**CHAMBER OF COMMERCE**
**OF THE**
**UNITED STATES OF AMERICA**

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Information Quality Guidelines Staff
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Dear Sir or Madam:

The U.S. Chamber of Commerce (Chamber) submits this Request for Correction (Request) to the U.S. Environmental Protection Agency (EPA) under the Data Quality Act[1] and the Office of Management and Budget (OMB)[2] and EPA Information Quality Guidelines[3] (referred to collectively herein as the Guidelines). The Chamber is the world's largest business federation, representing more than three million businesses of every size, sector, and region. This Request includes three attachments which are incorporated herein by reference and are part of this Request.

## I.  OVERVIEW OF REQUEST FOR CORRECTION

This Request seeks the correction of erroneous physical and chemical property information contained in EPA databases that EPA disseminates and makes publicly accessible. The databases, including: CHEMDAT8, RCRA, SCDM, SCDM Win, SIMS, STF, SPHEM, CHEM9, HHRAP, HHRAPCF, TreatDB, KowWin, PhysProp, Chemfate, Water9, and PBT Profiler, which are identified, documented, and discussed in the Attachments to this Request provide the public and policymakers inconsistent and contradictory numerical data entries for physical-chemical constants characteristic of various chemicals that are used in commerce or that occur in the environment. As

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[1] Section 515, Treasury and General Government Appropriations Act for Fiscal Year 2001; Public Law 106-554; 44 U.S.C. §3516, note.

[2] *Guidelines for Ensuring and Maximizing the Quality, Objectivity, Utility, and Integrity, of Information Disseminated by Federal Agencies*, Office of Management and Budget, *Federal Register* 67 (February 22, 2002): 8452.

[3] *Guidelines for Ensuring and Maximizing the Quality, Objectivity, Utility, and Integrity, of Information Disseminated by the Environmental Protection Agency*. October 2002. U.S. Environmental Protection Agency. <http://www.epa.gov/quality/informationguidelines/documents/EPA_InfoQualityGuidelines.pdf>.

indicated in Attachment 1[4], use of this erroneous information leads, for example, to widely varying—and hence unreliable or ambiguous—determinations of human health risk impacts (such as in a determination of residual risks required under Section 112(f) of the Clean Air Act and environmental cleanup goals that are based on sediment quality objectives[5]).

Chamber members are affected by dissemination of this inconsistent and erroneous information in two primary ways. First, various Chamber members produce, use, or are otherwise associated with one or more of the chemicals whose erroneous information is listed in the databases; and second, use of the erroneous data found in the EPA databases results in significant financial impacts to Chamber members, such as when they are involved with contaminant cleanup activities. For example, as clearly indicated in Attachment 1, there is no doubt that, due to data inconsistency errors, estimates of contaminated site cleanup costs can easily be in error by tens of millions of dollars.

The Data Quality Act required OMB to issue governmentwide guidelines that *ensur[e] and maximiz[e] the quality, objectivity, utility, and integrity* of all information disseminated by federal agencies[6]. Each federal agency was then required to issue its own implementing guidelines by October 2002[7,8]. Each agency's guidelines were required to include an administrative mechanism that allows affected parties to seek and obtain the correction of information that does not comply with the Guidelines[9,10]. OMB makes clear that the purpose of this administrative correction mechanism is to facilitate public review of agency information practices[11].

## II.     INCONSISTENT DATABASES AND IMPACT

In numerous instances (see, for example, the numerical values and numerical value ranges listed for the chemicals identified in Table 1 of Attachment 1 and Tables 1 and 3 of Attachment 2), depending on which EPA database is consulted, widely differing numerical values—sometimes

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[4] I. Linkov, M. Ames, E. Crouch, *Uncertainty in $K_{ow}$: Implications for Risk Assessment and Remedial Decisions*, (Cambridge, MA: Cambridge Environmental Inc., March 2004).
[5] A Sediment Quality Objective can be thought of as a level of a contaminant in sediment that is established with an adequate margin of safety for the reasonable protection of the beneficial uses of water or the prevention of nuisances.
[6] *Ibid*, Footnote 1, Section 515(a).
[7] *Ibid*, Footnote 1, Section 515(b)(2)(A).
[8] *Ibid*, Footnote 2, Section IV, 5.
[9] *Ibid*, Footnote 1, Section 515(b)(2)(B).
[10] *Ibid*, Footnote 2, Section IV, 3.
[11] *Ibid*, Footnote 2, Section III, 3.

differing by a factor of a million, in some instances even by a factor upward of 10 billion or more—are assigned to the same exact physical or chemical property parameter associated with the same exact chemical. In simple terms, the same exact chemical may be assigned greatly different values between databases.

Specifically, the Attachments: 1) note the identity of some relevant EPA databases; 2) indicate, by example, some specific instances of data inconsistencies; 3) discuss the potential impacts of the data inconsistencies on assessments of human health risks and other environmental impacts, as well as on cleanup decisions; and 4) discuss, again by example, the cost impact discrepancies that arise as a result of such database inconsistencies.

## A.  EXAMPLES OF INCONSISTENCIES BETWEEN DATABASES

### 1.  Henry Laws Constant

The numerical value listed for the Henrys Law Constant[12] in the SCDM database for 3, 3'-dimethoxybenzene (a chemical intermediate used in the production of dyes and pigments) differs by a factor of more than ten billion from its numerical value listed in the CHEM9 database[13].

### 2.  HHRAP Database

In the HHRAP database, the numerical value of the octanol-water partition coefficient[14] (Kow) for aldrin (an insecticide) differs by a factor of more than one billion from the same property listed for the same chemical in the STF database[15].

As documented in the attachments, errors such as these are two of but many that can be found among the various EPA databases.

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[12] A measure of the ratio of the concentration of a compound in air or vapor to the concentration of the compound in water under equilibrium conditions.
[13] See Table 3 of Attachment 2.
[14] A coefficient representing the ratio of the solubility of a compound in octanol (a non-polar solvent) to its solubility in water (a polar solvent). Log Kow is generally used, for example, as a relative indicator of the tendency of an organic compound to adsorb to soil.
[15] *Ibid*, Footnote 13.

B.    EXAMPLES OF INCONSISTENCIES WITHIN THE SAME DATABASE

In the CHEM9 EPA database (a compound properties processor based upon an EPA compound database of more than 1,000 compounds), there are multiple instances in which a chemical compound is listed twice and the two entries specify different numerical values for various of the same physical/chemical property parameters that characterize the chemical. For example, in CHEM9, a numerical value is listed for the vapor pressure (in mm Hg) of bis(2-chloroethyl) ether (a chemical used in organic syntheses and for other purposes). But then, in the same database, the same chemical is listed again, this time under the name dichloroethyl ether, and an entirely different value for its vapor pressure is indicated. Similarly, in CHEM9, the chemical Freon 12 is entered twice with two different Henrys Law Constant values given, depending on which entry is consulted.

C.    IMPACT OF DATA INCONSISTENCIES

As documented in the Attachments, these inconsistent and erroneous data entries have serious consequences. The data are used, for example, in performing tasks such as assessing the bioconcentration of chemicals, the movement of chemicals in the environment, human health risks, and environmental cleanup requirements. Despite these data errors, these EPA databases are readily and publicly available and are used by EPA, other federal, state, and local regulators, and others to freely and arbitrarily select what numerical value to use to evaluate an environmental impact or issue. Given the existence of documented data errors such as those noted in this Request, and as clearly established in the Attachments, serious mistakes and erroneous conclusions will arise, for example, in regard to estimates of environmental and human health impacts, necessary prevention measures, and remediation costs.

