Prediction of Soil Sorption Coefficients of Hydrophobic Organic Pollutants by Adsorbability Index

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Synopsis. The adsorbability index proposed by Abe et al. to predict the activated carbon adsorption of organic compounds from aqueous solution was well correlated with the soil sorption coefficients of polycyclic aromatic hydrocarbons (PAHs), alkylbenzenes, chlorobenzenes, chlorinated alkanes and alkenes, heterocyclic and substituted PAHs, and halogenated phenols. The adsorbability index was also found to be well correlated with the first-order molecular connectivity index and the total molecular surface areas of these compounds.

The adsorbability index, AI, has recently been proposed by Abe et al.[1] from a quantitative structure–activity relationship analysis based on the molecular refraction to predict the activated carbon adsorption of 157 compounds from aqueous solutions (Freundlich adsorption constant: K). Their results indicated the good linear relationship between $\log K$ and AI with the correlation coefficient, r, of 0.986. Then, we investigated whether the adsorbability index was applicable to predict the soil sorption as well as the activated carbon adsorption. As a quantitative measure of the soil adsorption a soil sorption coefficient, K_{om},[2–15] has been used, which is defined as the ratio between the concentrations of a given chemical sorbed by the soil and dissolved in the soil water normalized to the total organic carbon content of the soil. The soil sorption coefficient, K_{om}, is also one of the important parameters to describe the environmental fate of chemicals. Besides the experimental determination of K_{om}, the values of K_{om} can be estimated from the water solubility[4,7,8,11,13–15] or 1-octanol/water partition coefficient,[4,7–11] but the estimation needs their accurate data.

Recently, Sabljić[2] showed the first-order molecular connectivity index, χ, as a good structure parameter that described most adequately a relationship between the molecular structure of 72 hydrophobic organic compounds and their adsorption by soil. Furthermore, he indicated that χ was well correlated with the total molecular surface areas, TSA, of the compounds. Then, attempts were made to determine a relationship between AI and TSA of the 72 hydrophobic organic compounds reported by Sabljić,[2] which included polycyclic aromatic hydrocarbons (PAHs), alkylbenzenes, chlorobenzenes, chlorinated alkanes and alkenes, heterocyclic and substituted PAHs, and halogenated phenols.

Results and Discussion

The adsorbability index, AI, of a given molecule can be readily calculated from Eq. 1[1] by adding the values of A and I shown in Table 1,

$$\mathrm{AI} = \Sigma A + \Sigma I \tag{1}$$

where A and I indicate the factors of the respective increasing and decreasing adsorbabilities of the atom or functional group in the molecule onto the activated carbon from aqueous solution.

The AI values calculated from Eq. 1 are shown in Table 2 for the 72 hydrophobic organic compounds.[2] The AI values in Table 2 are obtained by only the A values, since the I values can be ingnored for the compounds used in this work. The logarithm of K_{om} was expressed by the following regression equation:

$$\log K_{om} = 0.62\,\mathrm{AI} + 0.16 \quad (r = 0.967,\ s = 0.341), \tag{2}$$

where s is the standard deviation. The graphical representation of this fit is given in Fig. 1. This led to the conclusion that the adsorbability index gave good prediction of the soil sorption coefficients as well as

Table 1. Adsorbability Index (AI)[a]

	A			I
C	0.26	Aliphatic		
H	0.12	-OH	(alcohols)	−0.53
N	0.26	-O-	(ethers)	−0.36
O	0.17	-CHO	(aldehydes)	−0.25
S	0.54	N	(amines)	−0.58
Cl	0.59	-COOR	(esters)	−0.28
Br	0.86	>C=O	(ketones)	−0.30
NO_2	0.21	-COOH	(fatty acids)	−0.03
-C=C-	0.19	Aromatics		
Iso	−0.12	-OH, -O-, N, -COOR, >C=O, -COOH		0
Tert.	−0.32	α-Amino acids		−1.55
Cyclo	−0.28			

a) Ref. 1.

