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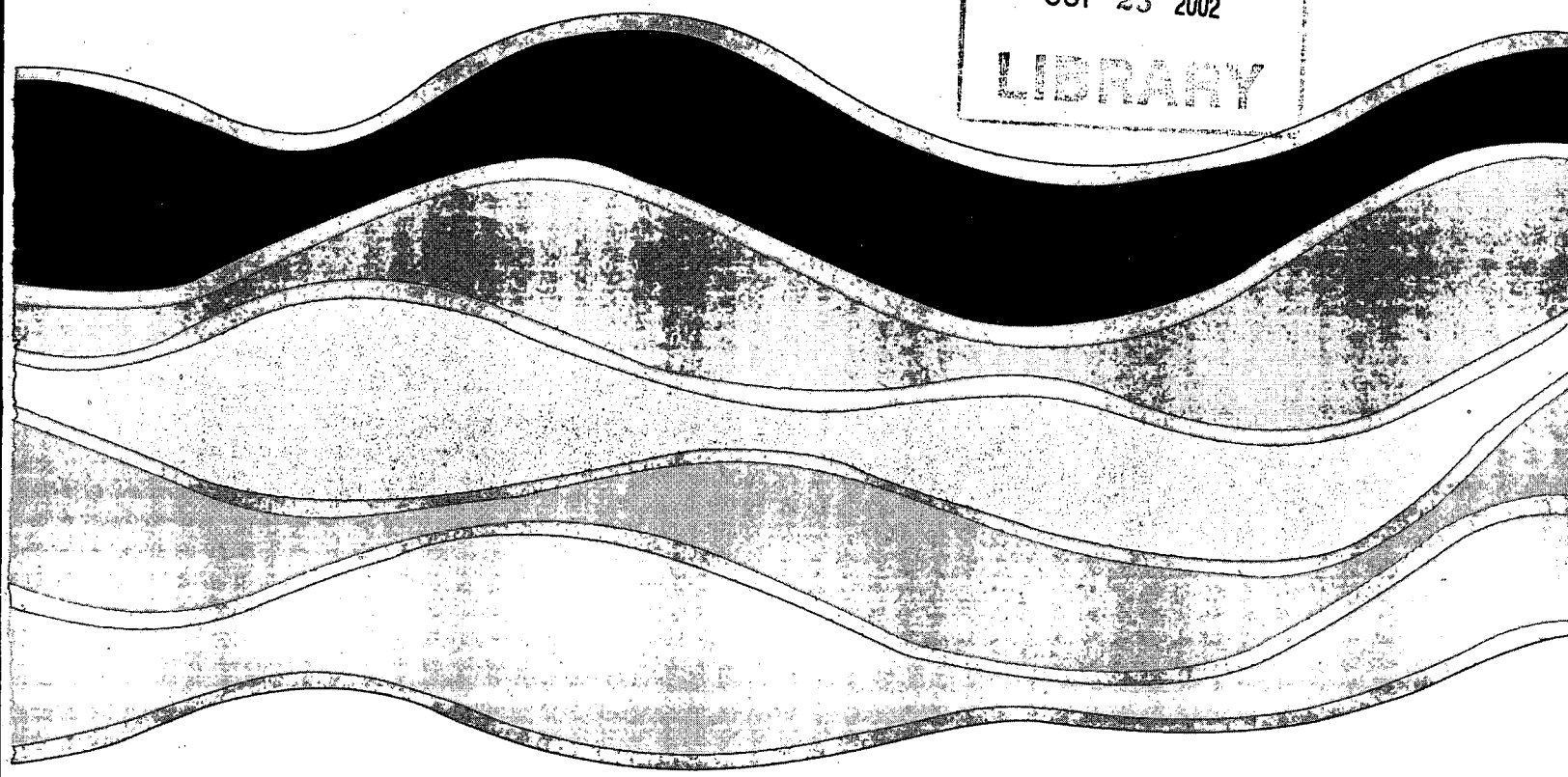

SELECTION OF ENVIRONMENTAL FATE PROPERTIES FOR A SUITE OF ORGANIC COMPOUNDS EMPLOYED BY NORTHERN RIVER BASINS STUDY CONTAMINANT FATE AND FOOD CHAIN MODELLING

B. BROWNLEE

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Selection of Environmental Fate Properties for a Suite of Organic Compounds Employed in Northern River Basins Study Contaminant Fate and Food Chain Modelling

B. Brownlee

Aquatic Ecosystem Protection Branch
National Water Research Institute
Environment Canada
Burlington, Ontario

Aquatic Ecosystem Protection Branch Technical Note

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Management Perspective

From mid-1994 until the completion of the Northern River Basins Study (NRBS) in early 1996, the NRBS Modelling Sub-Committee worked with private sector consultants on contaminant fate and food chain modelling for the Athabasca, Wapiti and Smoky Rivers in the northern river basins of Alberta. In the earlier stages of the modelling activities it was necessary to select physical-chemical properties for the contaminants being modelled. This Note provides background information as to how these properties were selected.

