

Prediction of soil organic carbon partition coefficients by soil column liquid chromatography

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Abstract

To avoid the limitation of the widely used prediction methods of soil organic carbon partition coefficients (K_{OC}) from hydrophobic parameters, e.g., the *n*-octanol/water partition coefficients (K_{OW}) and the reversed phase high performance liquid chromatographic (RP-HPLC) retention factors, the soil column liquid chromatographic (SCLC) method was developed for K_{OC} prediction. The real soils were used as the packing materials of RP-HPLC columns, and the correlations between the retention factors of organic compounds on soil columns (k_{soil}) and K_{OC} measured by batch equilibrium method were studied. Good correlations were achieved between k_{soil} and K_{OC} for three types of soils with different properties. All the square of the correlation coefficients (R^2) of the linear regression between $\log k_{soil}$ and $\log K_{OC}$ were higher than 0.89 with standard deviations of less than 0.21. In addition, the prediction of K_{OC} from K_{OW} and the RP-HPLC retention factors on cyanopropyl (CN) stationary phase (k_{CN}) was comparatively evaluated for the three types of soils. The results show that the prediction of K_{OC} from k_{CN} and K_{OW} is only applicable to some specific types of soils. The results obtained in the present study proved that the SCLC method is appropriate for the K_{OC} prediction for different types of soils, however the applicability of using hydrophobic parameters to predict K_{OC} largely depends on the properties of soil concerned.

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1. Introduction

Soil organic carbon partition coefficient (K_{OC}) is an important parameter used to estimate the mobility of an organic compound in soil [1]. As the traditional laboratory methods for the determination of K_{OC} are time consuming, many alternative approaches have been proposed to predict K_{OC} [2]. Since soil organic matter (SOM) is considered the dominant sorptive phase for the sorption of organic compounds on soils, prediction of K_{OC} from hydrophobic parameters is widely used [2]. The *n*-octanol/water partition coefficients (K_{OW}) and the retention factors on high performance liquid chromatographic (HPLC) stationary phases are frequently used to predict K_{OC} . The retention factors on several HPLC

columns with the chemically bonded octadecyl, ethyl, diol, aminopropyl, cyanopropyl (CN) and humic acid stationary phases were compared for prediction of K_{OC} [3–5]. Among these phases, because the properties of the humic acid are close to those of SOM and it was considered the most promising model material of SOM. However, the variability in properties of SOM existed in different types of soils can result in considerable uncertainties in K_{OC} prediction [6,7]. In addition, many studies showed that organic compounds were sorbed effectively not only by SOM, but also by soil minerals [8–10], thus the contribution of minerals to overall sorption of organic compounds on soil is another important factor that affects the accuracy of K_{OC} prediction. It is clear that the sorption of an organic compound on a specific type of soil is dependent on the natures of this soil. The approaches of using hydrophobic parameters to predict K_{OC} ignore the specific properties of soils, therefore it only can be used to roughly screen the sorption potential of organic

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compounds on soils, but in some cases, e.g., sorption of organic compounds on soil with low organic carbon content, these approaches are not appropriate.

In this study, for avoiding the limitation of the hydrophobic parameters for K_{OC} prediction, soil column liquid chromatography (SCLC) [11–13] was developed for K_{OC} prediction. In this method, the real soil was used as HPLC column packing, and the retention factors (k_{soil}) of organic compounds on soil columns were measured on-line by HPLC. The correlations between the K_{OC} values measured by batch equilibrium experiments and k_{soil} were investigated for three types of soils with apparently different properties. The results were compared with those of the hydrophobic parameters, i.e., *n*-octanol/water partition coefficients (K_{OW}) and HPLC retention factors on cyanopropyl (CN) phase (k_{CN}), and the limitations of using the hydrophobic parameters to predict K_{OC} were discussed.

2. Experimental

2.1. Materials

Three EUROSIL samples, i.e., EUROSIL 1#, 2# and 5#, from the Environment Institute of the Joint Research Center Ispra (the European Commission's DG, XI) were selected in this study. The properties and the sources of the three soils are presented in Table 1 [14].