## III. CONCLUSIONS DRAWN FROM THE USE OF INCONSISTENT DATA

The Attachments clearly establish that: 1) EPA databases contain inconsistencies; 2) the inconsistencies can and do cause the occurrence of erroneous estimates and assessments of human health risks and environmental impacts; 3) the inconsistencies result in widely varying estimates of cost impacts to business and industry stakeholders—these cost estimate variations, as discussed above, easily amount to tens of millions of dollars; 4) the databases are used for important regulatory purposes (e.g., to establish sediment quality objectives relevant to the management of contaminated sites); 5) the data, databases, and models are publicly disseminated by EPA; 6) the inconsistent data between databases or within the same database leads to widely varying and arbitrary outcomes in regulatory decisions; and 7) any deliberate selection of a database to achieve desired results permits regulatory outcomes to be manipulated.

## IV. APPLICABLE LAWS, REGULATIONS, AND GUIDANCE

The database inconsistencies identified herein represent a fundamental flaw in the information disseminated by EPA to support risk-based and other highly important decisions. These databases violate the Data Quality Act and the Guidelines as set forth below:

### A. The Databases are Subject to the Guidelines

In order to be covered by the Guidelines there must have been an agency dissemination of information after October 1, 2002. Each requirement is readily met in this instance. First, dissemination is defined as *agency initiated or sponsored distribution of information to the public*[16],[17]. The EPA databases are being disseminated because they are posted on EPA's Web site and are being used or relied upon to support regulatory decisions, including the establishment of health risks and environmental cleanup requirements. Second, information is defined as *any communication or representation of knowledge such as facts or data, in any medium or form*….[18],[19]. EPA's databases clearly qualify as

[16] *Ibid*, Footnote 2, Sections V, 8.
[17] *Ibid*, Footnote 3, Section 5.3.
[18] *Ibid*, Footnote 2, Sections V, 5.
[19] *Ibid*, Footnote 3, Section 5.3.

information because, among other purposes, they communicate data that EPA and others use to estimate risk.  Finally, since EPA's databases continue to be maintained and disseminated by EPA, they have been disseminated after October 1, 2002.

Accordingly, the dissemination of the databases is clearly covered by the Guidelines.

## B.      The Databases are not Objective

The information contained in the EPA databases (as discussed herein and in the Attachments) violates the Guidelines because it is not objective.  Specifically the information is not presented[20,21] in an accurate, clear, complete, and unbiased manner, nor, as a matter of substance[22,23], is it accurate, reliable, and unbiased.

## C.      The Information in the Databases is Influential

The EPA databases at issue qualify as influential information because the information will have or does have a clear and substantial impact on important public policies or private sector decisions[24,25.] For example, the information is used to establish regulatory requirements, develop human health risk assessments, and establish

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[20] Objectivity has two distinct components:  presentation and substance. The presentation component of the objectivity standard requires that all information disseminated by the agency must be presented in an *accurate, clear, complete, and unbiased manner*.  As OMB explains: *This involves whether the information is presented within a proper context.  Sometimes, in disseminating certain types of information to the public, other information must also be disseminated to ensure an accurate, clear, complete, and unbiased presentation.  Also, the agency needs to identify the sources of the disseminated information (to the extent possible, consistent with confidentiality protections) and, in a scientific…or statistical context, the supporting data and models, so that the public can assess for whether there may be some reason to question the objectivity of the sources.  Where appropriate, data should have full, accurate, transparent documentation, and error sources should be identified and disclosed to users.*  The values for chemical and physical data presented in the EPA databases or computed by models (see Attachments) fail to meet this objective presentation standard because they are inconsistent across the databases and models.  Because the numbers are inconsistent, some are obviously incorrect.  Further, because they are inconsistent and at least partially incorrect, they are also unclear, incomplete, and potentially biased.

[21] *Ibid*, Footnote 3, Section 5.1.

[22] The substance of all information disseminated by the agency must meet a general standard of objectivity, defined as *a focus on ensuring accurate, reliable, and unbiased information.*  The information at issue is not accurate or reliable because it is inconsistent across the various EPA databases.  Because the numbers are inconsistent, some are obviously incorrect (and potentially biased).

[23] *Ibid*, Footnote 3, Section 5.1.

[24] *Ibid*, Footnote 2, Section V, 9.

[25] *Ibid*, Footnote 3, Section 6.2.

environmental cleanup requirements.  As previously discussed in this Request, and as documented in Attachment 1, the information that underpins these activities has huge financial implications for business and industry stakeholders—easily amounting to many millions of dollars.

1.      **The Influential Information is Subject to the Safe Drinking Water Act Standard**

The Guidelines require that influential information concerning an analysis of risks to human health, safety, or the environment must meet the standard for risk assessments adopted by Congress in the Safe Drinking Water Act Amendments of 1996 (SDWA) that has been adopted governmentwide by OMB[26] and adopted by EPA[27].  This standard for risk assessments clearly applies to the EPA databases at issue.  Under the standard, EPA must ensure that the databases that it disseminates are based on the *best available, peer-reviewed science and supporting studies conducted in accordance with sound and objective scientific practices…*[28], and that *…all data is collected by accepted methods or best available methods…*[29]  Since the data in EPA's databases are inconsistent, and necessarily incorrect in at least some instances, it is clear that this SDWA standard has not been met.

2.      **The Influential Information Must be Transparent and Reproducible**

In addition, because the information is influential scientific or statistical information under the Guidelines[30,31] it must include sufficient transparency to ensure its reproducibility.  Because the databases produce varying results that are necessarily erroneous in some instances, the databases and any decisions based on them are not reproducible.

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[26] *Ibid*, Footnote 2, Section V, 3(b)(ii)(C).
[27] *Ibid*, Footnote 3, Section 6.4.
[28] *Federal Register* 67 (February 22, 2002): 8457.
[29] *Ibid*.
[30] *Ibid*, Footnote 2, Section V, 9.
[31] *Ibid*, Footnote 3, Section 6.2.

### D. The Databases Lack Utility

The databases violate the Guidelines because they lack the requisite utility[32,33]. The Guidelines require that all information disseminated by federal agencies must be *useful to its intended users, including the public.*[34,35]. EPA's databases are not useful to the public or the agency because they contain inconsistencies that make them, in at least some instances, incorrect.

### E. Chamber Members are Impacted by the Inconsistent Data

As previously stated, the Chamber is an affected party because its members (inclusive of numerous industrial, manufacturing, and chemical companies) are impacted by the use of EPA's databases. Moreover, the existence of erroneous and/or inconsistent parameters in these databases can have huge financial implications (see Attachments) for Chamber members.

## V. CORRECTION REQUEST

For the following chemicals and/or chemical mixtures: Total PCBs; aldrin; arochlor; benzene; benzo(a)anthracene; benzo(a)pyrene; bis(2-ethylhexl)phthalate; dibutylphthalate; dichlorodifluoromethane; 2,4-dichlorophenoxyacetic acid; 7,12-dimethylbenz(a)anthracene; 3,3'-dimethoxybenzidine; 1,4-dioxane; ethylene dibromide; hexachlorobutadiene; hexachloropentadiene; hexachloroethane; methyl methacrylate; PCBs; pentachlorophenol; pyrene; pyridine; 1,2,3-trichloropropane; and vinyl chloride, which are found in one or more of the following databases as identified in Table 1 of Attachment 1 and Tables 1 and 3 of Attachment 2: CHEMDAT8; RCRA; SCDM; SCDM Win; SIMS; STF; SPHEM; CHEM9; HHRAP; HHRAPCF; TreatDB; KowWin; PhysProp; Chemfate; Water9; PBT Profiler; and ATSDR, the Chamber requests that EPA, to the extent that it disseminates information about these chemicals and chemical mixtures and to the extent that it disseminates these databases, assure that the databases consistently and uniformly indicate the same, correct numerical value for any listed physical or chemical property parameter associated with

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[32] *Ibid*, Footnote 2, Section 2.
[33] *Ibid*, Footnote 3, Section 5.1.
[34] *Ibid*, Footnote 2, Section V, 2.
[35] *Ibid*, Footnote 3, Section 5.1.

the identified chemicals and chemical mixtures regardless of what database is consulted (or what model is used) to estimate the relevant numerical value for these parameters (such as the octanol-water partition coefficient) that are characteristic of these chemicals and chemical mixtures, as identified, documented, and discussed in this Request and in the Attachments to this Request.

