FINAL DRAFT REPORT

Intermedia Transfer Factors for Contaminants Found at Hazardous Waste Sites

BENZO(a)PYRENE
[B(a)P]

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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 B(a)P. 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 B(a)P. 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 Benzo(a)pyrene

Description	Symbol[a]	Mean Value	Coefficient of Variation	Number of Values
Molecular Weight (g/mol)	MW	252.3	4.6×10^{-5}	3
Octanol-Water Partition Coefficient	K_{ow}	2.2×10^6	0.72	7
Melting Point (K)	T_m	450.7	0.0028	4
Vapor Pressure (Pa)	VP	7.1×10^{-7}	0.068	3
Solubility (mol/m^3)	S	1.0×10^{-5}	0.63	8
Henry's Law Constant (Pa-m^3/mol)	H -	0.092	1.0	1
Diffusion Coefficient in Pure Air (m^2/d)	D_{air}	0.44	0.08	e
Diffusion Coefficient in Pure Water (m^2/d)	D_{water}	5.3×10^{-5}	0.25	e
Organic Carbon Partition Coefficient	K_{oc} -	2.5×10^6	0.91	5
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} -	0.015	1.0	1
Biotransfer Factor in Plants Relative to Contaminant Air Concentration [m^3 (a)/kg (pFM)]	K_{pa} -	5.9×10^5	14	e
Biotransfer Factor in Milk Relative to Cattle-Diet Contaminant Intake (d/kg)	B_k -	8.8×10^{-3}	11	e
Biotransfer Factor in Meat Relative to Cattle-Diet Contaminant Intake (d/kg)	B_t -	0.029	13	e
Biotransfer Factor in Eggs Relative to Hen-Diet Contaminant Intake (d/kg)	B_e -	17	14	e
Biotransfer in Breast Milk Relative to Contaminant Intake by the Mother (d/L)	B_{bmk} -	0.44	10	e
Bioconcentration Factor in Fish Relative to Contaminant Water Concentration	BCF -	330	0.41	3
Skin Permeability Coefficient (cm/h)	K_{p_w} -	0.012	2.4	e
Skin-Water/Soil Partition Coefficient [ppm (skin)/ppm (water)]	K_m -	3.0×10^4	0.27	e
Reaction Half-Life in Air (d)	T_{half_a}	0.063	1.5	3
Reaction Half-Life in Ground-Surface Soil (d)	T_{half_g}	230	0.27	7
Reaction Half-Life in Root-Zone Soil (d)	T_{half_s}	230	0.27	7
Reaction Half-Life in the Vadose-Zone Soil (d)	T_{half_v}	880	1.1	4
Reaction Half-Life in Ground-Water Zone Soil (d)	T_{half_q}	880	1.1	4
Reaction Half-Life in Surface Water (d)	T_{half_w}	2.3	2.1	7
Reaction Half-Life in the Sediment (d)	T_{half_d}	1200	1.1	2

[a]Values followed by a "-" include default equations that can be used for estimations
[b]$K_d = [(K_{oc}) \times$ (fraction organic matter)], a site and soil zone specific parameter
[e]estimated 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 (mg/kg)/(mg/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 cm^3 (soil)/cm^3 (skin), we divide equation K_m by the sorption coefficient K_d for soil, or

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

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:

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

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:

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

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

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

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

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

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

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 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

$$\text{GSD} = \exp\left\{ \ln(1+CV^2) \right\} \qquad \text{(Eqn. 6)}$$

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

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

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

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:

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

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

Other Names

Benzo[def]chrysene; 1,2-benzopyrene; 3,4-benzopyrene; 6,7-benzopyrene; 3,4-benzpyrene; 3,4-benz(a)pyrene; benz(a)pyrene; BP; B(a)P

Background

Benzo(a)pyrene [B(a)P] is a polyaromatic hydrocarbon (PAH). B(a)P is produced ubiquitously as the result of incomplete combustion. Formation occurs when gasoline, garbage, or any animal or plant material burns. It is often found in the smoke and soot of tar-production plants; coking plants; asphalt-production plants; facilities that burn organic material such as wood, coal and oil. B(a)P is also in cigarette smoke; charcoal-broiled meat and smoked foods. Smoke and soots, when released into the atmosphere, combine with the dust particles in the air and are carried into water, soil and crops (WHO, 1983). Other sources of B(a)P are coal tar pitch used to cement electrical parts and the wood preservative creosote. Photolysis of B(a)P is rapid and is considered the primary fate mechanism in air, water and surface soil (USEPA, 1978). As of 1990, B(a)P has been found in 10% (110 out of 1,117) of the NPL hazardous waste sites in the US (ATSDR, 1990).

