ ($R^2 = 0.95$, $n = 10$) [15]; (h) $\log K_{oc} = 0.9994 \log K_{ow} - 0.6387$ ($R^2 = 0.89$, $n = 56$) (this study).
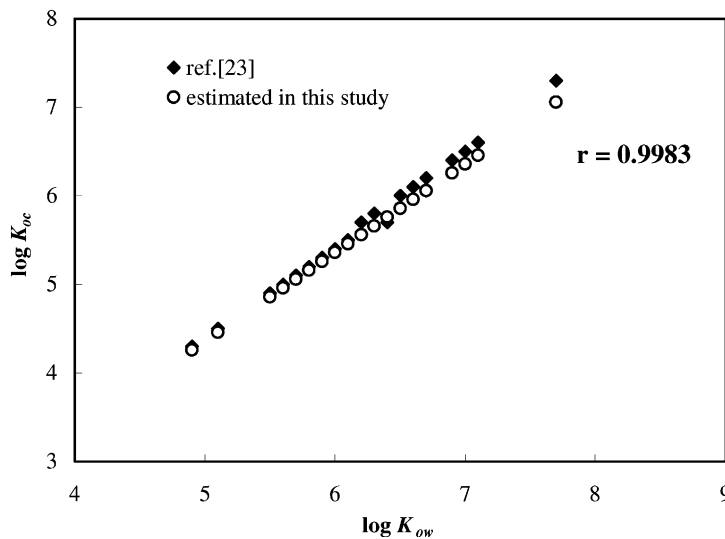
Fig. 3. Correspondence between $\log K_{oc}$ of [23] and $\log K_{oc}$ of this study, $\log K_{oc} = 1.071 \log K_{ow} - 0.98$ ($R^2 = 0.964$, $n = 45$) [23].
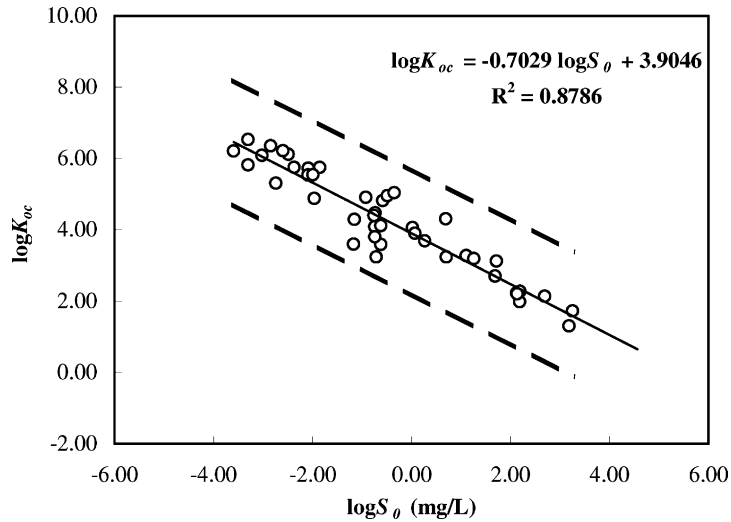
Fig. 4. Correlation plots of log S_0 and log K_{oc} ($n = 49$).

4.1.3. The correlation of K_{ow} with S_0

Fig. 5 shows the relationship of K_{ow} and S_0 with 95% of confidence interval ($n = 82$, $R^2 = 0.9135$, S.E.=0.64), and it has the more negative relationship than the relationship of K_{oc} and S_0. The Eq. (8) suggested by Means et al. [16] corresponded well with the present result.

