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Prediction of Bioaccumulation Potential of Some Aromatic Hydrocarbons in Indicator Species of Ecotoxicity

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The bioconcentration is considered to be the partitioning of compounds between the lipid phase of an organism and water (Veith et al.1980). Also it has been defined as the ability of some chemicals to move through the food chain resulting in higher and higher concentrations at each trophic level (Kenaga and Goring, 1980).

The use of bioconcentration factors (BCF) as an estimate of bioaccumulation potential of chemicals in aquatic and terrestrial organisms, has become increasingly important in hazard evaluation programs. The BCF provides a conservative prediction of chemical residues in small animals of the aquatic and terrestrial ecosystem (Burmaster et al. 1991), as well as a mechanism for ranking the bioaccumulation potential of organic chemicals in the environment. Consequently, the bioconcentration test is a requisite component for evaluating possible environmental hazards of new chemicals (Mace 1990). The most common method for estimating a chemical's BCF relies on established correlations between BCF and hydrophobicity of the chemical. As a consequence, bioconcentration factors have been correlated with various partition coefficients, most exactly the 1-octanol/water partition coeficient (log Kow). A positive relationship has been demonstrated between the log Kow value and the log bioaccumulation factor in roots, bacteria, daphnia, earthworms, sediments, soil, mussel and fish (Geyer et al.1984).

There are several equations relating these two parameters for a specific set of biological organisms and for a specific set of chemicals which log Kow match a value range. Depending on biological animal, the chemical to test and the log Kow value range, we will choose the most accurate equation available (Geyer et al.1991).

For compounds with log Kow < 6, linear relationships have been found:
log BCF = 0.542 log Kow + 0.124 (Neely et al, 1974).
log BCF = 0.85 log Kow - 0.70 (Veith and Macek, 1980)
log BCF = 1.00 log Kow - 1.32 (Mackay, 1982)
log BCF = 0.79 log Kow - 0.40 (Veith and Kosian, 1983).
For compounds with a range of log Kow > 6, curvilinear relationships between log BCF and log Kow have been observed (4) (l0), and sigmoidal (Spacie and Hemelink, 1982) besides the parabolics (Tulp and Hutzinger,1978), which have also been proposed. Also has been found

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Table 1. Values of tR, STD, the corresponding capacity factor and log Kow from literature.

COMPOUND	MEAN t_R	STD DEV.	CAPACITY FACTOR $k' = \frac{t_R - t_0}{t_0}$	log Kow
BENZENE	6.80	0.115	1.51	2.13
TOLUENE	9.36	0.242	2.45	2.69
CHLOROBENZ.	10.10	0.257	2.73	2.84
BROMOBENZ.	10.50	0.224	2.88	2.99
IODOBENZ.	12.84	0.386	3.74	3.15
ETHYLBENZ.	14.19	0.271	4.24	3.25

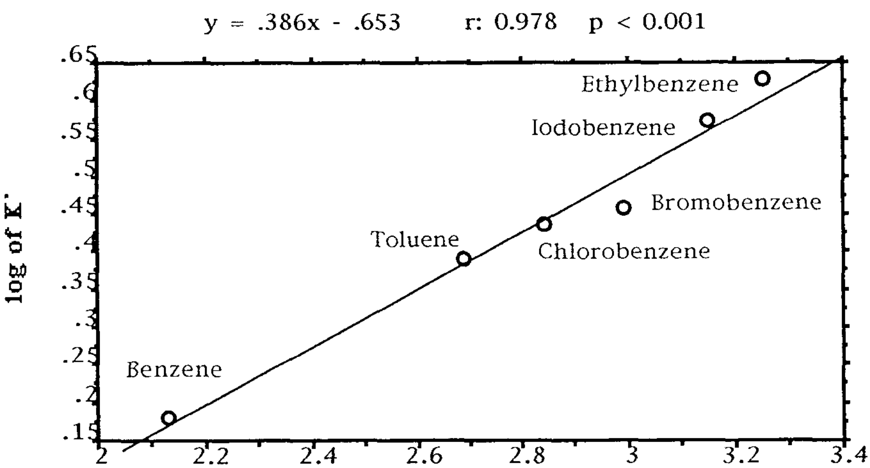

Figure 1. Plotting of the chromatographic data of capacity factors (K') against the partition coefficients (Log Kow).

relationships comparing bioconcentration factors of two biological organisms:

log fish BCF = 0.043 + 1.001(log daphnia BCF)

log daphnia BCF = 0.987 + 0.679(log fish BCF) (Kenaga and Goring, 1980).