Table 2. Values of the Soil Sorption Coefficients (K_{om}), the Adsorbability Indexes (AI) of the 72 Hydrophobic Organic Compounds

Compound	log K_{om}[a]	AI[b]	(log K_{om}) Error(%)[c]	(TSA) Error(%)[d]
Dibenz(*a*,*h*)anthracene	6.31	9.49	3.6	−5.9
3-Methylcholanthrene	6.25	9.09	6.7	−4.8
Dibenzo(*a*,*i*)carbazole	6.14	8.92	6.7	−9.4
2,3,4,5,6,2′,5′-Heptachlorobiphenyl	5.95	8.75	5.5	5.6
Naphthacene	5.81	7.83	13.2	−6.5
DDT[e]	5.38	8.81	−5.2	8.9
7,12-Dimethylbenz(*a*)athracene	5.37	8.83	−5.6	−0.9
2,4,5,2′,4′,5′-Hexachlorobiphenyl	5.34	8.28	0.2	4.8
6-Aminochrysene	5.21	8.21	−1.4	−4.9
2,3,4,2′,3′,4′-Hexachlorobiphenyl	5.05	8.28	−5.5	4.8
Pyrene	4.92	6.88	9.5	−11.2
9-Methylanthracene	4.81	6.67	10.1	−3.6
DDE[f]	4.70	8.29	−13.5	5.1
2,5,2′,5′-Tetrachlorobiphenyl	4.67	7.34	−1.5	2.8
2,4,5,2′,5′-Pentachlorobiphenyl	4.63	7.81	−8.7	3.9
2,3,4,2′,5′-Pentachlorobiphenyl	4.50	7.81	−11.9	3.9
Aldrin	4.45	8.00	−15.8	6.5
2-Aminoanthracene	4.45	6.55	4.6	−5.3
Anthracene	4.42	6.17	9.3	−7.4
2,4,4′-Trichlorobiphenyl	4.38	6.87	−1.5	1.7
Phenanthrene	4.36	6.22	7.3	−8.1
Acridine	4.22	6.05	6.7	−7.9
Dibenzothiophene	4.05	5.76	7.3	−5.6
2-Methylnaphthalene	3.93	5.01	16.4	−3.8
2,4′-Dichlorobiphenyl	3.90	6.40	−6.5	0.3
Pentachlorophenyl	3.73	5.37	5.9	3.4
2,2′-Dichlorobiphenyl	3.68	6.40	−12.9	0.3
Hexachlorobenzene	3.59	5.67	−3.0	3.6
3,4,5-Trichlorophenyl	3.56	4.43	17.9	0.1
Pentachlorobenzene	3.50	5.20	2.7	2.2
Butylbenzene	3.39	4.85	6.0	7.0
1,2,3-Trichlorobenzene	3.37	4.26	16.4	−1.5
2,4,5-Trichlorophenol	3.36	4.43	13.0	0.1
2,3,4,6-Tetrachlorophenol	3.35	4.90	4.0	1.9
1-Naphthol	3.33	4.68	7.5	−6.9
2-Chlorobiphenyl	3.23	5.93	−19.5	−1.2
Hexachlorocyclohexane	3.21	6.08	−23.2	10.7
1,2,3,5-Tetrachlorobenzene	3.20	4.73	2.8	0.6
1,2,4,5-Tetramethylbenzene	3.12	4.85	−2.1	7.8
Naphthalene	3.11	4.51	4.4	−8.8
2,4,6-Trichlorophenol	3.02	4.43	3.2	0.1
1,3,5-Trichlorobenzene	2.85	4.26	1.1	−1.5
1,3,5-Trimethylbenzene	2.82	4.35	−1.9	4.8
1,2,3-Trimethylbenzene	2.80	4.35	−2.7	4.8
2,4-Dichlorophenol	2.75	3.96	4.3	−2.1
1,2,4-Trichlorobenzene	2.70	4.26	−4.4	−1.5
2,3-Dichlorophenol	2.65	3.96	0.7	−2.1
Bromobenzene	2.60	3.59	7.7	−6.6
1,4-Dimethylbenzene	2.52	3.85	−1.7	1.0
1,4-Dichlorobenzene	2.40	3.79	−5.2	−4.0
Toluene	2.39	3.35	5.8	−4.2
Tetrachloroethene	2.32	3.07	10.5	1.8
1,2-Dichlorobenzene	2.26	3.79	−11.7	−4.0
1,3-Dimethylbenzene	2.26	3.85	−13.4	1.0
1,3-Dichlorobenzene	2.23	3.79	−13.2	−4.0
4-Bromophenol	2.17	3.76	−15.5	−4.5
1,2-Dibromo-3-chloropropane	2.11	3.69	−16.7	7.9
Chlorobenzene	2.10	3.32	−6.3	−7.2
1,1,1-Trichloroethane	2.02	2.65	10.2	6.8
Trichloroethene	2.00	2.60	10.9	−0.8
Ethylbenzene	1.98	3.85	−29.4	0.6
Benzene	1.92	2.85	−1.0	−11.4
1,1,2-Trichloroethane	1.87	2.65	3.0	4.8

