

# Estimating the Organic Carbon Partition Coefficient and Its Variability for Hydrophobic Chemicals

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Numerous correlations have been developed between the organic carbon/water partition coefficient  $K_{OC}$  and various molecular properties and descriptors, but most notably the octanol/water partition coefficient  $K_{OW}$  and water solubility. From an analysis of the theory underlying in this partitioning and an examination of the existing database, it is suggested that the preferred approach is to correlate the quantity  $\log(K_{OC}/K_{OW})$ , which is essentially the ratio of activity coefficients in octanol and organic carbon, with a molecular property or with  $\log K_{OW}$  rather than  $\log K_{OC}$  with  $\log K_{OW}$ . Such an approach is presented for estimating  $K_{OC}$  for hydrophobic chemicals, including an expression of uncertainty limits, based on a correlation derived between  $\log(K_{OC}/K_{OW})$  and  $\log K_{OW}$ . In its simplest form the correlation is that  $K_{OC} = 0.35K_{OW}$  subject to variation by a factor of 2.5 in either direction. It is suggested that new experimental data be assessed for consistency and achievement of true equilibrium by comparison with this correlation.

## Introduction

Since most sorption of hydrophobic organic substances is to the natural organic matter present in these media, the usual approach is to assume that all sorption is to that matter and to invoke a partition coefficient between organic carbon ( $K_{OC}$ ) or organic matter ( $K_{OM}$ ) and water.  $K_{OC}$  is then  $K_P/\phi$ , where  $K_P$  (L/kg) is the ratio of concentrations in the solid phase (mg/kg) and in water (mg/L) and  $\phi$  is the mass fraction organic carbon. Numerous measurements of  $K_{OC}$  and  $K_{OM}$  have been reported in the literature, and many correlations have been derived between them and various molecular descriptors. Gawlik et al. (1) reviewed 24 correlations of  $K_{OC}$  with water solubility, 76 with the octanol/water partition coefficient  $K_{OW}$ , 35 with RP-HPLC retention time, and 38 with topological indices or other molecular properties. They concluded that it was not possible to recommend any single correlation as being preferred universally for all compounds. Major difficulties thus face the environmental scientist when selecting among these correlations and even when assessing conflicting experimental data for the same substance.

Part of this difficulty lies in the expected variability in  $K_{OC}$  resulting from the complex and variable nature of organic

matter. There has been considerable research into the chemical nature, structure, and properties of sediments and soil organic matter (2–4). It is viewed as a combination of fulvic and humic acids and humin, with an average carbon content of approximately 58% (5). Organic matter is variable in properties and consists of aggregates of material that may be in a continuous state of degradation, rearrangement, and replenishment. Hydrophobic solutes appear to bind readily and rapidly with the outer surface region in a few hours to a few days and then diffuse slowly into (and out of) the hydrophobic interior region and narrow cavities in the organic matter during time periods of weeks (6). The measured concentration in the solid phase is thus expected to vary with time explaining much of the variability in reported data. Chiou et al. (4) have also shown differences between the sorptive behavior of soils and sediments, with sediment  $K_{OC}$  values being about twice those of soils. Additionally PAHs exhibit higher partitioning to soil/sediment organic matter than other nonpolar solutes such as PCBs apparently because of more favorable PAH–organic matter interactions (4). It should also be noted that material other than organic carbon has sorptive capacity; thus even when the organic carbon content is zero, a finite value of  $K_P$  is expected. Finally, the water associated with the solids after filtering or centrifuging will contain dissolved solute. The quantity of this solute can become appreciable when  $K_{OC}$  is low, i.e.,  $\log K_{OC}$  less than about 2.5, especially when the organic carbon content of the sorbent is low.

Studies by Chiou et al. (4) and others indicate that for any given chemical, an inherent variability in  $K_{OC}$  values is expected as a result of different environmental conditions and equilibration times. Thus it is unlikely that a highly accurate, generally applicable correlation for  $K_{OC}$  or  $K_{OM}$  can be established. In this study we review and criticize existing correlation approaches, set out a theoretical basis for correlations, and suggest an approach that includes a measure of variability. A method is recommended by which new experimental data can be assessed for consistency, taking in account equilibration time.

