

FINAL DRAFT REPORT

Intermedia Transfer Factors for Contaminants Found at Hazardous Waste Sites

2,3,7,8-TETRACHLORODIBENZO-*p*-DIOXIN (TCDD)

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FORWARD

The Department of Toxic Substances Control (DTSC), within the California Environmental Protection Agency, has the responsibility for managing the State's hazardous-waste program to protect public health and the environment. The Office of Scientific Affairs (OSA) within the DTSC provides scientific assistance in the areas of toxicology, risk, environmental assessment, training, and guidance to the regional offices within DTSC. Part of this assistance and guidance is the preparation of regulations, scientific standards, guidance documents, and recommended procedures for use by regional staff, local governmental agencies, or responsible parties and their contractors in the characterization and mitigation of hazardous-waste-substances-release sites. The CalTOX model has been developed as a spreadsheet model to assist in exposure and health-risk assessments that address contaminated soils and the contamination of adjacent air, surface water, sediments, and ground water.

The modeling effort includes multimedia transport and transformation models, exposure scenario models, and efforts to quantify and reduce uncertainty in multimedia, multiple-pathway exposure models. Use of the CalTOX model requires that we determine the intermedia transfer factors (ITFs) that define concentration relationships between an exposure medium and the environmental medium that is the source of the contaminant. ITFs are chemical and physical parameters which serve as inputs in the CalTOX model analysis.

This report provides a set of ITFs needed to run the CalTOX model for TCDD. For this chemical, we have conducted a critical review of existing literature for measured values and estimation methods in order to compute an arithmetic mean (\bar{x}), a coefficient of variation (CV), and plausible range for each ITF.

OVERVIEW

The purpose of this report is to provide a set of chemical-specific intermedia-transfer factors (ITFs) for TCDD. We have carried out a critical review of the existing literature in order to identify a mean value, coefficient of variation (CV) and value range for the ITFs listed in Table 1. For values used to define a given parameter, our highest priority was given to experimental values reported in the primary scientific literature, that is, peer-reviewed journals. For parameters that are not readily available from the primary literature, widely cited secondary references such as Lyman et al. (1982, 1990), Verschueren (1984), Howard et al. (1990, 1991), Mackay et al. (1992), the CRC Handbook (1989-90) and the Merck Index (1983, 1989) are used to establish parameter values. When measured values are not available from either the primary literature or secondary references, estimates of ITF parameter values are based on estimation equations that are available in the primary literature. Typically, these estimation methods relate ITFs to other measured contaminant parameters using quantitative-structure-activity-relationship (QSAR) methods. In these cases, parameter values estimated from a QSAR method are treated as the arithmetic mean and the estimation error of the method is used to determine the CV. Table 1 summarizes the units required by the CalTOX model, the values of chemical specific physico-chemical properties, distribution coefficients, biotransfer and bioconcentration factors, and transformation half-lives obtained in this study.

CalTOX Chemical-Specific Input Requirements

The CalTOX model uses three sets of input data—one describing the chemical-specific properties of the contaminants, a second providing properties of the environment or landscape receiving the contaminants, and a third that defines for exposure assessment the characteristics of individuals in various age/sex categories and the characteristics of the micro-environments in which they live or from which they obtain water and food. Each of the inputs in these sets must be described in terms of a mean value with an estimated coefficient of variation, which describes the uncertainty or variability associated with that parameter. This report addresses mean value, CV, and range of values needed to characterize chemical-specific inputs.

Physicochemical Properties

Physicochemical properties include molecular weight, octanol-water partition coefficient, melting point, vapor pressure, Henry's law constant, diffusion coefficients in air and water, and the organic-carbon partition coefficient. The octanol-water partition coefficient provides a measure of the extent of chemical partitioning between water and octanol at equilibrium and is used as a basis for estimating other ITF parameters. The melting point is the temperature at which a compound makes the transition from a solid to a liquid phase. Vapor pressure is the pressure exerted by a chemical vapor in equilibrium with its solid or liquid phase. Water solubility is the upper limit on a chemical's dissolved concentration in pure water, at a specified temperature.

Table 1. Summary of Chemical Properties for 2,3,7,8 Tetrachlorodibenzo-*p*-dioxin

Description	Symbol ^a	Mean Value	Coefficient of Variation	Number of Values
Molecular Weight (g/mol)	MW	322	6.2×10^{-5}	4
Octanol-Water Partition Coefficient	K_{ow}	4.6×10^6	0.73	6
Melting Point (K)	T_m	578	0.0025	10
Vapor Pressure (Pa)	VP	1.6×10^{-6}	1.6	3
Solubility (mol/m ³)	S	1.9×10^{-7}	1.6	4
Henry's Law Constant (Pa·m ³ /mol)	H -	2.5	1.5	4
Diffusion Coefficient in Pure Air (m ² /d)	D_{air}	0.42	0.080	e
Diffusion Coefficient in Pure Water (m ² /d)	D_{water}	5.1×10^{-5}	0.25	e
Organic Carbon Partition Coefficient	K_{oc} -	5.4×10^6	1.6	7
Distribution Coefficient in Ground-Surface and Root-Zone Soil	K_{d_s} -	b	e	e
Distribution Coefficient in Vadose-Zone Soil	K_{d_v} -	b	e	e
Distribution Coefficient in the Ground-Water Zone	K_{d_q} -	b	e	e
Distribution Coefficient in Ground Water Sediment	K_{d_d} -	b	e	e
Partition Coefficient in Plants Relative to Soil Concentration [ppm (pFM) / ppm (sFM)]	K_{ps} -	0.34	0.20	4
Biotransfer Factor in Plants Relative to Contaminant Air Concentration [m ³ (a)/kg (pFM)]	K_{pa} -	2.6×10^4	0.85	2
Biotransfer Factor in Milk Relative to Cattle-Diet Contaminant Intake (d/kg)	B_k -	4.5×10^{-3}	0.98	4
Biotransfer Factor in Meat Relative to Cattle-Diet Contaminant Intake (d/kg)	B_t -	0.24	0.14	1
Biotransfer Factor in Eggs Relative to Hen-Diet Contaminant Intake (d/kg)	B_e -	37	14	e
Biotransfer in Breast Milk Relative to Contaminant Intake by the Mother (d/kg)	B_{bmk} -	0.92	10	e
Bioconcentration Factor in Fish Relative to Contaminant Water Concentration	BCF -	1.9×10^4	1.1	7
Skin Permeability Coefficient (cm/hr)	K_{p_w} -	0.010	2.4	e
Skin-Water Partition Coefficient [ppm (skin)/ppm (water)]	K_m -	5.4×10^4	0.27	e
Reaction Half-Life in Air (d)	T_{half_a}	30	1.7	3
Reaction Half-Life in Ground-Surface Soil (d)	T_{half_g}	2200	0.86	6
Reaction Half-Life in Root-Zone Soil (d)	T_{half_s}	6700	1.8	8
Reaction Half-Life in the Vadose-Zone Soil (d)	T_{half_v}	6700	1.8	8
Reaction Half-Life in Ground-Water Zone Soil (d)	T_{half_q}	1500	0.44	4
Reaction Half-Life in Surface Water (d)	T_{half_w}	430	1.2	4
Reaction Half-Life in the Sediment (d)	T_{half_d}	2100	0.61	4

^aValues followed by a "-" include default equations that can be used for estimations

^b $K_d = [(K_{oc}) \times (\text{fraction organic matter})]$, a site and soil zone specific parameter

^eestimated parameter value

Henry's law constant is a measure at equilibrium of the ratio of chemical activity in the gas above a liquid to chemical activity in the liquid. Diffusion coefficients describe the movement of a molecule in a liquid or gas medium as a result of differences in concentration within the medium. They are used to calculate the dispersive component of chemical transport. The higher the diffusion coefficient, the more likely a chemical is to move in response to concentration gradients. The organic-carbon partition coefficient provides a measure of chemical partitioning between organic carbon (in soils, rocks, and sediments) and water. The higher the K_{OC} the more likely a chemical is to bind to the solid phase of soil or sediment than to the liquid phase.