Sommaire à l'intention de la Direction

Du milieu de 1994, jusqu'à la réalisation, au début de 1996, de l'étude sur les bassins hydrographiques du Nord (*Northern River Basins Study - NRBS*), le sous-comité sur la modélisation du NRBS a travaillé de près avec des experts-conseils du secteur privé sur les conséquences des contaminants et sur les modèles de chaîne alimentaire dans les bassins des rivières Athabasca, Wapiti et Smoky, dans le Nord de l'Alberta. Durant les premières étapes des activités portant sur la modélisation, il a été nécessaire de choisir les propriétés physiques et chimiques des contaminants faisant l'objet de la modélisation. Le présent document explique la sélection de ces propriétés.

Introduction

This note is an edited version of a series of Technical Memoranda originally written by the author to the members of the Northern River Basins Study (NRBS) Modelling Sub-Committee (MSC) in October, 1994 and March, 1995. The purpose of these memoranda was to finalize the environmental fate properties for a set of compounds which were selected for contaminant fate and food chain modelling for NRBS. The members of the MSC were:

Dr. B. Brownlee, National Water Research Institute, Burlington
Mr. R. Crosley, Environment Canada, Calgary
Dr. M. MacKinnon, Syncrude Research, Edmonton
Dr. D. Muir, Fisheries and Oceans Canada, Winnipeg
Mr. L. Noton, Alberta Environmental Protection, Edmonton

ex officio Members:

Mr. M. Digel, Golder Associates, Calgary
Mr. G. MacDonald, Golder Associates, Calgary
Ms. M.E. Starodub, CanTox Inc., Mississauga

There are numerous references to the "Golder Table" in this Note. This table was provided by M. Digel, Golder Associates, in December, 1994, and was an initial compilation of physical-chemical properties for the compounds which had been selected for modelling. The compounds were:

2,3,7,8-Tetrachlorodibenzofuran (2378TCDF)
Dehydroabietic Acid (DHA)
12,14-Dichlorodehydroabietic Acid (12,14DCDHA)
3,4,5-Trichlorocatechol (345TCC)
3,4,5-Trichloroguaiacol (345TCG)
3,4,5-Trichloroveratrole (345TCV)
Phenanthrene

The final report on chemical fate modelling (Golder 1997) summarizes the environmental fate constants used at the outset of the model.

Golder Associates Ltd. 1997. Northern River Basins Study Project Report No. 112. Contaminant Fate Modelling, Athabasca, Wapiti and Smoky Rivers. Northern River Basins Study, Edmonton, Alberta.

Part One

ESTIMATED PROPERTIES AND RATES FOR MODELLED COMPOUNDS

The following three tables contain results of application of property estimation software from Syracuse Research Corportion (PCKOC, BIODEG and HENRY).

Table 1. Organic Carbon-Based Partition Coefficients (log Koc) Estimated Using PCKOC.

Compound	Formula	Mol. Wt.	log Koc
2,3,7,8-Tetrachlorodibenzofuran	C12H4Cl4O	305.98	4.91
Dehydroabietic acid	C20H28O2	300.44	4.34
12,14-Dichlorodehydroabietic acid	C20H26Cl2O2	369.33	4.79
3,4,5-Trichlorocatechol	C6H3Cl3O2	213.45	3.30
3,4,5-Trichloroguaiacol	C7H5Cl3O2	227.48	2.94
3,4,5-Trichloroveratrole	C8H7Cl3O2	241.50	2.59
Phenanthrene	C14H10	178.24	4.32

Selection of biodegradation rates is less straightforward. The results in the table below are useful as relative rates but need to be augmented with a few "absolute" rates (or rate ranges) to serve as reference points. Estimations for some additional compounds are included as possible reference points.

Table 2. Biodegradation Probabilities Estimated Using BIODEG.

Compound	CAS No.	Biodegradation Probability	
		Linear Regression	Non-linear Regression
2378TCDF	51207-31-9	0.1151	0.0054
DHA	1740-19-8	0.5320	0.5181
12,14DCDHA	65281-77-8	0.1256	0.0058
345TCC	56961-20-7	0.3272	0.0099
345TCG	57057-83-7	0.3976	0.0857
345TCV	16766-29-3	0.4680	0.4674
Phenanthrene	85-01-8	1.0000	0.9997

... continued

Table 2. Concluded.