$$\log K_{ow} = -0.686 \log S_0 + 4.59 \ (R^2 = 0.914, \ n = 22) \ [14] \tag{8}$$
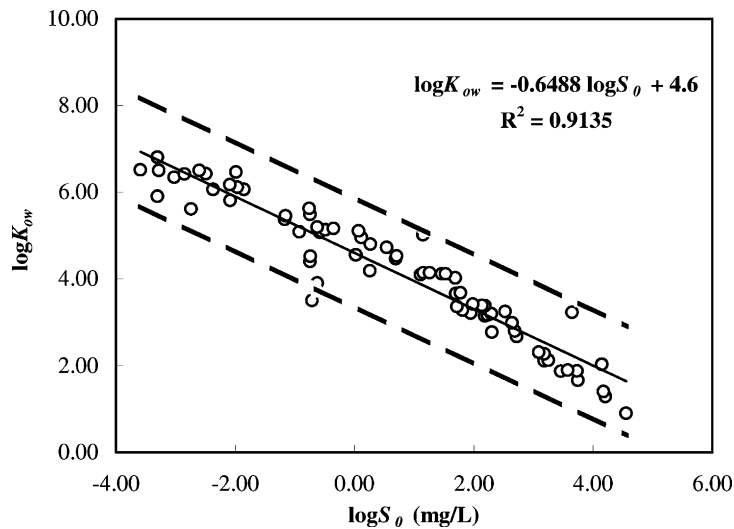
Fig. 5. Correlation plots of log S_0 and log K_{ow} ($n = 82$).

As described above, there was a clear mutual correlation among K_{oc}, K_{ow} and S_0. Judging from the statistical test results about the deviations of each correlation coefficient with 5% level of significance, there were not differences in level of significance in estimating K_{oc} with K_{ow} or S_0. Considering the precision, number and distribution range of data, it is useful to estimate the K_{oc} with K_{ow} or S_0 with the estimation equations of the present study.

4.2. Estimation of K_{oc} of PCDD/F

To evaluate the solubility enhancement of dioxins in the presence of DHM by Eq. (4), the distribution coefficient to organic carbon, K_{oc}, is needed. The data about the physical properties of dioxins isomers are shown in some articles; however, it is insufficient to estimate the behavior characteristics of every dioxins isomer because of partiality of data to 2,3,7,8-TCDD that shows the highest toxicity, and large deviations of data. For that reason, the K_{oc} of each dioxins isomer was estimated by the regression equation gained from previous section with K_{ow} that was estimated with the software presented by Environmental Science Center [25]. The K_{ow} of 2,3,7,8-substituted isomers ranges in 7.02–8.6 of PCDDs and 6.5–8.8 of PCDFs, and is increased with increasing the chlorination degree. The estimation result of K_{oc} with estimated K_{ow} and K_{oc} cited from other researches are shown in Table 1. As shown in Table 1, the K_{oc} of dioxins is depended on the amount of chlorine substituted, and thus the K_{oc} of eight-chlorinated isomers has the highest values in the same manner to K_{ow}. Since the estimated K_{oc} in this study are in the ranges of other researches' values or similar to them, as shown in Table 1, it could be surmised that the estimated K_{oc} gained by regression equation of this study are not unreasonable to be used in the evaluation of solubility enhancement of PCDD/F.

4.3. Solubility enhancement of PCDD/F in the presence of DHM

As the amount of substituted chlorine increased, the pure solubility (S_0) decreased while the K_{ow} and the K_{oc} increased. Fig. 6(A) and (B) showed the solubility enhancement (S_w/S_0) of a part of 2,3,7,8-substituted isomers calculated with the Eq. (4) using the K_{oc} in Table 1. As shown in Fig. 6(A) and (B), when the amount of substituted chlorine and DHM concentration increased, actual solubility, S_w increased extraordinary comparing to pure solubility, S_0. In the case of OCDD affected most by DHM in Fig. 6(A), the solubility in 5 mg-OC/l of DHM increased about 450 times more than that in 0 mg-OC/l of DHM. The enhancement ratio of OCDD in 5 mg-OC/l of DHM was 35 times as large as that of 2,3,7,8-TCDD. As shown of PCDFs in Fig. 6(B), DHM affected the solubility of OCDF more deeply than any one of the other PCDFs, which was the same to PCDDs. As a result, it means that the isomer showing high solubility enhancement has a high possibility to leach out with DHM.