The Chamber considers compliance with the Data Quality Act to be a foremost responsibility of federal agencies and a chief manner in which agencies can improve the quality of regulations and other information. We therefore appreciate the opportunity to file this Request and thank EPA for its consideration of our proposed corrective actions.

Sincerely,

William L. Kovacs

Attachments

[Attachment 1]

PEER REVIEW DRAFT

**Uncertainty in $K_{ow}$: Implications for Risk Assessment and Remedial Decisions**

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Key Words: $K_{ow}$, risk assessment, uncertainty analysis, data quality

**ABSTRACT**

The assessment of human health and ecological risks at chemically contaminated sites often includes the use of chemical transport and fate models as well as models to assess exposure/toxicity. These models require input data on a variety of physical and chemical properties for each compound of concern. Small changes in some of these parameters can result in significant differences in estimated human health or ecological risks, and possibly in the extent of any risk-based remediation efforts. The octanol-water partition coefficient ($K_{ow}$) for hydrophobic organic compounds is one such parameter, particularly because it is often used to estimate additional partitioning and bioaccumulation parameters. Unfortunately, there is considerable uncertainty in the $K_{ow}$ values for many compounds of concern. Some risk assessments include quantitative, probabilistic treatments of $K_{ow}$ and/or advanced chemical analyses to allow the use of site-specific $K_{ow}$ values. However, most risk assessments rely on deterministic calculations with parameter values taken from tabulations either compiled by the U.S. EPA or other regulatory agencies, from literature sources, or from a combination of these. The EPA has published or recommended the use of several databases and documents that report $K_{ow}$ values for compounds of interest, but for some chemicals there is a wide range of tabulated $K_{ow}$ values even among these sources. This paper assesses the implications of using various values of $K_{ow}$ to calculate sediment quality objectives (SQOs) for a PCB-contaminated site in the coastal waters of Puget Sound. A simplified food chain model was implemented using the range of $K_{ow}$ values available from, or recommended by the U.S. EPA. The output of this model provides exposure point concentrations used for estimating human health risks through ingestion of locally caught game fish. SQOs were calculated as the maximum PCB concentration in sediments that would be associated with a health-protective level of risk. The SQOs obtained for the lowest $K_{ow}$ value reported in EPA tabulations are as much as a factor of five higher than those obtained with the highest $K_{ow}$ value. For the site considered in this study, this range of SQOs is estimated to correspond to a difference in remediation costs of $48 million. Standardization of $K_{ow}$ estimates among EPA databases and estimation programs would result in

more consistent selection of remedial alternatives among sites and would ease the process of regulatory risk assessment review.

## INTRODUCTION

The octanol-water partition coefficient ($K_{ow}$) describes the equilibrium ratio of the concentrations of a chemical substance in n-octanol and in water. This partition coefficient is widely used in risk assessments to approximate the distribution of chemicals between aqueous and organic media. Further, $K_{ow}$ is widely used to estimate other physical properties and toxicities. For example, in exposure modeling, it is used to estimate dermal permeabilities and absorption from the gastro-intestinal tract and lung. Environmental models utilize $K_{ow}$ to estimate soluble concentrations in water, bioconcentration coefficients between environmental media and living organisms, and soil and sediment adsorption coefficients.

In principle, $K_{ow}$ is a well-defined and measurable property. In practice, the $K_{ow}$ value for many hydrophobic organic compounds is not well characterized—a fact well known to both chemists and risk assessors (Renner, 2002). A complicating factor arises for mixtures of closely related compounds, for example PCBs or dioxins, that are often treated as a single "chemical" in risk assessments. For such mixtures, there is no single correct value of $K_{ow}$ that can be applied in all circumstances.

It is possible for the uncertainty due to these two factors to be quantitatively characterized and incorporated in modeling. Advanced chemical analysis can be used to support selection of a site-specific $K_{ow}$ or to allow treatment of each specific chemical form separately. However, this is seldom practical and can rarely be carried through completely because ecotoxicological benchmarks are often available only for mixtures of such chemicals. Quantitative probabilistic analysis can be used to account for the uncertainty in $K_{ow}$, but this method is also rarely applied.

A more difficult situation to address arises when poor quality data enter the tabulations due to either the referencing of inappropriate experimental results, inadequate documentation procedures, or simple errors in reporting. Pontolillo and Eganhouse (2001) examined more than 700 publications reporting $K_{ow}$ values for DDT and DDE. They found variations of up to four orders of magnitude in reported $K_{ow}$ values for these compounds and little indication of a decline in the range of variation over the last five decades. Even the "recommended values" were found to range over more than two orders of magnitude. Eganhouse and Pontolillo (2002) concluded that many values recommended in literature tabulations are based on examination of erroneous and incomplete data compilations. The authors concluded that estimation of critical environmental parameters on the basis of $K_{ow}$ is inadvisable and could result in erroneous risk assessment results.

This paper complements the study of Pontolillo and Eganhouse (2001) by evaluating the variation of $K_{ow}$ for polychlorinated biphenyls (PCBs) in EPA compiled or recommended databases, and by assessing the potential cost implications of the use of a range of these values for a site-specific remediation. The selection of PCBs for this evaluation is especially suitable

because they are a primary risk driver for many contaminated sites, because there is considerable variation in $K_{ow}$ values for PCBs among available databases, and because PCBs, though actually a class of related compounds, are often treated as a single "chemical". The term PCB does not identify a specific compound but instead refers to any of 209 PCB congeners each of which has its own $K_{ow}$. The EPA chemical property databases (which term hereafter is used to include estimation programs often included with such databases) include values for PCBs identified either as an unspecified mixture of congeners or as mixtures specified by their commercial Aroclor number. Ranges of $K_{ow}$ values for both total PCBs and Aroclor 1254 are evaluated in the modeling that follows.

## CASE STUDY

The case study presented in this paper is based on conditions at the Hylebos Waterways Superfund Site located in the southern basin of Puget Sound, near Tacoma, Washington. In 1983, EPA placed the Commencement Bay Nearshore/Tideflats Site on the National Priorities List of sites requiring investigation and cleanup under the Superfund Program. The nearshore/tideflats area was shown to be contaminated with a large number of hazardous substances at concentrations greatly exceeding those found in Puget Sound reference areas. At Hylebos Waterway, one of the nine problem areas in Commencement Bay, PCBs were identified as the primary chemical of concern.