Compound	CAS No.	Biodegradation Probability	
		Linear Regression	Non-linear Regression
245TCphenol	95-95-4	0.2479	0.0079
Catechol	120-80-9	0.9368	0.9616
Dibenzofuran	132-64-9	0.9279	0.9946
2378TCDD	1746-01-6	0.2648	0.0608

Notes:
1.The CAS numbers are included here since they have not been included in the compilation and they can be useful for literature searching.
2. Biodegradation probability is the probability that the compound will degrade FAST. Greater than 0.5 = YES, less than 0.5 = NO.
3. For comparison, estimates for a few model compounds in Howard et al. (1991) have been included: 2,4,5-trichlorophenol, catechol, dibenzofuran, and 2378TCDD.
4. Overall, the program would likely overestimate the *in situ* rates for phenanthrene and 2378TCDF relative to 345TCG.

These estimates can be used in two ways:

1. From the Golder table literature values are available for water column and sediment biodegradation rates for DHA (lake) and phenanthrene. Equating the probabilities above to relative rates, rates can be calculated for the other compounds.
2. Some field values are available for water column disappearance rates for 345TCG (B. Brownlee and L. Noton unpublished results). Again, rates can be calculated for the other compounds based on relative rates derived from the probabilities. Summer water column disappearance rates (15-20°) for 345TCG are about 0.7 d^{-1}. Winter water column disappearance rates (0°) are about 0.15 d^{-1}.
3. Kinetic analysis of field data of L. Noton for 345TCC, 345TCV, DHA and 12,14DCDHA does not look feasible.
4. For the water column, the same rates can be used for 345TCC, 345TCG, 345TCV and DHA; faster rates (x2) for phenanthrene; slower rates (x1/2) for 12,14DCDHA; and very low or zero for 2378TCDF. This would give a much faster rate for DHA disappearance in a river than in a lake (1.65E-02 d^{-1} from Brownlee et al. 1977). The difference between winter and summer rates would provide a rough temperature correction.
5. For sediment biodegradation rates, there are no field data for the Athabasca and few literature data. Our compilation has sediment biodegradation rates for

phenanthrene and DHA, and we can assume that 2378TCDF will be very slow (half-life of >> 1 yr).

Table 3. Henry's Law Constants Estimated Using HENRY.

Compound	Henry's Constant ($atm \cdot m^3 \cdot mol^{-1}$) Bond Method	Group Method	Henry's Constant (dimensionless) Bond Method	Group Method
2378TCDF	1.238E-05	5.351E-05	5.062E-04	2.188E-03
DHA	1.780E-07	NA	7.276E-06	NA
12,14DCDHA	9.772E-08	NA	3.995E-06	NA
345TCC	2.373E-11	4.994E-11	9.702E-10	2.042E-09
345TCG	1.349E-08	3.300E-07	5.516E-07	1.349E-05
345TCV	7.670E-06	2.180E-03	3.136E-04	8.913E-02
Phenanthrene	5.134E-05	2.561E-05	2.099E-03	1.047E-03

Notes:

1. Units of $atm \cdot m^3 \cdot mol^{-1}$ can be approximately converted to $Pa \cdot m^3 \cdot mol^{-1}$ by multiplying by E+05 (10^5).
2. The software gives two values, one based on the bond contribution description and the other on the group contribution description.
3. In some cases the two methods (bond and group) give quite different results, e.g., 345TCV, and it is not clear which is preferable. A value of ca. 4.0E-04 was calcluated from literature values of vapor pressure and solubility (Brownlee et al. 1993). In log terms, this is closer to the group value.
4. For comparison, the value in the Golder table for H for 2378TCDF is 1.5 $Pa \cdot m^3 \cdot mol^{-1}$, or about 1.5E-05 $atm \cdot m^3 \cdot mol^{-1}$, quite close to the values calculated.
5. Similarly for phenanthrene, the estimated values of 2.6-5.1E-05 $atm \cdot m^3 \cdot mol^{-1}$ are well within the range in the Golder table (2.5E-05 to 1.3E-04).
6. This good agreement for 2378TCDF and phenanthrene indicates that the estimation software can give credible values.

PHOTOLYSIS

Two compounds (2378TCDF and phenanthrene) have reasonably short photochemical half-lives and, under open water conditions, photodegradation could be important if there is much light penetration. There are limited field results that indicate that such is not the case. For the Athabasca River in August, 1994 the 10% light level at 300 nm was calculated to be 7 cm for unfiltered and 10 cm for filtered water (B. Brownlee unpublished results). Unless the percent of time a molecule spends in the top 5-10 cm of the water column can be calculated, photolysis should be neglected in the first phase of modelling.

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Part Two

SELECTED PROPERTIES AND RATES. 2378TCDF and Phenanthrene

The discussion below draws heavily on the Mackay et al. (1992) compilation, especially when referring to ranges or typical values. Single values are referenced individually.