Table 1
Properties of soil samples

	EUROSIL	EUROSIL	EUROSIL
	1#	2#	5#
Sand (kg/kg)	0.033	0.134	0.716
Silt (kg/kg)	0.219	0.641	0.127
Clay (kg/kg)	0.75	0.226	0.06
C_{org} (kg/kg)	0.0329	0.0239	0.0443
CEC (cmol _c /kg)	32.4	28.9	24.1
pH (in 0.01M CaCl ₂)	5.7	7.2	3.2
Source	Italy	Greece	Germany

Twenty-one test organic compounds (listed in Table 2), which include *s*-triazine, phenoxyalkanoic acid, triazole, imidazole, organophosphate, carbamate, phenole and aniline, were obtained from Aldrich (Milwaukee, WI), Bayer AG (Bayer Landwirtschaftszentrum, Monheim, Germany), Fluka (Buchs, Switzerland), and Sigma (St. Louis, MO). They were of the highest purity available and were checked by RPLC on C₁₈ column to find no impurity peaks existed. They were separately dissolved in HPLC grade methanol (Shangdong Yuwang Chemical Factory, Jinan, China), in a typical concentration of about 0.1 mg/ml. The white diatomite gas chromatographic support 102 with particle size of 60–80 mesh was from Shanghai Reagent Company. Pure water was prepared using a Millipore S.A. 67120 water system. CaCl₂ (purity > 96%) was from Anshan Chemical Reagent Company.

Table 2

The logarithmic values of *n*-octanol/water partition coefficients ($\log K_{OW}$), capacity factors on HPLC cyanopropyl phase (CN) ($\log k_{CN}$), soil/water partition coefficients ($\log K_{OC}$)^a and capacity factors on soil columns ($\log k_{soil}$) for all tested compounds

Chemical	$\log K_{OW}$	$\log k_{CN}$	$\log K_{OC}$			$\log k_{soil}$		
			1#	2#	5#	1#	2#	5#
Atrazine	2.50	-0.12	2.15	1.97	2.49	0.26	-0.07	-0.15
Terbutryn	3.65	0.15	3.55	2.88	3.05	0.96	0.74	0.60
Prometryn	3.10	0.09	2.54	2.63	2.93	0.83	0.60	0.23
Triadimefon	3.11	0.23	2.83	2.56	3.05	0.57	0.48	0.20
Triadimenol	3.15	0.08	2.58	2.44	2.72	0.43	0.20	0.06
Triazoxide	2.04	0.08		3.07			0.72	
Fuberidazole	2.67	0.13		2.64			0.70	
Fenamiphos	3.30	0.17	2.77	2.46	3.04	0.64	0.55	0.42
Azinphos-methyl	2.96	0.29	3.30	2.89	3.23	1.12	0.53	0.40
Isofenphos	4.04	0.45		3.11			0.90	
Fenthion	4.84	0.53	3.72	3.67	3.67	1.58	1.43	1.22
Methiocarb	3.34	0.06	2.74	2.64	2.82	0.75	0.70	0.42
Aniline	0.94	-0.45	2.38	1.50	2.14	0.07	-0.44	-0.29
4-Methylaniline	1.39	-0.34	2.14	2.13		0.29	-0.18	
Phenol	1.46	-0.43	1.31	1.75	1.54	-0.82	-0.27	-1.04
4-Chlorophenol	2.39	-0.23	2.14	1.97	2.33	0.31	0.29	-0.32
2,4-Dichlorophenol	3.06	0.01	2.61	2.65	2.91	0.57	0.50	0.23
Disulfoton	3.95	0.49	3.42	3.33	3.50	1.16	1.04	0.81
Carbendazime	1.51	-0.27		2.32			0.40	
Fenoxaprop-ethyl		0.60	3.31			1.18		
2,4-D	2.81	-0.90	2.18			-0.01		

^a K_{OC} : Freundlich adsorption coefficient (K_f) normalized to the organic carbon content (f_{OC}) of a soil, K_f is calculated from $\log x/m$ (g/g) = $\log K_f + n \log C_{aq}$ (g/ml) [14] at $C_{aq} = 1$ g/ml.