Formula

$C_{20}H_{12}$
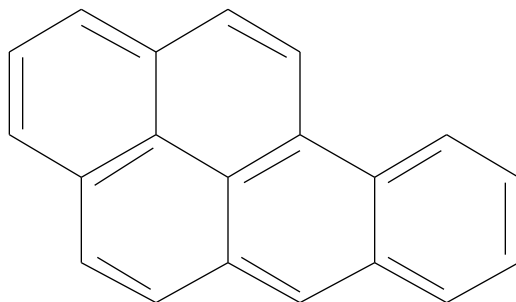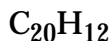
MW: Molecular Weight

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

 Reported Values

252.3	reported by WHO (1983)
252.32	reported by CRC Handbook [Weast et al. (1987)]
252.32	reported by Mackay et al. (1992)

From the above 3 reported values above, we obtain the following statistics for the molecular weight of B(a)P:

Arithmetic mean (coefficient of variation):
$MW = 252.3 \ (4.6 \times 10^{-5})$ g/mol

Range: 252.3 to 252.32 g/mol

K_{ow}: Octanol-Water Partition Coefficient

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

Experimental Values

9.8×10^5 reported at 23 °C as a log P of 5.99 by Mallon and Harrison (1984) using a shake flask-UV method

1.1×10^6 reported as a log K_{ow} of 6.04 by Radding et al. (1976) using a shake flask-UV method (1975) [Also cited in Mackay et al. (1992)]

1.1×10^6 reported at 23 °C as a log P of 6.06 by Mallon and Harrison (1984) estimated using a HPLC-UV method

1.6×10^6 reported as a log K_{ow} of 6.20 by Hanai et al. (1981) estimated using a HPLC-k' method [Also cited in Mackay et al. (1992)]

2.0×10^6 reported as a log K_{ow} of 6.31 by Smith et al. (1978)

3.2×10^6 reported as a log K_{ow} of 6.50 by Bruggeman et al. (1982) estimated using a RP-TLC method [Also cited in Mackay et al. (1992)]

5.4×10^6 reported at 25 °C as a log K_{ow} of 6.73 by Webster et al. (1985) estimated using a Waters Bondapak HPLC method

From the 7 measured values above we obtain the following statistics for the octanol-water partition coefficient of B(a)P at 25 °C:

Arithmetic mean (coefficient of variation):
$K_{ow} = 2.2 \times 10^6 \ (0.72)$

Range: 5.4×10^5 to 9.8×10^6

Other Values

6.8×10^6 reported as a log K_{ow} of 6.74 by Sarna et al. (1984) estimated using a HPLC-RT method in a Waters μBondapak column [Also cited in Mackay et al. (1992)]

5.8×10^7 reported as a log K_{ow} of 7.76 by Sarna et al. (1984) estimated using a HPLC-RT method in a Bio-Rad Biosil column [Also cited in Mackay et al. (1992)]

9.8×10^7 reported as a log K_{ow} of 7.99 by Sarna et al. (1984) estimated using a HPLC-RT method in a BCH LiChrosorb column [Also cited in Mackay et al. (1992)]

T_m: Melting Point

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

Experimental Values

449.6   reported as 176.4 °C by Murray et al. (1974) using a Mettler FP51 melting point apparatus [Also cited in Mackay et al. (1992)]

449.7 to 452   reported as 176.5 °C by Mailhot & Peters (1988) [Also cited in Mackay et al. (1992)]

451.3   reported as 178.1 °C by Karcher et al. (1983)

From the 4 values reported above, we obtain the following statistics for the melting point of B(a)P:

     Arithmetic mean (coefficient of variation):
         T_m = 450.7 (0.0028) K

     Range: 449.6 to 452 K

VP: Vapor Pressure at Standard Temperatures

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

Experimental Values

6.6×10^{-7} reported at 25 °C as a log VP of -3.951 (Pa) by Hinkley (1990) estimated using capillary gas chromatography referenced to p,p' DDT and corrected from the liquid to the solid state