2378TCDF

Water Solubility 0.000419 mg/L

From Mackay et al. (1992). This value is experimental (Friesen et al. 1990, generator column).

log Kow 6.53

From Sijm et al.(1989). This is an experimental value using a slow stirring method.

log Koc 6.5

For log Koc, a value of 7.5 seems too high if we use a value of 6.5 for log Kow which would suggest a value in the range 6.0-6.5. Field values of log Koc for 2378TCDD are 6.0-6.6. Sijm et al. (1989) reported log Kow=6.42 for 2378TCDD and log Kow=6.53 for 2378TCDF. Since log Kow are similar for 2378TCDD and 2378TCDF, their log Koc should also be similar. A value of 6.5, the same as Kow, meets these criteria.

Henry's Law Constant 1.5 $Pa \cdot m^3 \cdot mol^{-1}$ (1.5E-05 $atm \cdot m^3 \cdot mol^{-1}$)

This value from Mackay et al. (1992) appears to be reliable and is between the values from the estimation software (HENRY).

Photolysis Zero

The rates in Mackay et al. (1992) indicate a short half-life, with a rate in full sunlight of about 11/day. However, as mentioned above, light penetration is apt to be low. At 300 nm, the 10 percent light level is probably 5-10 cm. The photolysis rate can be set to zero initially.

Water Column Biodegradation half-life > 1 yr

The only value available for comparison is for 2378TCDD with an aquatic aerobic half-life of 1.2-1.6 years (Howard et al. 1991).

Sediment Biodegradation half-life > 1 yr

See above.

PHENANTHRENE

Water Solubility 1.0 mg/L

Mackay et al. (1992) have many values near 1.0 so a value of 1.0 is reasonable.

log Kow 4.46

The modal value (n=52) from Mackay et al. (1992) as in the Golder table.

log Koc 4.31

Similar to log Kow. It is the mean value (n=19) from Mackay et al. (1992) in the Golder table.

Henry's Law Constant 3.9 $Pa \cdot m^3 \cdot mol^{-1}$ (3.9E-05 $atm \cdot m^3 \cdot mol^{-1}$)

Several values in Mackay et al. (1992) are near 4.0 $Pa \cdot m^3 \cdot mol^{-1}$. Baker and Eisenreich (1990) give a value of H at 15° of 0.69 which should permit temperature correction of H.

Photolysis Zero

Howard et al. (1991) give half-lives for phenanthrene of 3 hr in summer and 25 hr in winter. However, by the argument given above for the 2378TCDF photolysis rate, this rate should be set to zero initially.

Water Column Biodegradation Rate 0.01 d^{-1}

This is near the fast end of the range of values given in Howard et al. (1991). The rationale is the high probability computed by the estimation software (BIODEG).

Sediment Biodegradation Rate 0.01 d^{-1}

Same rationale as for the water column rate.

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Part Three

SELECTED PROPERTIES AND RATES. Dehydroabietic and 12,14-Dichlorodehydroabietic Acids

DEHYDROABIETIC ACID

Water Solubility 0.00125 mg/L

The calculated value from the Golder table.

log Kow 6.1

The same as log Koc described below. The value in the Golder table (7.42) seems to high by at least an order of magnitude.

log Koc 6.09

This was arrived at as follows. First, NRBS field results from 1992 and 1993 were used to calculate log Koc. The results are summarized in Table 4. The actual value above comes from the estimation software (PCKOC), without correcting for the carboxyl group. An earlier value, proposed in September, 1994, was log Koc=4.34, which includes a correction for the carboxyl group. Referring to Table 4, the value above is at the upper end of the range for field values, so probably there is some effect from the carboxyl group but the magnitude is unknown. Two further points: (1) this value (6.09) falls well within the range of calculated field Koc values for structurally similar abietic acid (Table 4), (2) for all of the resin acids, the log Koc values for the Hinton Combined Effluent are lower than the river values by one to three orders of magnitude indicating that one or the other is not at equilibrium, most likely the effluent.

Henry's Law Constant 1.8E-02 $Pa \cdot m^3 \cdot mol^{-1}$ (1.8E-07 $atm \cdot m^3 \cdot mol^{-1}$)

The value from the estimation program (HENRY).

Photolysis Zero

Set to zero for the same reason as 2378TCDF and phenanthrene. However, DHA appears to be photoactive (Anderson et al. 1992).

Water Column Biodegradation 1.65E-02 d^{-1}

This is the value Brownlee et al. (1977). Several assumptions were made in estimating that value. The rate is probably too slow for a river with biofilm to degrade organic compounds but it is the only one available.

Sediment Biodegradation 9.00E-05 d^{-1}

See above.

Bioconcentration Factor 96±35 (n=10)

This value is from Niimi and Lee (1992) for rainbow trout and is based on the concentration of free DHA measured in tissue for whole fish. Conjugated DHA was also analyzed. Elimination rates were also measured. They concluded that the half-lives of these acids were < 4 d.