## Theory Underlying Partitioning

The most reliable correlation equations for  $K_{OC}$  are likely to be those which have a sound basis in the thermodynamic theory underlying the partitioning phenomenon. The two most commonly used correlations are with the octanol/water partition coefficient ( $K_{OW}$ ) and water solubility ( $S_w$ ).

When a chemical achieves equilibrium in a two-phase system such as organic carbon and water, it will have equal chemical potentials or fugacities ( $f$ ) in both phases. The fugacity in the aqueous phase can be expressed approximately on a Raoult's law basis as

$$f = x_w \gamma_w P_L^S = a P_L^S \quad (1)$$

where  $x_w$  is the mole fraction of the chemical dissolved in water and  $P_L^S$  is the reference fugacity or approximately the vapor pressure of the pure chemical in the liquid state.  $P_L^S$  is measurable for liquids, whereas for solids and gases it must be estimated.  $\gamma_w$  is the activity coefficient of the dissolved chemical which varies with chemical structure and is dependent on concentration, but for small mole fractions  $\gamma$  is assumed to be constant. The activity coefficient is an expression of the chemical's hydrophobicity and describes the tendency of the chemical to partition from water into the gas phase, the activity  $a$  being the product of  $x_w$  and  $\gamma_w$ .

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The concentration  $C$  (mol/m<sup>3</sup>) of a chemical in water is  $x_w/v_w$ , where  $v_w$  is the molar volume of water (approximately  $18 \times 10^{-6}$  m<sup>3</sup>/mol). Other common units for concentration are mg/L or g/m<sup>3</sup>, both of which are  $M_i C$  or  $M_i x_w/v_w$  or  $M_i f/(v_w \gamma_w P_L^S)$ , where  $M_i$  is the molecular mass of the chemical (g/mol). By analogy, the fugacity in the organic carbon phase can be expressed as

$$f = x_c \gamma_c P_L^S \quad (2)$$

where  $x_c$  denotes the mole fraction and  $\gamma_c$  the activity coefficient. Values of  $x_c$  and  $\gamma_c$  are difficult to measure individually, but their product can be measured readily.

The concentration of the chemical (g/m<sup>3</sup>) in the organic carbon phase is  $M_i x_c/v_c$ , where  $v_c$  is the molar volume of the wet organic carbon phase (which is also uncertain), but more commonly concentration is expressed in the more readily measurable units of mg/kg OC which is  $M_i x_c/(v_c \rho_c)$  or  $M_i f/(v_c \rho_c \gamma_c P_L^S)$ , where  $\rho_c$  is the density of organic carbon (g carbon/cm<sup>3</sup> wet phase or kg/L). The organic carbon/water partition coefficient  $K_{OC}$  (L/kg) expressed as the ratio of concentrations in the OC phase (mg/kg) to that in water (mg/L) is thus

$$K_{OC} = \frac{v_w \gamma_w}{v_c \rho_c \gamma_c} \quad (3)$$

The group  $v_c \rho_c$  is also the molecular mass  $M_c$  (g/mol) of the OC phase, and since  $v_w$  is  $M_w/\rho_w$ , where  $M_w$  is the molecular mass of water and  $\rho_w$  its density,  $K_{OC}$  is also given by

$$K_{OC} = \frac{M_w \gamma_w}{M_c \gamma_c \rho_w} \quad (4)$$

The commonest correlation for  $K_{OC}$  is with the octanol/water coefficient  $K_{OW}$ , for which extensive databases and reliable estimation methods exist. The fugacity of a chemical in the octanol phase of an octanol/water two-phase system, by analogy with water, is

$$f = x_o \gamma_o P_L^S \quad (5)$$

The octanol/water partition coefficient is thus

$$K_{OW} = \frac{v_w \gamma_w}{v_o \gamma_o} = \frac{M_w \gamma_w \rho_o}{M_o \gamma_o \rho_w} \quad (6)$$

where the subscript O refers to the octanol phase.