7.3×10^{-7} extrapolated to 25 °C and corresponding to 7.3×10^{-7} (Pa) by Murray et al. (1974) using the Knudsen effusion weight loss method at 358 < T < 341 K

7.5×10^{-7} reported at 25 °C as 7.51×10^{-7} (Pa) by Stephenson and Malanowski (1987) [Also cited in Mackay et al. (1992)]

From the 3 measured values above, we obtain the following statistics for the vapor pressure of B(a)P at 25 °C:

Arithmetic mean (coefficient of variation):
$VP = 7.1 \times 10^{-7}$ (0.068) Pa

Range: 6.6×10^{-7} to 7.5×10^{-7} Pa

Other Values

3.8×10^{-7} reported at 20 °C as K_{ow} of 9.2×10^{-8} torr by Bidleman et al. (1986) estimated using a GC-RT method and corrected from the liquid state regression to the solid state [Also cited in Mackay et al. (1992)]

1.5×10^{-5} reported at 25 °C as log P (in torr) of -6.948 by Bidleman and Foreman (1984) estimated using a GC-RT method [Also cited in Mackay et al. (1992)]

1.1×10^{-4} reported at 25 °C as log P (in torr) of -6.076 by Bidleman and Foreman (1984) estimated using a GC-RT method [Also cited in Mackay et al. (1992)]

S: Solubility in Water

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

Experimental Values

5.0×10^{-4} reported at 25 °C as 5.0×10^{-4} mg/L by Eadie et al. (1990) estimated using thin layer chromatography and liquid scintillation counting [also cited in Mackay et al. (1992)]

8.0×10^{-4} reported at 25 °C as an average of log S (in mol/L) of -8.5 by Whitehouse & Cooke (1982) estimated using an HPLC/UV method [also cited in Mackay et al. (1992)]

1.6×10^{-3} reported at 25 °C as 0.0016 g/m^3 by Billington et al. (1988) estimated using a RP-HPLC method [also cited in Mackay et al. (1992)]

3.8×10^{-3} reported at 25 °C as 0.0038 mg/L by Lee et al. (1992) using contaminated coal tar mixtures and a shake-flask equilibration GC-ITD method

3.8×10^{-3} reported at 25 °C as 3.8×10^{-3} mg/L by Bruggeman et al (1982) estimated using a RP-TLC/UV method [also cited in Mackay et al. (1992)]

3.8×10^{-3} reported at 25 °C as a log S (in mol/L) of -7.82 by Yalkowsky and Valvani (1980) using a shake-flask UV method [also cited in Mackay et al. (1992)]

4.8×10^{-3} reported at 25 °C as 1.9×10^{-8} mol/L by Barone et al. (1967) using shake flask/fluorescence [also cited in Mackay et al. (1992)]

Unit Conversion

Arithmetic mean (coefficient of variation) of B(a)P solubility

$$= 2.6 \times 10^{-3} \ (0.63) \ \text{mg/L}$$

$$= 1.0 \times 10^{-5} \ (0.63) \ \text{mol/m}^3$$

From the 8 measured values above, we obtain the following statistics for the water solubility of B(a)P at 25 °C:

Arithmetic mean (coefficient of variation):
$$S = 1.0 \times 10^{-5} \ (0.63) \ \text{mol/m}^3$$

Range: 2.0×10^{-6} to 1.9×10^{-5} mol/m^3

H: Henry's Law Constant

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

Experimental Values

0.092   reported at 24 °C as 0.092 Pa-m^3/mol by ten Hulscher et al. (1992) using a gas purge technique at $10 < T < 55$ °C

From the measured value above, and assuming the CV is 1, we obtain the following statistics for Henry's law constant at 24 °C:

Arithmetic mean (coefficient of variation):
$$H = 0.092 \ (1.0) \ \text{Pa-m}^3/\text{mol}$$

Other Values

0.050   reported at 25 °C as 5×10^{-2} Pa-m^3/mol by EPA (1990)

0.056   calculated at 25 °C and corresponding to 5.6×10^{-2} Pa-m^3/mol by Eastcott et al. (1988) using a direct concentration ratio technique [Also cited in Mackay et al. (1992)]

0.11   calculated at 25 °C corresponding to 0.11 Pa-m^3/mol by SRC (1988) using a direct concentration ratio technique