2.2. Column packing

Air-dried soil samples were gently ground and then sieved. The fraction of soil particles with sizes of 60–100 mesh was carefully mixed with diatomite particles in a mass ratio of 2:3 (soil:diatomite) to prepare column packing, so that usable columns could be packed even for poorly aggregated soils or clay soils. Certain amount of the mixture (approximately 1.4 g) was divided into seven portions, incrementally and tightly dry packed into a stainless steel HPLC column (50 mm × 5 mm i.d.) at the same packing height (7 mm) for each portion with a homemade pressurizing device. Both column ends contained a piece of nylon membrane (Millipore) of 0.45 μm pore size and a stainless steel flow-rate allocation disc. The packed soil columns had bulk densities and porosities of 1.31 g/ml and 0.53 for EUROSIL 1#, 1.11 g/ml and 0.57 for EUROSIL 2#, and 1.35 g/ml and 0.51 for EUROSIL 5#, respectively. A reference column was packed with pure diatomite particles with the similar procedure, its bulk density and porosity were 1.10 g/ml and 0.60, respectively.

2.3. Soil column methodology

Packed column was installed in an HPLC system which consisted of a Waters 515 HPLC pump, a Waters 2487 Dual λ UV detector, and an injection valve (Rheodyne, 7725i) fitted with a sample loop. The column was placed in a thermostat set at 30 °C (±1 °C). The solute concentration in the column effluent was measured on-line by a UV detector at the maximum wavelength of each compound. The chromatogram was processed on a personal computer equipped with DL 800 workstation.

Experiments were performed by injecting about 2–5 μl of solute solution. Flow rate of mobile phase was 0.2 ml/min for all experiments. The dead time was measured from the retention time of NaNO₂ as a non-retained solute. The solute retention time was determined from the first moment of the chromatogram, and the retention factor of a compound on soil column was calculated from the retention time of the solute and the dead time.

2.4. Mobile phases used for column experiments

SCLC is a dynamic method, it allows the soluble species in the soil to be removed by continuous flow of mobile phase. However, for batch equilibrium method which is a static method, the soluble species are released from soil, and the resulting change in composition of aqueous phase during sorption tests can affect the sorption equilibrium in a batch (closed) system. In this study, the K_{OC} values of test compounds measured by batch experiments were cited from literature [14], where the K_{OC} values were measured under the aqueous phase containing a small part of soil solution, therefore for avoiding the uncertainties resulted

from the difference of the aqueous phases between batch and SCLC experiments, the mobile phases of soil columns have been prepared to simulate the aqueous phases used in batch sorption experiments. According to the previous study [15], 220 ml of 0.01 M CaCl₂ solution was mixed with 45 g of soil (solution/soil ratio was 5/1), and the mixtures were shaken for 12 h. After centrifugation the clear solutions were filtered through 0.45 μm membrane filter. Then the soil solutions were diluted 10 times using 0.01 M CaCl₂ solution and then used as the mobile phases for the corresponding soil columns.

3. Results and discussion

3.1. Contribution of diatomite support to retention

The retention factor of a compound on the reference column is a measure of its sorption on the diatomite. The water/diatomite adsorption coefficients were calculated from the retention factors (k_0) on the reference column by $K_0 = k_0\theta_0/\rho_0$, where θ_0 and ρ_0 are the bulk density and porosity of the reference column, respectively. The partial retention values on net diatomite in soil column were further calculated from $\phi_d K_0(\rho/\theta)$, where ρ and θ are, respectively, the bulk density and porosity of the soil column, and ϕ_d is the mass contents of diatomite in column. Then the percent contributions of the diatomite to retention of organic compounds were finally calculated from $\phi_d K_0(\rho/\theta)/k \times 100$, where k is the retention factor of a compound on overall soil column packing. For most organic compounds, the contributions were lower than 5%, except those of fenoxapropethyl on EUROSIL 1#, isofenphos on EUROSIL 2# and disulfoton on EUROSIL 5#, where they were 5.91, 5.26 and 8.36%, respectively. Therefore, it was concluded that the co-existed diatomite has minor contributions to the retention on soil columns. The logarithmic values of the retention factors of tested compounds on the three soil columns ($\log k_{soil}$) are listed in Table 2.

