Influence of the Polarity of Organic Matter on the Sorption of Acetamide Pesticides

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Understanding and quantifying the sorption of agrochemicals onto soils is essential to predict their fate and transport in the environment. While many correlations exist between partition coefficients of organic pollutants onto soils and the quantity of soil organic matter, only recently studies have revealed the importance of the nature of soil organic matter. Here we report on the uptake of three acetamide pesticides onto four model organic sorbents. The organic carbon referenced sorption coefficient, K_{oc}, decreased with the increasing polarity index (PI) ($O + N/C$) of the organic sorbent. A regression of K_{ow}, solubility, and polarity index indicated that such correlations are very specific to the pollutant class. Apart from the quality of the organic sorbent properties, the hydrophobicity of the pesticide and the presence of functional groups also contribute to sorption. The more polar the solute and/or the organic sorbent the more likely it is that interactions other than hydrophobic will contribute to sorption, causing the currently used $K_{oc} - K_{ow}$ correlations to fail.

Keywords: *Acetamide pesticides; alachlor; metolachlor; propachlor; organic sorbents; sorption; desorption*

INTRODUCTION

Sorption of weakly polar organic compounds (WPOCs) to soil organic matter (SOM) is often described by linear relationships of the following form,

$$\log K_{oc}(K_{om}) = a \log K_{ow}(C_w) + b \qquad (1)$$

where K_{oc} and K_{om} are the organic carbon and organic matter referenced partition coefficients, K_{ow} is the octanol–water distribution coefficient, and C_w is the solubility in water (Karickhoff *et al.*, 1979; Kenaga and Goring, 1980; Means *et al.,* 1980; Briggs, 1981; Chiou *et al.*, 1983). Equation 1 implies that partitioning (into octanol) and sorption (onto an organic sorbent) are similar processes and predicts that a pollutant specific K_{oc} be independent of the source and properties of the organic carbon. The dependence of each process on molecular properties of sorbate and sorbent may actually be quite different. For example, octanol may be viewed as an isotropic medium while a sorbing organic surface is not. The sorbing surface is relatively rigid, and thus the conformation and structure of the molecule will affect sorption much more than partitioning into an organic solvent. Molecules with similar functional groups but different spatial arrangements may have similar solvent partition coefficients, yet display different surface interactions. Differences in natural organic matter (NOM) properties may spur differences similar to the partitioning to different organic solvents. For example, if one considers the partitioning of organic compounds to octanol, K_{ow}, and hexane, K_{hexane}, the ratio of K_{ow}/K_{hexane} would increase when polar functional groups are present in the compound (Schwarzenbach *et al.*, 1993). Accordingly, one should anticipate variations on $K_{oc} - K_{ow}$ correlations as a function of NOM properties.

The properties of NOM in subsurface environments vary with time, location, and depth (Thurman, 1985; Chen and Pawluk, 1995; Weber *et al.*, 1995). Humification processes vary as a function of the chemical microenvironment that organic debris encounter, generating NOM with a variety of properties. NOM from different sources may differ in their aromaticity, polarity, and the availability of specific surface sites capable to interact with WPOCs. Largely decomposed soils, that are highly humic, contain more of lignin-like organic matter that is less polar than nondecomposed soils that contain more cellulose-like material (Garbarini and Lion, 1986; Kile *et al.*, 1995). Diagenetic alteration of organic matter can result in organic structures that resist further chemical and biological transformation, thus the partitioning exhibits more site-limited sorption behavior (Weber *et al.*, 1995). One should expect the properties and molecular structure of NOM to influence sorption in very different ways and to skew the expected correlation between K_{oc} and K_{ow}.

Recent work has indicated that the "quality" of the soil organic matter influences the partitioning of hydrophobic organic compounds (Garbarini and Lion, 1986; Gauthier *et al.*, 1987; Rutherford *et al.*, 1992; Xing *et al.*, 1994a–c; Kile *et al.*, 1995; Koelmans *et al.*, 1995). For example, reported K_{oc} values for metolachlor sorption onto soils vary from 28 to 663 (Jordan, 1978; Pusino *et al.*, 1992; Jayasundera, 1995). The wide range of experimentally determined K_{oc} values, reported for the same organic compound in different high organic soils, is also evidence that the "quality" of the organic matter is important in determining the sorption behavior of a given compound. Studies have shown that the K_{oc} of hydrophobic organic compounds was not only a function of the soil organic carbon content but also a function of the oxygen and nitrogen content and the degree of aromaticity (Xing *et al.*, 1994b,c; Rutherford *et al.*, 1995; Kile *et al.*, 1995). In addition, Xing *et al.* (1994c) have hypothesized that the sorption of the BTX compounds

