CORRELATION STUDIES FOR SOIL SORPTION OF PCB CONGENERS

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Introduction

Polychlorinated biphenyls (PCBs) are some of the most prevalent environmental pollutants. The soil water distribution coefficient (K_d) is an important parameter which determine the mobility of PCBs in the environment. For prediction purposes the sorption of a variety of pollutants to soil and sediments has been normalized to the content of soil organic carbon (f_{OC}): $K_{OC} = K_d / f_{OC}$. The octanol water partition coefficient (K_{OW}) has been used in predicting K_{OC} for non-polar compounds (Briggs, 1981): $\log K_{OC} = a + b \log K_{OW}$ (I). Only limited data is available on K_{OW} of PCB congeners. However, K_{OW} may be derived from thermodynamic data (Miller et al.,1984): $\log K_{OW} = a + b T_b$ (II), where the boiling point (T_b) of PCB congeners again may be derived from gas chromatography (GC) data (Purnell, 1962):
$T_b = a + b \log \alpha$ (III), with the relative retention volume (α) obtained isothermally on a non-polar GC-column. By combining I, II and III it appears that the soil sorption of PCB congeners can be predicted from their GC retention: $\log K_{OC} = a + b \log \alpha$.

In the present paper experimental data for the soil sorption of 50 PCB congeners is presented. Predictions from GC retention are compared with predictions from molecular structure and octanol water partition.

Materials and methods.

The soil sorption of PCBs from an aquoeus solution of Aroclor 1232 (200 µg/L) was measured in triplicate using 20 g soil and 800 mL water. After 24 hrs equilibration at 23 °C the centrifuged water phase was solid phase extracted on C-18/silica and analysed by capillary column GC-ECD. Three horizons of a Dystric Gleysol were used with f_{OC} in the range of 0.03%-1.87% .

Data for K_{OC} of PCB congeners occuring in higher chlorinated Aroclor mixtures was recalculated from previosly published results (Paya-Perez et al., 1990; Cortes et al., 1990).

The relative GC retention volume (α) was determined

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isothermally at 4-6 different temperatures for 50 resolved PCB congeners on a 60 m x 0.25 mm (0.25 µm) SE-54 column by injection of Aroclor mixtures and pure congeners. By interpolation from linear plots of log α vs. 1/T for each congener α was determined at 200 °C.

Data for K_{OW} of PCB congeners was taken from the literature (Rapaport and Eisenreich, 1984).

Results and discussion.

The experimental data was found to be in agreement with published results obtained under different experimental conditions. Significant (p < 0.001) correlations of K_{OC} were obtained with α and with K_{OW} (Figure 1 and 2):

log K_{OC} = 5.03 + 0.959 log α (r^2 = 0.88, SE = 0.10, n = 50)

log K_{OC} = 3.56 + 0.310 log K_{OW} (r^2 = 0.80, SE = 0.13, n = 32)
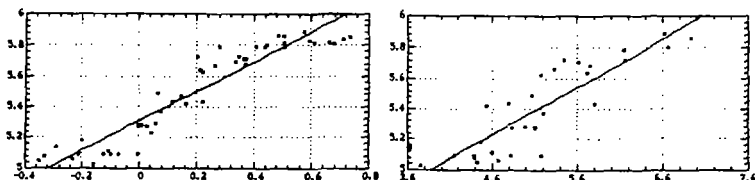

Figure 1. log K_{OC} vs. log α Figure 2. log K_{OC} vs. log K_{OW}

The values for α obtained at 200 °C showed a strong correlation with relative retention times obtained from the GC operated with a temperature programme (r^2 = 0.989). This allows for the use of published GC data (Mullin et al., 1984) for predicting soil sorption:

log K_{OC} = 4.39 + 1.563 log RRT (r^2 = 0.88, ES = 0.11).

Soil sorption could also be nicely predicted from the molecular structure of PCB congeners. Linear regressions between K_{OC} and the number of chlorine atoms in the molecule were obtained for each substitution class of PCBs (Figure 3a-d):

non-ortho: log K_{OC} = 4.85 + 0.183 N_{Cl} (r^2 = 0.94, SE = 0.10, n = 5)

mono-ortho: log K_{OC} = 4.66 + 0.222 N_{Cl} (r^2 = 0.84, SE = 0.11, n = 16)

di-ortho: log K_{OC} = 4.57 + 0.214 N_{Cl} (r^2 = 0.89, SE = 0.10, n = 18)

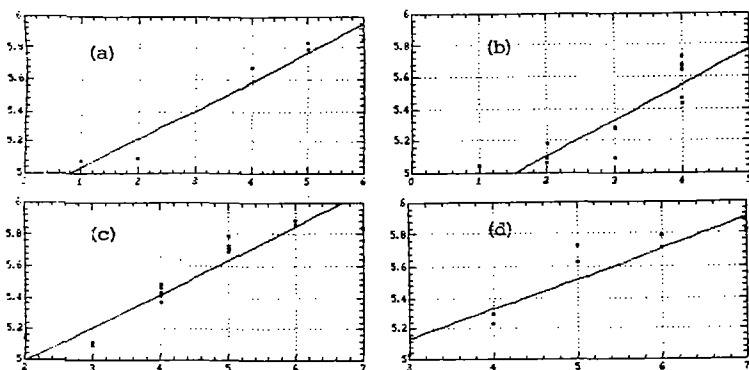*tri-ortho*: log K_{OC} = 4.56 + 0.192 N_{Cl} (r^2 = 0.86, SE = 0.11, n = 11)

Figure 3. log K_{oc} vs. N_{Cl} for non-ortho (a), mono-ortho (b),
di-ortho (c) and tri-ortho (d) substituted PCB.

Data for K_d of each soil horizon showed significantly better
correlations with α ($r^2 > 0.94$), K_{OW} ($r^2 > 0.88$) and molecular
structure ($r^2 = 0.90$-0.98). This underlines the limitations in
attributing soil sorption exclusively to soil organic carbon,
thereby disregarding possible variations in the composition of soil
organic matter and the influence of other soil parameters such as
specific surface area and clay minerals.

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