COMPARISON OF THE OCTACHLORODIBENZO-p-DIOXIN (OCDD) BIOACCUMULATION POTENTIAL IN AQUATIC BIOTA ESTIMATED BY DIFFERENT METHODS

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ABSTRACT
The bioconcentration factors (BCF) of octachlorodibenzo-p-dioxin (OCDD) in aquatic biota were estimated by 3 different methods: 1) Prediction the BCF values of OCDD in sludge, algae, water flea, and mussel using quantitative structure activity relationships (QSAR) from its n-octanol/water partition coefficient (log K_{OW}) and/or its water solubility. 2) Estimation of the BCF values from measured OCDD concentrations in biota and water. 3) Estimation of the BCFs from measured OCDD concentrations in biota and sediment using the sediment-soil adsorption coefficient (K_{OC}) to calculate the OCDD concentration in the water phase.

KEYWORDS
Octachlorodibenzo-p-dioxin; OCDD, bioconcentration factor; BCF; QSAR; sludge; algae; daphnia; mussel; fish

1. INTRODUCTION

Octachlorodibenzo-p-dioxin (OCDD) is the most persistent, most lipophilic congener of all the polychlorinated dibenzo-p-dioxins (PCDDs) with an octanol/ water partition coefficient (log K_{OW}) of 9.80 [1], lowest water solubility between 0.4 and 0.074 ng/L [2], and the highest sediment-soil adsorption coefficient corrected for the organic C content (log K_{OC}) of 9.40 [3]. It is usually the most prevalent PCDD found in pentachlorophenol (PCP), sludge, sediments, fly ash, fresh water, and marine biota (mussel, fish etc.) and in human blood, milk and adipose tissue. The 2,3,7,8-TCDD toxicity equivalence factor (TEF) of OCDD has been estimated by Birnbaum et al. [4] to be only 0.01 to 0.001. However, because of the relatively high concentrations of OCDD compared to the lower chlorinated dibenzo-p-dioxins the toxic equivalence of OCDD in many environmental biota may be relatively high. Beside toxicity, biotic and abiotic degradation, bioaccumulation potential of a chemical in aquatic organisms, such as algae, mussel, and fish is one of the important criteria in assessing the hazard. The aim of this study was to predict the BCF values of OCDD from quantitative structure activity (QSAR) equations and comparison of these values with BCF data estimated from experimental laboratory, lake enclosures and environmental monitoring studies.

2. MATERIAL AND METHODS

2.1 Prediction of the Bioconcentration Potential of OCDD Using QSAR: METHOD A

The steady-state bioconcentration factors (BCF) of OCDD in sludge, algae (*Chlorella fusca*), water flea (*Daphnia magna*), and mussel (*Mytilus edulis*) were calculated from its n-octanol/water partition coefficient (log K_{OW} = 9.8) and/or its water solubility (7.4 x 10^{-5} µg/L) using linear regression equations which were developed recently by the authors of this paper (Table 1).

2.2 BCF Estimation from Measured OCDD Concentrations in Biota and Water: METHOD B

The BCF values of OCDD were calculated by dividing OCDD concentrations (pg/kg) in biota (C_B) by the OCDD concentration (pg/L) in the water (C_W). The concentration data were taken from the literature and are given with references in Table 2.

2.3 BCF Estimation from Measured OCDD Concentrations in Biota and Sediment: METHOD C [20]

In case the OCDD concentration in water was not reported because it was too low and/or could not be determined we calculated the OCDD concentration in the water phase from the measured concentration in the sediment using the sediment-soil adsorption coefficient K_{OC} = 2.5 x 10^9 [3]:

$$K_{OC} = \frac{C_S * 100}{C_W * \%OC} \qquad (7)$$

C_S: Chemical (OCDD) concentration in the sediment (dry wt. basis)
%OC: Organic carbon content in the sediment (% C dry wt. basis)

The chemical (OCDD) concentration in the water (C_W) is then:

$$C_W = \frac{C_S * 100}{K_{OC} * \%OC} \qquad (8)$$

The % OC of the sediment or sludge can be determined directly or by multiplying the value of ignition loss (corresponds to the organic matter %) with a factor of 0.6, since the organic carbon is about 60 % of the organic matter. The C_W values were then used to calculate the BCFs. The bioconcentration factors of OCDD by biota on a wet wt. basis (BCF_W) and on a lipid wt. basis (BCF_L) are summarized in Table 2.