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Table 1. Physical and Chemical Properties of Alachlor, Metolachlor, and Propachlor (Montgomery, 1993)

Pesticide	Structure	Properties	
Alachlor		Mol. weight	269.8
		Physical state	solid
		Solubility (mgL⁻¹)	242
		log K_{ow}	2.63
		Mol. surface area[a]	290 (A⁰)²
Metolachlor		Mol. weight	283.8
		Physical state	liquid
		Solubility (mgL⁻¹)	530
		log K_{ow}	2.93
		Mol. surface area[a]	327.9 (A⁰)²
Propachlor		Mol. weight	211.7
		Physical state	solid
		Solubility (mgL⁻¹)	613
		log K_{ow}	1.61
		Mol. surface area[a]	246 (A⁰)²

[a] The surface areas were calculated with HYPER-CHEM using the Van der Waals interactions method.

Table 2. Elemental Analysis of the Model Organic Sorbents

sorbent	C, %	H, %	N, %	O,[a] %	ash, %	surface area[b] (m² g⁻¹)
lignin (organosolv)	65.65	5.52	0.11	28.7	0.0	1.8
lignin (alkali)	58.69	4.69	0.04	30.6	7.1	5.2
collagen	55.96	8.52	12.48	23.0	0.0	>0.5
chitin (practical grade)[a]	44.6	6.82	6.74	38.1	3.7	5.1
cellulose	44.4	6.20	0.0	49.4	0.0	2.4

[a] Xing et al., 1994b. [b] BET surface area (N_2 area).

were influenced by the physical conformation of the sorbing organic phase.

These studies demonstrate the importance of the quality of the soil organic matter, in the partitioning of organic compounds to the organic matter. Several researchers have attempted to model the sorption behavior of organic compounds to organic matter by introducing "organic matter quality" functions into linear correlations (Garbarini and Lion, 1981; Xing *et al.*, 1994c). These correlations have been specifically developed using highly hydrophobic compounds and are not directly applicable to other types of pollutants. Unlike hydrocarbons, agrochemicals are complex organic compounds that possess functional groups capable of interacting with NOM. Thus, as the number of possible interactions between WPOCs and NOM increase, one should expect larger deviations of K_{oc} values.

Studies using different compound classes are needed to analyze the nonlinear relationship between K_{oc} and the quality of the organic matter. The goal of this study was to determine the influence of organic sorbent polarity on the sorption of acetamide pesticides. Organic sorbents are chosen to represent model input sources for soil organic matter with a range of degree of humification and polarity.

MATERIALS AND METHODS

Pesticides. Alachlor and propachlor were received gratis from Dr. Cathleen Hapeman of USDA and had a purity of 99.0% and 94%, respectively. Metolachlor was obtained gratis from Ciba-Geigy Corporation and had a purity of 99.0%. All were of analytical grade and were used without further purification. Their physical and chemical properties are listed in Table 1. Stock solutions were prepared by dissolving each in distilled water and filtering through a 0.45 μm membrane filter. Organic solvents were not used to aid the dissolution of the pesticides to eliminate any cosolvent effects on partitioning to organic sorbents.

Organic Sorbents. Four commercial biopolymers that represent model input sources of soil organic matter were selected as organic sorbents for this study. Lignin (alkali) and cellulose were obtained from Aldrich (Milwaukee, WI), and chitin and collagen were obtained from Sigma (St. Louis, MO); all were used without further purification. The elemental analysis of the organic sorbents were provided by the manufactures and are listed in Table 2. The mass percent of C, H, N, and O for cellulose was calculated from the formula $(C_6H_{10}O_5)_n$.

Pesticide Analysis. Standard pesticide solutions and centrifuged and filtered clear supernatants from adsorption and desorption experiments were analyzed by HPLC using a

Waters HPLC system equipped with an Altech Altima column (i.d. = 4.6 mm, L = 150 mm, C18, 5 μm) preceded by a guard column, a multiwavelength programmable UV-detector, and Millenium software. Samples were eluted and analyzed using the following mobile phase and wavelengths, respectively: alachlor, 60% acetonitrile in water at 220 and 265 nm; metolachlor, 70% methanol in water at 220 and 266 nm; propachlor, 58% methanol in water at 220 and 230 nm.