Also used in  $K_{OC}$  correlations is the solubility of pure chemical in water, which is reached when its fugacity equals that of the pure liquid saturated with water, and is approximately the pure liquid vapor pressure if water is sparingly soluble in the liquid. In such cases

$$f \cong P_L^S = x_w \gamma_w P_L^S \quad (7)$$

which implies that  $x_w$  is approximately  $1/\gamma_w$  and the solubility  $S_w$  in g/m<sup>3</sup> (or mg/L) is  $M_i x_w/v_w$  or  $M_i/(v_w \gamma_w)$ . For solids the fugacity is that of the solid phase  $P_S^S$ ; thus  $x_w$  is  $(P_S^S/P_L^S)/\gamma_w$  or  $F/\gamma_w$ , where  $F$  is the fugacity ratio which can be estimated from the melting point and the entropy of fusion. In units of g/m<sup>3</sup> (or mg/L), the solubility is  $F M_i/(v_w \gamma_w)$ . For liquids  $F$  can be regarded as 1.0.

**Existing Correlations.** Most of the reported correlations are between log  $K_{OC}$  and log  $K_{OW}$  or log  $S_w$ . Unfortunately, the low water solubilities and high  $K_{OW}$  values of highly hydrophobic compounds are difficult to measure accurately, and this may contribute to a loss of correlation. A major problem with the solubility correlations is the need to include

an estimate for  $F$  for solid substances. This "correction" is frequently and wrongly ignored. The most attractive approach is to use  $K_{OW}$  for correlation purposes, largely because it avoids the necessity of estimating  $F$  and also because of the availability of an extensive database (MedChem Master file) for nearly 10 000 chemicals (7). For other chemicals,  $K_{OW}$  can be estimated from structural properties (8). An additional advantage of using  $K_{OW}$  is that it contains the quantity  $\gamma_o$ , activity coefficient of the chemical in octanol. As molar volume increases, it is likely that  $\gamma_o$  increases reflecting growing molecular dissimilarity or nonideality. It is possible that  $\gamma_c$ , the corresponding coefficient in organic carbon, also increases, and thus any increasingly nonideal behavior in organic carbon may be compensated for in part by the increase in  $\gamma_o$ .

In a systematic study, Sabljic et al. (9) examined  $K_{OC}$  versus  $K_{OW}$  relationships for different chemicals, and general and class-specific models for predicting  $K_{OC}$  from  $K_{OW}$  data were derived. For the predominantly hydrophobic chemicals, however, Sabljic et al. (9) noted that the  $K_{OC}$  data had large uncertainties, particularly in the log  $K_{OW}$  range from 4 to 7.5. They derived a model based on first-order molecular connectivity indices. Such correlations may give an apparently superior fit to those with  $K_{OW}$  as a result of inclusion of some erroneous experimental data in the  $K_{OW}$  correlations. As more accurate and critically reviewed  $K_{OW}$  data become available, it is likely that  $K_{OW}$  will become the favored molecular descriptor.

Because of the wide variation in  $K_{OC}$ , the correlation is usually of the form

$$\log K_{OC} = A \log K_{OW} + B \quad (8)$$

For example, Karickhoff (10) obtained values of  $A$  of 1.0 and  $B$  of  $-0.35$  for PAHs from benzene to pyrene. For most of the other proposed correlations (1),  $A$  is less than 1.0, typically 0.8. The factors which control  $A$  are examined below.

## Discussion

**Development of Estimation Methodology.** As eqs 3 and 6 show, both  $K_{OC}$  and  $K_{OW}$  contain the term  $\gamma_w$ . This quantity varies from less than 1.0, for highly polar substances, to values of  $10^6$  or more for nonpolar hydrophobic substances. A relationship between  $K_{OC}$  and  $K_{OW}$  is thus highly autocorrelated, being strongly influenced by the variable  $\gamma_w$  which is present in both quantities. Subtle contributions of, or changes to, the other terms such as  $\gamma_o$  or  $\gamma_c$  tend to be obscured. This problem can be avoided by correlating  $K_{OC}/K_{OW}$  which, from eqs 3 and 6, is  $v_o \gamma_o/(v_c \rho_c \gamma_c)$  or  $v_o \gamma_o/(M_c \gamma_c)$ . The key quantities in these ratios that vary from chemical to chemical are  $\gamma_c$ , which expresses (inversely) the affinity of the chemical for the OC phase, and  $\gamma_o$ , which is similar but applies to the octanol phase. Two situations may arise:

First is the special case in which  $\gamma_o/\gamma_c$  (and hence  $K_{OC}/K_{OW}$ ) is constant for chemicals with different molecular properties (or  $K_{OW}$ ). Then, from eqs 3, 6, and 8,  $A$  is 1.0 and  $B$  is log( $v_o \gamma_o/v_c \rho_c \gamma_c$ ).