12,14-DICHLORODEHYDROABIETIC ACID

Water Solubility no data

If a value is required, then the DHA value shoud be a good approximation.

log Kow 6.38

The value from the Golder table calculated by the method of Hansch and Leo (1978). A value of 6.5, the same as the log Koc below, could also be used.

log Koc 6.54

The same argument as for DHA above.

Henry's Law Constant 9.8E-03 $Pa \cdot m^3 \cdot mol^{-1}$ (9.8E-08 $atm \cdot m^3 \cdot mol^{-1}$)

The value from the estimation program (HENRY).

Photolysis Zero

Set to zero because of low light penetration. However, since DHA appears to be photoactive it is possible that 12,14-DCDHA is also photoactive.

Water Column Biodegradation Rate 1.65E-02 d-1

The same value as for DHA.

Sediment Biodegradation Rate $9.0E-05\ d^{-1}$

The same value as for DHA.

Bioconcentration Factor 92 ± 29 (n=10)

Taken from Niimi and Lee (1992) with the same conditions as for DHA. The authors don't specify the isomer of dichloro-DHA, but the 12,14-isomer is the usual one.

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PCKOC. Soil/Sediment Adsorption Program by W.M. Meylan and P.H. Howard, Lewis Publishers, Boca Raton, FL, 1992.

Table 4. Field Koc Values for Resin Acids.

Site	Water Column Conc. (ng/L)	Suspended Sed. Conc. (ng/g)	foc	log Koc
1992 Dehydroabietic Acid				
u/s Hinton	ND (L 63)	140	0.025	> 4.95
Hinton Comb. Eff.	8000	36000	0.266	4.23
Haul Bridge	125	1400	0.031	5.56
Obed	ND (L 160)	1200	0.029	> 5.41
Emerson	32	1300	0.035	6.06
Knight	76	1200	0.036	5.64
Windfall	ND (L 80)	980	0.034	> 5.56
1993 Dehydroabietic Acid				
Hinton Comb. Eff.	30000 [a]	37000	0.311	3.60
1992 12,14-Dichlorodehydroabietic Acid				
u/s Hinton	ND (L 36)	0.2	0.025	> 2.35
Hinton Comb. Eff.	120	4400	0.266	5.14
Haul Bridge	3.4	140	0.031	6.12
Obed	ND (L 69)	140	0.029	> 4.84
Emerson	NDR (2.2)	260	0.035	6.53
Knight	ND (L 2.5)	190	0.036	> 6.32
Windfall	ND (L 27)	97	0.034	> 5.02
1993 12,14-Dichlorodehydroabietic Acid				
Hinton Comb. Eff.	ND (L 10000) [a]	2600	0.311	> 2.92
Haul Bridge	130 [b]	710	0.046	5.07
Obed	140 [b]	5100	0.046	5.90
Emerson	80 [b]	770	0.062	5.19
1992 Abietic Acid				
u/s Hinton	ND (L 150)	31	0.025	> 3.92
Hinton Comb. Eff.	1500	16000	0.266	4.60
Haul Bridge	10	425	0.031	6.14
Obed	ND (L 330)	660	0.029	> 4.84
Emerson	ND (L 10)	350	0.035	> 6.00
Knight	ND (L 12)	380	0.036	> 5.94
Windfall	ND (L 140)	440	0.034	> 4.97
1993 Abietic Acid				
Hinton Comb. Eff.	90000 [a]	28000	0.311	3.00
Haul Bridge	200 [b]	6400	0.046	5.84
Obed	270 [b]	29000	0.046	6.37
Emerson	90 [b]	4600	0.062	5.92
Lesser Sl. R. Mouth	1670 [b]	96	0.090	2.81
ANC Effluent	3200 [b]	760000	0.401	5.77

[a] From Northdat.
[b] From Alberta Environmental Protection data for 1993 winter synoptic.

Part Four

SELECTED PROPERTIES AND RATES. 3,4,5-Trichlorocatechol/guaiacol/veratrole

3,4,5-TRICHLOROCATECHOL

Water Solubility 16.5 mg/L

The calculated value from the Golder table.

log Kow 3.7

The experimental value from Xie et al. 1984, as in the Golder table.

log Koc 3.3

The calculated value from the estimation program (PCKOC). This also agrees well with the calculated value provided by CanTox (ASTER 1994). However, it is lower by about one unit than the log Koc (Kp) of 4.35 found by Remberger et al. (1986). Sediment seems to have a rather high affinity for chlorocatechols, perhaps for reasons other than simple organic carbon-based partitioning.

Henry's Law Constant 8.1E-03 $Pa \cdot m^3 \cdot mol^{-1}$ (8.1E-08 $atm \cdot m^3 \cdot mol^{-1}$)

H resulting from the values for vapour pressure and solubility calculated by CanTox in the Golder table.