Sorption of Pesticides onto Organic Sorbents. Sorption experiments were conducted in autoclaved amber glass vials using 25 g L⁻¹ solutions of organic sorbents (solution to solid ratio was 40:1). The vials were sealed with screw caps with a Teflon lining. The ionic strength was maintained at 0.01 M NaCl. The suspensions were mixed, end over end, using a shaker. Aliquots (1.5 mL) were removed after 1 h, 4 h, 1 day, 3 days, 6 days, 10 days, and 14 days of equilibration and were centrifuged (14000 rpm, 20 min) using polypropylene tubes that were previously tested for adsorption of the pesticide. The supernatant was filtered through a 0.25 μm membrane filter and the pesticide in the solution phase analyzed as above. The amount sorbed was determined by the difference method. Sorption onto vials and centrifuge tubes was negligible for all the experiments. All experiments were conducted at constant room temperature (25 °C). Each experiment was conducted at least two times, and the mean value of duplicate vials was used for analysis. The mean error was less than 1% in all cases.

Sorption/Desorption of Metolachlor by Organic Sorbents. Isotherms were obtained using batch equilibration as described above. To determine the sorption behavior of metolachlor, 10−25 g L⁻¹ sorbent concentrations (solution to solid ratio was 40:1 to 50:1) (in duplicate) were equilibrated with metolachlor stock solution, for each sorbent. For all the sorbents studied, the initial metolachlor concentrations varied from ∼130 to 430 μM. After the initial equilibration period, 4 mL of supernatant was replaced with 4 mL of 0.01 M NaCl adjusted to pH 5. The organic sorbents were resuspended by inverting the tubes, and the solutions were transferred back to the vials. The suspensions were allowed to equilibrate for a further 48 h. After equilibration, 5 mL aliquots were centrifuged (14000 rpm for 20 min), and the supernatants were analyzed.

DSC Presentation and Analysis. Differential scanning calorimetry (DSC) is an enthalpy change method in which the difference in energy inputs into a substance and a reference material is measured as a function of temperature while the substance and the reference material are subject to a controlled temperature program. The DSC system used measures temperatures and heat flow associated with material transitions, providing quantitative and qualitative data on endothermic (heat adsorption) and exothermic (heat evolution) processes. In this study, DSC analyses were performed with a 910S DSC system used with a microprocessor-based TA Instruments thermal analyzer, Thermal Analyst 2000, to control, collect and analyze the data. The organic sorbent samples were weighed in aluminum crucibles using a Cahn Model 4700 electrobalance with an accuracy of 0.001 mg. Samples were run in nonhermetic, crimped pans to improve thermal contact between the sample and the container and reduce the thermal gradients in the sample. The furnace of the DSC was under a liquid N_2 flow of 200 mL min⁻¹ as the purge gas. The analyses were performed from 30 to 400 °C. The temperature gradient was 10 °C min⁻¹. The organic sorbent samples were
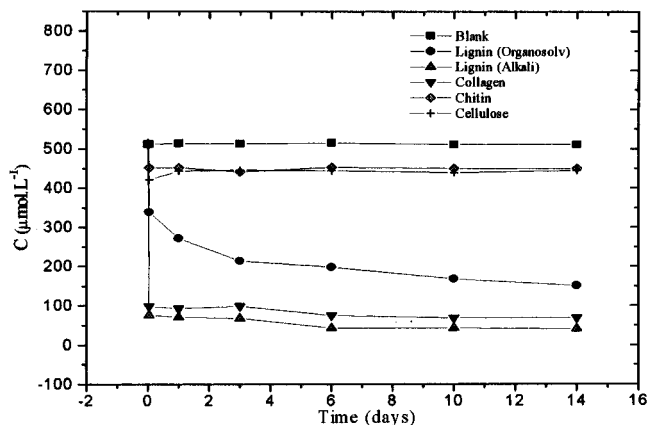
Figure 1. Time study of metolachlor adsorption to organic sorbents. The solution to solid ratio was 40:1 (sorbent concentration = 25 g L^{-1}), and the ion concentration was adjusted to 0.01 M NaCl.

put in the aluminum crucibles with a predetermined amount of metolachlor placed on the underside of the lid. The samples were first loaded with metolachlor vapors, generated *in situ*, by heating to a temperature of 180 °C and cooling down to 30 °C before heating to a 400 °C to obtain the DSC graphs.