The Solid-Water Distribution Coefficients

The distribution or sorption coefficient, K_d , is the concentration ratio, at equilibrium, of chemical attached to solids and/or particles (mol/kg) to chemical concentration in the solution, mol/L. When K_{OC} is multiplied by the fraction organic carbon in a soil or sediment, we obtain an estimate of the soil/water or sediment/water partition coefficient. CalTOX requires, as input, distribution coefficients for ground-surface, root-zone, and vadose-zone soil; ground-water-zone rock or soil, and surface-water sediments.

Biotransfer Factors and Bioconcentration Factors

The CalTOX model requires, as input, general relationships that can be used to estimate partition coefficients between air and plants; between soil and plants; between animal feed intake and animal-based food products; between surface water and fish; between the human mother's uptake and breast milk; between skin and water; and between skin uptake and concentration in skin water.

The chemical-specific plant-air partition coefficient, K_{pa} , represents the ratio of contaminant concentration in above-ground plant parts, in mg/kg (fresh mass), to contaminant concentration in the gas-phase of the atmosphere mg/m^3 (air). The plant-soil partition coefficient, K_{ps} , expresses the ratio of contaminant concentration in plant parts, both pasture and food, in mg/kg (plant fresh mass) to concentration in wet root-zone soil, in mg/kg.

The biotransfer factors B_t , B_k and B_e are the steady-state contaminant concentrations in, respectively, fresh meat, milk, and eggs; divided by the animals' daily contaminant intake. These factors are expressed in units of $(\text{mg}/\text{kg})/(\text{mg}/\text{d})$, or kg/d . Unlike bioconcentration factors, which express steady-state concentration ratios between animal tissue and a specific environmental medium, biotransfer factors express the steady-state relationship between intake and tissue or food-product concentrations.

Lactating women can transfer to breast milk their intake of contaminants from all intake routes—ingestion, inhalation, and dermal contact. B_{bmk} is the biotransfer factor for milk-concentration versus the mother's intake. This relationship may also be

described as the ratio of contaminant concentration in mother's milk divided by the mother's daily intake of that contaminant, in units of d/kg (milk).

The bioconcentration factor BCF provides a measure of chemical partitioning between fish tissue based on chemical concentration in water.

Chemical specific exposure factors used in CalTOX include the skin-water and skin-soil partition coefficients. K_m is the skin-water partition coefficient in cm^3 (water)/ cm^3 (skin) . In order to estimate the skin-soil partition factor, K_m^{soil} , with units $\text{cm}^3(\text{soil})/\text{cm}^3(\text{skin})$, we divide equation K_m by the sorption coefficient K_d for soil, or

$$K_m^{\text{soil}} = \frac{K_m}{K_d}$$

K_{p_w} is the steady-state permeability coefficient in cm/hour for a contaminant from water on skin through stratum corneum and can either be based on a measured value or estimated values.

Chemical-Specific Transformation Process Half-Lives

Chemical transformations, which may occur as a result of biotic or abiotic processes, can have a profound effect on the persistence of contaminants in the environment. Experimental methods and estimation methods are available for defining these fate processes in a variety of media. Specific information on the rates and pathways of transformation for individual chemicals of concern should be obtained directly from experimental determinations, if possible, or derived indirectly from information on chemicals that are structurally similar. CalTOX makes use of media- and reaction-specific reaction half-lives to establish rate constants for transformation removal processes that include photolysis, hydrolysis, oxidation/reduction, and microbial degradation.

Transformation-rate half-lives are among the more uncertain parameters in the CalTOX model. There are typically few available measurements or ranges of estimated values in the primary and secondary literature. Most of the available half-life values are obtained from limited measurements for environmental media that are not necessarily representative of those in California. These values often involve scientific judgment as much as measurement. In making use of these data, we expanded the range of the reported values by a factor of 5 when only 2 or 3 representative values are presented and by a factor of 10 when only one value is provided. If 4 or more measured values are available, these uncertainty factors are not applied. In order to express the lack of reliability associated with a limited number of measured values for a parameter, these uncertainty factors are used to express both large uncertainty and significant variability.

Statistical Methods

Each of the inputs to CalTOX must be described by a mean value and an estimated coefficient of variation which describes the uncertainty or variability associated with that parameter. For input values that are derived from a number of measured values, the mean and coefficient of variation are obtained from the arithmetic mean and the arithmetic standard deviation of the inputs. For estimated input values, the mean and coefficient of variation are obtained from an estimation equation and the residual error of the estimation equation. The methods we used to obtain these values are described here.

Mean and Coefficient of Variation

The arithmetic mean (\bar{x}) is used to represent all inputs that are derived from a number of measured values—even those that might have geometric distributions. The (\bar{x}) is computed by summing the reported values and dividing this sum by the total number of observations:

$$\text{Arithmetic mean } (\bar{x}) = \frac{\sum_{i=1}^n x_i}{n} \quad (\text{Eqn. 1})$$

Where $\sum_{i=1}^n x_i$ is the sum of the observed values and n is the number of observations. In this case, the coefficient of variation (CV) is computed by dividing the arithmetic standard deviation (S_n) by the mean. Standard deviation and CV are computed according to the following equations:

$$\text{standard deviation } (S_n) = \sqrt{\frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n}} \quad (\text{Eqn. 2})$$

$$\text{coefficient of variation } (CV) = \frac{S_n}{\bar{x}} \quad (\text{Eqn. 3})$$

It should be noted that, based on the central limit theorem of statistics, the confidence associated with the estimate of \bar{x} from above becomes large as the number of samples used to estimate \bar{x} also becomes large. Therefore, the reliability of the estimates of *mean* and *CV* of a parameter are low when the sample size is small. It is beyond the scope of this document to explicitly address the reliability of these estimates.

Nonetheless, in order to give an indication of potential reliability problems, we list the number of measurements used to estimate the mean and CV of each parameter in the last column of Table 1.

Estimation Equations and the Residual Errors of the Estimation Method

Estimates of some CalTOX inputs are based on regression equations that relate a parameter value to some measure of structure or activity associated with the contaminant. These methods are referred to as quantitative structure-activity relationship (QSAR) methods. The reliability of a parameter-value estimated in this way is defined by the precision of these QSAR methods.

Our estimate of precision in QSAR estimation methods is based on calculating, S_e , the *standard error of the estimate* (or standard deviation of the residuals). This error calculation is based on the regression equations and fragment models used to derive a parameter value. To illustrate, when the value of parameter such as the organic-carbon partition coefficient (K_{oc}) is estimated using a regression or correlation analysis, the S_e is calculated using the following approach (Hamburg, 1970). First, since it is typical that it is the $\log K_{oc}$ (not K_{oc} itself) that is estimated from a regression equation, we calculate the S_e of $\log K_{oc}$ according to

$$S_e \text{ of } \log K_{oc}^{est} = \sqrt{\frac{\sum_{i=1}^n (\log K_{oc}^{msd} - \log K_{oc}^{est})^2}{(n-2)}} \quad (\text{Eqn. 4})$$

where n is the number of chemicals used in the estimation protocol and K_{oc}^{est} refers to the estimated property (K_{oc} in this case) and K_{oc}^{msd} refers to the corresponding measured values used to carry out the regression. In order to calculate the S_e of K_{oc} we make use of the transformation

$$\text{GSD} (K_{oc}^{est}) = 10^{(S_e \text{ of } \log K_{oc}^{est})} \quad (\text{Eqn. 5})$$

to calculate the geometric standard deviation of S_e (GSD) of K_{oc}^{est} , which is simply the GSD of the K_{oc} estimate, that is $\text{GSD} (K_{oc}^{est})$. It has been shown by Atchison and Brown (1957) that the relationships between the GSD and CV for log normal distributions are as follows

$$\text{GSD} = \exp\{\sqrt{\ln(1+CV^2)}\} \quad (\text{Eqn. 6})$$

$$CV = \sqrt{\left(\exp\{[\ln(\text{GSD})]^2\} - 1\right)} \quad (\text{Eqn. 7})$$

Since the implicit assumption of a regression for estimating the log of K_{oc} is that any estimated value, $\log(K_{oc}^{est})$, is centered on normal distribution with standard deviation equal to S_e of $\log K_{oc}$ it follows that the corresponding estimated value of K_{oc} is centered on a log normal distribution with GSD (K_{oc}^{est}) and with

$$CV(K_{oc}^{est}) = \sqrt{\exp\{[\ln(\text{GSD}(K_{oc}^{est}))]^2\} - 1} \quad (\text{Eqn. 8})$$

This approach is used to estimate CVs for the estimation equations presented in this document.