Table 2. (Continued)

Compound	log K_{om}[a]	AI[b]	(log K_{om}) Error(%)[c]	(TSA) Error(%)[d]
Tetrachloromethane	1.85	2.62	3.0	4.1
1,1,2,2-Tetrachloroethane	1.66	3.12	−27.0	7.9
Trichloromethane	1.65	2.15	9.0	−0.5
1,2-Dibromoethene	1.65	2.67	−10.7	1.2
1,2-Dibromoethane	1.56	2.72	−19.1	0.7
Dichloromethane	1.44	1.68	16.1	−7.2
1,2-Dichloropropane	1.43	2.68	−28.1	7.5
1,3-Dichloropropane	1.42	1.90	5.2	7.1
1,2-Dichloroethane	1.28	2.18	−18.8	0.5

a) Ref. 2. b) Calcd from Eq. 1. c) Error(%)={1−(log $K_{om\,calcd}$ from Eq. 2)/(log K_{om})}×100. d) Error(%)={1−(TSA_{calcd} from Eq. 4)/(TSA)}×100. e) 1,1-Bis(4-chlorophenyl)-2,2,2-trichloroethane. f) 2,2-Bis(4-chlorophenyl)-1,1-dichloroethylene.

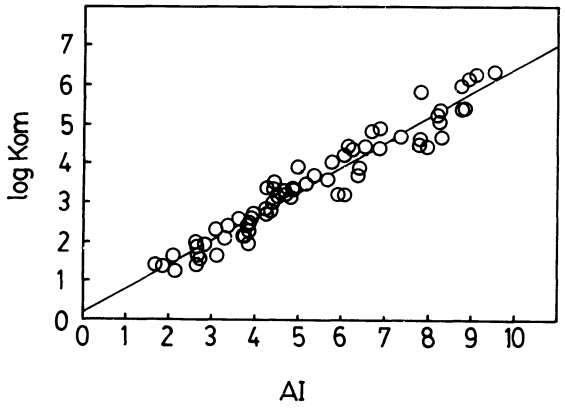

Fig. 1. Relationship between log K_{om} and adsorbability index, AI.

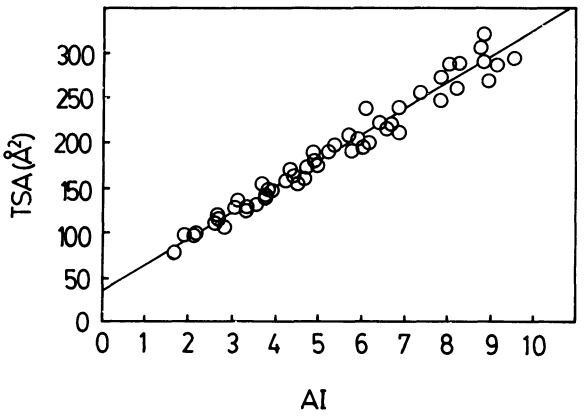

Fig. 2. Relationship between total molecular surface areas, TSA, and adsorbability index, AI.

the first-order connectivity index (χ) as shown by Eq. 3.[2]

$$\log K_{om} = 0.53\chi + 0.54 \quad (3)$$
$$(r = 0.976,\ s = 0.298)$$

Therefore, the adsorbability index for prediction of the activated carbon adsorption was also found to be effective for prediction of the soil adsorption coefficient.

On the other hand, the regression analysis showed that the relationships between AI, TSA, and χ were expressed as the following linear functions:

$$TSA = 29.4AI + 35.3 \quad (4)$$
$$(r = 0.985,\ s = 10.9)$$

$$\chi = 1.16AI - 0.68 \quad (5)$$
$$(r = 0.988,\ s = 0.377)$$

$$TSA = 24.1\chi + 58.5 \quad (6)$$
$$(r = 0.956,\ s = 19.4),$$

The AI index was well correlated with both TSA and χ. The correlation of TSA with AI (Eq. 4) was superior to that of TSA with χ (Eq. 6) reported by Sabljić.[2] Figure 2 shows the relationship between TSA and AI according to Eq. 4. The adsorbability index was found to be a parameter that strongly depends on the total molecular surface areas.

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