Second,  $\gamma_o/\gamma_c$  may vary with molecular properties (or with  $K_{OW}$ ): e.g.,  $\gamma_c/\gamma_o$  may increase with increased molecular mass or  $K_{OW}$ , and a relationship may exist of the form

$$\gamma_o/\gamma_c = Y K_{OW}^n$$

where  $Y$  and  $n$  are constants or

$$\frac{\gamma_o v_o}{\gamma_c v_c \rho_c} = Y K_{OW} = (K_{OC}/K_{OW})$$

where  $Y$  is  $Y v_o/v_c \rho_c$ . This leads to the correlation

$$\log K_{OC} = (1 - n) \log K_{OW} + \log Y$$

If  $\gamma_c/\gamma_o$  is weakly dependent on  $K_{OW}$ , for example, to the power  $n$  of 0.2, we obtain

$$\log K_{OC} = 0.8 \log K_{OW} + \log Y \quad (9)$$

The preponderance of correlations with  $A$  in the range 0.6–0.8 suggests that this second situation applies. The implication is that with increasing molecular size or  $K_{OW}$ ,  $\gamma_c$  increases more than  $\gamma_o$ , or at least the ratio  $\gamma_c/\gamma_o$  increases. Chiou et al. (4) have shown that  $\gamma_c$  is lower for PAHs than other nonpolar solutes such as PCBs, i.e., PAHs behave more ideally in organic matter. It is therefore likely that the ratio  $\gamma_c/\gamma_o$  and its dependence on molecular size also depend on chemical class. Thus, general correlations covering a wide range of chemicals are likely to be less accurate than class-specific correlations.

**Data Analysis.** Most of the data treated here for hydrophobic chemicals were obtained from the set compiled by Sabljic et al. (9) (81 data points). Data were also obtained from Karickhoff (10) (5 data points), Chin et al. (11) (4 data points), Chiou et al. (12) (11 data points), Pussemier et al. (13) (11 data points), and Schwarzenbach and Westall (14) (6 data points). When the organic matter partition coefficient  $K_{OM}$  was reported, it was adjusted to  $K_{OC}$  as  $1.724K_{OM}$  (5).

A conventional plot of  $\log K_{OC}$  versus  $\log K_{OW}$  for the data yielded the correlation ( $n$  = number of data points;  $r^2$  = coefficient of determination;  $s$  = standard error of estimate):

$$\log K_{OC} = 0.81 \log K_{OW} + 0.09 \quad (10)$$

$$n = 118; r^2 = 0.89; s = 0.42$$

Figure 1 is a plot of  $\log(K_{OC}/K_{OW})$  as a function of  $\log K_{OW}$  for the same data. Plots of  $\log(K_{OC}/K_{OW})$  versus molecular weight, molecular volume, and molecular area were generally similar (since  $K_{OW}$  is related to these molecular descriptors) and are not included here. Figure 1 shows that 78% of the data (92 data points) lie in the range of  $K_{OC}/K_{OW}$  of 0.1–1.0 with 3% (4 data points) exceeding 1.0 and 19% (22 data points) less than 0.1. Linear regression yielded

$$\log(K_{OC}/K_{OW}) = -0.19 \log K_{OW} + 0.09 \quad (11)$$

$$n = 118; r^2 = 0.31; s = 0.42$$

Although eqs 10 and 11 are algebraically similar, the high  $r^2$  value of 0.89 for eq 10 is largely a result of the strong autocorrelating influence of  $\gamma_w$  on both  $K_{OC}$  and  $K_{OW}$  values. This autocorrelation masks the variability in  $K_{OC}$  shown in Figure 1.

The primary reason for the negative slope in eq 11 and the slope of 0.81 in eq 10 is a group of 15 data points, with  $K_{OC}/K_{OW} < 0.1$ , to the lower right of Figure 1. They are PCBs (8 data points), chlorobenzenes (tri, tetra, penta, and hexa), DDT, DDE, and aldrin. The only data point with  $K_{OC}/K_{OW}$  significantly above 1.0 was mirex. As shown in Table 1, which summarizes data from a handbook by Mackay et al. (15), for chemicals such as DDT, DDE, aldrin, and mirex, there is a wide range in the reported  $K_{OC}$  values. Clearly, any correlation is readily distorted if an erroneously low value of  $K_{OC}$  is used. This has the effect of reducing the slope  $A$  in eq 8.