The fundamental assumption of these relationship is that organic chemical hydrophobicity is the principal driving force of bioconcentration (Neely et al. 1974); that is, organic chemical bioconcentration is simply the thermodynamically driven partitioning between water and the lipid phase of the animal (Lu and Metcalf 1975, Veith et al.1979).

Table 2. Reported values of log Kow experimental and log BCF (2) obtained by Connell and Veith equations.

LOG BCF (l), Calculated or experimented by other authors.
LOG BCF (2), Calculated from log Kow experimental,by Eq.I and Il.

COMPOUND	LOG Kow	LOG BCF(1)	SPECIES	REFERENCE	LOG BCF(2)
THIOUREA	-1.17	1.73	ALGAE	GEYER,1984	——
BENZENE	2.11	1.60 1.10	ALGAE BLUEGILL	GEYER,1984 VEITH,1980	1.273 1.093
TOLUENE	2.69	2.57 1.16-1.30	ALGAE BLUEGILL	GEYER,1984 VEITH,1980	1.522 1.584
CHLOROBEN.	2.84	3.44 2.65	DAPHNIA FISH	NEELY,1974 CALL,1977	1.632 1.714
BROMOBENZ.	2.99	1.18-1.84	FISH	VEITH,1980	1.755 1.841
IODOBENZ.	3.15	1.90-2.31	FISH	VEITH,1980	1.900 1.977
ETHYLBENZ.	3.25	2.34	FISH	VEITH,1980	1.996 2.062

In this work, we use two valid equations for fishes relating both parameters in an equilibrium system.The BCF values obtained from equations are compared with Kow values experimentally obtained (OECD technique) for a set of Aromatic Hydrocarbons. This way we have obtained a measure of bioaccumulation potential of these chemicals in the indicator organisms of Ecotoxicity.

MATERIALS AND METHODS

The partition coefficient (log Kow) of six aromatic hydrocarbons was determined by the reverse-phase liquid chromatography (method 117 OECD). This method allows us to obtain the capacity factor value for each compound from chromatographic retention time (Mancha and Díaz,1991). These values along with the partition coefficients data compiled from the bibliography, are shown in Table 1.

The capacity factors are plotted against the log Kow gleaned from the literature. From this diagram we can obtain the Kow value for any test compound pertaining to the same group substances of reference used.