RESULTS AND DISCUSSION

Pesticide Sorption Behavior to Organic Sorbents. Figure 1 shows the time studies conducted to establish the equilibration time for the sorption of metolachlor. More than 95% of the final adsorption (14 days) to all the organic sorbents other than lignin (O) was reached within the first day. Alachlor and propachlor behaved similarly (data not shown). Equilibration time for all three pesticides was set as 48 h. Furthermore, after the initial loss, no other significant losses were observed in the time study, indicating that under our conditions, neither chemical nor biological degradation occurred.

Adsorption/Desorption Isotherms of Metolachlor. In the concentration range studied, both adsorption and desorption of metolachlor onto lignin (A) and collagen followed a linear isotherm (Figure 2). The sorption behavior of metolachlor to chitin and cellulose followed a linear isotherm at low equilibrium concentrations but deviated, in positive direction, from linearity at higher concentrations (Figure 3). To compare the uptake capacity among the four organic sorbents, the partition coefficients (K_d's) were calculated from the linear portion of each isotherm using the following linear relation,

$$x/m = K_d \cdot C \qquad (2)$$

where x/m is the uptake of the pesticide per unit mass of organic sorbent and C is the equilibrium concentration in solution. The organic carbon referenced partition coefficient, K_{oc}, was determined as

$$K_{oc} = K_d/f_{oc} \qquad (3)$$

The calculated K_d values for adsorption to lignin, collagen, chitin, and cellulose are 460, 225, 3.2, and 3.5 L kg^{-1}, respectively, indicating that metolachlor uptake by different organic sorbents varied.

Metolachlor can be sorbed by organic matter through (1) charge transfer (π) or van der Waals bonds between the aromatic nuclei of the herbicide and the aromatic rings of the organic matter surface, and/or (2) H-bonds between the carbonyl oxygen in the amide group of the
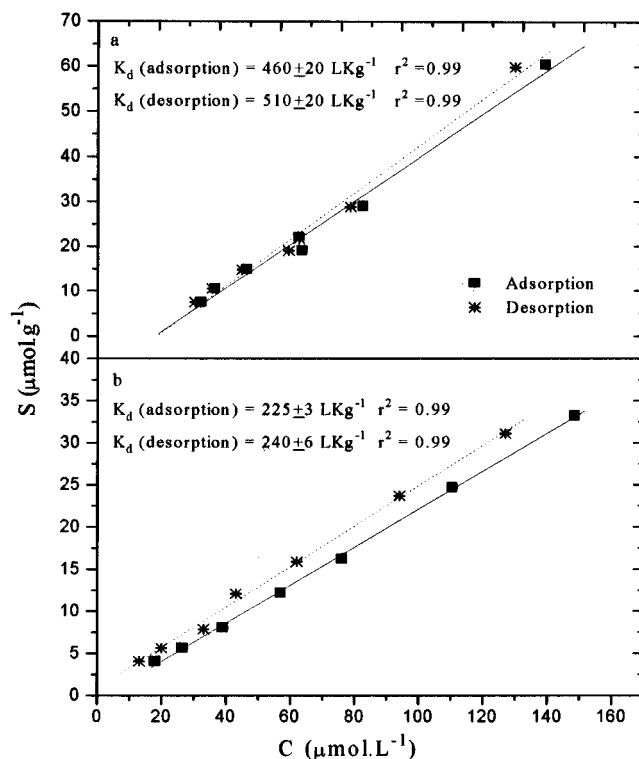