Photolysis Zero

Set to zero for the same reason as 2378TCDF and phenanthrene.

Water Column Biodegradation 0.7 d^{-1}

Based on summer field results from surveys by NWRI and AEP for 345TCG (B. Brownlee and L. Noton unpublished results).

Sediment Biodegradation No value yet

Applying the water column-to-sediment ratio of half-lives for DHA (Brownlee et al. 1977) to the half-life above, results in a half-life of 180-200 days for 345TCC in sediment.

3,4,5-TRICHLOROGUAIACOL

Water Solubility 9.1 mg/L

The calculated value from the Golder table (Kolset and Heiberg 1988).

log Kow 4.2

The experimental value from Xie et al. 1984, as in the Golder table.

log Koc 3.6

The calculated value from the estimation program (PCKOC), without correcting for the aromatic ether fragment.

Henry's Law Constant 1.6E+01 $Pa \cdot m^3 \cdot mol^{-1}$ (1.6E-04 $atm \cdot m^3 \cdot mol^{-1}$)

H resulting from the values for vapour pressure and solubility in the Golder table. The vapour pressure value is from Bidleman and Renberg (1985).

Photolysis Zero

Set to zero for the same reason as 2378TCDF and phenanthrene.

Water Column Biodegradation 0.7 d^{-1}

Based on summer field results from surveys by NWRI and AEP for 345TCG (B. Brownlee and L. Noton unpublished results).

Sediment Biodegradation No value available

See above discussion for 345TCC.

Bioconcentration Factor 268±77 (n=5)

From Niimi et al. (1990).

3,4,5-TRICHLOROVERATROLE

Water Solubility 2.5 mg/L

From Neilson et al. (1984).

log Kow 4.6

From Neilson et al. (1984). Alternate value is 5.25, also from Neilson et al. (1984).

log Koc 3.9

The calculated value from the estimation program (PCKOC), without correcting for the aromatic ether fragments.

Henry's Law Constant 4.0E+01 $Pa \cdot m^3 \cdot mol^{-1}$ (4.0E-04 $atm \cdot m^3 \cdot mol^{-1}$)

H calculated in Brownlee et al. (1993) from literature values for vapour pressure (Bidleman and Renberg 1985) and solubility (Neilson et al. 1984).

Photolysis Zero

Set to zero for the same reason as 2378TCDF and phenanthrene.

Water Column Biodegradation 0.7 d^{-1}

Based on summer field results from surveys by NWRI and AEP for 345TCG (B. Brownlee and L. Noton unpublished results).

Sediment Biodegradation No value yet

See above discussion for 345TCC.

Bioconcentration Factor 3160

From Neilson et al. (1984) for zebra fish (whole body).

The calculated values of H selected for 345TCC/TCG/TCV (8.1E-08, 1.6E-04, and 4.0E-04 atm/m3/mol) are higher than the values predicted by the estimation program (2.4E-11, 1.3E-08 and 7.7E-06 atm/m3/mol; bond contribution method).

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Xie, T.-M., B. Hulthe and S. Folestad. 1984. Determination of partition coefficients of chlorinated phenols, guaiacols and catechols by shake-flask GC and HPLC. Chemosphere 13:445-459.

Part Five

SELECTED PROPERTIES AND RATES. ADDITIONAL INFORMATION

PHENANTHRENE

Sediment Biodegradation Rate 0.01-0.03 d^{-1}

This is the same as previously selected and comes from Grosser et al. (1995) who found half-life for mineralization of 14C-labelled phenanthrene in acclimated soil (coal tar refinery site) of 20 to 60 days.

DEHYDROABIETIC ACID

Water Solubility 4.9 mg/L

This experimental value is from Nyrén and Back (1958) and is much higher than the value of 0.00125 mg/L from the Golder table.

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Grosser, R.J., D. Warshawsky and J.R. Vestal. Mineralization of polycyclic and *N*-heterocyclic compounds in hydrocarbon-contaminated soils. Environ. Toxicol. Chem. 14:375-382.

Nyrén, V. and E. Back. 1958. The ionization constant, solubility product and solubility of abietic and dehydroabietic acid. Acta Chem. Scand. 12:1516-1520.

Annotated Bibliography

3,4,5-Trichlorocatechol/guaiacol/veratrole

Allard, A.-S., M. Remberger and A.H. Neilson. 1985. Bacterial *O*-methylation of chloroguaiacols: Effect of substrate concentration, cell density and growth conditions. Appl. Environ. Microbiol. 49:279-88.

This may be useful for estimating biodegradation rates. However field data (AEP) are probably more useful.

Remberger, M., P-A. Hynning and A.H. Neilson. 1993. Release of chlorocatechols from a contaminated sediment. Environ. Sci. Technol. 27:158-164.

