*Review*

# Potential causes of organic carbon normalized partition coefficient (K$_{OC}$) variability for organic compounds: A review

### Ahmad Gholamalizadeh Ahangar

Department of Soil Science, College of Agriculture, University of Zabol, Zabol, Iran. E-mail: a_ahangar2002@yahoo.com or ahmadgholamalizadehahangar@gmail.com Tel: +98 542 2235115. Fax: +98 542 2235115.

**Even though the most widely-used sorption model is the organic carbon normalized partition coefficient (K$_{OC}$) partitioning model and this model provides a good approximation of sorption properties in many cases, it is unreasonable to expect such a simple model to accurately describe a process as complex as sorption of organic pollutants to soil. The one main shortcomings of the K$_{OC}$ model is; it assumes all organic matter is equally sorptive. Although some studies have reported correlations between K$_{OC}$ and particular C types, especially aromatic C and alkyl C. Here, alternative causes of K$_{OC}$ variability are reviewed. Sorption by soil minerals and blocking of sorption sites by minerals or by the lipid fraction of organic matter also altering the physical conformation of the soil organic matter are other possible of K$_{OC}$ variability which is making it more sorptive.**

**Key words:** Sorption, nuclear magnetic resonance spectroscopy (NMR spectroscopy), clay minerals, soil lipids, conditioning effect, organic carbon normalized partition coefficient (K$_{OC}$)

## INTRODUCTION

The toxicity, degradability and mobility of organic pollutants in soils are largely controlled by their sorption to soil particles. For non-ionic species, the sorption process is most commonly described as a linear (that is, concentration-independent) partitioning between the solution and soil organic matter (Chiou, 1989). In this most simple of models, just one parameter, organic carbon normalized partition coefficient (K$_{OC}$), the C-normalized partition coefficient, quantifies the sorption interaction (Chiou, 1989). In the simplest case, K$_{OC}$ is seen as a property of the sorbate molecule alone, and is independent of soil properties other than C content (Chiou, 1989; Wauchope et al., 2002). In this sense K$_{OC}$ is analogous to K$_{OW}$, the octanol-water partitioning coefficient, and indeed good correlations between K$_{OC}$ and K$_{OW}$ have been reported (Chiou et al., 1979, 1983). However, numerous studies have identified situations where the simple organic matter partitioning model does not provide an adequate description of the sorption interaction in soils (Wauchope et al., 2002). These include situations where the criteria for a partitioning

interaction are not fulfilled (e.g. sorption is not inde-pendent of concentration, sorption is not fully reversible, sorption kinetics are very slow, or there are significant competition effects between sorbate molecules) and situations where either organic matter is not the sole sorbent (that is, soil minerals contribute significantly to sorption) or different sources of organic matter have different sorption affinities (Wauchope et al., 2002). In such cases K$_{OC}$ is no longer a "universal" constant, but rather a measure of the affinity of the organic matter in that particular soil for the organic species in question. A number of more sophisticated models have been developed in an attempt to better describe and predict sorption behaviour (Allen-King et al., 2002). Most models include multiple organic matter components with different sorption properties. In such models, variability in K$_{OC}$ between soils is explained by differences in the relative proportions of different organic matter components. The models mostly differ in the proposed composition of the highly sorptive and usually non-partitioning component, which has variously been attributed to black carbon

(Chiou, 1995; Koelmans et al., 2006), "carbonaceous geosorbents", including coal and kerogen as well as black carbon (Cornelissen et al., 2005), aliphatic domains (Mao et al., 2002; Salloum et al., 2002) and "condensed" (Weber and Huang, 1996) or "glassy" (Xing and Pignatello, 1997) domains.

In a review of published $K_{OC}$ measurements, Wauchope et al. (2002) found that where

$K_{OC}$ had been determined for a large number of soils, the coefficient of variation in $K_{OC}$ was generally around 30 to 60% and that the ratio of maximum to minimum $K_{OC}$ values amongst the soils was generally around 3 to 10. They suggest that around half of this variability in $K_{OC}$ can be ascribed to experimental error, whereas the rest reflects differences in the nature of organic matter between soils.