0.50   calculated at 25 °C and corresponding to 0.5 Pa-m^3/mol by Mabey et al. (1982) using a direct concentration ratio technique [Also cited in Mackay et al. (1992)]

0.81   calculated at 25 °C and corresponding to 0.81 Pa-m^3/mol by Capel et al. (1991) using a direct concentration ratio technique [Also cited in Mackay et al. (1992)]

Estimation Method

$$H = \frac{VP\ (Pa)}{S\ (mol/m^3)} = \frac{7.1 \times 10^{-7}}{3 \times 10^{-5}} = 2.4 \times 10^{-2}\ (1.3)\ Pa\text{-}m^3/mol$$

D$_{air}$: Diffusion Coefficient in Pure Air

The units used for the diffusion coefficient in pure air are $\frac{meters^2}{day}$ (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:

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

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 263 cm^3/mol, molecular weight (M_x) of 252.3 g/mol, and a temperature equal to 298 K, the above expression gives:

$$D_{air} = 2.0 \times 10^{-5}\ T^{1.75} = 0.44\ m^2/d$$

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

Based on the estimated value and estimation error reported above, we obtain the following statistics for the estimated air diffusion coefficient of B(a)P at 25 °C:

   Arithmetic mean (coefficient of variation):
        D$_{air}$ = 0.44 (0.08) m^2/d

D_{water}: Diffusion Coefficient in Pure Water

The units used for the diffusion coefficient in pure water are $\dfrac{meters^2}{day}$ (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:

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

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 263 cm^3/mol, a temperature (T) of 298 K, and M_y (molec. wt. of water) equal to 18 g/mol., this expression gives:

$$D_{water} = 1.76 \times 10^{-7} \, T = 5.3 \times 10^{-5} \, m^2/d \text{ at 25 °C}$$

Original data for this estimation, 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 CV of 0.25 from a 25% estimation error.

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

Arithmetic mean (coefficient of variation):
$D_{water} = 5.3 \times 10^{-5}$ (0.25) m^2/d

K_{oc}: Organic-Carbon Partition Coefficient

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

Experimental Values

3.2×10^4 reported at 5 °C as a surface soil log K_{oc} of 4.5 by Simmleit and Herrmann (1987) using 0 to 25 cm deep Upper Franconian loam (10-15% fraction organic carbon [f_{oc}]) and carbonate well water (200 mg $CaCO_3/L$)

8.9×10^5 reported as a log K_{oc} of 5.95 measured by Landrum et al. (1984) using dissolved Aldrich Chemical humic acid

1.8×10^6 reported at 26.3 °C as a sediment (dry wt. [sDM])/water log K_{oc} of 6.26 by Kayal & Connell (1990) using samples from Brisbane R. Austrailia (7.8 pH, 3.38% f_{oc}) [Also cited in Mackay et al. (1992)]

4.6×10^6 reported as a log K_{oc} of 6.66 by Eadie et al. (1990) using ambient concentrations of B(a)P in Lake Michigan water and suspended sediments (13% f_{oc}) from 1984 and 1986

5.1×10^6 reported as a soil/sediment log K_{oc} of 6.71 by Smith et al. (1978)

From the 5 measured values above, we obtain the following statistics for the soil organic carbon partition coefficient for B(a)P:

Arithmetic mean (coefficient of variation):
$$K_{oc} = 2.5 \times 10^6 \ (0.91)$$

Range: 3.2×10^4 to 5.1×10^6

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}.

$$K_{oc} = 0.41 \times K_{ow}$$
$$K_{ow} = 2.2 \times 10^6$$

$$K_{oc} \text{ (est)} = 9.0 \times 10^5 \ (1)$$

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 $\dfrac{\text{mg/kg (dry surface and root-zone soil)}}{\text{mg/kg (water)}}$ 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 $\dfrac{\text{mg/kg (dry vadose-zone soil)}}{\text{mg/kg (water)}}$ 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 $\dfrac{\text{mg/kg (dry aquifer material)}}{\text{mg/kg (water)}}$ 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 $\dfrac{\text{mg/kg (dry surface-water sediment)}}{\text{mg/kg (water)}}$ 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 $\dfrac{\text{mg/kg (plant fresh mass [pFM])}}{\text{mg/kg (soil fresh mass [sFM])}}$ (ppm [pFM]/ppm [sFM])

Reported Value

0.015   reported as a soil/plant bioaccumulation factor of log -1.25 mg/kg (dry plant) per mg/kg (dry soil) by Travis and Arms (1988) and attributed to Edwards (1983) who reviewed bio-uptake and bio-monitoring studies for PAH's. We assume plants are 25% dry mass and root-zone soil is 10% water by weight.