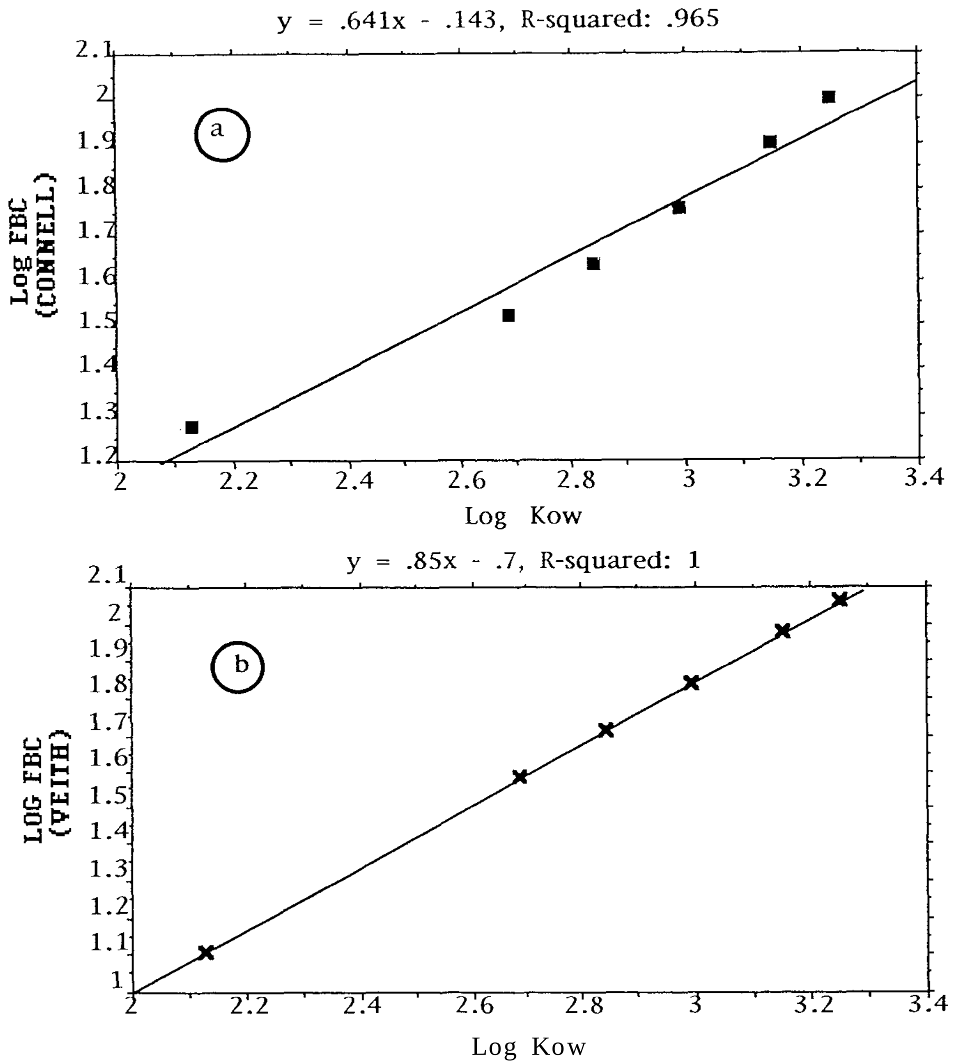

Figure 2. Plot BCF-Kow. (a): using CONNEL equation (I)
(b): using VEITH equation (II)

The regression line characterising the relationship log K' - log Kow is represented by the solid line in Fig.1, and expressed as : y = 0.386 x - 0.653. A multiple correlation coefficient of 0.978 and a covariance of 0.63 were obtained from the regression. and F test indicated a confidence level of 0.999.

Using data from log Kow of the aromatic hydrocarbons studied, we have investigated the relationship between log Kow and log BCF. This log BCF values were obtained by substitution of that log Kow value in the Hauker and Connell equation (equation I) and Veith and Macek equation (equation II). This, together with more recent additional BCF data experimented or calculated by others authors (Neely et al., Mackay, Geyer et al., Zaroogian et al.) for the compounds is presented in Table 2.

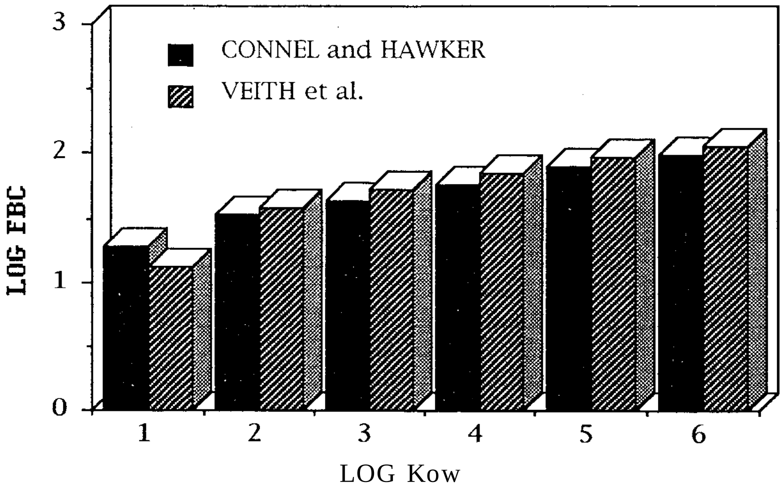

Figure 3. Bar chart showing the relationship log BCF - log Kow for each compound by Connell and Veith equations.

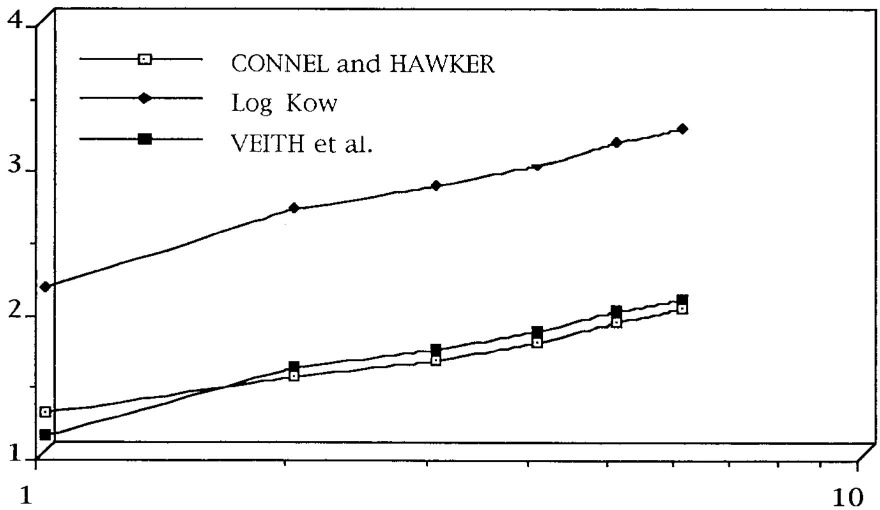

Figure 4. Diagram with the values of log BCF according to the I and II equations and the corresponding values of log Kow.