According to dioxins distribution patterns in the leachate of incineration residue landfill site and test column packed with incineration fly ash or bottom ash, the more chlorinated dioxins were actually leached with a higher concentration [2,3,29–31]. From Kim and Lee, leaching test of the fly ash discharged from municipal solid waste incinerator extracted with DHM [32], the effect of DHM on the leachability of dioxins was very clear; the leachability of OCDF was remarkably increased with increasing the DHM concentration. As a result,

Table 1
Estimation and comparison of $\log K_{oc}$ of PCDD/F

	$\log K_{oc}$ of PCDD/F				$\log K_{ow}$[g]	Solubility, $\log S_0$[h]
	This study[a]	From [26,27]	From [28]	Others		
1,2,3,7-TCDD	–	4.26–6.55	–	–	–	
1,3,6,8-TCDD	–	2.05–6.74	–	–	–	
2,3,7,8-TCDD	6.38	3.06–8.5	5.52	6.4[b], 7.42[c], 7.39[d], 5.68[e], 6.6[f]	7.0	−4.71
1,2,3,4,7-PCDD	–	4.85–6.38	5.91	–	–	
1,2,3,7,8-PCDD	6.86	–	–	–	7.5	
1,2,3,4,7,8-HxCDD	7.16	5.02–7.1	–	–	7.8	−5.35
1,2,3,6,7,8-HxCDD	7.16	–	6.3	–	7.8	
1,2,3,7,8,9-HxCDD	7.16	–	–	–	7.8	
1,2,3,4,6,7,8-HpCDD	7.56	5.47–7.8	6.69	–	8.2	−5.62
OCDD	7.96	5.92–7.9	7.08	–	8.6	−7.13
2,3,7,8-TCDF	5.86	5.2–7.5	5.2	–	6.5	−3.38
1,2,3,7,8-PCDF	6.36	–	–	–	7.0	
2,3,4,7,8-PCDF	6.36	5.59–7.4	5.59	–	7.0	−3.63
1,2,3,4,7,8-HxCDF	6.86	7.4	–	–	7.5	−5.08
1,2,3,6,7,8-HxCDF	6.86		–	–	7.5	−4.75
1,2,3,7,8,9-HxCDF	6.86		–	–	7.5	
2,3,4,6,7,8-HxCDF	6.86		–	–	7.5	
1,2,3,4,6,7,8-HpCDF	7.36	6.0–7.9	6.37	–	8.0	−5.87
1,2,3,4,7,8,9-HpCDF	8.16	5.0–6.7	–	–	8.8	
OCDF	8.16	6.0–7.4	6.75	–	8.8	−5.94

[a] Calculated with K_{ow} estimated with software in [25].

[b] From [10].

[c] From [8].

[d] From [9].

[e] From [11].