Figure 2. Adsorption−desorption isotherms of metolachlor by (a) lignin (alkali) and (b) collagen.
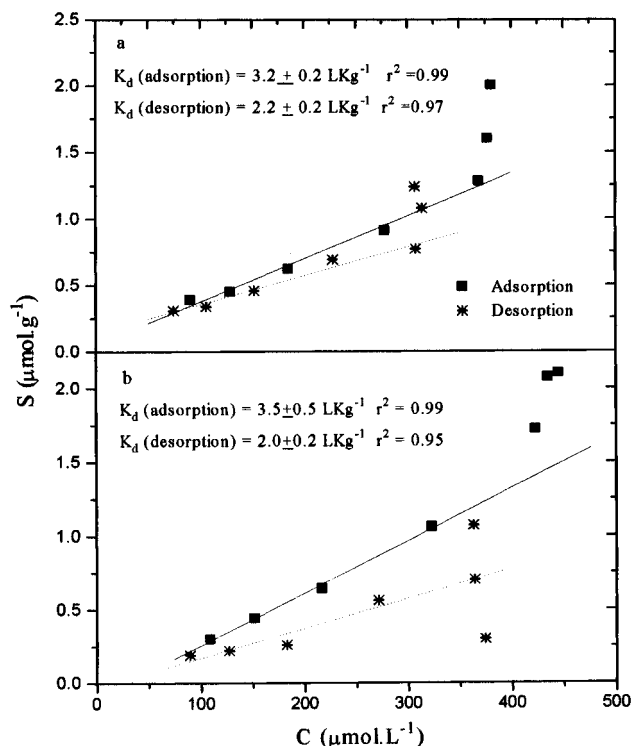

Figure 3. Adsorption−desorption isotherms of metolachlor by (a) chitin and (b) cellulose.

herbicide and the H from carboxyl and hydroxyl groups that are present in the organic matter surfaces. The linear isotherms obtained for lignin and collagen suggest partitioning as a major sorption mechanism. Furthermore, an experiment was conducted in the presence of multiple solutes with isotherms exactly the same in the single versus the multiple solute system, suggesting that the sorption was not site-limited (Jayansudera, 1995).

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The uptake capacity of chitin and cellulose was less than that of lignin and collagen. The deviation from linearity, observed at higher concentrations, may imply the bonding of metolachlor molecules to already sorbed molecules. The absence of aromatic moieties in both chitin and cellulose and the polar nature of the surfaces may lead to other specific interactions with metolachlor, such as H-bonding, as the dominating mechanism of sorption to these sorbents. The higher uptake by collagen, as compared to chitin and cellulose, can also be attributed to its expansion properties allowing for an internal sorption as that observed for polymer-like materials (Sposito, 1989).

The desorption isotherms from all organic sorbents studied showed hysteresis. For lignin and collagen $K_{d(desorption)}$ increased to 510 and 240 from $K_{d(adsorption)}$ of 460 and 225 L kg^{-1}, respectively. However, the $K_{d(desorption)}$ decreased to 2.2 and 2.0 from $K_{d(adsorption)}$ 3.2 and 3.5 L kg^{-1} for chitin and cellulose, respectively. The increase in $K_{d(desorption)}$ for lignin and collagen can be due to the slow diffusion from internal sorption. In a separate study, after a 48 h equilibration period, 13.2% of the adsorbed fraction to lignin was desorbed and only a 11% was desorbed when the sorption equilibration period was increased to 240 h. It is expected that for longer equilibration times, "aging" will lead to a decrease in the labile fraction, and thus, the extent of desorption.

The dissolved organic carbon content (DOC) measured in 25 g L^{-1} solutions of lignin, collagen, chitin, and cellulose were >1000, >700, 45, and 120 ppm, respectively. Dialysis bag experiments indicated that the amount of DOC present could not explain the decrease in $K_{d(desorption)}$ observed in the case of chitin and cellulose and the increase in $K_{d(desorption)}$ for lignin and collagen. Therefore, the hysteresis effects could not be directly related to the cosolvent effects due to the presence of DOC. However, metolachlor−DOC interactions in the chitin and cellulose systems might be more favorable than in the lignin and collagen systems where a true partitioning may take place. It can also be hypothesized that metolachlor molecules were adsorbed to the surface bound organic matter of chitin and cellulose and that DOC−metolachlor was released into solution during desorption causing the decrease in $K_{d(desorption)}$.