3. RESULTS AND DISCUSSION

The steady-state BCF values of OCDD in sludge, algae, Daphnia, and mussel predicted from log K_{OW} and/or water solubility are recorded in Table 1. In Table 2 BCF data from experimental laboratory, lake enclosures, and environmental monitoring studies are summarized. It is obvious that in the experimental studies under controlled conditions with OCDD relatively low BCF values were found after aqueous exposure. However, in all the reported BCF studies the aqueous exposure concentration of OCDD exceeded the water solubility of this chemical or a cosolvent was used to add the test chemical to the water. In both cases it is likely that the extremely lipophilic OCDD was not completely dissolved in the water. The experimentally determined low uptake of OCDD by aquatic organisms is then not due to a low bioaccumulation potential, but to a low bioavailability. In other experiments [14] the time of uptake was so short that no steady-state concentration in the organism could be reached.

4. CONCLUSIONS

The bioaccumulation potential of OCDD in aquatic biota such as sludge and mussel calculated from environmental monitoring studies using the K_{OC} value are in satisfactory agreement with the predicted BCF values by QSAR. These BCF values of OCDD are some orders of magnitude higher than all the experimentally determined BCF values using measured water concentration data.

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TABLE 1

STEADY-STATE BIOCONCENTRATION FACTORS (BCF) OF OCTACHLORODIBENZO-p-DIOXIN (OCDD) BY BIOTA FROM WATER PREDICTED FROM QSAR (LIPOPHILICITY, log K_{OW}: 9.80 and/or WATER SOLUBILITY, WS: $7.4 * 10^{-5}$ µg/L)

B I O T A	E Q U A T I O N	No.	REF.	BIOCONCENTRATION FACTOR	
				BCF_W [a)]	BCF_L [b)]
SLUDGE	$\log BCF_{OC} = 0.70 * \log K_{OW} + 0.74$	(1)	[5]	$4.0 * 10^7$ c)	$1.3 * 10^8$ d)
ALGAE	$\log BCF_W = 0.68 * \log K_{OW} + 0.164$	(2)	[6]	$1.1 * 10^7$	$5.5 * 10^7$ e)
(*Chlorella fusca*)	$\log BCF_W = 4.55 - 0.46 * \log WS$ (µg/L)	(3)	[7]	$2.9 * 10^8$	$1.5 * 10^9$ e)
WATER FLEA (*Daphnia magna*)	$\log BCF_W = 0.895 * \log K_{OW} - 1.53$	(4)	[5]	$1.7 * 10^7$	$9.7 * 10^8$ f)
MUSSEL	$\log BCF_W = 0.858 * \log K_{OW} - 0.808$	(5)	[8]	$5.9 * 10^7$	$5.9 * 10^9$ g)
(*Mytilus edulis*)	$\log BCF_W = 4.94 - 0.682 * \log WS$ (µg/L)	(6)	[8]	$4.0 * 10^7$	$4.0 * 10^9$ g)

a) BCF_W: Wet wt. Basis.

b) BCF_L: Lipid Basis = (BCF_W * 100)/Lipid %.

c) BCF_d: Dry wt. Basis, assuming 30 % Organic Carbon (OC).

d) BCF_{OC}: Bioconcentration Factor on Organic Carbon Content Basis ($BCF_{OC} \triangleq K_{OC}$).

e) BCF_d: Dry wt. Basis.

f) Assuming 1.8 % Lipid.

g) Assuming 1 % Lipid.