3.2. Correlations between K_{OC} and k_{soil}

Correlations between $\log K_{OC}$ and $\log k_{soil}$ were investigated by the following form:

$$\log K_{OC} = a \log k_{soil} + b \quad (1)$$

where a and b are the regression coefficients. The $\log K_{OC}$ values measured using batch equilibrium experiments are taken from reference [14] and presented in Table 2 for the three soils. The regression results were:

$$\begin{aligned} \text{EUROSIL 1\# : } \log K_{OC} &= 1.05 \log k_{soil} + 2.07, \\ R^2 &= 0.89, \text{ S.D.} = 0.21, F = 121 \end{aligned} \quad (2)$$

$$\begin{aligned} \text{EUROSIL 1\# : } \log K_{OC} &= 1.11 \log k_{soil} + 2.04, \\ R^2 &= 0.89, \text{ S.D.} = 0.18, F = 146 \end{aligned} \quad (3)$$

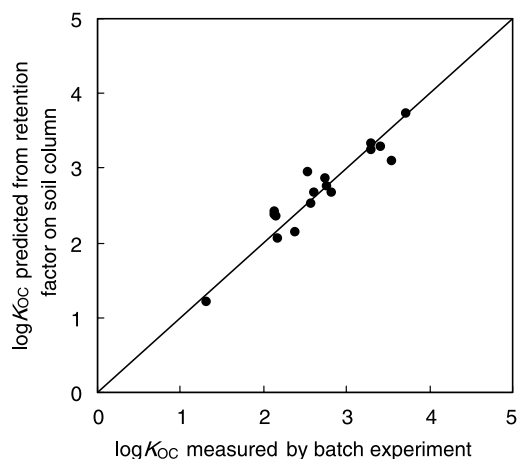


Fig. 1. $\log K_{OC}$ measured by batch experiments vs. $\log K_{OC}$ predicted from retention factor on soil column for EUROSOIL 1#.

$$\text{EUROSOIL 1\# : } \log K_{OC} = 0.98 \log k_{soil} + 2.62, \\ R^2 = 0.93, \text{ S.D.} = 0.15, F = 174 \quad (4)$$

where R^2 is the correlation coefficient, S.D. is the standard deviation of regression, and F is the significance factor.

The above regression results indicate that good linear free energy relationships existed between $\log K_{OC}$ and $\log k_{soil}$ for all the three soils. The correlations between K_{OC} measured by batch experiments and predicted from retention factors are plotted in Figs. 1–3 for EUROSOILS 1#, 2# and 5#, respectively. Although the tested compounds span a wide range of chemical properties, all the data points in the three figures are evenly distributed around the 1:1 line, and there are no apparent exceptions. These results indicate that the K_{OC} values of compounds for a specific type of soil can be accurately predicted from k_{soil} on soil column packed with this soil.

In addition, the possibility to use the retention factors on a soil column to predict the K_{OC} values for other soils of different natures was studied. The cross correlations between $\log K_{OC}$ and $\log k_{soil}$ for the three soils were investigated.

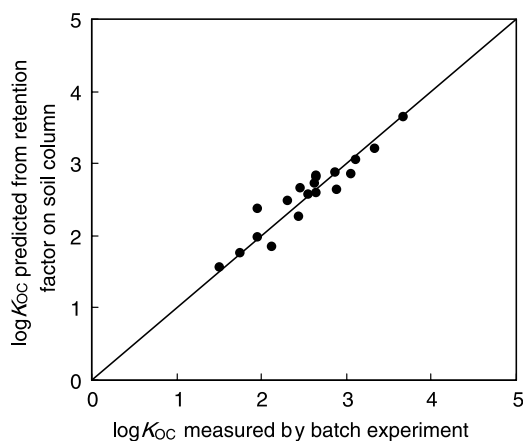


Fig. 2. $\log K_{OC}$ measured by batch experiments vs. $\log K_{OC}$ predicted from retention factor on soil column for EUROSOIL 2#.