This has distribution (in percent) of 345TCC between particulate, colloidal, DOC-bound and soluble fractions.

Remberger, M., A.-S. Allard and A.H. Neilson. 1986. Biotransformation of chloroguaiacols, chlorocatechols and chloroveratroles in sediments. Appl. Environ. Microbiol. 51:552-558.

345TCC K_p 22.2 mL/kg Organic C; 345TCV K_p 1.6 mL/kg Organic C.

The latter value is the same as Allard et al. (1988) in the Cantox list.

Suntio, L.R., W.Y. Shiu and D. Mackay. 1988. A review of the nature and properties of chemicals present in pulp mill effluents. Chemosphere 17:1249-1290.

A good compilation of the earlier literature.

Xie, T.-M. 1983. Determination of trace amounts of chlorophenols and chloroguaiacols in sediment. Chemosphere 12:1183-1191.

345TCG log K_{ow} 4.45 (calculated by method of Leo and Hansch).

Xie, T.-M. and D. Dryssen. 1984a. Simultaneous determination of partition coefficients and acidity constants of chlorinated phenols and guaiacols by gas chromatography. Analytica Chim. Acta 160:21-30.

3345TCG log K_{ow} 4.13-4.14.

Xie, T.-M., B. Hulthe and S. Folestad. 1984b. Determination of partition coefficients of chlorinated phenols, guaiacols and catechols by shake-flask GC and HPLC. Chemosphere 13:445-459.

345TCG log K_{ow} 4.11 (GC) and 4.18 (HPLC).
345TCC log K_{ow} 3.79 (GC) and 3.71 (HPLC).

Xie, T.-M., K. Abrahamsson, E. Fogelqvist and B. Josefsson. 1986. Distribution of chlorophenolics in a marine environment. Environ. Sci. Technol. 20:457-463.

345TCG log K_{ow} 4.00 (field corrected for ambient pH).

Food Chain

Koelmans, A.A. and C.S. Jiménez. 1994. Temperature dependence of chlorobenzene bioaccumulation in phytoplankton. Chemosphere 28:2041-2048.

This may be useful for other organochlorines as well.

Niimi, A.J., H.-B. Lee and G.P. Kissoon. 1990. Kinetics of chloroguaiacols and other chlorinated phenolic derivatives in rainbow trout (Salmo gairdneri). Environ. Toxicol. Chem. 9:649-653.

345TCG mean BCF 268±77 (mean log BCF 2.41).

Rogers, I.H., J.A. Servizi and C.D. Levings. 1988. Bioconcentration of chlorophenols by juvenile chinook salmon (Oncorhyncus tshawytscha) overwintering in the upper Fraser River: Field and laboratory tests. Water Poll. Research J. Canada 23:100-113.

BCF can be calculated from water and fish concentrations for 345TCG.

2378TCDF

Dung, M.H. and P.W. O'Keefe. 1994. Comparative rates of photolysis of polychlorinated dibenzofurans in organic solvents and in aqueous solutions. Environ. Sci. Technol. 28:549-554.

2378TCDF half-life in water at 300 nm is 0.45 h^{-1}.

Endicott, D.D. and P.M. Cook. 1994. Modelling the partitioning and bioaccumulation of TCDD and other hydrophobic organic chemicals in Lake Ontario. Chemosphere 28:75-87.

2378TCDF biota (lake trout) to sediment ratio, BSR, of 0.43.

Fletcher, C.L. and W.A. McKay. 1993. Polychlorinated dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs) in the aquatic environment - A literature review. Chemosphere 26:1041-1069.

2378TCDF bioavailability index (same idea as BSR above) 0.06. Data from Kuehl et al (1987b).

Hinton, S.W., R. Brinck and L. Walbridge. 1993. Mass transfer of TCDD/DF from suspended sediment particles. Water Sci. Technol. 28(8/9):181-190.

This reference has some useful experimental data on 2378TCDF partitioning.

Kukkonen, J. and J. Pellinen. 1994. Binding of organic xenobiotics to dissolved organic macromolecules: comparison of analytical methods. Science of the Total Environ. 152:19-29.

This reference gives the water-DOM partition coefficient for 2378TCDD. The DOM was natural humic substances and chlorolignin.

Loonen, H., J.R. Parsons and H.A.J. Govers. 1994. Effect of sediment on the bioaccumulation of a complex mixture of polychlorinated dibenzo-p-dioxins (PCDDs) and polychlorinated dibenzofurans (PCDFs) by fish. Chemosphere 28:1433-1446.

This reference gives BCFs for guppies in the absence and presence of sediment, and biota-sediment accumulation factors.

Muir, D.C.G., W.L. Fairchild and D.M. Whittle. 1992. Predicting bioaccumulation of chlorinated dioxins and furans in fish near Canadian bleached kraft mills. Water Poll. Res. J. Canada 27:487-507.