The aim of this review is to draw much attention to some other causes of $K_{OC}$ variability which in spite of their importance less much attention has been paid to them. Besides chemistry of soil organic matter and the masking role of soil minerals, some other possibility can be considered as causes of $K_{OC}$ variability. Blocking of sorption sites by the lipid fraction of organic matter is also altering the physical conformation of the soil organic matter, making it more sorptive.

## SOM HETEROGENEITY

It is well documented that $K_{OC}$ varies widely for organic matter types as different and distinct as plant biopolymers (cellulose, lignin, cuticle), peat, coal and shale (Chefetz et al., 2000; Chen et al., 1996; Salloum et al., 2002). It has also been shown that different humic fractions from the same soil can have different $K_{OC}$ values (Chefetz et al., 2000; Chen et al., 1996; Gunasekara and Xing, 2003; Kang and Xing, 2005; Mao et al., 2002; Salloum et al., 2001) and that modification of organic matter can affect $K_{OC}$ of humic substances (Gunasekara et al., 2003; Simpson et al., 2003). However, it is less certain the extent to which differences in the nature of organic matter are responsible for variations in $K_{OC}$ between soils. The most simple and obvious way to prove a link between organic matter chemistry and $K_{OC}$ would be show to a correlation between $K_{OC}$ and a parameter that measures some aspect of organic matter chemistry. Such correlations have been shown for model systems (Chefetz et al., 2000; Salloum et al., 2002) and humic extracts (Mao et al., 2002), but their relevance to whole soils is questionable.

The role of the variability of organic matter chemistry on sorption properties has been widely investigated. Research has focused on both variability of organic matter composition between soils and heterogeneity of organic matter within soils. Grathwohl (1990) carried out the first comprehensive study of the influence of organic matter chemistry on the sorption of non-ionic compounds,

although some previous studies had already identified that $K_{OC}$ varied for different organic matter sources (Garbarini and Lion 1986; Gauthier et al., 1987). Grathwohl (1990) showed that Koc for organic matter in unweathered high-grade coals and shales was more than an order of magnitude higher than for soils or low-grade coals. He also found that weathering of geological organic matter (coal and kerogen) decreased its sorptivity. Both effects resulted in a positive correlation between Koc and the atomic H/O ratio.

Many studies have tried to find a correlation between soil/sediment organic matter (SOM) structural properties and the sorption of soil organic matter. Gauthier et al. (1987) examined the structure and composition of four humic substances using 13C CPMAS NMR, and found that the degree of aromacity played a key role in the sorption affinity of humic and fulvic acids. A number of other studies have also found strong correlations between aromacity and binding coefficients for a variety of sorbents and sorbates (Abelmann et al., 2005; Chin et al., 1997; Perminova et al., 1999).

A number of studies have found aliphatic C to be the dominant sorbing phase (Chefetz et al., 2000; Chen et al., 2007; Salloum et al., 2002), whereas other studies suggest that aromatic C plays the dominant role (Abelman et al., 2005; Ahmad et al., 2001; Golding et al., 2005; Xing, 1997).

Kile et al. (1999) reported that $K_{OC}$ for carbon tetrachloride for 19 soils and 9 sediments was negatively correlated with the proportion of "polar organic carbon" (O-alkyl C + carbonyl C). On the other hand, Ahmad et al. (2001) found a strong correlation of $K_{OC}$ for two pesticides (carbaryl and phosalone) with aromatic C across 27 soils from Australia and Pakistan. Xing (1997) also reported a correlation between $K_{OC}$ and aromaticity for a small set of four soils. It should be noted that Kile et al. (1999) found no correlation between $K_{OC}$ and aromatic C for their data set.

We have restricted our attention to soils collected from a single ~2 ha site, the soils of which are formed from a mineralogically and texturally uniform parent material (Ahangar et al., 2008a). Previous studies have found $K_{OC}$ to vary less at these scales than at larger scales (Coquet and Barriuso, 2002; Novak et al., 1997).

