Bull. Environ. Contam. Toxicol. (1984) 33:561–567

Bulletin of Environmental Contamination and Toxicology

Partition Coefficients as a Measure of Bioconcentration Potential of Crude Oil Compounds in Fish and Shellfish

Masana Ogata, Kuniyasu Fujisawa, Yasuo Ogino, and Emiko Mano

Department of Public Health, Okayama University Medical School, 2-5-1 Shikatacho, Okayama City 700, Japan

The ability of some chemicals to move through the food chain resulting in high concentration is defined as the ratio of the concentration of chemicals in biota to that of exposure water mesured at equilibrium. The relationship between the chemicals and their abilities of bioconcentration of several chlorinated hydrocarbons in trout muscle was found (Neely et al.1974) to follow a straight line relationship with partition coefficient.

This paper deals with the correlation between the partition coefficient and the concentration factor of alkyl benzenes in crude oil for gold fish and also the correlation between the partition coefficients and concentration factor of alkyl dibenzothiophene for shellfish reared in oil suspension and that caught in the sea on the basis of previous reports (Ogata et al. 1980a, Ogata et al. 1980b).

MATERIALS AND METHODS

The partition coefficient of the chemical between n-octanol and water was either taken from the tabulation of Leo et al.(1971).

Method on contamination of aromatic hydrocarbons for goldfish: Goldfish were reared in water containing 1 mg/l concentrations of compounds, their concentration being measured by gas chromatograph,which ranged from 0.017 to 0.8 ppm.

Pretreatment for gas chromatography: Goldfish(2g) was minced weighed and packed in a Lour-Lock syringe containing 10 ml of air. Water sample of 5 ml collected from the bottom of the fish tank with a Lour-Lock syringe containing 10 ml of air through a glass tube. That was added with 2 ul of 1.3.5-trimethyl benzene as an internal standard and 15 g of ammonium sulfate. The solution was shaken, warmed to 80 C for 5 min in an electric water bath, and allowed to stand for 5 min. One milliliter of evaporated gas was introduced into an air sampler for gas chromatography (Sudo 1965,

Ogata et al. 1975). The concentration of each substance in sampler was quantified by a standard curve.
The apparatus employed was the Shimazu GC-4BM gas chromatograph with FID detector. Analysis was made under the following conditions, column liquid phases ; 5 % Benton 34 + 5 % DIDP, on celite 60-80 mesh ; size of column ; 0.3 cm x 5 m, column temperature ; 100°C(Benzoic compounds; Benzene - Sthylene) 130°C(Isopropylbenzoic compounds; Isopropylbenzene - Diisopropylbenzene), carrier gas ; N_2 60 ml/min. Concentration factor of the short necked clam reared in oil suspension and the oyster or mussel caught in the sea, measured by gas chromatography, were calculated from the data of our previous report (Ogata et al. 1980a, Ogata et al. 1980b).

RESULTS AND DISCUSSION

Partition coefficients and bioconcentration at equilibrium of compounds; The logarithms of biocon-

Table 1. Partition coefficients and bioconcentration factor for aromatic compounds in goldfish.

Aromatic compounds in exposure water	Log partition coefficient	Log Biocon. factor
Benzene	2.13	0.63
Toluene	2.69	0.92
Etylbenzene	3.15	1.19
p-Xylene	3.15	1.17
m-Xylene	3.20	1.17
o-Xylene	2.77	1.15
Stylene	2.59	1.13
Isopropyl benzene	3.66	1.55
α-Methylstyrene	3.35	1.47
p-Methylstyrene	3.35	1.50
m-Methylstyrene	3.35	1.55
β-Methylstyrene	3.35	1.53
m-Diisopropyl benzene	4.10	2.11
o-Diisopropyl benzene	4.10	2.14
Anthracene	4.45	2.21
Pyrene	4.88	2.66
o-terphenyl	5.28	2.77

Biocon.:Bioconcentration

centration factors of aromatic compounds for gold fish reared in water containing these compounds are shown in Table 1.
The uptake rates (K_1), clearance rates (K_2) and bioconcentration factor (K_1/K_2) of alkyl dibenzothiophenes for short necked clam are shown in Table 2.

Table 2. Bioconcentration factor of alkyl dibenzothiophene(alk-DBT) measured from uptake rate and clearance rate for short necked clam reared in oil suspension.