In some cases the error term, CV for example, is calculated by combining through the operations of multiplication and division the CVs of two or more parameters. For example the CV in the ration $H = VP/S$ is combined from the CV (VP) and CV (S). In this case, if the input parameters are independent, the combined CV is calculated using the following equation:

$$CV_{\text{combined}} = \sqrt{\frac{\sum_{i=1}^n CV_i^2}{n}} \quad (\text{Eqn. 9})$$

where n is the number of parameters used in the multiplication/division and CV_i is the coefficient of variation in the i th input parameter.

2,3,7,8-Tetrachlorodibenzo-p-dioxin

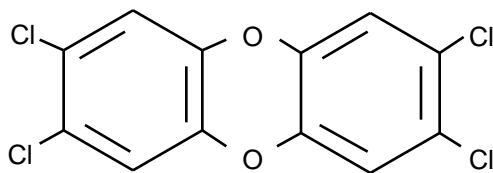
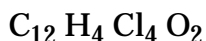
Other Names:

TCDD; 2,3,7,8-TCDD; 2,3,7,8-tetrachlorodibenzo-1,4-dioxin; 2,3,7,8-tetrachlorodibenzo (b,e) (1,4) dioxin; TCDBD; 2,3,6,7-tetrachlorodibenzo-p-dioxin; tetradoxin; dioxin; dioxine (Sax and Lewis, 1989)

Background:

TCDD is a trace contaminant of chlorophenols and products synthesized from chlorophenols. It has been associated with the manufacture of hexachlorophene; 2,4,5-T; 2,4-D and other pesticides having these compounds as precursors. Other sources of TCDD are pulp and paper manufacturing, incineration of municipal and industrial wastes, accidental transformer fires and accidental industrial explosions (Sittig, 1985). Similar to some of the chlorinated hydrocarbon insecticides, TCDD is fairly persistent and immobile in soil. Vertical movement of TCDD does not occur in a wide range of soil types (Kearney et al., 1973a). Although pesticides currently produced commercially contain lower concentrations of dioxin containing contaminants; past production, disposal and industrial waste sites remain as sources of exposure.

Formula:



MW: Molecular Weight

The units used for molecular weight are grams/mole (g/mol).

Reported Values

321.96	reported as 321.96 g/mol by Merck et al. [CRC Handbook (1989)]
321.974	reported as 321.974 g/mol by IUPAC (1979)
322	reported as 322 g/mol by WHO IARC (1977)
322.0	reported as 322.0 g/mol by Mackay et al. (1992)

From the 4 values reported above, we obtain the following statistics for the molecular weight of TCDD:

Arithmetic mean (coefficient of variation):
 MW = 322 (6.2×10^{-5}) g/mol

Range: 321.96 to 322 g/mol

K_{ow}: Octanol-Water Partition Coefficient

The units used for K_{ow} are $\frac{\text{mg/liter (octanol)}}{\text{mg/liter (water)}}$ and K_{ow} is therefore unitless.

Reported Values

- 1.4 × 10⁶ reported as a K_{ow} of 1.4 × 10⁶ by Kenaga (1980)
- 2.49 × 10⁶ to 6.38 × 10⁶ reported at 22 °C as a K_{ow} of 2.485 × 10⁶ to 6.375 × 10⁶ by Marple et al. (1986) using 2 separate cell types and the equilibration-GC/Low Resolution Mass Spectrometry (LRMS) method for 15 to 31 days
- 2.63 × 10⁶ reported as a log K_{ow} of 6.42 by Sijm et al. (1989a) using the slow stirring-GC/MSD method [Also cited in Mackay et al. (1992)]
- 4.37 × 10⁶ reported at 25 °C as a log K_{ow} of 6.64 by Isnard and Lambert (1989)
- 1.05 × 10⁷ reported as a log K_{ow} of 7.02 by Burkhard and Kuehl (1986) estimated using a reverse-phase HPLC-RT method [Also cited in Mackay et al. (1992)]

From the 6 measured values above we obtain the following statistics for the octanol-water partition coefficient of TCDD:

Arithmetic mean (coefficient of variation):
 K_{ow} = 4.6 × 10⁶ (0.73)

Range: 1.4 × 10⁶ to 1.05 × 10⁷

T_m: Melting Point

The units used for melting point are kelvins (K).

Reported Values

- 575 to 578 reported as a MP of 575 to 578 K by Sittig (1985)

576 to 578	reported as a MP of 303 to 305 °C by Crummett and Stehl (1973)
578	reported as a MP of 578 K by Boer et al. (1972)
578	reported as a MP of 305 °C by Schroy et al. (1985)
578 to 579	reported as a MP of 578 to 579 K by Pohland & Yang (1972) [Also cited in Mackay et al. (1992)]
579	reported as a MP of 579 K by Branson et al. (1985) [Also cited in Mackay et al. (1992)]
580	reported as a MP of 580 K by Crosby (1985)

From the 10 reported values above, we obtain the following statistics for the melting point of TCDD:

Arithmetic mean (coefficient of variation):
 $T_m = 578 (0.0025) \text{ K}$

Range: 575 to 580 K

VP: Vapor Pressure at Standard Temperatures

The units used for vapor pressure are pascals (Pa).

Experimental Values

9.87×10^{-8}	reported at 25 °C as 7.4×10^{-10} torr by Podoll et al. (1986) using an average of 5 measurements and the ^{14}C -gas saturation method [Also cited in Mackay et al. (1992)]
2.02×10^{-7}	reported at 25 °C as an vapor pressure of 2.02×10^{-7} Pa by Schroy et al. (1985) estimated using 303 to 328 K, an Antoine equation and a gas saturation-GC/MS method
4.5×10^{-6}	reported at 25 °C as 4.5×10^{-6} Pa by Rordorf (1985) by the gas saturation-GC method [Also cited in Mackay et al. (1992)]

From the 3 measured values above, we obtain the following statistics for vapor pressure at 25 °C:

Arithmetic mean (coefficient of variation):
 $\text{VP} = 1.6 \times 10^{-6} (1.6) \text{ Pa}$

Range: 9.87×10^{-8} to 4.5×10^{-6} Pa

Estimation Method

Schroy et al. (1984) has developed an Antoine equation relating vapor pressure to temperature for TCDD in the temperature range 303 to 328 K. This equation yields the following estimation for the VP of TCDD in Pascals at 25 °C:

$$\ln VP = 34.57083 - \frac{14903.438}{273.15 + T (^{\circ}\text{C})}$$

$$VP (\text{est}) = 2.02 \times 10^{-7} \text{ Pa at } 25 ^{\circ}\text{C}$$

S: Solubility in Water

The units used in the solubility values below are $\frac{\text{mg}}{\text{liter (water)}}$ (mg/L).

Experimental Values

- 7.97×10^{-6} reported at 25 °C as 7.97×10^{-6} mg/l by Adams and Blaine (1986) using an ^3H -TCDD method
- 1.25×10^{-5} reported at 25 °C as 12.5 parts per trillion by Marple et al. (1986a) using ^{14}C -gas chromatogram/low resolution mass spectroscopy (GC/LRMS) method
- 1.93×10^{-5} reported at 25 °C as 19.3 parts per trillion by Marple et al. (1986a) using the GC/LRMS method [Also cited in Mackay et al. (1992)]
- 2×10^{-4} reported at 25 °C as 2×10^{-7} g/100g water by Crummett and Stehl (1973) using a GC/electron capture detector (GC/ECD) method [Also cited in Mackay et al. (1992)]

Unit Conversion

Arithmetic mean (coefficient of variation) of TCDD solubility

$$= 6 \times 10^{-5} (1.6) \text{ mg/L}$$

$$= 1.86 \times 10^{-7} (1.6) \text{ mol/m}^3$$

From the 4 measured values above, we obtain the following statistics for the water solubility of TCDD at 25 °C:

Arithmetic mean (coefficient of variation):

$$S = 1.9 \times 10^{-7} (1.6) \text{ mol/m}^3$$

Range: 2.48×10^{-8} to 6.21×10^{-7} mol/m³

H: Henry's Law Constant

The units used for Henry's Law constant are $\frac{\text{Pascals}\cdot\text{m}^3}{\text{mole}}$ (Pa·m³/mol).