In 1989, EPA issued a Record of Decision (ROD, USEPA, 1989a) which established Sediment Quality Objectives (SQOs) at the site for a wide range of hazardous substances, as well as a ten-year remediation plan for meeting those values using a combination of sediment cleanup, source controls, and natural recovery. A site-specific biota-to-sediment accumulation factor (BSAF) was calculated based on available fish tissue and sediment data. This BSAF was used to establish the SQO for PCBs at 150 ppb, which was deemed to be health protective for local subsistence anglers. Using the same BSAF and revised input parameters for fish consumption rates and the toxicity factor for PCBs, EPA revised the SQO to 300 ppb in July 1997. The average PCB concentration in a reference area used for comparison was approximately 30 ppb.

The Washington State Department of Ecology (WSDOE) used sediment data from Commencement Bay to demonstrate approaches for identifying PCB sediment contamination hotspots and for calculating urban bay, area-weighted, average PCB sediment concentrations (WSDOE, 2002). Using sediment sampling stations in Commencement Bay and the geographic information system ArcView (Environmental Systems Research Institute, Inc.) in conjunction with the Spatial Analyst extension, WSDOE mapped out areas in Commencement Bay associated with particular PCB concentrations.

Although site-specific BSAFs were empirically determined for the area and were used by the EPA and WSDOE for calculating SQOs at this site, such a process is not often practical. More frequently, SQOs are based on biotransfer parameters and modeling using tabulated data that are more easily obtained than site-specific information. We use this particular site for our convenience, since it provides readily available data allowing the assessment of the impact of

employing a range of tabulated $K_{ow}$ values on derived SQO levels and remediation costs. In our case study, PCB partitioning and fate were modeled using the TrophicTrace risk model (USACE, 2004). Other site-specific information required for the modeling (*e.g.*, the spatial extent and level of PCB contamination, sediment characteristics, exposure parameters for local population, etc.) was taken from site-specific measurements and estimates.

Both WSDOE (1997) and USEPA (1989a) present the volumes and remedial costs associated with meeting a specified remedial action level. Required sediment remediation volumes and the approximate costs for various SQOs obtained in our case study were calculated by multiplying the ratio of the remediation costs to volumes from the WSDOE and EPA assessments by the measured volume of contamination above calculated SQOs.

## METHODS

### $K_{ow}$ for Total PCBs and Aroclor 1254

Several databases and software packages reporting physical-chemical properties for PCBs are posted or referenced on the EPA web site. In addition, there are several guidance documents and databases referenced by the EPA and used in human health and ecological risk assessments that contain recommended $K_{ow}$ values for PCBs. Even though there are many original publications reporting $K_{ow}$ values for PCBs, only values obtained from the databases and software packages available from, or recommended by the EPA have been used in the case study. These tabulations list $K_{ow}$ values for PCBs (with no further specification), values for commercially available congener mixtures known as Aroclors, and/or values for individual congeners. Aroclor 1254 is the mixture that is tabulated most often in the databases, so $K_{ow}$ values for both unspecified PCB mixtures and Aroclor 1254 were used in the case study. Table 1 shows the log $K_{ow}$ values used in the case study.[1]

### Conceptual Model

The conceptual model used in the analyses is a simple food chain in which the contaminant of concern is total PCBs. A common polychaete, *Nereis virens* (sandworm), represents the prey base for a generic forage fish. It is assumed that the generic game fish feed solely on the generic forage fish. The human receptors are tribal anglers eating the generic game fish.

### Bioaccumulation Model

The analysis applies a steady-state bioaccumulation model based on the approach of Gobas *et al.* (Gobas, 1993; Gobas *et al.*, 1995). The model predicts PCB accumulation in fish through direct gill uptake of PCBs from water and dietary consumption of contaminated prey. The model is

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[1] Values of $K_{ow}$ are often tabulated as their base 10 logarithm (*e.g.*, a $K_{ow}$ of 1,000,000 will be tabulated as a log $K_{ow}$ of 6.00) because $K_{ow}$ values are very large numerically and vary over a wide range among different compounds. We follow this convention here.

implemented in the software package TrophicTrace (USACE, 2004). Model input parameters include: sediment concentrations for PCBs, weight and lipid content of aquatic organisms, food ingestion rate and body weight of fish, total organic carbon in sediment, and $K_{ow}$. Water concentrations are calculated from sediment concentrations using equilibrium partitioning. This is a conservative assumption (*i.e.* likely to overestimate risk) because equilibrium is not likely to be reached in a marine ecosystem. Default TrophicTrace data as well as site-specific information used to define input parameters are given in Table 2. Site-specific information was used when available. Several sources provide equations for the rate constants used in the model (Gobas, 1993; Gobas *et al.*, 1995; Burkhard, 1998).

**Human Health Exposure and Risk Model**

The potential non-cancer human health risk was estimated using the hazard quotient approach defined as:

$$HQ = \frac{IR_f * C_f * ED}{BW * RfD * AT * 10^6} \qquad (1)$$

where:

| | | |
|---|---|---|
| *HQ* | = | toxicity hazard quotient, |
| *IR$_f$* | = | annual average fish ingestion rate (g/day), |
| *C$_f$* | = | concentration of PCBs in fish tissue (µg/kg), |
| *ED* | = | exposure duration (days), |
| *BW* | = | body weight (kg), |
| *RfD* | = | reference dose (mg/kg-day), |
| *AT* | = | averaging time (days), and |
| $10^6$ | = | unit conversion factor. |

This equation was used to calculate a concentration of PCBs in fish tissue that would result in an acceptable risk level based on the use of the following exposure parameters.

*Fish Ingestion rate*: For the purposes of this study, we used a mean fish ingestion rate of 42 grams/day based on a survey of fish consumption among members of two Puget Sound tribes (WSDOE, 1997). Game fish from contaminated areas was assumed to comprise 50% of the anglers' fish diet.

*Exposure duration*: An exposure duration of 7300 days (*i.e.* 365 day/yr for 30 yr) was used to characterize a long-term fish ingestion scenario.

*Body weight*: Body weight is set to 70 kg as is commonly used in USEPA risk assessments (USEPA, 1997a).

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*Reference Dose*: The reference dose for Aroclor 1254 of 0.00002 mg/kg-day was selected for the assessment of both Aroclor 1254 and total PCBs following USEPA guidance for food chain exposures (1996). The value is from the EPA's Integrated Risk Information System (IRIS) database (2004), and is specified as a point estimate also following USEPA guidance (1989b).

*Averaging time*: An averaging time of 7300 days (*i.e.* 365 day/yr for 30 yr) was used to characterize long-term non-cancer health risks.

*Risk Levels*: Choice of a risk level is a policy decision. Most regulatory programs in the U.S. set a risk criteria for non-carcinogens at HQs below 1. For the purpose of this study, the risk-based cleanup levels are based on an HQ value of 1.

## Remedial Cost Estimation

Remedial costs are usually estimated based on the volume of contaminated sediments requiring removal and site-specific dredging/disposal scenarios. For this case study the remedial costs were estimated as the product of the area contaminated above the derived SQO, an assumed dredging depth, and an average dredging cost per unit volume. The spatial extent of contamination was taken from site study documents (WSDOE, 2002). The average dredging/disposal cost per unit volume was calculated using the ratio of overall remedial costs estimated by the EPA (1997a) to the volume of sediment requiring removal estimated by the WSDOE (1997).

## Software Implementation

TrophicTrace software (USACE, 2004) was used in this study to calculate SQOs from the PCB concentration in fish tissue determined by the exposure and risk model above. TrophicTrace is an Excel (Microsoft Corp.) add-in that provides a spreadsheet tool for calculating potential human health and ecological risks associated with bioaccumulation of contaminants in dredged sediments. It implements the risk assessment algorithms described above. The TrophicTrace software has been peer-reviewed and is currently used in several site-specific risk assessments (USACE, 2003; Bridges, 2004).