Alkyl DBT		Uptake rate k_1/day	Clearance rate k_2/day	Bioc k_1/k_2
DBT	a*	32.94	0.23	146.24
	a	51.68	0.22	238.75
Mono-alkyl	b	44.78	0.23	195.77
DBT	c	63.34	0.22	288.66
	a	51.44	0.21	242.56
Di-alkyl	b	54.38	0.25	217.49
	c	56.84	0.23	244.94
DBT	d	66.39	0.24	281.48
	e	59.67	0.23	258.51
	a	38.07	0.10	384.58
Tri-alkyl	b	45.77	0.14	322.45
	c	41.19	0.14	303.89
DBT	d	30.52	0.13	231.08
	e	45.98	0.20	227.85

*:isomers

The logarithms of the bioconcentration factor of alkyl dibenzothiophene for experimentally polluted short necked clam and naturally polluted oyster and mussel caught in the sea are also shown in Table 3.
The regression equation between partition coefficient and the bioconcentration of aromatic compounds for gold fish reared in these compounds was Log(bioconcn.factor)=0.714Log(partition coeff) -0.920 with a correlation coefficient of 0.98 as shown in Table 4 and Fig 1.
The regression equations between the partition coefficient and the bioconcentration of dibenzothiophene for short necked clam being reared in crude oil suspension

Table 3 Logarithm of partition coefficients and bioconcentration factor of alk-DBT for short necked clam reared in oil suspension and shellfish caught in the sea.

Alkyl DBT		Log parti. coeff.	Log bioconcentration for experimental and natural polluted shellfish		
			Short necked clam	Oyster	Mussel
DBT	a	4.42	2.17	3.12	3.13
	a	5.08	2.38	3.29	3.27
Mono-alkyl	b	4.73	2.29	3.31	2.87
DBT	c	4.78	2.46	3.58	3.22
	a	5.49	2.38	3.57	3.58
Di-alkyl	b	5.50	2.34	3.41	3.05
	c	5.50	2.39	3.62	3.41
DBT	d	5.52	2.45	3.78	3.12
	e	5.52	2.41	3,98	3.27
	a	5.77	2.58	3.72	3.61
Tri-alkyl	b	5.89	2.51	3,87	3.62
	c	5.86	2.48	3.67	3.32
DBT	d	5.61	2.36	4.13	3.39
	e	5.52	2.36	4.45	3.34

Parti. Coeff. : Partition Coefficient

is Log(bioconcn.factor)=0.163Log(partition coeff.) + 1.524, with correlation coefficient of 0.71. Regression equation between partition coefficient and bioconcentration for mussel is Log(bioconcn. factor)=0.494 Log(partition coeff.) + 1.026, with a correlation coefficient of 0.62 for mussel. And equation between partition coefficient and bioconcentration for oyster caught in the sea was Log(bioconcn. factor)=0.311 Log(partition coeff.) +1.631 with correlation coefficient of 0.64 for oyster. The hypothesis that population correlation coefficient (ρ) is zero is dinied within 5% level by t-test in all cases. In t-test of b=(b;regression coefficient),the correlation was significant at 5% levels in all cases of regression equations as shown in Table 3. The straight line of best fit was drawn through the points of partition coefficient and bioconcentration factor of alkyl benzene and its regression equation shown in Figure 1 for aromatic compounds.