No experimental values for Henry's-law constant are available in the current literature, estimation methods are therefore considered below.

Estimation Method 1

Henry's law constant may be estimated by dividing the vapor pressure by the solubility, as in the following equation:

$$H = \frac{VP \text{ (Pa)}}{S \text{ (mol/m}^3\text{)}}$$

- | | |
|-------|--|
| 0.152 | calculated at 25 °C and reported as 0.152 Pa·m ³ /mol by Crosby (1985) using vapor pressure and solubility values [also cited by Mackay (1992)] |
| 0.21 | calculated at 25 °C and reported as 2.1 × 10 ⁻⁶ atm·m ³ /mol by Schroy et al. (1985a) using vapor pressure and solubility values [also cited by Mackay (1992)] |
| 1.60 | calculated at 25 °C and reported as 12 torr·M ⁻¹ by Podoll et al. (1986) using vapor pressure and solubility values [also cited by Mackay (1992)] |
| 7.9 | calculated at an indefinite temperature and reported as as 0.0032 dimensionless by Jury (1990) using vapor pressure and solubility values |

<p>From the 4 estimated values above, we obtain the following statistics for Henry's law constant at 25 °C:</p> <p style="text-align: center;">Arithmetic mean (coefficient of variation): H = 2.5 (1.5) Pa·m³/mol</p> <p style="text-align: center;">Range: 0.15 to 7.9 Pa·m³/mol</p>
--

Estimation Method 2

We estimate Henry's law constant using values derived in this report:

$$H = \frac{VP}{S} = \frac{1.6 \times 10^{-6} \text{ Pa}}{1.9 \times 10^{-7} \text{ mol/m}^3}$$

$$H \text{ (est)} = 8.6 \text{ Pa}\cdot\text{m}^3/\text{mol}$$

$$CV_{\text{pooled}} = 1.6$$

D_{air}: Diffusion Coefficient in Pure Air

The units used for the diffusion coefficient in pure air are $\frac{\text{meters}^2}{\text{day}}$ (m^2/d).

Estimation Method

Based on the Fuller et al. (1966) method described in Lyman et al. (1982), the estimated diffusion coefficient in air (m^2/d) is given by:

$$D_{\text{air}} = 8.6 \times 10^{-3} T^{1.75} \frac{\sqrt{(29 + M_x)/(29 \times M_x)}}{[2.7 + V_x^{1/3}]^2}$$

Molar volume (V_x) can be estimated by the LeBas incremental method as described in Lyman et al. (1982) With a molar volume, V_x , of $275.6 \text{ cm}^3/\text{mol}$, molecular weight (M_x) of 322 g/mol , and a temperature equal to 298 K ; the above expression gives:

$$D_{\text{air}} = 1.97 \times 10^{-5} T^{1.75} = 0.42 \text{ m}^2/\text{d}$$

The reported average absolute estimation error is 5 to 10% (Fuller et al., 1966). This estimation error is equivalent to the CV reported below.

Based on the estimated value and the estimation error reported above, we obtain the following statistics for the estimated air diffusion coefficient of TCDD at $25 \text{ }^\circ\text{C}$:

Arithmetic mean (coefficient of variation):

$$D_{\text{air}} = 0.42 (0.08) \text{ m}^2/\text{d}$$

D_{water}: Diffusion Coefficient in Pure Water

The units used for the diffusion coefficient in pure water are $\frac{\text{meters}^2}{\text{day}}$ (m^2/d).

Estimation Method

Based on the Wilke and Chang (1955) method described in Reid et al. (1987) the diffusion coefficient in water (m^2/d) is given by:

$$D_{\text{water}} = \frac{6.5 \times 10^{-7} \sqrt{f \times M_y} T}{h_y V_x^{0.6}}$$

Wilke and Chang (1955) recommend an association factor, f , of 2.6 when the solvent is water. The viscosity of water, h_y , is 0.89 cP at 25 °C. Molar volume (V_x) can be estimated by the LeBas incremental method as described in Lyman et al. (1982). With a V_x equal to 275.6 cm³/mol, a temperature (T) of 298 K (25 °C), and M_y (MW of water) equal to 18 g/mol., this expression gives:

$$D_{\text{water}} = 1.72 \times 10^{-7} T = 5.11 \times 10^{-5} \text{ m}^2/\text{d at } 25 \text{ }^\circ\text{C}$$

Data provided in Reid et al. (1987) can be used to determine the standard error of the estimator for this estimation method. From this data we calculate a 25% estimation error corresponding to a CV of 0.25.

Based on the estimated value and the estimation error reported above, we obtain the following statistics for the estimated water diffusion coefficient of TCDD at 25 °C:

Arithmetic mean (coefficient of variation):

$$D_{\text{water}} = 5.1 \times 10^{-5} (0.25) \text{ m}^2/\text{d}$$

K_{oc} : Organic-Carbon Partition Coefficient

The units used for K_{oc} are $\frac{\text{mg/kg (organic carbon)}}{\text{mg/kg (water)}}$ and K_{oc} is therefore unitless.

Experimental Values

- 5.75×10^4 derived from a log K_{oc} of 4.76 measured by Puri et al. (1989) from the sandy silt (45%/35%) soil (pH 8.5) of Visalia, CA [Also cited in Mackay et al. (1992)]
- 7.24×10^5 reported as a log K_{oc} of 5.86 measured by Puri et al. (1989) from a silt/clay (53%/33%) soil (pH 7) of Times Beach, MO [Also cited in Mackay et al. (1992)]
- 1.74×10^6 reported as a log K_{oc} of 6.24 measured by Puri et al. (1989) from a sandy soil (pH 4) of Eglin Air Force Base, FL [also cited in Mackay et al. (1992)]
- 2.00×10^6 reported as a log K_{oc} of 6.3 measured by Lodge and Cook (1989) from sediment collected in Lake Ontario [Also cited in Mackay et al. (1992)]

- 3.98×10^6 reported as a log K_{oc} of 6.6 measured by Walters and Guiseppi-Elie (1989) with ^{14}C labeled soil using batch equilibrium and a gas chromatogram/electron capture detector (GC/ECD) in a methanol/water solution [Also cited in Mackay et al. (1992)]
- 4.61×10^6 reported as a K_d of 30400 ml/g by Walters et al. (1989) using ^{14}C -TCDD and soil (pH=6.8, f_{oc} =0.0066) in a batch equilibrium GC/ECD method
- 2.45×10^7 reported as a log K_{oc} of 7.39 measured by Jackson et al. (1986) using average values in 10 soils from NJ and MO

From the 7 measured values above, we obtain the following statistics for the organic carbon partition coefficient of TCDD:

Arithmetic mean (coefficient of variation):
 $K_{oc} = 5.4 \times 10^6$ (1.6)

Range: 5.75×10^4 to 2.45×10^7

Estimation Method

Karickhoff (1981) has described empirical estimation methods for obtaining K_{oc} from K_{ow} . The most general of these is that K_{oc} is equal to 0.41 times K_{ow} .

$$K_{oc} = 0.41 \times K_{ow}$$

$$K_{ow} = 4.6 \times 10^6$$

$$K_{oc} \text{ (est)} = 1.9 \times 10^6 \text{ (1)}$$

The reported CV is based on data provided by Karickhoff (1981). This estimation error does not include uncertainty in the value of K_{ow} .