## RESULTS

## Discrepancies in Recommended $K_{ow}$ Values

A review of databases and software packages available from, or recommended by the EPA, reveals several sources reporting $K_{ow}$ values for total PCBs and/or Aroclor 1254 (Table 1). Reported log $K_{ow}$ values for total PCBs range from 3.9 to 8.23. The range of reported log $K_{ow}$ values for Aroclor 1254 is also quite wide (from 3.34 to 6.98).

Some of the differences in $K_{ow}$ values are evident among different EPA offices. The STF model developed by the Office of Research and Development (ORD) recommends a log $K_{ow}$ value of

8.23 for total PCBs; the Office of Air Quality Planning and Standards (OAQPS) provides a value of 7.31 in their Water 9 software; the Office of Pollution Prevention and Toxics (OPPT) gives a value of 6.3 in the PBT Profiler software; and the Office of Solid Waste and Emergency Response (OSWER) reports a value of 6.04 in the PHEM manual and in the SCDMWin database.

Significant differences can also be found among the software/tabulation products generated within the same office. For example, both Water 9 and Chem9 software were developed by OAQPS, but the $K_{ow}$ values for Aroclor 1254 that they generate differ by almost 3 orders of magnitude (log $K_{ow}$ values of 6.03 and 3.34, respectively). The tabulated $K_{ow}$ value for total PCBs reported in the paper version of the OSWER SCDM database is 6.7, while its software implementation (SCDMWin) reports a value of 6.04. The PhysProp, KowWin, and ChemFate Software products were all developed by the Syracuse Research Corporation for EPA, but recommended $K_{ow}$ values for total PCBs from these databases also range widely (from 3.9 to 7.1 for total PCBs).

It is possible that some of the differences are due to different intended purposes for the software/tabulations—different values of log $K_{ow}$ may more accurately represent the fate of PCBs in different situations. However, no warnings are provided in any of the software/tabulations on the applicability of the values obtained.

**Financial Implications of Selecting Different $K_{ow}$ Values**

Figure 1 presents the Sediment Quality Objectives for PCBs calculated using log $K_{ow}$ values from 6.0 to 7.2. This range does not include extreme values recommended in some databases (*e.g.*, the low values of 3.34 and 3.9, or the high value of 8.23). Selection of log $K_{ow}$ values from different databases can result in SQO levels that differ by more than a factor of seven. The case study cost associated with remediation requirements to achieve these health-based SQO levels range from approximately $7.5 million for a log $K_{ow}$ value of 6.0, to $55 million for a log $K_{ow}$ value of 7.2.

**DISCUSSIONS AND CONCLUSIONS**

Our review of $K_{ow}$ values available in EPA recommended databases reveals a range of values that covers more than four orders of magnitude for total PCBs and more than 3 orders of magnitude for Aroclor 1254. These ranges are even wider than the two order of magnitude range found for recommended $K_{ow}$ values for DDT and DDE by Pontolillo and Eganhouse (2001).

We have demonstrated the implication of selecting different $K_{ow}$ values for developing sediment quality objectives (SQOs) at a Superfund site using a standard approach applied through a peer-reviewed software package that was developed and recommended for such use by the Army Corps of Engineers. Even ignoring all other uncertainties in the modeling, variation of the $K_{ow}$ value for PCBs over the range available from the EPA produced extreme differences in cleanup

criteria and costs (a range of 7 to 1 in the latter, even without the use of the most extreme values).

One cannot predict which $K_{ow}$ values might be used in particular cases. However, it may be presumed that citation of an EPA source (such as those listed in Table 1) would provide adequate justification for any particular $K_{ow}$ value used in the modeling of a Superfund site. In this case at least, since it is possible to select a value from EPA sources that gives such a wide range of outcomes, the results have to be considered substantially arbitrary (even assuming no arbitrariness in other parts of the process). Moreover, without standardization of the source of estimates for values of parameters (*i.e.* selection of a single value for a particular chemical), the results at otherwise identical sites may also differ arbitrarily for the same reason.

There are many ways to deal with parameter uncertainties in risk assessment. Probabilistic methods can be used to explicitly characterize uncertainty in values resulting from different measurement techniques or an unknown mixture of components at a site (Linkov *et al.*, 2001). Site-specific calibrations can be used to narrow uncertainty distributions (USEPA, 1999). However, these methods assume that the empirical inputs, including those from databases, are valid. Eganhouse and Pontolillo (2002) concluded that to a large extent, the lack of data quality procedures and the proliferation of erroneous data and references may be responsible for the wide range of $K_{ow}$ values for DDT and DDE reported in the literature and recommended by agencies. Our study highlights the significance of their conclusion. Rigorous data quality and peer review procedures are required to ensure a consistent use of meaningful $K_{ow}$ values and of other possibly uncertain parameters in risk assessments and remedial action planning.

## ACKNOWLEDGEMENTS

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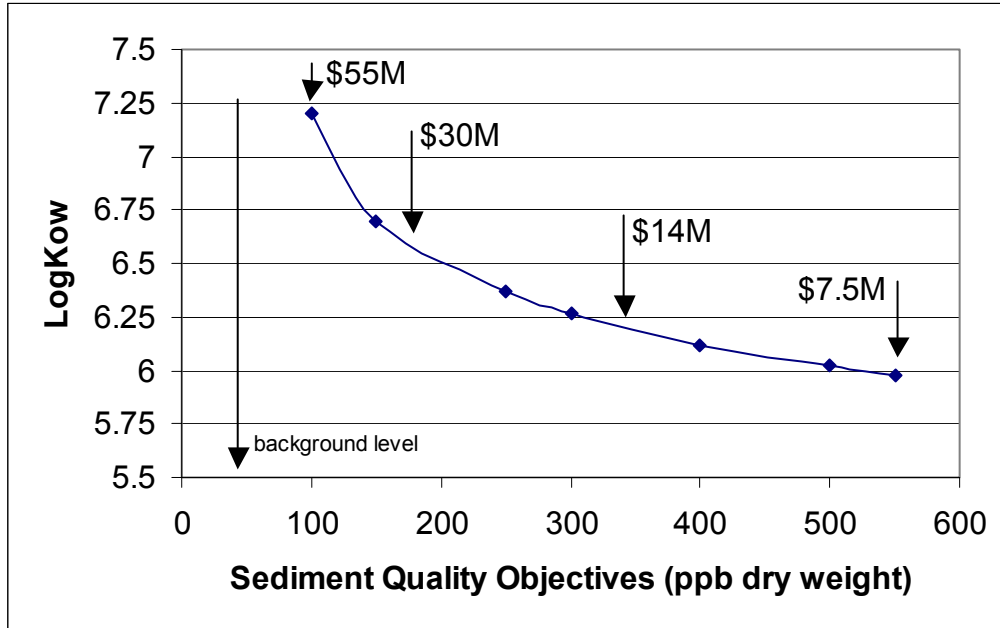
Figure 1.  Sediment Quality Objectives calculated for different $K_{ow}$ values.  Arrows indicate potential costs of remediation to selected SQO levels.