We show that $K_{OC}$ was positively correlated with aryl C (r2 = 0.59, significance level 0.001) and negatively correlated with O-alkyl C (r2 = 0.84, significance level <0.001) for diuron. This is only the second report of correlations between whole soil $K_{OC}$ and NMR-derived measures of organic matter chemistry. We suggest that this success may be a consequence of limiting this study to a very small area (Ahangar et al., 2008a). There is growing evidence that interactions between organic matter and clay minerals strongly affect $K_{OC}$. However, because the soil mineralogy varies little across the field, the influence of these interactions is greatly diminished, allowing the effect of organic matter chemistry on $K_{OC}$ to

be seen clearly.

These findings confirm that the chemistry as well as the amount of organic matter influences the sorption affinity of these soils. Aromatic C is identified as having the highest affinity for diuron, a finding consistent with previous similar studies on soils (Ahmad et al., 2001; Xing, 1997), and humic substances (Chen et al., 1996; Chin et al., 1997; Perminova et al., 2001; Xing and Chen, 1999). Conversely, the negative correlation between O-alkyl C and $K_{OC}$ identifies this C type as having the lowest affinity for diuron, a finding consistent with the results of Kile et al. (1999).

## SOM, MINERAL INTERACTION

The presence of soil minerals can influence sorption properties of a soil, both directly and indirectly. It has been reported that smectites can sorb comparable amounts of phenanthrene as soil clays containing a significant amount organic matter (Hundal et al., 2001). Sorption to clay minerals has been also reported for pesticides (Teppen et al., 2006). On the other hand, soil minerals may indirectly reduce $K_{OC}$ by blocking organic matter sorption sites or by causing conformational changes in its structure (Bonin and Simpson, 2007; Celis et al., 2006; Jones and Tiller, 1999; Njoroge et al., 1998; Pusino et al., 1992; Salloum et al., 2001).

Njoroge et al. (1998) found that that Kd for 1, 2, 4-trichorobenze and tetrachloroethene decreased by about 100-fold down a soil profile. This decrease was much greater than could be explained on the basis of SOM content of the lower horizons. They attributed the decrease in Koc with soil depth to the association of the SOM with the clay mineral of the soils and the possible effect of this intimate association on SOM accessibility, sorptivity or both.

Salloum et al. (2001) found that Koc values for isolated humic acid and humin from soils in most instances are higher than those for the source soil samples, and suggested the cause may be SOM-mineral interactions that decrease sorption affinity of the whole soils. Bonin and Simpson (2007) reported that de-ashing a soil humin fraction increased its Koc, indicating that soil clay minerals can influence the availability of sorption domains on SOM.

We investigated the effect of organic matter-mineral interactions on sorption by comparing sorption properties of soils before and after HF-treatment (Ahangar et al., 2008b). HF-treatment improves spectral quality by concentrating the organic matter, and also removing paramagnetic species that broaden NMR signals and decrease observability (Skjemstad et al., 1994; Schmidt et al., 1997; Smernik et al., 2000; Mathers et al., 2002)

The increases in $K_{OC}$ observed here on HF-treatment (average factor of 2.5 for diuron and 2.3 for phenanthrene) were very similar to the average increase

Smernik et al. observed for a larger and more diverse set of soils from Sri Lanka (Smernik et al., submitted). We attribute this increase mainly to the removal of organic matter-mineral interactions for the HF-treated soils.

A clear influence of organic matter chemistry on $K_{OC}$ was observed for diuron for both whole soils and HF-treated soils and for phenanthrene for the HF-treated soils. The positive correlations with aryl-C and negative correlations with O-alkyl C observed in all cases are again consistent with a number of literature reports (Ahmad et al., 2001; Kile et al., 1999; Xing, 1997). On the other hand, there was no clear influence of organic matter chemistry on $K_{OC}$ for phenanthrene for the whole soils. This is also consistent with the results for diuron $K_{OC}$ for the whole soils from Sri Lanka (Smernik et al., submitted).