K_{d_s} : Distribution Coefficient in Ground-Surface and Root-Zone Soil

The units used for K_{d_s} are $\frac{\text{mg/kg (dry surface and root-zone soil)}}{\text{mg/kg (water)}}$ and K_{d_s} is therefore unitless.

Estimation Method

This is a site specific parameter and depends on the fraction organic carbon in the surface and root-zone soil and on the value of K_{oc} . K_{d_s} is the product of the soil organic carbon partition coefficient (K_{oc}) and the fraction organic carbon in the surface and root-zone soil (f_{oc_s}) (Karickhoff, 1981).

$$K_{d_s} = K_{oc} \times f_{oc_s}$$

$$f_{oc_s} = \frac{\text{kg organic carbon (dry surface and root-zone soil)}}{\text{kg (soil)}}$$

Based on the estimation reported above, we obtain the following equation for the distribution coefficient in surface and root-zone soil. K_{d_s} is a site and soil-zone specific parameter depending on the fraction organic carbon in the surface and root-zone soil or:

$$K_{d_s} = K_{oc} \times f_{oc_s}$$

K_{d_v} : Distribution Coefficient in Vadose-Zone Soil

The units used for K_{d_v} are $\frac{\text{mg/kg (dry vadose-zone soil)}}{\text{mg/kg (water)}}$ and K_{d_v} is therefore unitless.

Estimation Method

This is a site specific parameter and depends on the fraction organic carbon in the vadose-zone soil and on the value of K_{oc} . K_{d_v} is the product of the soil organic carbon partition coefficient (K_{oc}) and the fraction organic carbon in the vadose-zone soil (f_{oc_v}) (Karickhoff, 1981).

$$K_{d_v} = K_{oc} \times f_{oc_v}$$

$$f_{oc_v} = \frac{\text{kg organic carbon (dry vadose-zone soil)}}{\text{kg (soil)}}$$

Based on the estimation reported above, we obtain the following equation for the distribution coefficient in vadose-zone soil. K_{d_v} is a site and soil-zone specific parameter depending on the fraction organic carbon in the vadose-zone or:

$$K_{d_v} = K_{oc} \times f_{oc_v}$$

K_{d_q}: Distribution Coefficient in the Ground-Water Zone

The units used for K_{d_q} are $\frac{\text{mg/kg (dry aquifer material)}}{\text{mg/kg (water)}}$ and K_{d_q} is therefore unitless.

Estimation Method

This is a site-specific parameter and depends on the fraction organic carbon in the ground-water zone and on the value of K_{oc}. K_{d_q} is the product of the soil organic carbon partition coefficient (K_{oc}) and the fraction organic carbon in the ground-water zone (f_{oc_q}) (Karickhoff, 1981).

$$K_{d_q} = K_{oc} \times f_{oc_q}$$

$$f_{oc_q} = \frac{\text{kg organic carbon (dry aquifer material)}}{\text{kg (solid)}}$$

Based on the estimation reported above, we obtain the following equation for the distribution coefficient in the ground-water zone. K_{d_q} is a site and soil-zone specific parameter depending on the fraction organic carbon in the ground-water zone or:

$$K_{d_q} = K_{oc} \times f_{oc_q}$$

K_{d_d}: Distribution Coefficient in Sediment Particles

The units used for K_{d_d} are $\frac{\text{mg/kg (dry surface-water sediment)}}{\text{mg/kg (water)}}$ and K_{d_d} is therefore unitless.

Estimation Method

This is a site specific parameter and depends on the fraction organic carbon in the surface-water sediment and the value of K_{oc}. K_{d_d} is the product of the soil organic carbon partition coefficient (K_{oc}) and the fraction of organic carbon in surface-water sediment (f_{oc_d}) [Karickhoff, 1981].

$$K_{d_d} = K_{oc} \times f_{oc_d}$$

$$f_{oc_d} = \frac{\text{kg organic carbon (dry surface-water sediment)}}{\text{kg (soil)}}$$

Based on the estimation reported above, we obtain the following equation for the distribution coefficient in surface-water sediment particles. K_{d_d} is a site and soil-zone specific parameter depending on the fraction organic carbon in surface-water sediment or:

$$K_{d_d} = K_{oc} \times f_{oc_d}$$

K_{ps} : Partition Coefficient for Plant-Tissue (Above Ground Fresh Mass) Relative to Soil Concentration (Fresh Soil)

The units used for K_{ps} are $\frac{\text{mg/kg (plant fresh mass [pFM])}}{\text{mg/kg (soil fresh mass [sFM])}}$ (ppm [pFM]/ppm [sFM]).

Experimental Values

- 0.2539 reported as a plant/soil contamination ratio corresponding to 0.2539 ppm (pFM)/ppm (sFM) by Cocucci et al. (1979) using potato plants grown in contaminated soil in Seveso, Italy 1 year after soil contamination
- 0.3116 reported as a plant/soil contamination ratio corresponding to 0.3116 ppm (pFM)/ppm (sFM) by Cocucci et al. (1979) using onion plants grown in contaminated soil in Seveso, Italy 1 year after soil contamination
- 0.3794 reported as a plant/soil contamination ratio corresponding to 0.3794 ppm (pFM)/ppm (sFM) by Cocucci et al. (1979) using narcissus plants grown in contaminated soil in Seveso, Italy 1 year after soil contamination
- 0.4049 reported as a plant/soil contamination ratio corresponding to 0.4049 ppm (pFM)/ppm (sFM) by Cocucci et al. (1979) using carrot plants grown in contaminated soil in Seveso, Italy 1 year after soil contamination

From the 4 values above, we obtain the following statistics for the partition coefficient in plant tissue relative to contaminant soil concentration of TCDD:

Arithmetic mean (coefficient of variation):
 $K_{ps} = 0.34$ (0.20) ppm (sFM)/ppm (pFM)

Range: 0.2539 to 0.4049

Other Values

- 0.0015 to 0.0075 is the range of values of this partition factor from surface soil to edible plant parts due to rain splash, K_{ps}^{rain} in Dreicer et al. (1984)

Estimation Method

Based on a review of reported measurements of bioconcentration for 29 persistent organochlorines in plants, Travis and Arms (1988) have correlated plant-soil bioconcentration (on a dry-mass basis) in above-ground plant parts with octanol-water partition coefficients. This bioconcentration factor, B_v , on a dry-weight basis is expressed as:

$$\log B_v = 1.58 - 0.58 \log K_{ow} \pm 0.73 \quad (n = 29, r^2 = 0.525)$$

We calculated the error term, ± 0.73 , from the mean square error of the estimator for this regression from the data provided by Travis and Arms (1988). When adjusted to a fresh-mass basis (assuming that the plant dry-mass fraction equals 0.2), this estimation equation gives the plant-soil partition coefficient, K_{ps} . Expressing the ratio of contaminant concentration as mg/kg in above-ground plant fresh mass relative to contaminant concentration in mg/kg (dry soil) in the root-zone, K_{ps} , is:

$$K_{ps} = 7.7 K_{ow}^{-0.58} \text{ ppm (sDM) / ppm (pFM)}$$

Assuming fresh root-zone soil is 10% water by mass, the K_{ps} in the root-zone soil becomes:

$$K_{ps} = 7.0 K_{ow}^{-0.58} \text{ ppm (sFM) / ppm (pFM)}$$

Arithmetic mean (coefficient of variation) of K_{ps} estimation:

$$K_{ps} \text{ (est)} = 0.0098 \text{ (4.0) ppm (sFM) / ppm (pFM)}$$

$$CV = 4$$

The estimation error reported above corresponds to a CV of 4.