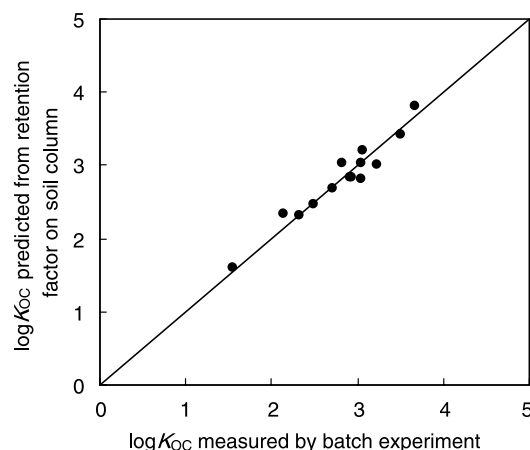


Fig. 3. $\log K_{OC}$ measured by batch experiments vs. $\log K_{OC}$ predicted from retention factor on soil column for EUROSOIL 5#.

The R^2 of the regression correlation between $\log K_{OC}$ values for EUROSOIL 1# and $\log k_{soil}$ on EUROSOIL 5# column was 0.90, and that between $\log K_{OC}$ values for EUROSOIL 5# and $\log k_{soil}$ on EUROSOIL 1# column was 0.93. However, all the other R^2 s for the pairs of EUROSOIL 2# and EUROSOIL 1# or EUROSOIL 5# were lower than 0.80. These results show that the retention factors on soil column cannot be arbitrarily extended to be used to predict the K_{OC} values for other soils with different properties.

3.3. Comparing k_{soil} with hydrophobic parameters for K_{OC} prediction

K_{OW} and retention factor on CN phase (k_{CN}) are frequently used hydrophobic parameters to predict K_{OC} [3,16], and the k_{CN} has been proposed as an alternative method of K_{OC} prediction by OECD [17]. The correlations were achieved in the form of Eq. (1) by replacing $\log k_{soil}$ with $\log k_{CN}$ or $\log K_{OW}$, respectively. The values of $\log K_{OW}$ [18] and $\log k_{CN}$ [14] of the test compounds were taken from the corresponding references, and are presented in Table 2.

For EUROSOIL 1#, the regression results were:

$$\log K_{OC} = 0.49 \log K_{OW} + 1.28, \\ R^2 = 0.65, \text{ S.D.} = 0.39, F = 23 \quad (5)$$

$$\log K_{OC} = 1.29 \log k_{CN} + 2.67, \\ R^2 = 0.65, \text{ S.D.} = 0.38, F = 23 \quad (6)$$

In comparing with the regression results of the correlation between $\log K_{OC}$ and $\log k_{soil}$ Eq. (2), the regression results between $\log K_{OC}$ and $\log K_{OW}$ (Eq. (5)) or $\log k_{CN}$ (Eq. (6)) were apparently poor. The main component of EUROSOIL 1# is clay (0.75 kg/kg), and its clay/OC ratio is 22.8, and in view of the study of Hasset et al. [8] who found the contribution of clay to overall sorption was apparent at clay/OC ratios of more than 10, so the clay has significant, even possibly dominant contribution to the overall sorption

of compounds on EUROSIL 1#. As both the mechanisms of distribution of organic compounds in *n*-octanol/water and in HPLC mobile phase/stationary phase systems are partitioning, the poor correlations between the K_{OC} and the two hydrophobic parameters mean an apparently different mechanism, which should be adsorption, involved in sorption of organic compounds on EUROSIL 1#. Therefore, it can be concluded that the hydrophobic parameters are not applicable for K_{OC} prediction for soil with high clay content, where adsorption has dominant contribution to the overall sorption of organic compounds on soil.

For EUROSIL 2#, the regression results between $\log K_{OC}$ and $\log K_{OW}$, $\log k_{CN}$ were:

$$\begin{aligned} \log K_{OC} &= 0.43 \log K_{OW} + 1.37, \\ R^2 &= 0.68, \text{ S.D.} = 0.32, F = 34 \end{aligned} \quad (7)$$

$$\begin{aligned} \log K_{OC} &= 1.70 \log k_{CN} + 2.49, \\ R^2 &= 0.84, \text{ S.D.} = 0.23, F = 88 \end{aligned} \quad (8)$$