[f] From [12].
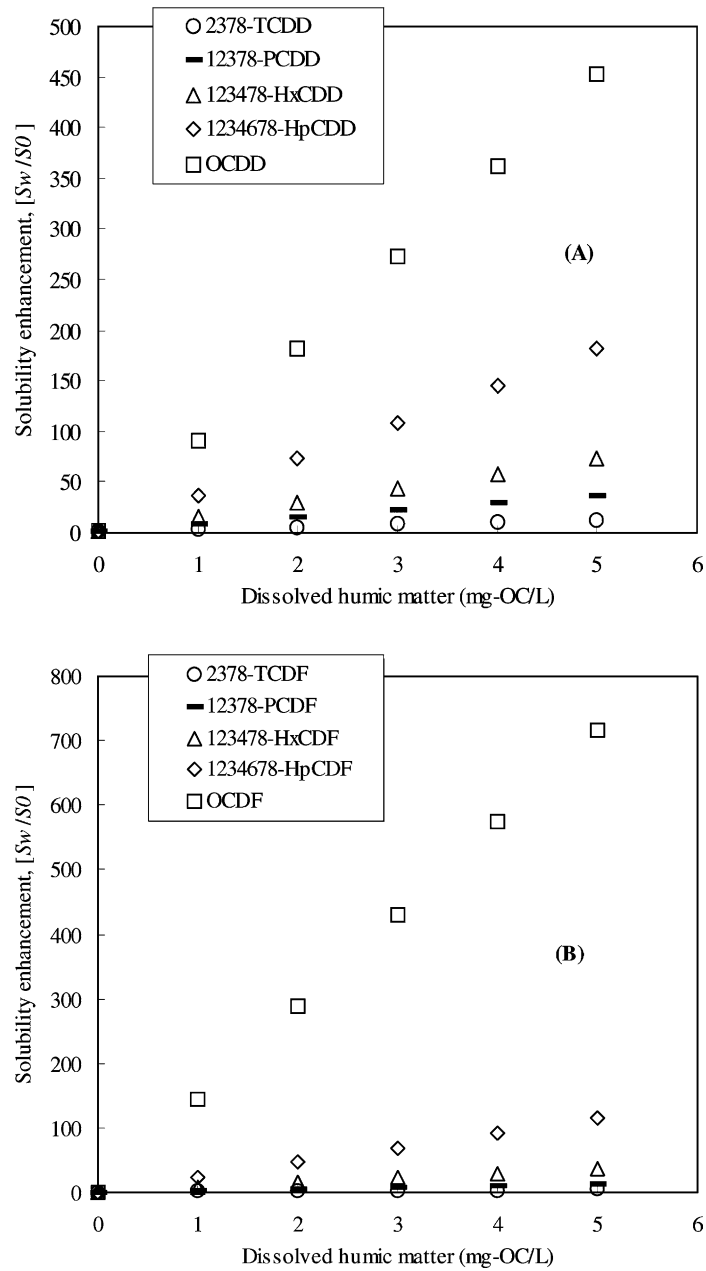
[g] Estimated with software in [23].

[h] From [28].

Fig. 6. Effect of the DHM on the solubility of PCDDs (A) and PCDFs (B).

this study is well revealing the leaching properties of every PCDD/F isomer in the presence of DHM.

5. Conclusion

Octanol-water partition coefficients (K_{ow}), water solubility (S_0), and dissolved humic matter (DHM)-water partition coefficients (K_{oc}) for 95 organic compounds were referred for estimating leachability of dioxins in the presence of DHM. The K_{oc} and K_{ow} values of dioxins were depended on chlorine content substituted. DHM in leachate influences on the solubility of dioxins, and thus the actual solubility (S_w) or leachability of dioxins increase extraordinarily as increasing DHM and chlorine content. It means that dioxins abundant wastes (fly ash) should not be codisposed with organic abundant wastes (sewage sludge, food waste or bottom ash, etc.) to minimize the leachability of dioxins.

Appendix A

The list of compounds with $\log K_{oc}$, $\log K_{ow}$ and $\log S_0$ (mg/l).

Compounds	Formula	$\log K_{oc}$	$\log K_{ow}$	$\log S_0$	Reference[a]
1,2,3-Trichlorobenzene	$C_6H_3Cl_3$	3.00	4.14	1.26	EST-20-502
		3.37	–[b]	–	EST-15-1360
1,2,4,5-Tetramethylbenzene	$C_{10}H_{14}$	–	4.72	0.54	EST-24-328
1,2,4-Trichlorobenzene	$C_6H_3Cl_3$	–	4.02	1.69	EST-16-4
1,2,4-Trichlorobenzene	$C_6H_3Cl_3$	2.70	4.02	1.69	EST-17-227
1,2,7,8-Dibenzopyrene	$C_{24}H_{14}$	3.08	6.62	−0.96	HWM
1,2-Dichlorobenzene	$C_6H_4Cl_2$	2.27	3.38	2.19	EST-17-227
1,2;5,6-Dibenzanthracene	$C_{22}H_{14}$	6.21	6.50	−2.60	EST-14-1524
1,2;7,8-Dibenzocarbazole	$C_{20}H_{13}N$	6.14	–	–	EST-16-93
1,3,5-Trimethylbenzene	C_9H_{12}	–	3.42	1.99	EST-16-4
1,3-Dichlorobenzene	$C_6H_4Cl_2$	2.23	3.38	2.13	EST-17-227
1,4-Dichlorobenzene	$C_6H_4Cl_2$	2.20	3.39	2.14	EST-17-227
1-Naphthol	$C_{10}H_8O$	3.33	–	–	EST-16-93
2,2′-PCB	$C_{12}H_8Cl_2$	3.68	4.80	0.27	EST-17-227
2,4′-PCB	$C_{12}H_8Cl_2$	3.89	5.10	0.07	EST-17-227
2,4,4′-PCB	$C_{12}H_7Cl_3$	4.38	5.62	−0.57	EST-17-227
		4.40	5.62	−0.94	EST-20-502
2,4,5,2′,4′,5′-PCB	$C_{12}H_4Cl_6$	5.34	6.72	–	EST-15-1360
2,4,5,2′,5′-PCB	$C_{12}H_5Cl_5$	4.87	6.11	−1.96	EST-20-502
2,4,6-Trinitrophenol	$C_6H_3O_7N_3$	–	2.03	4.15	EST-27-165
2,4-Dichlorophenol	$C_6H_4Cl_2O$	–	3.23	3.65	EST-27-165
2-Aminoanthracene	$C_{14}H_{11}N$	4.45	–	–	EST-16-93