$K_{OC}$  data (275 points) for 48 congeners of PCBs compiled by Mackay et al. (16) are plotted in Figure 2. The eight most studied congeners account for more than 50% of these data. The scatter in the data is impressive with 12% exceeding  $K_{OC}/K_{OW}$  of 1.0, 36% lying between 1.0 and 0.1, 39% lying between 0.1 and 0.01, and 13% lying below 0.01. It seems inconceivable that organic matter varies so greatly in

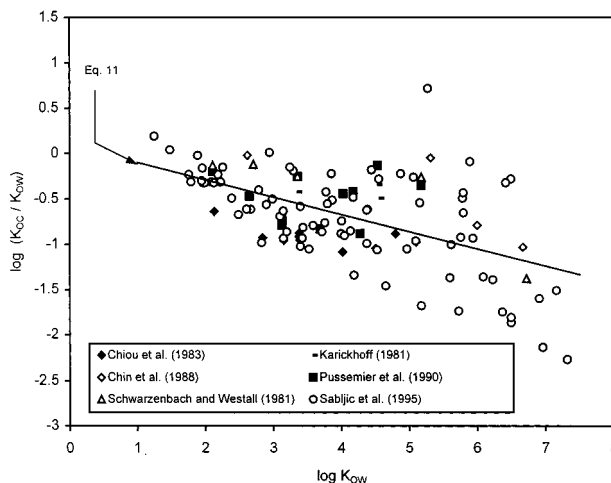


FIGURE 1. Plot of  $\log(K_{OC}/K_{OW})$  vs  $\log K_{OW}$  for hydrophobic chemicals for the initial data set compiled (regression eq 11).

TABLE 1. Variability in the Reported  $K_{OW}$  and  $K_{OC}$  for Selected Chemicals from Mackay et al. (15)<sup>a</sup>

chemical	log $K_{OC}$	
	range	data (numbers)
DDT	4.09–6.81	25
DDE	3.7–6.64	4
aldrin	2.6–4.7	8
mirex	3.08–6.42	7

<sup>a</sup> Including both measured and estimated values, obvious outliers were ignored.

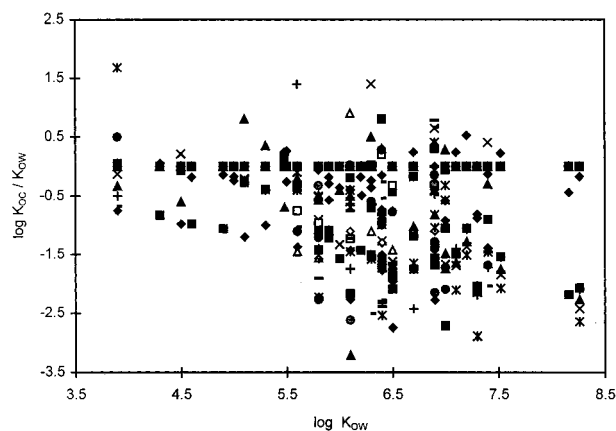


FIGURE 2. Scatter in  $\log(K_{OC}/K_{OW})$  as a function of  $\log K_{OW}$  for PCBs, using data from ref 16.

properties; thus we believe that many of these data points are erroneous. The principal cause is believed to be non-attainment of equilibrium: i.e., the equilibration times used in these estimations were insufficient. In a critical review of research over the past decade, Pignatello and Xing (6) have shown that the solid-phase to solution-phase partition coefficients are routinely measured and reported at non-equilibrium conditions. In most cases, the uptake or release of organics by natural particles is bimodal in that it occurs in fast and slow stages. Many reported  $K_{OC}$  values for soil represent principally the fast component rather than overall sorption (17). This has the effect of reducing these values, especially for hydrophobic chemicals which require longer equilibration times.