TABLE 2. BIOCONCENTRATION FACTORS (BCF) OF OCTACHLORODIBENZO-p-DIOXIN (OCDD) IN AQUATIC BIOTA FROM ENVIRONMENTAL MONITORING (EM), LAKE ENCLOSURES (LE), AND LABORATORY (LB) STUDIES

B I O T A	STUDY	CONCENTRATION OF OCDD IN				REF.	BIOCONCENTRATION FACTOR (BCF)				
		BIOTA (pg/kg)	WATER (pg/L)	SEDIMENT (ng/kg)	%OC		BCF_w a)	M b)	L c) (%)	BCF_L d)	REF.
SLUDGE	EM	$9.1*10^{6}$	14	-	45	[9]	$6.5*10^{5}$ p)	B	-	$1.4*10^{6}$ r)	T.W. s)
	EM	$7.4*10^{6}$	39	-	45	[9]	$1.9*10^{5}$ p)	B	-	$4.2*10^{5}$ r)	T.W.
	EM	$1.3*10^{6}$	8 e)	-	45	[10]	$1.6*10^{5}$ p)	B	-	$3.6*10^{5}$ r)	T.W.
	EM	$8.3*10^{6}$	$1*10^{-2}$ f)	-	45	[9,5]	$8.3*10^{8}$ p)	C	-	$1.8*10^{9}$ r)	T.W.
COMMON (BLUE)	LB g)	$1.2*10^{5}$ g)	$2.7*10^{3}$	-	-	[14]	$4.6*10^{1}$ g)	B	1.0	$4.6*10^{3}$ g)	[14]
MUSSEL (4-5 y)	EM	$1.4*10^{5}$ h)	$4*10^{-2}$ f)	$3.0*10^{3}$	3.1 h)	[11,12]	$3.5*10^{6}$	C	1.0	$3.5*10^{8}$	T.W.
(*Mytilus edulis*)	EM	$6.3*10^{4}$	$1*10^{-1}$ f)	$7.9*10^{3}$	3.0	[13]	$6.3*10^{5}$	C	1.0	$6.3*10^{7}$	T.W.
FISH											
Rainbow trout	LB	N.R. o)	$4.2*10^{5}$	-	-	[16]	$3.4*10^{1}$	D	6.9	$4.9*10^{2}$	[16]
Rainbow trout	LB	N.R.	$2.0*10^{4}$	-	-	[16]	$1.4*10^{2}$	D	6.9	$2.0*10^{3}$	[16]
Fathead minnow	LB	N.R.	$9*10^{3}$ m)	-	-	[16]	$2.2*10^{3}$	D	3.5	$6.3*10^{4}$	[16]
Fathead minnow	LB	N.R.	$9*10^{2}$ n)	-	-	[19]	$2.2*10^{4}$	D	3.5	$6.3*10^{5}$	[19]
White sucker	LE i)	$2.7*10^{6}$ i)	$<3*10^{2}$ i)	N.R.	N.R.	[15]	$>9*10^{3}$ i)	B	2	$>4.5*10^{5}$ i)	[15]
Bream (7-11 y)	EM k)	$3.8*10^{3}$ k)	$4.8*10^{-2}$ f)	$1.4*10^{4}$	12	[17]	$8.0*10^{4}$	C	4	$2.0*10^{6}$	T.W.
Carp (10 g)	LB l)	$2.5*10^{4}$ l)	$2.7*10^{-1}$ f)	$2.1*10^{4}$	3.1	[18]	$9.3*10^{4}$ l)	C	8.0	$1.2*10^{6}$ l)	T.W.
White sucker	LE i)	$2.7*10^{6}$ i)	$1.2*10^{-1}$ f)	$7.0*10^{4}$	22.5	[15,21]	$2.2*10^{7}$ i)	C	2	$1.1*10^{9}$ i)	T.W.

a) BCF_w: Wet wt. basis. b) M: Method A, B, C (see text); D: BCF=Uptake rate/Depuration rate [16]. c) L: Lipid Content (% wet wt.). d) BCF_L: Lipid basis. e) Corrected for blank. f) Calculated water conc. g) 64 days. h) Samplig site M3 [12]. i) 104 days. k) Moorfleet Canal. l) 55 days. m) Centrifuged water conc. n) "True solution" conc. [19]. o) N.R. Not reported. p) Dry wt. basis. r) Organic carbon basis. s) T.W. This work.

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