Compounds	Formula	$\log K_{oc}$	$\log K_{ow}$	$\log S_0$	Reference[a]
2-Chlorobiphenyl	$C_{12}H_9Cl$	3.23	4.51	0.71	EST-17-227
		–	4.54	0.71	EST-16-4
2-Methylnaphthalene	$C_{11}H_{10}$	4.93	4.11	1.46	EST-16-4
3-Chlorobiphenyl	$C_{12}H_9Cl$	–	4.95	0.12	EST-16-4
3-Methylcholanthracene	$C_{21}H_{16}$	6.11	6.42	−2.49	EST-14-1524
4,4′-DDE	$C_{14}H_8Cl_4$	6.64	7.00	−1.40	HWM
6-Aminochrysene	$C_{18}H_{13}N$	5.21	–	–	EST-16-93
7,12-Dimethylbenz(a)-anthracene	$C_{20}H_{16}$	5.39	5.98	−1.61	EST-14-1524
		5.68	6.94	−2.36	HWM
9-Methylnaphthalene	$C_{11}H_{10}$	4.81	5.07	−0.58	WR-13-241
DDT	$C_{14}H_9Cl_5$	5.14	6.19	–	EST-15-1360
N,N-Dimethylaniline	$C_8H_{11}N$	–	2.31	3.09	EST–16–4
N-Methylaniline	C_7H_9N	–	1.66	3.75	EST-16-4
Acetophenone	C_8H_8O	1.63	1.59	–	EST-15-1360
Acridine	$C_{13}H_9N$	4.22	–	–	EST-16-93
Aldrin	$C_{12}H_8Cl_6$	4.98	5.30	−0.74	HWM
		2.61	5.66	–	EST-14-553
Aniline	C_6H_7N	–	0.90	4.56	EST-16-4
Anisole	C_7H_8O	1.30	2.11	3.18	EST-17-227
Anthracene	$C_{14}H_{10}$	–	4.54	0.62	EST-16-4
		–	4.54	−1.47	EST-29-807
		4.15	4.45	−1.14	EST-18-187
		4.41	4.54	−1.14	WR-13-241
		4.43	4.54	0.07	EST-31-3558
		4.72	–		EST-20-1162
		4.93	4.55		WR-26-1645
		4.15	4.45	−2.15	HWM
Benz(a)anthracene	$C_{18}H_{12}$	–	5.91	−2.15	EST-29-807
		5.30	5.91	−1.85	EST-18-187
		6.14	5.60	−2.24	HWM
Benzene	C_6H_6	–	2.13	3.25	EST-16-4
		1.26	2.13	3.25	EST-17-227
		1.92	2.11	–	EST-15-1360
		1.98	–	–	EST-15-1360
		–	2.13	3.26	EST-24-328
Benzo(a)pyrene	$C_{20}H_{12}$	–	6.60	–	EST-19-1072
		5.95	6.50	−3.30	EST-18-187
		6.74	6.06	−2.42	HWM
		–	6.50	−2.82	Chem.-34-335
Benzo(b)fluoranthene	$C_{20}H_{12}$	5.74	6.06	−1.85	HWM
Benzo(ghi)perylene	$C_{22}H_{12}$	6.20	6.51	−3.59	HWM