 K_{pa} : Biotransfer Factors For Plant Leaves Relative to Contaminant Air Concentration

The units used for K_{pa} are $\frac{\text{mg/kg (plant fresh mass [pFM])}}{\text{mg/cubic meter of air (m}^3 \text{ [air])}} \text{ (m}^3 \text{ [a]/kg [pFM])}$

Experimental Value

1.03×10^4 to 4.11×10^4 reported at 25 to 35 °C as a theoretical log air to grass bioconcentration factor of 6.9 to 7.5 v/v by McCrady and Maggard (1993) using reed canarygrass [*Phalaris arundinacea* L.; 770g (pFM)/L (pFM)] and $^3\text{H-TCDD}$ for 8 days with and without photodegradation

From the 2 experimental values reported above, we obtain the following statistics for the partition coefficient in plant leaves relative to contaminant concentration in air for TCDD:

Arithmetic mean (coefficient of variation):
 $K_{pa} = 2.6 \times 10^4 (0.85) \text{ m}^3 \text{ [a]/kg [pFM]}$

Range: 1.03×10^4 to $4.11 \times 10^4 \text{ m}^3 \text{ [a]/kg [pFM]}$

Estimation Method

Based on the model of Riederer (1990) for foliar uptake of gas-phase contaminants (mg/m^3) relative to contaminant concentration in plant leaves (mg/kg fresh mass), we estimate a steady-state plant-air coefficient as:

$$K_{pa} (\text{m}^3 \text{ [a]/kg [pFM]}) = [0.5 + ((0.4 + 0.01 \times K_{ow})(RT/H))] \times 10^{-3} \text{ kg}/\text{m}^3$$

$$R = 8.313 \text{ Pa}\cdot\text{m}^3/\text{mol}\cdot\text{K}$$

$$T = 298 \text{ K}$$

$$H = 2.5 \text{ Pa}\cdot\text{m}^3/\text{mol}$$

$$K_{ow} = 4.6 \times 10^6$$

$$K_{pa} (\text{est}) = 4.6 \times 10^4 \text{ m}^3 \text{ [a]/kg [pFM]}$$

$$CV = 14$$

McKone (1993) has estimated that the CV associated with this partition estimation model is on the order of 14.

BIOTRANSFER FACTORS FOR FOOD PRODUCTS

The biotransfer factors B_t , B_k and B_e are the steady-state contaminant concentrations in, respectively; fresh meat, milk, and eggs; divided by the animals daily contaminant intake, and are expressed in units of $(\text{mg}/\text{kg})/(\text{mg}/\text{d})$ or d/kg .

B_k : Steady-State Biotransfer Factors for Whole Milk Relative to Contaminant Intake by Cattle

The units used for B_k are days/kg (milk) (d/kg [milk]).

Experimental Values

2.67×10^{-4} to 1.20×10^{-3} reported as a milk-fat uptake concentration of 4 to 18 ng/kg in cows grazing on dry hay contaminated with 10 ng/kg 2,3,7,8-TCDD by Riss et al. (1990); assuming milk is 4% fat and a feed consumption of 60 kg plant dry mass (pDM)/day

7.70×10^{-3} to reported as an average whole milk TCDD concentration of 63 and 73.5
 8.99×10^{-3} parts per trillion (ppt) by Jensen and Hummel (1982) using 500 ppt in
 feed for 16 and 21 days, respectively, and a feeding rate of 16 kg plant
 fresh mass (pFM)/d

From the 4 values above, we obtain the following statistics based the steady-state biotransfer factor for whole milk relative to contaminant intake by cattle and on combined variance for TCDD:

Arithmetic mean (coefficient of variation):

$$B_k = 4.5 \times 10^{-3} (0.98) \text{ days/kg (milk)}$$

Range: 2.67×10^{-4} to 8.99×10^{-3} days/kg (milk)

Estimation Method 1

Based on a review of biotransfer factors for 28 organic chemicals in milk Travis and Arms (1988) developed the following geometric-mean regressions for B_{k1} based on the octanol-water partition coefficient, K_{ow} ,

$$\log B_{k1} = \log K_{ow} - 8.1 \pm 0.84 (n = 28, r^2 = 0.55)$$

Using the data provided by Travis and Arms (1988), we calculated the error term, ± 0.84 , from the mean square error of the estimator for this regression. This estimation error corresponds to a CV of 6. From the above expression and $\log K_{ow}$ of 6.6, we obtain the following statistics for the B_{k1} of TCDD:

$$B_{k1} (\text{est}) = 0.037 \text{ days/kg (milk)}$$

$$CV = 6$$

Estimation Method 2

The transfer of organic chemicals from diet to milk has also been expressed in terms of the fat-diet partition coefficient, K_{fd} , which is the steady-state ratio of contaminant concentration in animal fat (or lipid) to contaminant concentration in animal diet with units kg(diet)/kg(fat). Kenaga (1980a) reviewed cattle-dietary feeding studies for 23 chemicals, and from these studies derived the following fat-diet equation relating K_{fd} to K_{ow} ,

$$\log K_{fd} = 0.5 \log K_{ow} - 3.457 \pm 1 (n = 23, r^2 = 0.62)$$

The estimation error in this expression, ± 1 , was calculated by Kenaga (1980a). From the above expression with $\log K_{ow}$ of 6.6, an assumed pasture intake by dairy cattle of 85 kg/d (McKone and Ryan, 1989), and an assumed fat content of 0.04 in milk; we obtain the following statistics for the B_{k2} of TCDD:

$$B_{k2} \text{ (est)} = 3.53 \times 10^{-4} \text{ days/kg (milk)}$$

$$CV = 14$$

The above estimation error corresponds to assumed CV of 14.

From the 2 estimations above and their corresponding CVs, we obtain the following statistics based the steady-state biotransfer factor for cow's milk relative to contaminant intake for TCDD:

$$B_k \text{ (est)} = 0.019 \text{ days/kg (milk)}$$

$$CV_{\text{pooled}} = 11$$

B_t : Steady-State Biotransfer Factor for Meat Relative to Contaminant Intake by Cattle

The units used for B_t are days/kg (meat) (d/kg [meat]).

Experimental Value

- 0.24 reported as a cattle feed/meat fat bioaccumulation by Jensen et al. (1981) using an average daily feed intake of 5.83 kg plant fresh mass (pFM)/d and a concentration of 24 parts per trillion (ppt) pFM and a TCDD fat concentration of of 84 ppt; assuming a cattle meat is 40% fat by weight

From the value above, and the experimental error, we obtain the following statistics for the steady-state biotransfer factor for meat relative to contaminant intake by cattle:

$$\text{Arithmetic mean (coefficient of variation):}$$

$$B_t = 0.24 (0.14) \text{ days/kg (meat)}$$

Estimation Method 1

Based on a review of biotransfer factors for 36 chemicals in meat, Travis and Arms (1988) developed the following geometric-mean regression for B_{t1} based on the octanol-water partition coefficient, K_{ow} ,

$$\log B_{t1} = \log K_{ow} - 7.6 \pm 0.95 \text{ (n = 36, } r^2 = 0.67)$$

Using the data provided by Travis and Arms (1988), we calculated the error term, ± 0.95 from the mean square error of the estimator for this regression. This estimation error corresponds to a CV of 11. From the above expression and a log K_{ow} equal to 6.6, we obtain the following estimation:

$$B_{t1} \text{ (est)} = 0.12 \text{ days/kg (meat)}$$

$$CV = 11$$

Estimation Method 2

The transfer of organic chemicals from diet to meat has also been expressed in terms of the fat-diet partition coefficient, K_{fd} , which is the steady-state ratio of contaminant concentration in animal fat (or lipid) to contaminant concentration in animal diet with units kg(diet)/kg(fat). Kenaga (1980a) reviewed cattle-dietary feeding studies for 23 chemicals, and from these studies derived the following fat-diet equation relating K_{fd} to K_{ow} :

$$\log K_{fd} = 0.5 \log K_{ow} - 3.457 \pm 1 \text{ (n = 23, } r^2 = 0.62)$$

The estimation error in this expression, ± 1 , was calculated by Kenaga (1980a). From the above expression with log K_{ow} equal to 6.6, an assumed pasture intake by beef cattle of 60 kg/d (McKone and Ryan, 1989), and an assumed fat content of 0.4 in meat; we obtain the following estimation:

$$B_{t2} \text{ (est)} = 0.0050 \text{ days/kg (meat)}$$

$$CV = 14$$

The above estimation error corresponds to a CV of 14.