As in the case of EUROSIL 1#, the regression results between $\log K_{OC}$ and $\log K_{OW}$ (Eq. (7)) or $\log k_{CN}$ (Eq. (8)) were poorer than those between $\log K_{OC}$ and $\log k_{soil}$ (Eq. (3)) for EUROSIL 2#. In comparing with K_{OW} (Eq. (7)), the regression results between k_{CN} and K_{OC} were much better (Eq. (8)) for EUROSIL 2#, and those between K_{OC} and k_{CN} for EUROSIL 2# (Eq. (8)) were also much better than those for EUROSIL 1# (Eq. (6)). These results can be explained on the basis of the properties of both CN phase and EUROSIL 2#. In comparing with EUROSIL 1#, the latter has lower clay content (0.226 kg/kg) and an apparently lower clay/OC ratio of 6.8, therefore the contribution of clay to sorption on EUROSIL 2# is not as significant as that on EUROSIL 1#, and it is possible that a considerable contribution of SOM exists in organic compound sorption on EUROSIL 2#. The CN phase, which contains both lipophilic ($-\text{CH}_2-\text{CH}_2-\text{CH}_2-$) and polar ($-\text{CN}$) moieties, is a moderately polar material. The dual moieties of the cyanopropyl stationary phase having both polar and non-polar sites allow the interactions of polar and non-polar groups of a molecule in a similar way as is the case for organic matter in soils. This enables the relationship between the retention factors on the CN column and the sorption coefficients on soil to be established.

Although a relatively good correlation was obtained between $\log K_{OC}$ and $\log k_{CN}$ for EUROSIL 2#, the R^2 (0.84) is still lower than that between $\log K_{OC}$ and $\log k_{soil}$ (0.90). The reasons may be fall into one of the two or both as described below. One is the CN phase cannot completely simulate the SOM of EUROSIL 2#, which have a more complex components and complicated properties. The other is a considerable contribution of clay to sorption still exists since the absolute content of clay in EUROSIL 2# is relatively high (0.226 kg/kg). For EUROSIL 5#, the

regression results between $\log K_{OC}$ and $\log k_{CN}$, $\log K_{OW}$ were:

$$\begin{aligned} \log K_{OC} &= 0.50 \log K_{OW} + 1.32, \\ R^2 &= 0.81, \text{ S.D.} = 0.25, F = 46 \end{aligned} \quad (9)$$

$$\begin{aligned} \log K_{OC} &= 1.81 \log k_{CN} + 2.70, \\ R^2 &= 0.93, \text{ S.D.} = 0.15, F = 155 \end{aligned} \quad (10)$$

From the values of R^2 and S.D. of the above regression results, we found the predictive accuracy of $\log k_{CN}$ was almost equivalent with that of $\log k_{soil}$ (Eq. (4)) for EUROSIL 5#. Although the correlation between $\log K_{OW}$ and $\log K_{OC}$ was not so good as that between $\log k_{CN}$ and $\log K_{OC}$, a relatively good result was also obtained ($R^2 = 0.81$).

Among the three soils, EUROSIL 5# has the maximum organic carbon content (0.0443 kg/kg) and the lowest clay content (0.06 kg/kg). The organic matter can be considered the dominant phase that contributes to overall sorption of compounds on soil. The partitioning of organic compound between water and SOM is the dominant mechanism for EUROSIL 5#. It should be the main reason for the good correlation existing between K_{OC} and the two hydrophobic parameters. As the case of EUROSIL 2#, due to the dual moieties of CN stationary phase whose properties are more similar to the soil SOM than *n*-octanol, for EUROSIL 5#, CN phase is also a better model material than *n*-octanol for prediction of K_{OC} .

4. Conclusion

The results obtained in this study indicate that the SCLC method is valid for all the three types of soils with significantly different properties, however, the applicability of using hydrophobic parameters to predict K_{OC} depends on the properties of soils. For soils containing high organic matter and low clay contents (e.g. EUROSIL 5#), the correlations between K_{OC} and hydrophobic parameters are relatively good, otherwise, the prediction of K_{OC} from hydrophobic parameters is limited, and its validity for K_{OC} prediction depends on the properties of SOM and the contents of clay and organic carbon in the soils investigated.

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