Table 1. Log $K_{ow}$ values for total PCBs and Aroclor 1254 used in the case study.

| Database | Log $K_{ow}$ Total PCBs | Log $K_{ow}$ Aroclor 1254 | Reference | Date of Download |
|---|---|---|---|---|
| KowWin (calculated) | 6.34 | 6.98 | USEPA, 2000 | 4/12/2004 |
| KowWin (experimental) | 6.29 | 6.79 | USEPA, 2000 | 4/12/2004 |
| PhysProp | 7.10 | 6.50 | SRC, 2004a | 4/12/2004 |
| ChemFate | 3.9 | | SRC, 2004b | 4/12/2004 |
| Water9 | 7.31 | 6.03 | USEPA, 2004a | 3/25/2004 |
| Chem9 | 7.31 | 3.34 | USEPA, 2004b | 3/20/2004 |
| SCDM[1] | 6.70 | | USEPA, 2004c | 3/30/2004 |
| SCDMWin | 6.04 | | USEPA, 1997b | 2/12/2004 |
| Superfund PHEM[2] | 6.04 | | USEPA, 1986 | NA |
| STF[3] | 8.23 | 6.04 | USEPA, 1991 | 2/24/2004 |
| HHRAPCF[4] | | 6.21 | USEPA, 1998 | NA |
| PBT Profiler | 6.3 | 6.8 | USEPA, 2004d | 3/30/2004 |
| ATSDR | | 6.50 | ATSDR, 2000 | NA |

[1] Superfund Chemical Data Matrix
[2] Public Health Evaluation Manual
[3] Soil Transport and Fate Database
[4] Human Health Risk Assessment Protocols for Combustion Facilities

Table 2.  Input Parameters

| Parameter | Mean value | Reference |
|---|---|---|
| **Sediment and Water** | | |
| Log-$K_{ow}$ | | Assumed, variable |
| Sediment Concentration (total PCBs, ng/g dry wt) | 300 | Cleanup level established by WSDOE, 1997 |
| Water Concentration (total PCBs, ng/l) | | Estimated based on equilibrium partitioning |
| TOC (%) | 3.4% | WSDOE, 1997 |
| **Sandworm** | | |
| Lipid Content (%) | 1.2% | Briggs and Kear, 1993; Rosman, 1999; Lemieux, *et al.*, 1997; Schrock, *et al.*, 1997 |
| **Generic Forage Fish** | | |
| Body Weight (g) | 3 | Assumed |
| Lipid Content (%) | 1% | Assumed |
| Site Use Factor (%) | 50% | Assumed |
| **Generic Game Fish** | | |
| Body Weight (g) | 250 | Site-specific |
| Lipid Content (%) | 3.5% | WSDOE, 1997 |
| Site Use Factor (%) | 50% | Assumed |
| **Human Ingestion** | | |
| Body Weight (kg) | 70 | WSDOE, 1997 |
| Reference Dose (mg/kg-day) | 0.00002 | IRIS, 2004 |
| Fish Ingestion (g/day) | 42 | WSDOE, 1997 |
| Exposure Duration (days) | 7300 | Assumed |
| Site Use Factor (%) | 50% | Assumed |

## IMPACT OF THE VARIABILITY IN PHYSICAL/CHEMICAL PARAMETERS ON RISK ASSESSMENTS

Physical-chemical constants are used in numerous fate and transport models (e.g., ground water, vapor intrusion, plant and animal uptake, etc.) to calculate human exposures in risk assessments. These constants, provided in numerous EPA databases, however, are not always consistent (as summarized in Marino, 1999). As a result, calculated human health risks, and alternatively, risk-based cleanup goals, can vary significantly depending on the source of the EPA physical-chemical constant. This represents a fundamental flaw in the data provided by EPA to support risk-based decisions.

The impacts of using different physical-chemical constants on the outcome of risk-based calculations were evaluated. This evaluation focused primarily on two parameters: octanol-water partition coefficient ($K_{ow}$) and Henry's Law Constant (HLC). For the chemicals considered in this evaluation, the $K_{ow}$ values varied by up to 150,000-fold and HLC values varied up to 6,000,000-fold (Table 1).

Although not directly used to calculate risks or risk-based cleanup goals, these physical-chemical constants are the foundation for several fate and transport models and are used as the basis for estimating other key parameters. In multi-pathway risk assessments, for example, $K_{ow}$ and HLC are used to calculate bioconcentration factors (BCF), beef biotransfer factors (Ba_beef), root concentration factors (RCF), soil organic carbon partitioning coefficients ($logK_{oc}$) (used to calculate soil-water partition coefficient), air-to-plant transfer factors, and more. If different $K_{ow}$ or HLC values are used for a particular chemical, the key parameter values can be significantly different (Table 2). Ultimately these values are used to estimate human exposures (and subsequently risk estimates) which are typically linearly related to the key parameter value. For example, if the calculated key parameter (e.g., BCF) varies by 10-fold, the calculated risks based on that key parameter would vary by 10-fold. Based on the values calculated for several chemicals using EPA-published $logK_{ow}$ values, BCF values varied from 1 to 38-fold, Ba_beef varied by over 150,000-fold, and RCF varied up to 6,000-fold (Table 2). These disparate values would significantly alter the conclusions of the risk assessment.

As noted above, physical-chemical constants are also used in various models provided by EPA. To illustrate how different physical-chemical constants for the same chemical can affect the model results, the "Johnson and Ettinger (1991) Model for Subsurface Vapor Intrusion into Buildings (Revised) (EPA, 2000)" was used. This model uses HLC to relate ground water concentrations, soil gas concentrations, and indoor air concentrations, to support risk-based decisions. Using the screening models available from EPA and modifying the input HLC values for benzene, hexachlorobutadiene and pentachlorophenol, the following were noted:

- Risk-based ground water concentrations varied up to 270-fold (Table 3), using default model inputs.

- Calculated risks for intrusion of soil gas into buildings varied up to 190-fold (Table 4), using default model inputs.

As shown in this simple evaluation, the dramatic disparities in physical-chemical constants provided in EPA guidance can significantly affect the outcomes of human health risk assessments, and consequently, the determination of risk-based cleanup goals. While some uncertainty may be expected in estimating the physical-chemical constants due to methodological extrapolations and uncertainties, the extreme variability presented in EPA databases is beyond the realm of uncertainty.

The impacts of the errors in the EPA databases on human health risk assessments and cleanup goals are significant and lack any scientific basis. As a result, calculated human health risks and cleanup goals based on some of the data provided in EPA databases cannot be considered reliable and may result in significantly flawed decisions.