From the 2 estimations above and their corresponding CVs, we obtain the following statistics based the steady-state biotransfer factor for cattle meat relative to contaminant intake for TCDD:

$$B_t \text{ (est)} = 0.061 \text{ days/kg (meat)}$$

$$CV_{\text{pooled}} = 11$$

B_e : Steady-State Biotransfer Factors for Egg Relative to Dietary Contaminant Intake by Chickens

The units used for B_e are days/kg (eggs) (d/kg [eggs]).

No reported measurements of egg-diet biotransfer for TCDD are available in the current literature. An estimation method is therefore considered.

Estimation Method

Based on measurements of polychlorodibenzodioxins (PCDDs) and polychlorodibenzo-furans (PCDFs) concentrations in soil versus concentrations in egg-fat and adipose tissue of foraging chickens, Stephens et al. (1990) have shown that contaminant concentrations in animal fat correlate with soil concentrations. In addition, they found the fat-soil partition factor in chicken fat is roughly six times higher than the fat-soil partition factor in cattle. However, the fraction of total intake represented by soil in the chicken diet is higher than in the cattle diet. Based on these observations and what is discussed in the above B_k and B_t sections, we (a) assume that the fat-diet partition factor in chickens is similar to that in cattle, (b) use $\log K_{fd} = \log K_{ow} - 4.9$ to estimate the K_{fd} for chickens, and (c) use the fat content of eggs (0.08) and feed intake of chickens (0.12 kg/d [fresh mass]) to obtain the following estimate of a biotransfer factor, B_e , from chicken diet to eggs with units d/kg (eggs):

$$\begin{aligned}\log B_e &= \log K_{ow} - 5.1 \\ \log K_{ow} &= 6.6\end{aligned}$$

$$B_e = 37 \text{ days/kg (eggs)}$$

We estimate the CV in this expression is 14.

Based on the estimation equation and the estimation error reported above, we obtain the following value for the estimated steady-state biotransfer factors for egg relative to dietary contaminant intake by chickens:

$$\begin{aligned}\text{Arithmetic mean (coefficient of variation):} \\ B_e &= 37 (14) \text{ days/kg (eggs)}\end{aligned}$$

B_{bmk} : Biotransfer Factor for Human Breast Milk Relative to Dietary Contaminant Intake by the Mother

The units used for B_{bmk} are days/kg (mothers milk) (d/kg [mothers milk]).

Estimation Method

No experimental results quantifying B_{bmk} are available in the current literature, an estimation method (Smith, 1987) is thus applied:

$$\begin{aligned}B_{bmk} &= 2 \times 10^{-7} K_{ow} \\ K_{ow} &= 4.6 \times 10^6\end{aligned}$$

$$B_{\text{bmk}} = 0.92 \text{ days/kg (mothers milk)}$$

The estimation error of the above method has a CV approximately equal to 10.

Based on the estimation equation and the estimation error reported above, we obtain the following value for the estimated biotransfer factor for human breast milk relative to dietary contaminant intake by the mother for TCDD:

Arithmetic mean (coefficient of variation):
 $B_{\text{bmk}} = 0.92 (10) \text{ days/kg (mothers milk)}$

BCF: Bioconcentration Factors for Fish Relative to Contaminant Water Concentration

The units used for BCF (fish/water) are $\frac{\text{mg/kg (fish)}}{\text{mg/liter (water)}}$, and BCF is therefore unitless.

Experimental Values:

- 2.67×10^3 reported as an average catfish (*Ictalurus punctuatus*)/water bioconcentration ratio of 2670 reported by Isensee (1978) using 0.66 and 239 parts per trillion TCDD in a model ecosystem for 6 days
- 7.39×10^3 reported as an average Mosquito fish (*Gambusia affinis*)/water bioconcentration ratio of 7393 reported by Isensee (1978) using 0.66 and 239 parts per trillion TCDD in a model ecosystem for 6 days
- 7.90×10^3 reported as a wet-weight fathead minnow/water BCF of 7900 by Adams (1986) using ^3H -TCDD at 1 ng/L for 28 days [also cited in Mackay et al. (1992)]
- 9.33×10^3 reported as a rainbow trout (*Salmo gairdneri*)/water log BCF of 3.97 by Branson et al. (1985) using 0.28 $\mu\text{g/L}$ [also cited in Mackay et al. (1992)]
- 1.30×10^4 reported as a Guppy (*Poecilia reticulata*)/water BCF of 1.3×10^4 by Opperhuizen et al. (1986)
- 2.67×10^4 reported as a rainbow trout (*Salmo gairdneri*)/water average BCF of 26700 by Mehrle et al. (1988) [also cited in Mackay et al. (1992)]
- 6.35×10^4 reported as a goldfish-lipid/water log BCF of 5.9 reported by Sijm et al. (1989) after 6 days and assuming a lipid content of 0.08 [also cited in Mackay et al. (1992)]

From the 7 measured values reported above, we obtain the following statistics for the bioconcentration in fish relative to contaminant concentration in water:

Arithmetic mean (coefficient of variation):
 $BCF = 1.9 \times 10^4$ (1.1)

Range: 2.67×10^3 to 6.35×10^4

Estimation Method

For fish, the BCF is taken as the ratio of concentration of a xenobiotic substance in fish flesh (or lipids) to the contaminant's concentration in water (Mackay, 1982). The BCF for neutral organic compounds can be estimated from regression equations based on selected physicochemical properties, particularly a compound's K_{ow} or aqueous solubility. Mackay (1982) recommends:

$$BCF = 0.048 \times K_{ow}$$

$$K_{ow} = 4.6 \times 10^6$$

$$BCF \text{ (est)} = 2.2 \times 10^5$$

$$CV = 0.6$$

The reported GSD is 1.8 which corresponds to an CV of 0.6.

K_{p_w} : Human Skin Permeability Coefficient Relative to Contaminant Concentration in Water

The units used for K_{p_w} are centimeters/hour (cm/hr).

Estimation Method

Because dermal transfer is considered a non steady-state event, diffusion models require input parameters which are difficult to measure, such as the stratum corneum diffusion coefficient (D_{sc}) [Flynn and Amidon, 1991]. Estimation of aqueous biotransfer of TCDD is calculated with the following equation based on the estimation method of McKone and Howd (1992).

$$K_{p_w} = MW^{-0.6} \left(0.33 + \frac{0.0025}{2.4 \times 10^{-6} + 3 \times 10^{-5} K_{ow}^{0.8}} \right)^{-1}$$

$$\log K_{ow} = 6.6$$

$$MW = 322 \text{ g/mol}$$

$$K_{p_w} = 0.010 \text{ cm/hr}$$

who report a CV equal to 2.4 in this estimate

Based on the estimation equation and the estimation error reported above, we obtain the following value for the estimated human skin permeability coefficient relative to contaminant water concentration for TCDD:

Arithmetic mean (coefficient of variation):

$$K_{p_w} = 0.010 (2.4) \text{ cm/hr}$$

K_m : Partition Coefficient for Human Skin Relative to Contaminant Concentration in Water or Soil

The units used for K_m are $\frac{\text{mg/kg (skin)}}{\text{mg/liter (water)}}$ (ppm [skin]/ppm [water]).

No experimental values for K_m are currently available in the literature, therefore an estimation method is considered.

Estimation Method

Experimental values quantifying dermal transfer of TCDD in water, or for water in a soil matrix, may depend on pH, particle size and organic carbon content (Flynn and Amidon, 1991). An estimation method based on McKone and Howd (1992) is therefore used here.

$$K_m = 0.64 + (0.25 K_{ow}^{0.8})$$

$$K_{ow} = 4.6 \times 10^6$$

$$K_m = 5.3 \times 10^4$$

The reported geometric standard deviation of 1.3 corresponds to a CV of 0.27.

Based on the estimation equation and the estimation error reported above, we obtain the following value for the partition coefficient into human skin relative to TCDD water or soil concentration:

Arithmetic mean (coefficient of variation):

$$K_m = 5.4 \times 10^4 (0.27)$$

T_{half_a}: Reaction Half-Life in Air

The units used for T_{half_a} are days.