From the reported value above, and the assumption that the CV is approximately 1, we obtain the following statistics for the plant-soil partition coefficient for B(a)P:

Arithmetic mean (coefficient of variation):
K_{ps} = 0.015 (1) ppm (pFM)/ppm (sFM)

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 [pDM]) in above-ground plant parts with octanol-water partition coefficients. This bioconcentration factor, B_v, on a dry-weight basis is expressed as:

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

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 (pFM) 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 in mg/kg in above-ground pFM relative to contaminant concentration in mg/kg (dry soil [sDM]) in the root-zone as:

$$K_{ps} = 7.7 \, K_{ow}^{-0.58} (CV = 4.0) \text{ ppm (plant FM)/ppm (soil DM)}$$

Expressing the ratio of contaminant concentration in mg/kg in above-ground pFM relative to contaminant concentration in mg/kg (sFM), and assuming fresh soil 10% by mass water in the root-zone soil, the K_{ps} estimation is:

$$K_{ps} \text{ (est)} = 7.0 \, K_{ow}^{-0.58}$$
$$K_{ow} = 2.2 \times 10^6$$

$$K_{ps} \text{ (est)} = 1.5 \times 10^{-3} \text{ ppm (pFM)/ppm (sFM)}$$

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 $\dfrac{\text{mg/kg (plant fresh mass [pFM])}}{\text{mg/cubic meter of air (m}^3 \text{ [air])}}$ (m^3 [a]/kg [pFM])

No reported measurements of K_{pa} for B(a)P are available in the current literature. An estimation method for this parameter is therefore applied.

Estimation Method

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

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

$$R = 8.313 \text{ Pa-m}^3/\text{mol-K}$$
$$T = 298 \text{ K}$$
$$H = 0.092 \text{ Pa-m}^3/\text{mol}$$
$$K_{ow} = 2.2 \times 10^6$$

$$K_{pa} \text{ (est)} = 5.9 \times 10^5 \text{ m}^3 \text{ [a]/kg [pFM]}$$

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

> Based on the estimation equation and the estimation error reported above, we obtain the following statistics for the partition coefficient in plant leaves relative to contaminant concentration in air for B(a)P:
>
> Arithmetic mean (coefficient of variation):
> $K_{pa} = 5.9 \times 10^5$ (14) m^3 [a]/kg [pFM]

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 (mg/kg)/(mg/d) or d/kg [media].

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]).

No experimental values for B_k are available in the current literature. Estimation methods are therefore considered.

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 6.34, we obtain the following statistics for the B_{k1} of B(a)P:

$$B_{k1} \ (\text{est}) = 0.0175 \ \text{d/kg (milk)}$$
$$CV = 6$$

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 (1980) 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 (1980). The above estimation error corresponds to a CV of 14. From the above expression with $\log K_{ow}$ of 6.34, 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 B(a)P:

$$B_{k2} \ (est) = 2.44 \times 10^{-4} \ d/kg \ (milk)$$
$$CV = 14$$

The estimation values reported above yield the arithmetic mean and CV reported below:

$$B_k \ (avg) = 0.0088 \ d/kg \ (milk)$$

We calculate the $CV_{combined}$ in this expression is 11.

Based on the estimation equation and the estimation error reported above, we obtain the following value for the estimated steady-state biotransfer factor for milk relative to dietary contaminant intake by dairy cattle for B(a)P:

Arithmetic mean (coefficient of variation):
$B_k = 0.0088$ (11) days/kg (milk)

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]).