Support for attributing the variability in  $K_{OC}$  values to nonattainment of equilibrium, for predominantly hydrophobic chemicals with high  $K_{OW}$  values, can also be found



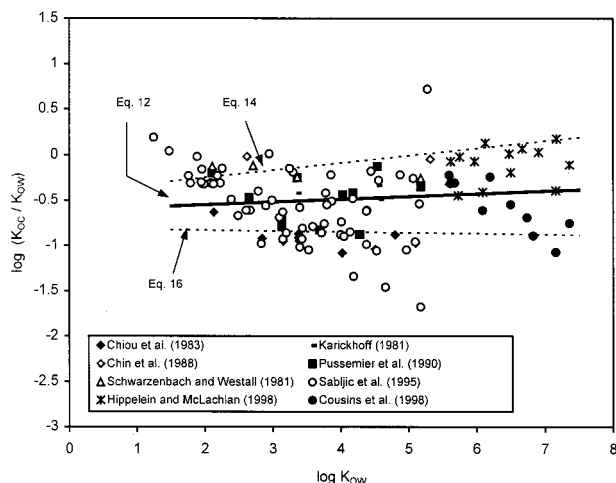


FIGURE 3. Plot of  $\log(K_{OC}/K_{OW})$  vs  $\log K_{OW}$  for hydrophobic chemicals for the modified data set as explained in the text (regression eq 12).

in some recent experimental studies (18, 19). For 10 different congeners of PCBs with  $\log K_{OW} > 5.5$ , the  $K_{OC}/K_{OW}$  data derived based on  $K_{SA}$  measurements of Cousins et al. (19) showed that on increasing the equilibration time from 3 to 83 days, the  $K_{OC}/K_{OW}$  values increased from between 0.005 and 0.43 to between 0.08 and 0.6. Further increase in equilibration time had little effect. The  $K_{OC}$  values were derived from the measured  $K_{SA}$  (soil-air) values and  $K_{AW}$  (air-water) partition coefficients for which also accurate estimates are available.

Of the 24 data points with  $\log K_{OW} > 5.5$  in Figure 1, a majority (14 data points) were PCBs. These data points were replaced by 23 data points for various congeners of PCBs with  $\log K_{OW} > 5.5$  obtained using  $K_{SA}$  measurements by Cousins et al. (19) and Hippelein and McLachlan (18). An equilibration time of approximately 3 months was used in both cases. A linear regression on this modified data (Figure 3) yielded

$$\log(K_{OC}/K_{OW}) = 0.03 \log K_{OW} - 0.61 \quad (12)$$

$$n = 117; r^2 = 0.02; s = 0.38$$

or equivalently

$$\log K_{OC} = 1.03 \log K_{OW} - 0.61 \quad (13)$$

The low correlation coefficient for eq 12 is the result of the random variability in  $K_{OC}$  values, as also shown by the residuals plot in Figure 4. This variability is masked in the conventional  $\log K_{OC}$  versus  $\log K_{OW}$  plot which, for the modified data set, also yielded eq 13 but with an  $r^2$  value of 0.95 and gives a false impression of predictability.

The residuals are uniformly distributed and are independent of  $K_{OW}$  for  $\log K_{OW}$  values greater than about 2.5 (Figure 4). The residuals for the new data introduced ( $\log K_{OW} > 5.5$ ), though random, are seen to be predominantly positive. This is due to the influence of the large number of data points between  $\log K_{OW}$  values of 3 and 5 for which we have no basis for reexamination. The residuals for  $K_{OW}$  values less than 2.5 are less scattered but mainly positive with a tendency to increase with reducing  $K_{OW}$  values, denoting underestimation of the predicted  $K_{OC}$  values. However, as mentioned earlier, the measured  $K_{OC}$  values for such chemicals are susceptible to overestimation due to the inclusion of dissolved solute in the water associated with the organic matter and the presence of sorption to nonorganic matter.

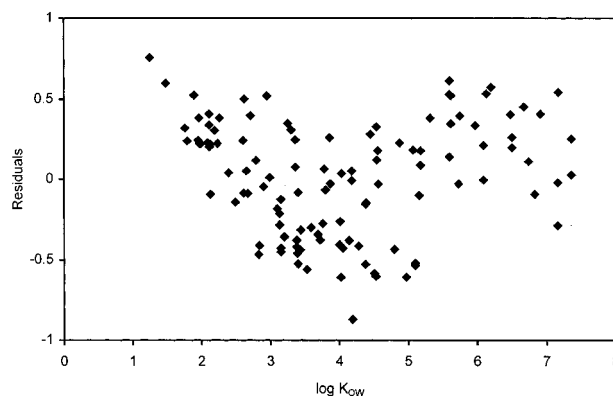


FIGURE 4. Plot of residuals between experimental and predicted values of  $\log K_{OC}$  using eq 12.