Differential Scanning Calorimetry. The DSC graphs for metolachlor desorption from lignin (A), chitin, and cellulose are presented in Figure 4. The DSC graph for collagen was not considered due to interference in the graph between collagen and metholachlor. The organic surfaces for the DSC study were loaded with metolachlor at a higher concentration than those for the isotherms. This was necessary to obtain a good DSC signal. The endothermic enthalpy peaks for metolachlor on the different organic sorbents were obtained at temperatures higher than that of metolachlor by itself and indicate binding of metholachlor onto the organic sorbent. The enthalpy of desorption is the result of different interactions between metolachlor molecules and the various organic sorbents and will result in different energies. A narrow peak and low energy obtained when metolachlor desorbed from lignin indicates that a physisorption mechanism was involved. For chitin a wider peak and low desorption energy was found which can be indicative of the contribution of several interactions with different adsorption energies. For cellulose, the peak is larger than that for lignin (A) and also has a higher desorption energy. This too
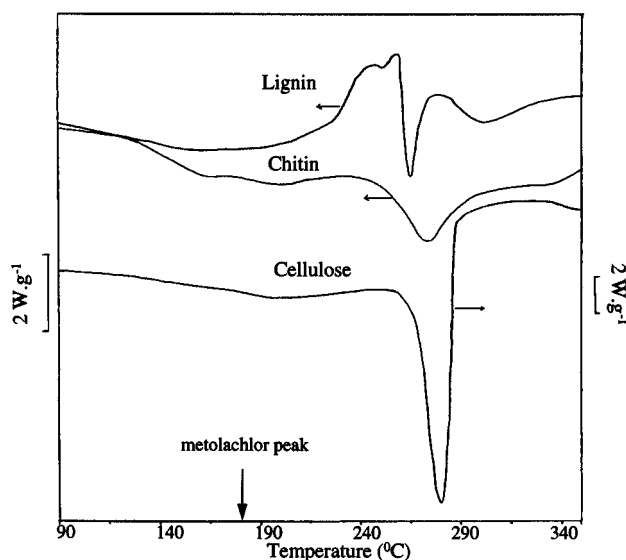

Figure 4. DSC graphs of metolachlor adsorbed onto different organic sorbents. Cellulose is plotted versus axis on the right in a different scale.
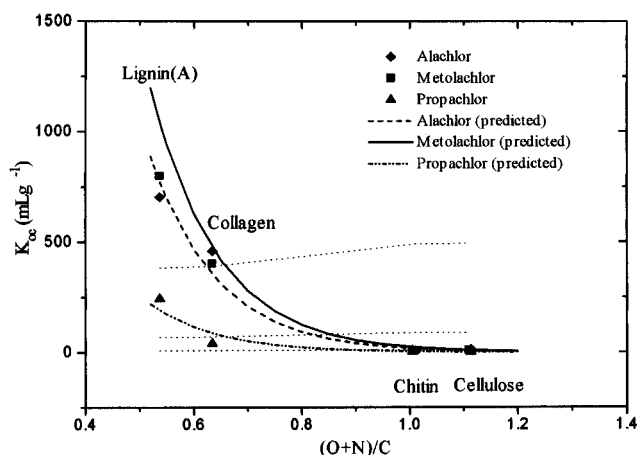

Figure 5. K_{oc}−polarity curves for alachlor, metolachlor, and propachlor using experimental and predicted data from log K_{oc} = 3.53 + 0.553 log K_{ow} − 0.091 log C_w − 3.51PI. The dotted lines represent predicted values using eq 5.

Table 3. Calculated Polarity Indexes (PI) for the Organic Sorbents and Partitioning Coefficients for the Pesticides Used

		alachlor		metolachlor		propachlor	
sorbent	PI $(O + N)/C$	K_d (mL g^{-1})	K_{oc}	K_d (mL g^{-1})	K_{oc}	K_d (mL g^{-1})	K_{oc}
lignin (A)	0.537	402	704	460	800	140	245
collagen	0.634	257	459	225	402	22.9	40.9
chitin	1.01	5.40	12.1	3.20	7.20	1.45	3.25
cellulose	1.11	6.45	14.5	3.50	7.90	0.57	1.28

indicates several interactions and stronger binding than that of chitin.