This presents an extensive compilation of bioaccumulation factors and biota/sediment accumulation factors from the literature and authors' field studies.

Rolff, C., D. Broman, C. Näf and Y. Zebühr. 1993. Potential biomagnification of PCDD/Fs - New possibilities for quantitative assessment using stable isotope trophic positions. Chemosphere 27:461-468.

This information should be useful for food chain modelling.

Tysklind, M., K. Lundgren and C. Rappe. 1993. Ultraviolet absorption characteristics of all tetra- to octachlorinated dibenzofurans. Chemosphere 27:535-546.

This paper gives UV spectral data for 2378TCDF in toluene.

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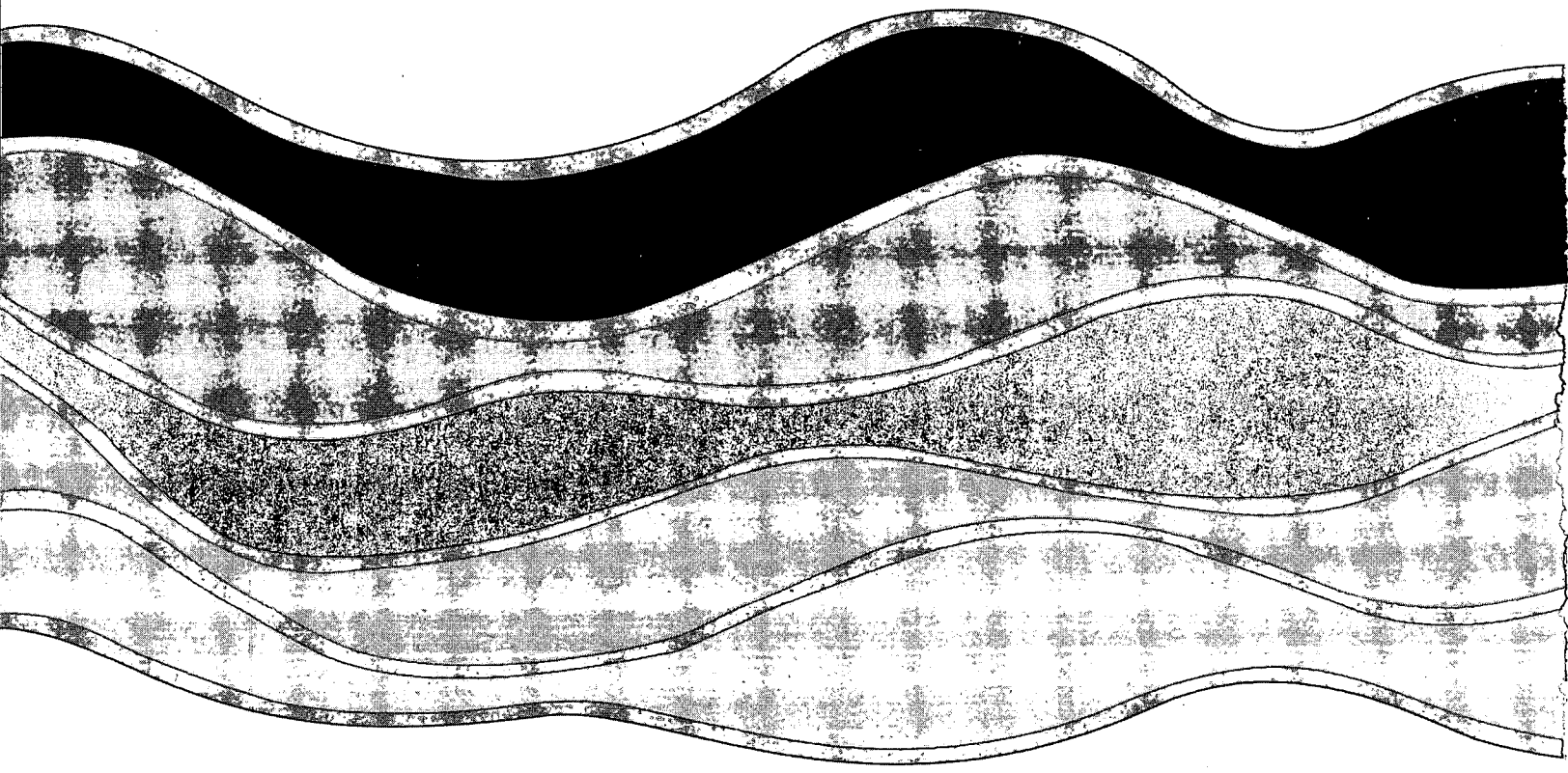

NATIONAL WATER RESEARCH INSTITUTE
P.O. BOX 5050, BURLINGTON, ONTARIO L7R 4A6

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