No reported values for the B_t of B(a)P are available in the current literature. Estimation methods are therefore considered

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},

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

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 errors corresponds to a CV of 11. From the above expression and a log K_{ow} equal to 6.34, we obtain the following estimation:

$$B_{t1} \text{ (est)} = 0.055 \text{ d/kg (meat)}$$
$$CV = 11$$

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 (1980) reviewed cattle-dietary feeding studies for 23 chemicals, and from these studies derived the following fat-diet equation relating K_{fd} to K_{ow}:

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

The estimation error in this expression, ± 1, was calculated by Kenaga (1980). The above estimation error corresponds to a CV of 14. From the above expression, with $\log K_{ow}$ equal to 6.34, an assumed pasture intake by beef cattle of 60 kg (pFM)/d (McKone and Ryan, 1989), and an assumed fat content of 0.4 in meat; we obtain the following estimation:

$$B_{t2} \text{ (est)} = 0.00345 \text{ d/kg (meat)}$$
$$CV = 14$$

The estimation values reported above yield the arithmetic mean and CV reported below:

$$B_t \text{ (avg)} = 0.029 \text{ d/kg (meat)}$$

We calculate the $CV_{combined}$ in this expression is 13.

Based on the estimation equation and the estimation error reported above, we obtain the following value for the estimated steady-state biotransfer factor for meat relative to dietary contaminant intake by dairy cattle for B(a)P:

Arithmetic mean (coefficient of variation):
$$B_t = 0.029 \text{ (13) days/kg (meat)}$$

B_e: Steady-State Biotransfer Factors for Eggs 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 B(a)P 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 to 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 observation 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 [plant fresh mass (pFM)]) to obtain the following estimate of a biotransfer factor, B_e, from chicken diet to eggs with units d/kg (eggs):

$$\log B_e = \log K_{ow} - 5.1$$
$$\log K_{ow} = 6.34$$

$$B_e = 17 \text{ d/kg (eggs)}$$

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 concentration relative to dietary contaminant intake by chickens for B(a)P:

Arithmetic mean (coefficient of variation):
$B_e = 17$ (14) d/kg (eggs)

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]).

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

Estimation Method

$$B_{bmk} = 2 \times 10^{-7} K_{ow}$$
$$K_{ow} = 2.2 \times 10^{6}$$

$$B_{bmk} = 0.44 \text{ d/kg (mothers milk)}$$

The CV of the above method is approximately 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 concentration relative to dietary contaminant intake by the mother for B(a)P:

Arithmetic mean (coefficient of variation):
$B_{bmk} = 0.44$ (10) d/kg (mothers milk)

BCF: Bioconcentration Factors for Fish Relative to Water Concentration

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

Experimental Values

224	reported at 23 °C as a fish BCF of 282 by McCarthy and Jimenez (1985) using ^{14}C B(a)P and Bluegill sunfish (*Lepomis machrochirus*) in a flow through chamber containing dissolved humic matter
282	reported at 23 °C as a fish BCF of 224 by McCarthy and Jimenez (1985) using ^{14}C B(a)P and Bluegill sunfish (*Lepomis machrochirus*) in a flow through chamber containing dissolved humic matter
480	reported as a fish BCF of 480 by Freitag et al. (1985) using Golden Ide (*Leuciscus idus melanotus*) for 3 days

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From the 3 measured values reported above, we obtain the following statistics for BCF in fish relative to contaminant concentration in water for B(a)P:

Arithmetic mean (coefficient of variation):
BCF (fish/water) = 330 (0.41)

Range: 224 to 480

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:

$$BCF = 0.048 \, K_{ow}$$
$$K_{ow} = 2.2 \times 10^6$$

$$BCF \text{ (est)} = 1.1 \times 10^5$$
$$CV = 0.6$$

The reported GSD is 1.8 which corresponds to an estimation error 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 nonsteady-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 B(a)P is calculated with the following equation based on the estimation method of McKone and Howd (1992).

$$K_{p\_w} = MW^{-0.6} \left[0.33 + \frac{0.0025}{2.4 \times 10^{-6} + 3 \times 10^{-5} \, K_{ow}^{0.8}} \right]^{-1}$$

$$K_{ow} = 2.2 \times 10^6$$
$$MW = 252.3 \text{ g/mol}$$

$$K_{p\_w} = 0.012 \text{ cm/hr}$$

who report a coefficient of variation equal to 2.4

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 B(a)P:

Arithmetic mean (coefficient of variation):
$$K_{p\_w} = 0.012 \, (2.4) \text{ cm/hr}$$

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

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

No reported measurements of K_m for B(a)P are available in the current literature. An estimation method for this parameter is therefore applied.

Estimation Method

Experimental values quantifying dermal transfer of B(a)P 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.