Pesticide Uptake as a Function of the Quality of the Organic Matter. The sorption behavior of acetamide pesticides was dependent on the "quality" of the organic matter. The partition coefficients, K_d and K_{oc}, were determined from Figures 2 and 3 for metolachlor and from similar equilibration experiments for alachlor and propachlor. The experimentally determined K_{oc} values were plotted against the polarity index (PI), $[(O + N)/C]$, of the organic sorbents (Figure 5). A decrease in K_{oc} with the increase in PI of the organic sorbent was observed in all three pesticides. Linear relations that relate the K_{ow} of a pesticide to the partitioning to soil organic matter are generally used

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to predict K_{oc} values (Karichhoff, 1979; Kenaga and Goring, 1980; Means *et al.*, 1980; Briggs, 1981; Chiou *et al.*, 1983). The following linear relation for the partitioning of nonionic organic compounds to soil organic matter (Chiou, 1989) was used to predict the K_{om} from K_{ow},

$$\log K_{om} = 0.904 \log K_{ow} - 0.779$$
$$(n = 12, \ r^2 = 0.989) \quad (4)$$

and then K_{oc} determined as follows (Hamaker and Thompson, 1972),

$$K_{om} = f_{oc}K_{oc} \quad (5)$$

In our experiments the sorbent is a pure organic phase ($f_{om} = 1$) and f_{oc} is the fraction of organic carbon in the sorbent. In predicting the K_{oc} values from eq 5, the soil organic carbon content is often assumed to be 57% C. The predicted K_{oc} values for alachlor, metolachlor, and propachlor are 68.7, 376, and 8.33, respectively, and are independent of sorbent properties. The K_{oc} values were also determined using the sorbent specific organic carbon contents, and these values are also plotted against PI in Figure 5. This data shows that the K_{oc} value of an organic compound is not only a function of the organic carbon content of the soil, but also a function of the its polarity index. The sorption capacity of all three pesticides to organic sorbents with a high PI was low. If the organic matter primarily consists of cellulose-like material, with a high polarity, the predicted K_{oc} will be greatly overestimated for metolachlor and alachlor but comparable for propachlor. If lignin-like material was present, the predicted K_{oc} values for all three pesticides will be underestimated.

Similarly, K_{oc} values were also predicted using other linear relations that are commonly used to model the fate of organic pollutants (results not shown) and compared with the experimentally determined values. Since none of these models account for the quality of the organic matter, depending on the system from which the model was derived, either overestimated or under-estimated K_{oc} values were obtained.

The correlation proposed by Xing *et al.* (1994a) of log K_{oc} vs log K_{ow} and PI using the sorption behavior of the BTX compounds on model organic sorbents was modified to model the sorption of acetamide herbicides onto organic sorbents. The adsorption of metolachlor and alachlor to the organic sorbents were almost the same although the K_{ow} of metolachlor was higher than that of alachlor. Our results indicate that not only the hydrophobicity but also solubility parameters are important when determining the sorption behavior of organic solutes, such as pesticides that possess functional groups, to organic phases.

The following equation was fitted to the experimentally determined log K_{oc} values and PI and log K_{ow} and log C_w from Table 1,

$$\log K_{oc} = 3.53 + 0.553 \log K_{ow} - 0.091 \log C_w - 3.51 \text{PI} \quad (6)$$

The predicted models using eq 6 are shown in Figure 5. This correlation can be used to predict the K_{oc} values of other acetamide pesticides to a reasonable extent. Due to the complex structures of pesticides and the wide variations in their properties, the application of this correlation to other pesticide groups cannot be justified. Also, these relations have been developed from experi-

ments by sorption onto pure organic compounds in the absence of a mineral matrix. Therefore, their application to whole soils, especially with low organic matter, must be approached with caution.

CONCLUSIONS

The sorption/desorption behavior and the uptake capacity of nonionic pesticides that posses polar functional groups by organic phases are a function of the properties of the sorbent as well as the sorbate. The K_{oc} of alachlor, metolachlor, and propachlor were a function of the degree of polarity of the organic sorbents. The uptake of the pesticides decreased with increasing sorbent polarity. It is hypothesized that while "partitioning" to the organic matter may be the dominant sorption mechanism for the less polar sorbents, more specific interactions such as hydrogen bonding may be involved apart from partitioning to sorbents with high PI.

The use of published linear relations of $K_{oc} - K_{ow}$, that recognize only the "quantity" of organic matter, to predict the sorption of pesticides can result in overestimated or underestimated partition coefficients. The significant difference in K_{oc} values obtained for soils of different origin can be attributed to the variations of the nature of the organic matter such as polarity and degree of aromaticity. Thus, to accurately predict sorption coefficients for WPOCs, further research needs to focus on the elucidation of mechanisms as a function of pollutants and sorbents properties.

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