We propose that the fickleness of the relationship between organic matter chemistry and $K_{OC}$ for whole soils may be a consequence of variability of the effect of organic matter-mineral interactions on $K_{OC}$. This would explain why the relationship between organic matter chemistry and $K_{OC}$ is more consistent for HF-treated soils than for whole soils. Further support for this hypothesis lies in the positive correlation between the increase in $K_{OC}$ on HF-treatment and the soil clay content.

## THE EFFECT OF SOIL LIPIDS

An alternative cause of $K_{OC}$ variability may be that not all organic matter is accessible to sorbate molecules. We recently showed that HF-treatment can increase soil $K_{OC}$ for diuron and phenanthrene by a factor of 2 to 3, and attributed this to organic matter-mineral interactions that block organic matter sorption sites in the whole soils (Ahangar et al., 2008b). A number of other studies are consistent with this interpretation (Celis et al., 2006; Bonin and Simpson, 2007).

It is not only interactions with minerals that may block sorption sites on organic matter. Kohl and Rice (1999) reported that removal of soil lipids increased the sorption affinity of three soils for aromatic sorbates. Lipid extraction was also found to increase sorption non-linearity. A number of similar findings have been reported recently. Chilom et al. (2005) found that lipid extraction increased the sorption affinity of polycyclic aromatic hydrocarbons (PAHs) for soils and sediments. Tremblay et al. (2005) reported lipid extraction increased $K_{OC}$ for phenanthrene by up to an order of magnitude for a sediment and its humin fraction, and also increased $K_{OC}$ for its humic acid fraction. Drori et al. (2006) found increases in KOC for three compounds on lipid extraction of soils. Finally, Wang and Xing (2007) reported increases in $K_{OC}$ for phenanthrene and 1-naphthol for a peat and its humic acid and humin fractions following lipid extraction.

We determined $K_{OC}$ for diuron and phenanthrene

before and after lipid extraction (Ahangar et al., 2009a). In every case, $K_{OC}$ was greater following lipid extraction, with the increase ranging from 10 to 54%. The average increase in $K_{OC}$ across the twelve soils was very similar for diuron (31%) and phenanthrene (29%). These findings are consistent with previous reports of $K_{OC}$ increasing following the removal of lipid from soils and soil fractions (Kohl and Rice, 1999; Chilom et al., 2005; Tremblay et al., 2005; Drori et al., 2006; Wang and Xing, 2007).

An alternative explanation for the increase in $K_{OC}$ on lipid extraction is that the structure of the organic matter is affected by exposure to the organic solvent. Lu and Pignatello (2002) reported that pre-treatment of soil with aqueous solutions of dichloromethane and benzene increased $K_{OC}$. They proposed a "conditioning effect", which increases the size of high sorption affinity nanopores within glassy domains of organic matter, to account for this increase. Wang and Xing (2007) proposed that the same conditioning effect is responsible for increases in sorption on pre-treatment with acetone. However, as Tremblay et al. (2005) point out, thes e treatments are also likely to at least partially solubilize lipids. They showed that re-addition of lipids reduced the sorption affinity of previously lipid-extracted materials, a finding that is not consistent with the conditioning effect hypothesis. We therefore suggest that the increases in sorption affinity on solvent extraction that we observed are most likely due to the removal of lipids that block organic matter sorption sites in soils (Ahangar et al., 2009a).

## SOM PHYSICAL CONFORMATION

The term "conditioning effect" was introduced to soil sorption studies by Xia and Pignatello (2001), and has its origins in the sorption of gases to synthetic polymers, where it is a well-established phenomenon. Exposure of "glassy" polymers to high pressures of gases such as $CO_2$ result in changes to their physical conformation, including swelling, that remain after the gas is removed (Kamiya et al., 1998; Wang et al., 1998). As a result of these changes, the polymer is more sortive of the gas in subsequent exposures. Xia and Pignatello (2001) reported a similar effect for sorption of trichloromethane to a peat soil: following exposure to high concentrations of trichloromethane, the soil was more sorptive in subsequent exposures. They interpreted this as evidence that some SOM components are "glassy".