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

$$K_{ow} = 2.2 \times 10^6$$

$$K_m = 3.0 \times 10^4 \text{ ppm (skin)/ppm (water)}$$

The reported geometric standard deviation of 1.3 in this estimation method corresponds to a CV of 0.27.

Based on the estimation equation and the estimation error reported above, we obtain the following statistics for the partition coefficient for human skin relative to contaminant water concentration for B(a)P:

Arithmetic mean (coefficient of variation):
$K_m = 3.0 \times 10^4$ (0.27) ppm (skin)/ppm (water)

T_{half_a}: Reaction Half-Life in Air

The units used for T_{half_a} are days.

Reported Values

0.015 to 0.046	reported as an estimated half-life of B(a)P in lower atmosphere by Howard et al. (1991) to be in the range of 0.37 to 1.1 hours based on photolysis as a removal process
0.023	reported as a calculated near surface half-life of 0.54 hours by Zepp and Scholtzhauer (1979) [also reported by Mackay et al. (1992)]

From the 3 estimations reported above, and the assumption that the actual range of values may be a factor of 5 higher or lower than this value, we obtain the following statistics on the reaction half-life for B(a)P in air:

Arithmetic mean (coefficient of variation):
T_{half_a} = 0.063 (1.5) days

Range: 0.0031 to 0.23 days

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

The units used for T_{half_g} are days.

Reported Values

151 to 309	reported at 20 °C as a soil biodegradation half-life of 151 to 309 days by Keck et al. (1989) using B(a)P: 33 ppm only, in a mixture of PAH's (10.8 ppm), and in creosote (13 ppm); individually measured in Kidman sandy loam [0.51% f_{oc}, 8.0 pH, 0.20 water by wt. (f_w)] in the dark; corrected for volatilization
173	calculated from degradation rate data by Lu et al. (1977) as 4×10^{-3} day^{-1} in soil using radiolabelled B(a)P in a Drummer soil (0.067 f_{oc}, 6.5 pH, 0.174 f_w) for 28 days
211	reported as a biodegradation half-life in soil of 211 days by Wild and Jones (1993) using 2 agricultural, 1 forest and a roadside soil (2.9-6.6 pH, 6-58% f_{oc}, and 0.25-0.65 f_w) contaminated with B(a)P (106-745 µg/kg); corrected for abiotic losses
218	reported at 20 °C as a zero order soil biodegradation half-life of 218 days by Bulman et al. (1987) using ^{14}C-B(a)P added to a Donneybrook sandy loam of Ontario, Canada (2.3% f_{oc}, 7.0 pH, 29.2% f_w) at 50 mg/kg for 400 days
229 to 309	reported at 20 °C as a biodegradation half-life of 229 to 309 days by Park et al. (1990) using a McLauren sandy loam and a Kidman sandy loam (4.8/7.9 pH, 1.1/0.5 f_{oc}, 12.4/16.3% f_w), respectively [This study is also cited in Howard et al. (1991)]

From the 7 measured values above, we obtain the following statistics for the reaction half-life for B(a)P in surface soil:

Arithmetic mean (coefficient of variation):
T_{half_g} = 230 (0.27) days

Range: 151 to 309 days

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

The units used for T_{half_s} are days.

Reported Values

151 to 309	reported at 20 °C as a soil biodegradation half-life of 151 to 309 days by Keck et al. (1989) using B(a)P: 33 ppm only, in a mixture of PAH's (10.8 ppm), and in creosote (13 ppm); individually measured in Kidman sandy loam (0.51% f_{oc}, 8.0 pH, 0.20 water by wt. [f_w]) in the dark; corrected for volatilization
173	calculated from degradation rate data by Lu et al. (1977) as 4×10^{-3} day^{-1} in soil using radiolabelled B(a)P in a Drummer soil (0.067 f_{oc}, 6.5 pH, 0.174 f_w) for 28 days
211	reported as a biodegradation half-life in soil of 211 days by Wild and Jones (1993) using 2 agricultural, 1 forest and a roadside soil (2.9-6.6 pH, 6-58% f_{oc}, and 0.25-0.65 f_w) contaminated with B(a)P (106-745 µg/kg); corrected for abiotic losses
218	reported at 20 °C as a zero order soil biodegradation half-life of 218 days by Bulman et al. (1987) using ^{14}C-B(a)P added to a Donneybrook sandy loam of Ontario, Canada (2.3% f_{oc}, 7.0 pH, 29.2% f_w) at 50 mg/kg for 400 days
229 to 309	reported at 20 °C as a biodegradation half-life of 229 to 309 days by Park et al. (1990) using a McLauren sandy loam and a Kidman sandy loam (4.8/7.9 pH, 1.1/0.5 f_{oc}, 12.4/16.3% f_w), respectively [This study is also cited in Howard et al. (1991)]