**Recommended Approach.** The large variability in reported  $K_{OC}$  values requires that the estimates derived based on correlations should include a measure of the associated uncertainty, and we have used 95% confidence boundaries for the purpose. A linear regression analysis was conducted on the modified data set used to obtain eq 12, and 95% confidence limits were obtained for the slope and intercept. The boundaries obtained using these limits are plotted in Figure 3 and correspond to the following equations:

upper limit

$$\log(K_{OC}/K_{OW}) = 0.08 \log K_{OW} - 0.41 \quad (14)$$

or equivalently

$$\log K_{OC} = 1.08 \log K_{OW} - 0.41 \quad (15)$$

lower limit

$$\log(K_{OC}/K_{OW}) = -0.01 \log K_{OW} - 0.81 \quad (16)$$

or equivalently

$$\log K_{OC} = 0.99 \log K_{OW} - 0.81 \quad (17)$$

Equations 14 and 16 show that the slope of the regressed line on the modified data (eq 12) is not significantly different from zero, which, when substituted in eq 12, justifies the frequently used approximation of  $K_{OC} = 0.4K_{OW}$ .

As noted by Cousins et al. (19), although their data set was obtained for the same group of chemicals (PCBs) and using exactly the same technique as Hippelein and McLachlan (18), the slopes of the regressions obtained using the two data sets independently were distinctly different (as can also be seen from their data plotted in Figure 3). This difference was attributed to the variability in the organic matter of the soils used. Both these data sets are however within the confidence boundaries defined by eqs 14 and 16. We thus recommend that in environmental and/or risk assessments,  $K_{OC}$  values for hydrophobic chemicals should be considered as a distribution bounded by eqs 14 (or 15) and 16 (or 17), rather than as discrete numbers derived from one of the numerous correlations in the literature. These equations should be applicable to all situations where partitioning into organic matter is expected to be the dominant process for chemical sorption. If the results are found to be sensitive to  $K_{OC}$  then, if needed, a more accurate estimate of its value should be sought for the specific environmental situation under consideration.

Because the coefficient on  $\log K_{OW}$  is not significantly different from zero, we suggest a simpler correlation that  $\log(K_{OC}/K_{OW})$  is  $-0.48$  with an upper limit of  $-0.05$  and a

lower limit of  $-0.86$ . This is equivalent to asserting that  $K_{OC}$  is  $0.33K_{OW}$  with an upper limit of  $0.89K_{OW}$  and a lower limit of  $0.14K_{OW}$ . A useful rule of thumb may thus be that  $K_{OC}$  is  $0.35K_{OW}$  with variation by a factor of 2.5 in either direction. If this rule of thumb is applied to the data used in developing the correlation equations above, about 80% of the data points in Figure 3 lie within these limits.

In conclusion, the variability in the composition of organic matter present in soils and sediments and the experimental difficulties and constraints in  $K_{OC}$  measurements are believed to explain the wide variability in the reported values. Therefore, considerable uncertainties are expected in  $K_{OC}$  values estimated from correlations.  $K_{OC}$  estimations based on  $K_{OW}$  values are preferable to those based on solubility. The suggested approach is to correlate  $K_{OC}/K_{OW}$  with a molecular property or  $K_{OW}$ , rather than  $\log K_{OC}$  with  $\log K_{OW}$ . This, in our opinion, gives a better indication of uncertainty in  $K_{OC}$ . It is suggested that  $K_{OC}$  estimates using correlations be viewed as a distribution, which includes this uncertainty, rather than a single value. When gathering and reporting experimental data for hydrophobic chemicals, it is desirable to calculate  $K_{OC}/K_{OW}$  and examine and report its magnitude. Values exceeding 1.0 and below 0.1 should be subjected to special scrutiny. Finally, when measuring  $K_{OC}$ , care must be taken to ensure that equilibrium is achieved. The time required could be several months and can be estimated using the correlation for the "slow" sorption rate constant as a function of molecular volume suggested by Cornelissen et al. (20).

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