**TABLE 1: Minimum and Maximum Physical/Chemical Parameters Provided in EPA Databases**

| Chemical | LogKow | | | Henry's Law Constant | | |
|---|---|---|---|---|---|---|
| | Min | Max | Ratio (Max/Min) | Min | Max | Ratio (Max/Min) |
| Benzene | 2.12 | 2.28 | 1.5 | $5.5 \times 10^{-3}$ | $5.5 \times 10^{-1}$ | 100 |
| Benzo(a) anthracene | 4.18 | 5.7 | 33 | $1.5 \times 10^{-9}$ | $3.4 \times 10^{-6}$ | 2,400 |
| Benzo(a) pyrene | 5.98 | 6.11 | 1.4 | $1.4 \times 10^{-9}$ | $1.6 \times 10^{-6}$ | 1,100 |
| Bis(2-ethylhexyl) phthalate | 2.12 | 7.3 | 150,000 | $1.1 \times 10^{-8}$ | $3.0 \times 10^{-7}$ | 28 |
| Dibutyl phthalate | 4.61 | 5.6 | 9.8 | $9.4 \times 10^{-10}$ | $1.8 \times 10^{-6}$ | 1,900 |
| Dichlorodifluoromethane | 2.16 | 2.4 | 1.8 | $2.5 \times 10^{-6}$ | $7.8 \times 10^{-1}$ | 320,000 |
| 2,4-Dichlorophenoxyacetic acid | 1.92 | 2.81 | 7.8 | $2.5 \times 10^{-6}$ | $4.0 \times 10^{-1}$ | 6,100,000 |
| 7,12-Dimethylbenz(a) anthracene | 5.98 | 7.46 | 30 | $2.7 \times 10^{-10}$ | $3.1 \times 10^{-8}$ | 120 |
| 1,4-Dioxane | -0.42 | 1.22 | 44 | $2.7 \times 10^{-7}$ | $2.3 \times 10^{-5}$ | 86 |
| Hexachlorobutadiene | 3.74 | 4.81 | 12 | $1.1 \times 10^{-5}$ | 4.6 | 410,000 |
| Hexachlorocyclopentadiene | 3.99 | 5.39 | 25 | $6.6 \times 10^{-4}$ | $1.1 \times 10^{1}$ | 16,000 |
| Hexachloroethane | 3.3 | 4.6 | 20 | $2.5 \times 10^{-6}$ | $2.2 \times 10^{-2}$ | 9,000 |
| Methyl methacrylate | -0.48 | 1.38 | 72 | $7.9 \times 10^{-6}$ | $2.4 \times 10^{-1}$ | 31,000 |
| PCBs | 6.04 | 8.23 | 155 | $2.7 \times 10^{-5}$ | $2.6 \times 10^{-3}$ | 97 |
| Pentachlorophenol | 5 | 5.09 | 1.2 | $2.4 \times 10^{-8}$ | $8.8 \times 10^{-5}$ | 3,600 |
| Pyridine | 0.65 | 0.67 | 1.1 | $8.9 \times 10^{-6}$ | $1.7 \times 10^{-3}$ | 190 |
| 1,2,3-Trichloropropane | 0.21 | 2.29 | 120 | $7.6 \times 10^{-6}$ | $2.8 \times 10^{-2}$ | 3,700 |
| Vinyl chloride | 0.06 | 1.5 | 28 | $2.0 \times 10^{-3}$ | $8.6 \times 10^{-2}$ | 43 |

Note:  LogKow ratios represent (Max $10^{logKow}$/Min $10^{logKow}$)
Based on work by Marino (1999)

**TABLE 2:  Ratio of Maximum/Minimum Values of Key Parameters Used
in Multi-Pathway Risk Assessments**

| Chemical | Beef Transfer Factor (Ba_Beef) | Bioconcentration Factor (BCF) | Root Concentration Factor (RCF) |
|---|---|---|---|
| Benzo(a)anthracene | 33 | NA | 15 |
| Bis (2-ethylhexyl phthalate | 150,000 | NA | 6,000 |
| 7,12-Dimethylbenz(a)anthracene | 30 | NA | 14 |
| 1,4-Dioxane | 44 | 18 | 1.3 |
| Hexachlorocyclopentadiene | 25 | NA | 12 |
| Hexachloroethane | 20 | NA | 9.4 |
| Methyl methacrylate | 72 | 26 | 1.4 |
| PCBs | 160 | NA | 49 |
| 1,2,3-Trichloropropane | 120 | 38 | 3.0 |
| Vinyl chloride | 28 | 12 | 1.5 |

Note:  All values calculated from $LogK_{ow}$
NA: Not Available - $LogK_{ow}$ is greater than 4.0
Based on work by Marino (1999).

**TABLE 3:  Risk Based Ground Water Concentrations Predicted Based on Henry's Law Constant
Using Johnson and Ettinger Model (EPA, 2000)**

| Chemical | Henry's Law Constant $(atm-m^3/mol-^oK)$ | Risk-Based Ground Water Concentration (ug/L) | Ratio of Max/Min Risk-Based Ground Water Concentration |
|---|---|---|---|
| Benzene | $5.5 \times 10^{-3}$ | 913 | |
| | $5.6 \times 10^{-3}$ | 910 | 1.5 |
| | $5.5 \times 10^{-1}$ | 608 | |
| Hexachlorobutadiene | $1.1 \times 10^{-5}$ | 68,100 | |
| | $8.2 \times 10^{-3}$ | 463 | 270 |
| | 4.57 | 250 | |
| Pentachlorophenol | $2.4 \times 10^{-8}$ | 263,000 | |
| | $2.6 \times 10^{-5}$ | 45,300 | 19 |
| | $8.8 \times 10^{-5}$ | 13,600 | |

**TABLE 4:  Inhalation Risks Predicted Based on Soil Gas Concentrations Based on Johnson and Ettinger Model (EPA, 2000)**

| Chemical | Henry's Law Constant $(atm\text{-}m^3/mol\text{-}^oK)$ | Incremental Risk From Vapor Intrusion to Indoor Air | Ratio of Max/Min Incremental Risk From Vapor Intrusion to Indoor Air |
|---|---|---|---|
| Benzene | $5.6 \times 10^{-3}$ | $2.0 \times 10^{-5}$ | |
| | $5.5 \times 10^{-1}$ | $2.0 \times 10^{-5}$ | 1 |
| Hexachlorobutadiene | $1.1 \times 10^{-5}$ | $1.8 \times 10^{-4}$ | |
| | 4.57 | $1.8 \times 10^{-4}$ | 1.2 |
| Pentachlorophenol | $2.4 \times 10^{-8}$ | $6.3 \times 10^{-2}$ | |
| | $8.8 \times 10^{-5}$ | $3.1 \times 10^{-4}$ | 190 |

Note:  Initial Soil Gas concentration of constituent is 200 ppmv.

| | Figure 1 | Figure 2 | | Figure 3 | | Figure 4 | Figures 5-8 | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Avg. No. Parameter Values/Chemical | Percent of Chemical With Equivalent Parameter Values from Different Datasets | | Coefficient of Variance (SD/Mean) | | Mean Coefficient of Variance | Percent of Pair Ratios | | | |
| | | All Equal | 1/2 Equal | Database Median CoV | Database 90th Percentile | | 1-10 | 10-100 | 100-1000 | >1000 |
| MolWT | 5.97 | 97% | 97% | 0.05% | 0.16% | 0.311% | 100% | 0% | 0% | 0% |
| HLC | 5.67 | 1.7% | 15% | 68% | 178% | 92% | 66% | 21% | 8.0% | 5% |
| LogKow | 5.78 | 30% | 53% | | | | | | | |
| Kow | | | | 35% | 116% | 47% | 91% | 7.5% | 0.7% | 0.5% |
| VapPRES | 5.73 | 3.3% | 35% | 27% | 155% | 62% | 85% | 6.4% | 3.7% | 5% |
| AqSOL | 3.82 | 22% | 65% | 18% | 82% | 37% | 92% | 5.2% | 2.7% | 0.0% |
| Dair | 2.30 | | | | | | | | | |
| Dwater | 2.30 | | | | | | | | | |

*[Attachment 3 - Summary worksheet]*

| Database | HLC | VapPRES | AqSOL | Kow |
|---|---|---|---|---|
| Table 1: Concordant and Dicordant Databases | | | | |
| CHEMDAT8 | c | c | | c, d |
| RCRA | | | c | |
| SCDM | d | d | d | |
| SIMS | c | c, d | | c |
| STF | d | | c, d | |
| SPHEM | | | | d |
| | | | | |
| Most concordant databases [c] | 27% | 78% | 50% | 82% |
| Least concordant (most discordant) [d] | 0.00% | 1.7% | 17% | 13% |