Compounds	Formula	$\log K_{oc}$	$\log K_{ow}$	$\log S_0$	Reference[a]
Benzo(k)fluoranthene	$C_{20}H_{12}$	5.74	6.06	−2.37	HWM
Benzoic acid	$C_7H_6O_2$	–	1.87	3.46	EST-27-165
Biphenyl	$C_{12}H_{10}$	3.27	4.09	1.16	EST-18-187
	$C_{12}H_{10}$	–	–	0.86	Chem. Hand
	$C_{12}H_{10}$	–	4.09	1.31	EST-16-4
Bromobenzene	C_6H_5Br	–	2.99	2.65	EST-16-4
Captan	$C_9H_8Cl_3NO_2S$	3.81	2.35	−0.30	HWM
Carbazole	$C_{12}H_9N$	–	3.28	1.81	Chem.-34-335
Chlordane	$C_{10}H_6Cl_8$	5.15	3.32	−0.25	HWM
Chlorobenzene	C_6H_5Cl	1.68	2.84	2.69	EST-17-227
		2.59	2.71	–	EST-15-1360
		–	2.84	2.69	EST-16-4
Chrysene	$C_{18}H_{12}$	5.30	5.61	−2.74	HWM
Dibenz(a,h)anthracene	$C_{22}H_{14}$	6.52	6.80	−3.30	HWM
Dibenzothiophene	$C_{12}H_8S$	4.05	–	–	JEQ-9-184
		–	4.55	0.02	Chem.-34-335
Dieldrin	$C_{12}H_8Cl_6O$	3.23	3.50	−0.71	HWM
Diethylstilbesterol	$C_{18}H_{20}O_2$	4.75	5.46	−2.02	HWM
Diphenylmethane	$C_{13}H_{12}$	–	4.14	1.16	EST-16-4
Ethylbenzene	C_8H_{10}	–	3.15	2.19	EST-16-4
		1.98	3.15	2.19	EST-17-227
Fluoranthene	$C_{16}H_{10}$	4.58	4.90	−0.69	HWM
		4.97	5.22	0.27	EST-31-3558
		5.26	5.22	–	WR-26-1645
		5.32	5.22	–	WR-26-1645
		–	5.22	−0.62	Chem.-34-335
Fluorine	$C_{13}H_{10}$	–	4.18	0.26	Chem.-34-335
Fluorobenzene	C_6H_5F	–	2.27	3.18	EST-16-4
Heptachlor	$C_{10}H_5Cl_7$	4.08	4.40	−0.74	HWM
Heptachlor epoxide	$C_{10}H_5Cl_7O$	2.34	2.70	−0.46	HWM
Hexachlorobenzene	C_6Cl_6	–	5.50	−0.12	EST-16-4
		3.59	5.23	−2.22	HWM
Hexachlorobiphenyl	$C_{12}H_4Cl_6$	6.08	6.34	−3.02	WR-13-241
Hexachlorophene	$C_{13}H_6Cl_6O_2$	4.96	7.54	−2.40	HWM
Indeno(1,2,3-cd) pyrene	$C_{22}H_{12}$	–	6.50	−3.28	HWM
Iodobenzene	C_6H_5I	–	3.25	2.53	EST-16-4
Isopropylbenzene	C_9H_{12}	–	3.66	1.70	EST-16-4
m-Chloroaniline	C_6H_6ClN	–	1.88	3.74	EST-16-4
m-Dichlorobenzene	$C_6H_4Cl_2$	–	3.38	2.13	EST-16-4
m-Toluidine	C_7H_9N	–	1.40	4.18	EST-16-4
m-Xylene	C_8H_{10}	–	3.20	2.30	EST-16-4
Methoxychlor	$C_{16}H_{15}Cl_3O_2$	4.90	5.08	−0.92	WR-13-241