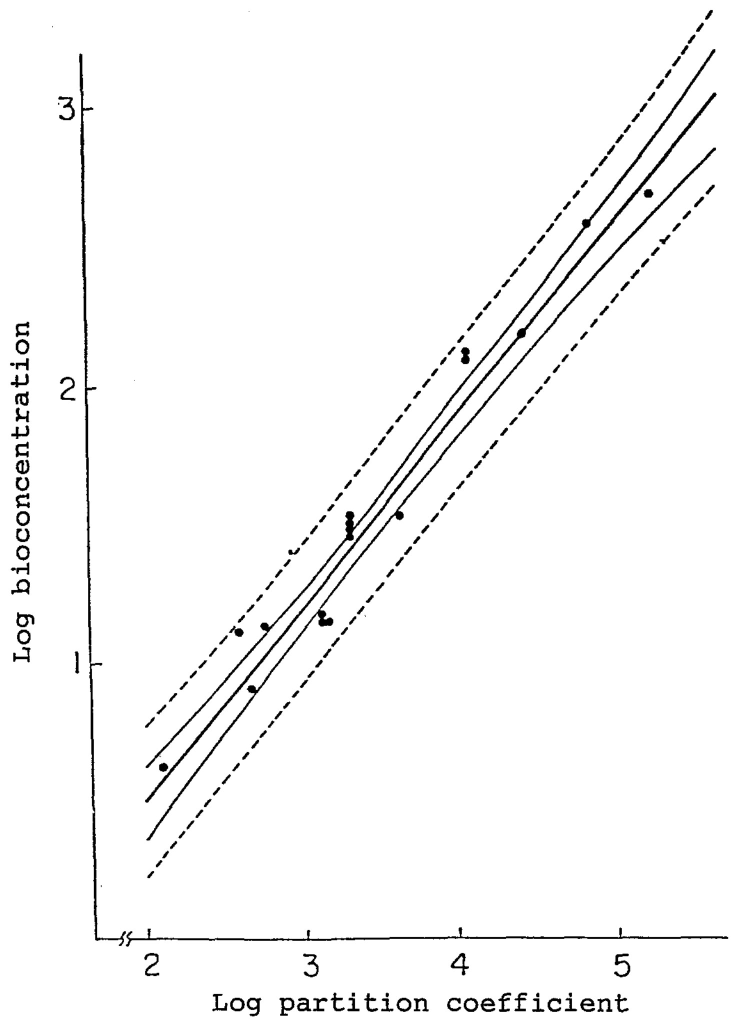

Fig 1. Linear regression between logarithms of partition coefficient and bioconcentration of alkyl benzenes in goldfish (r=0.98)

A straight line relationship was found between the partition coefficient of alkyl benzenes and their bioconcentration factor for goldfish. The results agree with the relation between the partition coefficient of chlorinated hydrocarbon and their bioconcentration factors for trout muscle as described by Neely 1974. However, there are no reports on relationship between the partition coefficient of chemicals and their bioconcentration factor for the biota caught in the sea.

Table 4. Correlation coefficients and factors of regression equation between logarithms of partition coefficients and those of bioconcentration of dibenzothiophene and alkyldibenzothiophene in fish and shellfish(A) and the t-test of correlation coefficient, slope of regression equation and intercept(B).

A: Correlation coefficient and regression equation

chemi -cals	biota	Orig. of Spec.	n	r1)	a2)	b2)	Ve3)
Aroma. Comp.	gold -fish	Exp.	17	0.98	0.71	-0.92	0.014
alkyl -DBT	short necked clam	Exp.	14	0.71	0.16	1.52	0.006
alkyl -DBT	oyster	Nat.	14	0.62	0.49	1.03	0.084
	mussel		14	0.64	0.31	1.63	0.031

B: t-test

chemi -cals	biota	Orig. of Spec.	V.S. Non. Corr.	slope	Inter.
Aroma. Comp.	gold -fish	Exp.	20.12**	20.12**	7.22*
alkyl -DBT	short necked clam	Exp.	3.45*	3.45*	5.99*
alkyl -DBTI	oyster	Nat.	2.75*	2.75*	1.06
	mussel		2.86*	2.86*	2.79*

1) r: Correlation coefficient, 2) y = ax + b
3) Ve: (Syy - Sxy /Sxx) / (n -2)
* : significant within 5% level,
**: significant within 1% level
Orig. of Spec.: Origin of specimens,
Aroma. Comp.: Aromatic compounds
Exp.: Experiment, Nat.: Natural, Inter.: Intercept
V.S. Non. Corr.: Versus none correlation

A straight line relationship was found between the Log parititon coefficient of alkyl dibenzothiophenes and their bioconcentration in the shellfish reared in oil suspension and also in those caught in the sea. Data indicate the bioconcentration of alkyl dibenzothiophenes and their partition coefficients follow a straight line relationship not only in experimental polluted shellfish but also in naturally polluted shellfish.

REFFERENCES

Leo A, Hansch C, Elkins D (1971) Partition coefficients and their uses. Chem Rev 71:525-563

Ogata M, Miyake Y (1975) Compound from floating petroleum accumulating in fish. Water Res 9: 1075-1078

Ogata M, Miyake Y (1980a) Gas chromatography combined with mass spectrometry for the identification of organic sulfur compounds in shellfish and fish. J Chromatogr Sci 18:594-605

Ogata M, Fujisawa K, Kira S, Yoshida Y (1980b) Accumulation and dissipation of organo sulfurs compounds in short necked clam and eel. Bull Environ Contam Toxicol 25:130-135

Sudo T, Kiyozumi O, Ito K, Oshima T (1965) Test method of volatile orgnic substance in Industrial Waste. Report on Institute of Hygiene, Mie Prefecture 150-155 (in Japanese)

Neely WB, Branson DR, Blau GE (1974) Partition coefficient to measure bioconcentration potential of organic chemicals in fish. Environ Sci & Technol 18:1113-1115

Received March 2, 1984; Accepted March 18, 1984