Concordance: Parmeter value ratios = $1.000 \pm 0.005$

| Maximum Parameter Value Ratios | | | | | |
|---|---|---|---|---|---|
| **Table 2: Chemicals with Highest Max/Min Parameter Value Ratios** | | | | | |
| Chemical | Chemical Class | HLC | VapPRES | AqSOL | Kow |
| DIMETHYL BENZ(A)ANT 7,12 | SVOC | 4.70E+07 | 1.45E+04 | | |
| DICHLOROPHENOXYACETIC ACID(2, | SVOC | 6.09E+06 | 4.83E+08 | | |
| Hexachlorobutadiene | SVOC | 4.06E+05 | | | |
| FREON 12, dichlorodifluoromethane | VOC | 3.19E+05 | | | |
| Methyl methacrylate | VOC | 3.07E+04 | | 8.00E+02 | 7.22E+01 |
| Bis (2-ethylhexyl) phthalate | SVOC | | 6.00E+06 | | 1.51E+05 |
| Benzo(a)pyrene | SVOC | | 1.14E+06 | | |
| Hexachlorobenzene | SVOC | | 1.00E+05 | 2.20E+01 | |
| Di-n-butyl phthalate | SVOC | | | 3.57E+01 | |
| Chloromethane | VOC | | | 7.51E+02 | |
| Pentachlorophenol | SVOC | | | 1.39E+02 | |
| PCBs | SVOC | | | | 1.55E+02 |
| Trichloropropane, 1,2,3- | SVOC | | | | 1.20E+02 |
| Dioxane, 1,4- | VOC | | | | 4.37E+01 |

Note: DIMETHYL BENZ(A)ANT 7,12 and FREON 12, dichlorodifluoromethane added/bromoform deleted

DMBA believed to be extra duplicate not referenced in original paper

Freon 12 added due to correction of STF HLC values.

| Table 3: Individual Parameter Values That Yielded Highest Max/Min Ratios | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Parameter | Constituent | Maximum Ratio | CHEMDAT8 | RCRA | Parameter Values SCDM | SIMS | STF | SPHEM |
| HLC | DIMETHYL BENZ(A)ANT 7,12 | 4.70E+07 | 1.27E-02 | NA | 3.11E-08 | 2.70E-10 | NA | NA |
| VapPRES | DICHLOROPHENOXYACETIC ACID(2, | 4.83E+08 | 2.90E+02 | 4.00E-01 | 6.00E-07 | 2.90E+02 | 1.00E-05 | 4.00E-01 |
| AqSOL | Methyl methacrylate | 8.00E+02 | NA | 1.60E+04 | 1.50E+04 | NA | 1.56E+04 | 2.00E+01 |
| Kow | Bis (2-ethylhexyl) phthalate | 1.51E+05 | 2.00E+05 | 2.00E+05 | 2.00E+07 | 2.00E+05 | 1.32E+02 | NA |

| Table 4: Risk Assessment Paramter Ratios Using LogKow Correlation Algorithms | | | | | | |
|---|---|---|---|---|---|---|
| **CASNUM** | **CHEMNAME** | **Ratio: Max/Min Calculated Values** | | | | **LogKow** | |
| | | Ba_beef | BCF | RCF | SSL Koc | Min | Max |
| 117-81-7 | Bis (2-ethylhexyl) phthalate | 1.51E+05 | NA | 5.97E+03 | 1.24E+05 | 2.12 | 7.3 |
| 1336-36-3 | PCBs | 1.55E+02 | NA | 4.85E+01 | 1.42E+02 | 6.04 | 8.23 |
| 96-18-4 | Trichloropropane, 1,2,3- | 1.20E+02 | 3.81E+01 | 2.97E+00 | 4.44E+01 | 0.2066 | 2.2873 |
| 80-62-6 | Methyl methacrylate | 7.22E+01 | 2.59E+01 | 1.40E+00 | 6.71E+01 | -0.479 | 1.38 |
| 123-91-1 | Dioxane, 1,4- | 4.37E+01 | 1.76E+01 | 1.30E+00 | 4.10E+01 | -0.42 | 1.2204 |
| 56-55-3 | Benz(a)anthracene | 3.31E+01 | NA | 1.46E+01 | 3.12E+01 | 4.18 | 5.7 |
| 57-97-6 | DIMETHYLBENZ(A)ANTHRACENE(7,1 | 3.00E+01 | NA | 1.37E+01 | 2.83E+01 | 5.98 | 7.4576 |
| 75-01-4 | VINYL CHLORIDE | 2.75E+01 | 1.24E+01 | 1.47E+00 | 1.38E+01 | 0.06 | 1.5 |
| 77-47-4 | Hexachlorocyclopentadiene | 2.51E+01 | NA | 1.17E+01 | 2.38E+01 | 3.99 | 5.39 |
| 67-72-1 | Hexachloroethane | 2.00E+01 | NA | 9.37E+00 | 1.07E+01 | 3.3 | 4.6 |

| CASNUM | CHEMNAME | Air-to-Plant Transfer Factor | Inhalation SSL Volatiliation Factor | Groundwater SSL Partition Factor | LogKow Min. | LogKow Max. | HLC Min. | HLC Max. |
|--------|----------|------------------------------|--------------------------------------|----------------------------------|-------------|-------------|----------|----------|
| 57-97-6 | DIMETHYL BENZ(A)ANT 7,12 | 1.76E+09 | 1.07E+03 | 2.83E+01 | 5.98E+00 | 7.46E+00 | 2.70E-10 | 1.27E-02 |
| 94-75-7 | 2,4 D | 1.52E+08 | NA | NA | 1.92E+00 | 3.23E+00 | 1.02E-08 | 6.21E-02 |
| 94-75-7 | DICHLOROPHENOXYACETIC ACID(2,4 | 5.44E+07 | NA | NA | 1.92E+00 | 2.81E+00 | 1.02E-08 | 6.21E-02 |
| 117-81-7 | Bis (2-ethylhexyl) phthalate | 9.18E+06 | 4.58E+02 | 5.53E+04 | 2.12E+00 | 7.30E+00 | 1.08E-08 | 3.01E-07 |
| 87-68-3 | Hexachlorobutadiene | 5.60E+06 | 1.41E+03 | 1.27E+01 | 3.74E+00 | 4.81E+00 | 1.13E-05 | 4.57E+00 |
| 75-71-8 | FREON 12, dichlorodifluoromethane | 5.78E+05 | 3.78E+02 | 7.90E+00 | 2.16E+00 | 2.40E+00 | 2.45E-06 | 7.81E-01 |
| 77-47-4 | Hexachlorocyclopentadiene | 4.97E+05 | 7.10E+02 | 2.56E+01 | 3.99E+00 | 5.39E+00 | 6.61E-04 | 1.06E+01 |
| 1336-36-3 | PCBs | 2.08E+04 | 2.79E+02 | 1.42E+02 | 6.04E+00 | 8.23E+00 | 2.69E-05 | 2.60E-03 |
| 56-55-3 | Benz(a)anthracene | 1.01E+05 | 2.05E+01 | 3.09E+01 | 4.18E+00 | 5.70E+00 | 1.38E-09 | 3.35E-06 |
| 57-97-6 | DIMETHYLBENZ(A)ANTHRACENE(7,12 | 4.32E+03 | 5.58E+00 | 2.83E+01 | 5.98E+00 | 7.46E+00 | 2.70E-10 | 3.11E-08 |
| 84-74-2 | Di-n-butyl phthalate | 2.19E+04 | 8.95E+00 | 9.36E+00 | 4.61E+00 | 5.60E+00 | 9.38E-10 | 1.81E-06 |

**Table 5: Risk Assessment Parameter Ratios Using Correlation Algorithms Requiring Both LogKow and HLC**

| CASNUM | CHEMNAME |
|--------|----------|
| 57-97-6 | DIMETHYL BENZ(A)ANT 7,12 |