From the 7 measured values above, we obtain the following statistics for the reaction half-life for B(a)P in root-zone soil:

Arithmetic mean (coefficient of variation):
T_{half_s} = 230 (0.27) days

Range: 151 to 309 days

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

The units used for T_{half_v} are days.

Reported Values

114 to 1059	reported as an estimated unacclimated aqueous aerobic biodegradation half-life of 114 days to 2.9 years by Howard et al. (1991) using scientific judgement and soil die-away data from Coover and Sims (1987) and Groenewegen and Stolp (1976)

228 to   reported as an anaerobic half-life of 228 days to 5.8 years by Howard et al.
2117   (1991) using scientific judgement based on aqueous aerobic
biodegradation half-life by Coover and Sims (1987) and Groenewegen
and Stolp (1976)

From the 4 reported values above, we obtain the following statistics for the
reaction half-life for B(a)P in the vadose-zone soil:

Arithmetic mean (coefficient of variation):
T_{half_v} = 880 (1.1) days

Range: 114 to 2117 days

T_{half_q}: Reaction Half-Life in Groundwater

The units used for T_{half_q} are days.

Reported Values

114 to   reported as an estimated unacclimated aqueous aerobic biodegradation
1059   half-life of 114 days to 2.9 years by Howard et al. (1991) using scientific
judgement and soil die-away data from Coover and Sims (1987) and
Groenewegen and Stolp (1976)

228 to   reported as an anaerobic half-life of 228 days to 5.8 years by Howard et al.
2117   (1991) using scientific judgement based on aqueous aerobic
biodegradation half-life by Coover and Sims (1987) and Groenewegen
and Stolp (1976)

From the 4 reported values above, we obtain the following statistics for the
reaction half-life for B(a)P in groundwater:

Arithmetic mean (coefficient of variation):
T_{half_q} = 880 (1.1) days

Range: 114 to 2117 days

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

The units used for T_{half_w} are days.

Reported Values

0.015 to 0.046	reported as an estimated aqueous half-life of 0.37 to 1.1 hours by Howard et al. (1991) using scientific judgement and data from an estimated photolysis half-life in air by Smith et al. (1978) and corrected to summer sunlight intensity Lyman et al. (1982)
0.022	reported as a photolytic aquatic rate constant of 1.3 hr^{-1} by Zepp (1980) [also cited in Mackay et al. (1992)]
0.029	reported as an aquatic photolysis rate constant of 2.8×10^{-4} second^{-1} by Callahan et al. (1979) [also cited in Mackay et al. (1992)]
0.045	reported as an estimated half-life in water of 0.045 day by Mill and Mabey (1985) under mid-December sunlight [also cited in Howard et al. (1991)]
3.2 to 13	reported as an estimated half-life in water of 3.2 to 13 days by Zepp and Scholtzhauer (1979) integrated over a full summer day at latitude 40°N with and without sediment partitioning, respectively [also reported in Mackay et al. (1992)]

From the 7 reported values above, we obtain the following statistics for the half-life for B(a)P in surface water:

Arithmetic mean (coefficient of variation):
T_{half_w} = 2.3 (2.1) days

Range: 0.015 to 13 days

T_{half_d}: Reaction Half-Life in Surface Water Sediment

The units used for T_{half_d} are days.

Reported Values

228 to 2117	reported as an estimated anaerobic half-life of 228 days to 5.8 years by Howard et al. (1991) using scientific judgement and an estimated unacclimated aqueous aerobic biodegradation half-life

From the 2 reported values above, and our assumption that Howard et al. (1991) have incorporated a reasonable range for this half-life, we obtain the following statistics for the half-life of B(a)P in sediment:

Arithmetic mean (coefficient of variation):
$$T_{half\_d} = 1200 \ (1.1) \ days$$

Range: 228 to 2117 days

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