Compounds	Formula	$\log K_{oc}$	$\log K_{ow}$	$\log S_0$	Reference[a]
Naphthalene	$C_{10}H_8$	–	3.36	2.17	EST-16-4
		3.11	3.36	–	EST-15-1360
		3.11	3.36	1.50	WR-13-241
		–	–	1.49	Chem. Hand
o-Chloroaniline	C_6H_6ClN	–	1.90	3.58	EST-16-4
o-Dichlorobenzene	$C_6H_4Cl_2$	–	3.38	2.19	EST-16-4
o-Toluidine	C_7H_9N	–	1.29	4.21	EST-16-4
o-Xylene	C_8H_{10}	–	2.77	2.31	EST-16-4
p-Dichlorobenzene	$C_6H_4Cl_2$	–	3.39	2.14	EST-16-4
p-Xylene	C_8H_{10}	–	3.15	2.30	EST-16-4
		–	3.18	2.17	EST-24-328
Parathion	$C_{10}H_{14}NO_5PS$	3.06	3.81	–	EST-15-1360
Pentachlorobenzene	C_6HCl_5	4.11	5.19	−0.62	HWM
Pentachloronitro benzene	$C_6Cl_5NO_2$	4.28	5.45	−1.15	HWM
Phenanthrene	$C_{14}H_{10}$	–	4.57	0.77	EST-16-4
		–	4.57	0.05	Chem.-34-335
		3.92	4.16	1.90	EST-18-187
		4.17	4.57	1.29	EST-31-3558
		4.36	4.57	0.11	WR-13-241
		4.73	4.34	–	WR-26-1645
		–	–	0.04	Chem. Hand
Phenanthridine	$C_{13}H_9N$	–	3.21	1.95	Chem.-34-335
Phentachlorophenol	C_6HCl_5O	–	5.01	1.15	EST-27-165
pp′-DDT	$C_{14}H_9Cl_5$	–	6.36	−1.19	EST-16-4
		5.06	6.36	−2.27	EST-20-502
		5.39	6.19	−2.26	HWM
		5.44	6.19	−2.47	EST-18-187
		5.61	–	–	EST-16-735
		5.72	–	–	EST-16-735
		5.72	5.75	–	WR-26-1645
		5.74	–	–	EST-16-735
		–	–	−2.23	Chem. Hand
Propylbenzene	C_9H_{12}	–	3.68	1.78	EST-16-4
Pyrene	$C_{16}H_{10}$	–	5.18	0.07	EST-16-4
		4.58	4.88	−0.89	HWM
		4.92	5.18	–	EST-15-1360
		4.92	5.18	−0.87	WR-13-241
		5.02	–	–	EST-21-243
		5.02	5.18	0.14	EST-31-3558
		5.23	5.18	–	WR-26-1645
		–	5.09	−0.87	EST-14-1524
t-Butylbenzene	$C_{10}H_{14}$	–	4.11	1.53	EST-16-4

Compounds	Formula	$\log K_{oc}$	$\log K_{ow}$	$\log S_0$	Reference[a]
Tetracene	$C_{18}H_{12}$	5.81	5.90	–	EST-15-1360
		5.81	5.90	−3.30	WR-13-241
Tetrachloroethylene	C_2Cl_4	2.32	2.60	–	EST-15-1360
Toluene	C_7H_8	–	2.69	2.71	EST-16-4
		–	2.65	2.73	EST-24-328
β-BHC	$C_6H_6Cl_6$	3.46	3.80	–	EST-15-1360
β-Hexachlorocyclohexane	$C_6H_6Cl_6$	3.58	3.90	−0.62	HWM

[a] EST-X-XX: Environmental Science and Technology, volume X, page XX; HWM: M.D. LaGrega, P.L Buckingham, J.C. Evans, Hazardous Waste Management, McGraw-Hill, 1990; Chem.-X-XX: Chemosphere, volume X page XX; WR-X-XX: Water Research, volume X, page XX; Chem. Hand: Chemistry Handbook, Basic Association of Japanese Chemical, 1993; JEQ-X-XX: J. Environ. Qual., volume X, page XX.

[b] Not shown in the reference.

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