The equation I relates equilibrium log Kow to log BCF for fish, and so, eliminates any influence of varying equilibrium time requirements and ensures that calculated BCF values are equilibrium values (fourth order polynomial in log Kow):

log BCF = $6.9 \times 10^{-3} \log(Kow)^4 - 1.85 \times 10^{-1} (\log Kow)^3 + 155 (\log Kow)^2 - 4.18 \log Kow + 4.79$ (Equation I).The line described by this equation is depicted in Fig 2(a).

The regression equation II (Veith and Macek, 1980) using a static water ecosystem, is:
log BCF = 0.85 log Kow - 0.70 (Equation II).

Limitations to the use of these equations may occur with compounds that do not penetrate through tissues or bioconcentrate at the same rates in organisms as expected from the average molecule, because of unusual steric configurations, molecular weights, or solubilities (Metcalf et al., 1973)

In Fig. 2(b) the relationship for the aromatic hydrocarbons between BCF and its Kow value is depicted. As can be seen from Fig.2(b), the BCF will be ≤ 100 (log BCF <2) if log Kow is <3 for both equations.

For compounds with log Kow > 3 (BCF > l00), moderate bioaccumulative properties have been seen. In both cases, BCF can be calculated from Kow with equation I or II.

RESULTS AND DISCUSSION

Using the Connell equation we obtain a correlation coefficient of 0.965. This correlation suggests that the log BCF can be estimated to within an order of magnitude for chemicals having a range of 10,000,000 in the partition coefficients. This conclusion was also drawn by Canton and Sloof (1979), and Esser and Moser (1982).

The values of BCF obtained after substituting the corresponding value of log Kow for each compound are grouped in Table 2 under log BCF(2). We can see the differences between other researchers, who have studied the same compounds in a specific biological species. (Geyer et al., 1991).The obtained bioconcentration factors are plotted against the measured octanol/water partition coefficient (Table 2) in Fig. 3. The BCF values of the chemicals increase with increasing values for Kow, which is consistent with the results of other researchers (Neely et al.1974, Veith et al. 1980, Geyer et al.,1984).The bar chart (Fig. 3) shows the uniformity in the results obtained from each equation for each compound.

The BCF value for benzene obtained from eq. II (Veith et al. 1980) is substantially lower than that expected on the basis of its relatively low Kow and its low BCF value obtained by eq.1 (Connell and Hawker,1988). We can observe the same results in diagram Fig. 4, where one can see that the lines obtained from each equation are parallel. They are also parallel with the line which represents the values of Kow for the same compounds.

As can be seen from Fig. 2. and the statistical results, a straight line can be used to represent the relationship between the partition coefficient and the bioconcentration factor. In other words, there is an obvious relationship between lipophilicity expressed as log Kow and log bioaccumulation potential of some organic chemicals belonging to the same group.

A summary of bioconcentration test results and log Kow values from a variety of experimental conditions from other studies as well as the data from this study is presented in Table 2. All these chemicals studied had comparatively small bioconcentration factors because the metabolism for the agent may be a very active process. Consequently, the total amount of material in the ecosystem is constantly being reduced, while the ratio between the fish and the environment will remain relatively constant. The variation of calculated values from the experimental ones for these chemicals was as much as one or two orders of magnitude.

Nevertheless, it does not invalidate calculated values for both parameters (BCF and Kow) as useful tools for preliminary potential hazard assessment. In every case, the equation which best adjusts to the range of values of Kow available, which in our case is equation II, is used. From the obtained experimental value for a group of organic chemicals belonging to the same chemical family, we can obtain a reliable value of the corresponding bioconcentration, by means of an equation. This equation relates both parameters taking into account the conditions of equilibrium. For a group of chemicals which possesses a range of values of Kow 2.5-6, a lineal equation which relates Kow and BCF gives us an approximate estimation of the bioconcentration factor in a specific organism.

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