Further investigations of the conditioning effect were carried out by Lu and Pignatello (2002) and Weber et al. (2002), who reported increased sorption affinity of a peat soil toward trichloromethane following conditioning with dichloromethane, and increased sorption affinity of a mineral soil toward chlorobenzenes following conditioning with benzene. In all cases, $K_{OC}$ increased by around 40%

(Lu and Pignatello, 2002). More recently, Sander et al. (2006) carried out detailed studies on the conditioning effect of trichloroethylene on two polymers, a peat and a humic acid. They confirmed that the conditioning effect occurred for a glassy polymer, but not a rubbery polymer. They found solvent conditioning increased sorption of the peat and the humic acid by a factor of up to two. Finally, Wang and Xing (2007) investigated the effect of acetone conditioning on the sorption properties of a peat and its humic fractions. They found that acetone-conditioning increased $K_{OC}$ for phenanthrene, but not for 1-naphthol.

We investigate the effect of conditioning of a whole soil and a lipid-extracted soil with a range of solvents of different polarities on the subsequent sorption of diuron and phenanthrene (Ahangar et al., 2009b). In particular, we aim to determine whether the increased sorption of the lipid-extracted soil over the whole soil may be due to an inadvertent conditioning effect occurring during lipid extraction. In our experiments, separate aliquots of the whole soil and the lipid-extracted soil were conditioned by shaking for five days with six separate solvents (water, acetonitrile, acetone, methanol, chloroform and dichloromethane) at a soil : solvent ratio of 1:20.

Organic carbon-normalized partitioning coefficients ($K_{OC}$) for two non-ionic compounds were consistently higher for the solvent-conditioned soils than for the untreated soils. The increase in $K_{OC}$ on solvent-conditioning was closely related to solvent polarity. The greatest increases in $K_{OC}$ (29 to 75%, average 49%) were for the least polar solvents. This was true for both whole soils and for lipid-extracted soils and for both compounds.

Importantly, increases in $K_{OC}$ on solvent-conditioning were similar for whole soils and lipid-extracted soils (average 32 and 30% increases, respectively, for the five solvents other than water). A key objective of this study was to determine whether the increase in $K_{OC}$ on lipid extraction using ASE may be due to a solvent-conditioning effect, rather than lipid removal, as we had previously proposed (Ahangar et al., 2009a). The results here support our original assertion, since solvent-conditioning effects were observed for the lipid-extracted soils, and were of the same magnitude as for the whole soils. If lipid extraction (ASE) had caused a solvent-conditioning effect, then there should have been no further increases in $K_{OC}$ on solvent-treatment. The question then arises as to why lipid extraction did not cause a solvent-conditioning effect, despite the fact that it involved treatment with 95% dichloromethane, a solvent shown here to cause a strong conditioning effect. We believe the most likely explanation is that ASE involved only a short exposure to dichloromethane; the ASE procedure was carried out for only 20 min, after which the bulk of the solvent was decanted off, and the remaining solvent removed by evaporation. Although the total exposure time to dichloromethane during ASE was therefore greater than 20 min, for most of the time the solvent would have been present at low concentrations.

By contrast, the solvent-conditioning procedure involved shaking the soil in the solvent for five days.

Therefore, the increase in $K_{OC}$ was similar for lipid-extracted soils as for whole soils, and showed the same relationship with solvent polarity. This shows that the removal of soil lipids using accelerated solvent extraction (ASE) did not have a conditioning effect on the organic matrix and supports our previous assertion that ASE increases $K_{OC}$ through the removal of lipids that block sorption sites and thereby reduce the sorption affinity of the whole soils.

## CONCLUSION

This review shows that most previous studies in this area have focussed solely on the effect of SOM chemistry on the sorption of non-ionic compounds. Much less attention has been paid to the interactions between SOM and the mineral phase and lipid components, or to SOM physical conformation. The role of SOM chemistry on sorption of non-ionic compounds has been over-emphasized. Other factors, identified previously, can alter the sorption properties of SOM to a degree that the effect of SOM chemistry is masked.

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