Reported Values

- | | |
|---------|--|
| 0.89 | reported as a calculated gas phase hydroxyl radical reaction rate constant of 9×10^{-12} cm ³ /molecule-sec by Atkinson (1987) using photo-oxidation as a removal process and assuming a hydroxyl radical air concentration of 1×10^6 molecules/cm ³ |
| 5 to 24 | reported as an atmospheric half-life of 5 to 24 days by Nash and Beall (1980) using various ³ H-TCDD contaminated herbicides in chamber and field bluegrass (<i>Poa pratensis</i> L.) plots for 70 to 280 days |

From the 3 values reported above, and our assumption that the range of actual values could be a factor of 5 higher or lower than this range, we obtain the following statistics on the reaction half-life for TCDD in air:

Arithmetic mean (coefficient of variation):

$$T_{half_a} = 30 (1.7) \text{ days}$$

Range: 0.18 to 120 days

Other Values

- | | |
|-----|---|
| 1.8 | reported as a TCDD contaminated plant photooxidation half-life of 44 hours by McCrady and Maggard (1993) using vapor-phase TCDD in chromatography jars for 8 days |
|-----|---|

T_{half_g}: Reaction Half-Life in Ground-Surface Soil

The units used for T_{half_g} are days.

Reported Values

- | | |
|-----|--|
| 365 | reported as a TCDD degradation half-life of approximately 1 year by Di Domenico et al. (1980) using an initial calculated regression at 32 sites in Seveso, Italy. A half-life of >10 years is estimated for deeper soils. |
|-----|--|

394 to 708	reported at 28 to 30 °C as a TCDD degradation of 29 to 46% by Kearney et al. (1972, 1973) using unlabelled TCDD on two soils (loamy sand and silty clay loam) at concentrations of 1, 10 and 100 ppm for 350 days; assuming first-order kinetics
3609	reported as an estimated soil reaction rate constant of 8×10^{-6} hr ⁻¹ by Mackay et al. (1985)
3650 to 4380	reported as a half-life in soil of 10 to 12 years by Young (1981) estimated using soil concentration measurements from 2,4,5-T contaminated soil at Eglin Air Force Base, Florida; samples taken beginning 4 years after final contamination event

From the 6 values above, we obtain the following statistics for the reaction half-life for TCDD in surface soil:

Arithmetic mean (coefficient of variation):

$$T_{\text{half}_g} = 2200 (0.86) \text{ days}$$

Range: 365 to 4380 days

T_{half_s}: Reaction Half-Life in Root-Zone Soil

The units used for T_{half_s} are days.

Reported Values

365	reported as a TCDD degradation half-life of approximately 1 year by Di Domenico et al. (1980) using an initial calculated regression at 32 sites in Seveso, Italy. A half-life of >10 years is estimated for deeper soils.
394 to 708	reported at 28 to 30 °C as a TCDD degradation of 29 to 46% by Kearney et al. (1972, 1973) using unlabelled TCDD on two soils (loamy sand and silty clay loam) at concentrations of 1, 10 and 100 ppm for 350 days; assuming first-order kinetics
3609	reported as an estimated soil reaction rate constant of 8×10^{-6} hr ⁻¹ by Mackay et al. (1985)
3650 to 4380	reported as a half-life in soil of 10 to 12 years by Young (1981) estimated using soil concentration measurements from 2,4,5-T contaminated soil at Eglin Air Force Base, Florida; samples taken beginning 4 years after final contamination event
3650 to 36500	reported as a half-life of 10 years by Nauman and Schaum (1987) in near surface soil (and 100 years if TCDD buried at greater depth)

From the 8 values above, we obtain the following statistics for the reaction half-life for TCDD in root-zone soil

Arithmetic mean (coefficient of variation):

$$T_{\text{half}_s} = 6700 \text{ (1.8) days}$$

Range: 365 to 36500 days

T_{half_v}: Reaction Half-Life in Vadose-Zone Soil

The units used for T_{half_v} are days.

Reported Values

365	reported as a TCDD degradation half-life of approximately 1 year by Di Domenico et al. (1980) using an initial calculated regression at 32 sites in Seveso, Italy. A half-life of >10 years is estimated for deeper soils.
394 to 708	reported at 28 to 30 °C as a TCDD degradation of 29 to 46% by Kearney et al. (1972, 1973) using unlabelled TCDD on two soils (loamy sand and silty clay loam) at concentrations of 1, 10 and 100 ppm for 350 days; assuming first-order kinetics
3609	reported as an estimated soil reaction rate constant of $8 \times 10^{-6} \text{ hr}^{-1}$ by Mackay et al. (1985)
3650 to 4380	reported as a half-life in soil of 10 to 12 years by Young (1981) estimated using soil concentration measurements from 2,4,5-T contaminated soil at Eglin Air Force Base, Florida; samples taken beginning 4 years after final contamination event
3650 to 36500	reported as a half-life of 10 years by Nauman and Schaum (1987) in near surface soil (and 100 years if TCDD buried at greater depth)

From the 8 values above, we obtain the following statistics for the reaction half-life for TCDD in vadose-zone soil:

Arithmetic mean (coefficient of variation):

$$T_{\text{half}_v} = 6700 \text{ (1.8) days}$$

Range: 365 to 36500 days

T_{half_q}: Reaction Half-Life in Groundwater

The units used for T_{half_q} are days.

Reported Values

836 to 1180	reported as an estimated half-life of 2.29 to 3.23 years by Howard et al. (1991) using scientific judgement and an aerobic biodegradation half-life in soil by Kearney et al. (1972)
1672 to 2360	reported as an estimated anaerobic half-life of 4.58 to 6.45 years by Howard et al. (1991) using scientific judgement and data from an unacclimated aqueous(water/sediment) aerobic biodegradation half-life by Ward and Matsumura (1978)

From the 4 values above, and our assumption that the range of actual values could be a factor of 5 higher or lower than this range, we obtain the following statistics for the reaction half-life for TCDD in groundwater:

Arithmetic mean (coefficient of variation):

$$T_{\text{half}_q} = 1500 (0.44) \text{ days}$$

Range: 836 to 2360 days

T_{half_w}: Reaction Half-Life in Surface Water

The units used for T_{half_w} are days.

Reported Values

1 to 6	reported at 25 °C as an aquatic photolysis half-life of 1 to 6 days by Dulin et al. (1986) using TCDD in quartz cylinders, 10/90% acetonitrile/water and calculated from absorbance, respectively; corrected for summer sunlight at 40° N
600	reported at 24 °C as a half-life of 600 days by Ward and Matsumura (1978) using lake water and sediment from Lake Mendota, WI in an anaerobic ¹⁴ C-TCDD water sediment die-away test [also cited in Howard et al. (1991)]
1111	reported as a water reaction rate constant of $2.6 \times 10^{-5} \text{ hr}^{-1}$ by Mackay et al. (1985)

From the 4 values above, we obtain the following statistics for the half-life for TCDD in surface water:

Arithmetic mean (coefficient of variation):

$$T_{\text{half_w}} = 430 (1.2) \text{ days}$$

Range: 1 to 1111 days

T_{half_d}: Reaction Half-Life in Sediment

The units used for T_{half_d} are days.

Reported Values

- | | |
|--------------|--|
| 600 | reported at 24 °C as a half-life of 600 days by Ward and Matsumura (1978) using lake water and sediment from Lake Mendota, WI in an anaerobic ¹⁴ C-TCDD water sediment die-away test [also cited in Howard et al. (1991)] |
| 1672 to 2360 | reported as an estimated anaerobic half-life of 4.58 to 6.45 years by Howard et al. (1991) using scientific judgement and data from an unacclimated aqueous (water/sediment) aerobic biodegradation half-life by Ward and Matsumura (1978) |
| 3609 | reported as an estimated sediment reaction rate constant of $8 \times 10^{-6} \text{ hr}^{-1}$ by Mackay et al. (1985) |

From the 4 values above, we obtain the following statistics for the half-life of TCDD in sediment:

Arithmetic mean (coefficient of variation):

$$T_{\text{half_d}} = 2100 (0.61) \text{ days}$$

Range: 600 to 3609 days

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