The Search for Reliable Aqueous Solubility (S_w) and Octanol-Water Partition Coefficient (K_{ow}) Data for Hydrophobic Organic Compounds: DDT and DDE as a Case Study

By James Pontolillo and Robert P. Eganhouse

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Units and Acronyms

g/L	grams per liter
mg/L	milligrams per liter
mol/L	moles per liter
°C	temperature in degrees Celsius

ARS	U.S. Agricultural Research Service
ASTM	American Society for Testing and Materials
BAF	bioaccumulation factor
BCF	bioconcentration factor
CAS	Chemical Abstracts Service
CASSI	Chemical Abstracts Search Service Index
DDE	dichlorodipheyldichloroethylene, $(ClC_6H_4)_2C{=}CCl_2$
DDT	dichlorodiphenyltrichloroethane, $(ClC_6H_4)_2CHCCl_3$
EPA	U.S. Environmental Protection Agency
IUPAC	International Union of Pure and Applied Chemistry
K_{oc}	organic carbon-normalized partition coefficient
K_{ow}	octanol-water partition coefficient
log K_{ow}	base-10 logarithm of octanol-water partition coefficient
NIST	National Institute of Standards and Testing
OECD	Organisation for Economic Co-operation and Development
POPs	persistent organic pollutants
p,p'-DDE	primary metabolite of *p,p'*-DDT
p,p'-DDT	dominant isomer in technical DDT
PPR	property-property relation
QSAR	quantitative structure-activity relation
S_{oct}	solubility in *n*-octanol
SPARC	SPARC Performs Automated Reasoning in Chemisty
SPR	structure-property relation
S_w	aqueous solubility
RP-HPLC	reversed phase-high performance liquid chromatography

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ABSTRACT

The accurate determination of an organic contaminant's physico-chemical properties is essential for predicting its environmental impact and fate. Approximately 700 publications (1944–2001) were reviewed and all known aqueous solubilities (S$_w$) and octanol-water partition coefficients (K$_{ow}$) for the organochlorine pesticide, DDT, and its persistent metabolite, DDE were compiled and examined. Two problems are evident with the available database: 1) egregious errors in reporting data and references, and 2) poor data quality and/or inadequate documentation of procedures. The published literature (particularly the collative literature such as compilation articles and handbooks) is characterized by a preponderance of unnecessary data duplication. Numerous data and citation errors are also present in the literature. The percentage of original S$_w$ and K$_{ow}$ data in compilations has decreased with time, and in the most recent publications (1994–97) it composes only 6–26 percent of the reported data. The variability of original DDT/DDE S$_w$ and K$_{ow}$ data spans 2–4 orders of magnitude, and there is little indication that the uncertainty in these properties has declined over the last 5 decades. A criteria-based evaluation of DDT/DDE S$_w$ and K$_{ow}$ data sources shows that 95–100 percent of the database literature is of poor or unevaluatable quality. The accuracy and reliability of the vast majority of the data are unknown due to inadequate documenta-tion of the methods of determination used by the authors. [For example, estimates of precision have been reported for only 20 percent of experimental S$_w$ data and 10 percent of experimental K$_{ow}$ data.] Computational methods for estimating these parameters have been increasingly substituted for direct or indirect experimental determination despite the fact that the data used for model development and validation may be of unknown reliability. Because of the prevalence of errors, the lack of methodological documentation, and unsatisfactory data quality, the reliability of the DDT/DDE S$_w$ and K$_{ow}$ database is questionable. The nature and extent of the errors documented in this study are probably indicative of a more general problem in the literature of hydrophobic organic compounds. Under these circumstances, estimation of critical environmental parameters on the basis of S$_w$ and K$_{ow}$ (for example, bioconcentration factors, equilibrium partition coefficients) is inadvisable because it will likely lead to incorrect environmental risk assessments. The current state of the database indicates that much greater efforts are needed to: 1) halt the proliferation of erroneous data and references, 2) initiate a coordinated program to develop improved methods of property determination, 3) establish and maintain consistent reporting requirements for physico-chemical property data, and 4) create a mechanism for archiving reliable data for widespread use in the scientific/regulatory community.

INTRODUCTION

Background

The fate of an anthropogenic organic compound released into the environment is primarily controlled by a combination of three factors: 1) prevailing **environmental conditions** at the point(s) of discharge, transport and subsequent residence, 2) the **physico-chemical properties** of the compound, and 3) **patterns of use** (that is, locus and timing of introduction; *1*). Thus, accurate determination of physico-chemical properties is critical to the formulation of valid environmental models and assessments. Conversely, the predictive/interpretive value of environmental studies can be seriously compromised if the physico-chemical data upon which they rely are of questionable or unknown quality (*2*). As litigation becomes an increasingly common aspect of environmental science, such studies may be challenged and even refuted (*3*).

Two of the most important physico-chemical properties relating to the environmental behavior of hydrophobic organic compounds are aqueous solubility and octanol-water partition coefficient (*1,4*). Both parameters have seen extensive use in medicinal chemistry (pharmokinetics, drug design, anesthesiology), chromatography, and pesticide chemistry. Aqueous solubility (S_w) is defined as the equilibrium distribution of a solute between water and solute phases at a given temperature and pressure. Because S_w is the maximum solute concentration possible at equilibrium, it can function as a limiting factor in concentration-dependent (for example, kinetic) processes (*5*). The octanol-water partition coefficient (K_{ow}) is defined as the ratio of the concentration of a chemical in *n*-octanol and water at equilibrium at a specified temperature. It is assumed that the molecular speciation of the solute is the same in both solvents and that the solutions are sufficiently dilute (*6*). In the case of hydrophobic organic compounds, demonstration of the latter condition can prove difficult because of analytical limitations (*7-9*).

S_w and K_{ow} values can be determined directly using a variety of methods. However, in the case of organic compounds that are sparingly soluble in water ($S_w \leq 10^{-5}$ mol/L) and have log K_{ow} values $\geq$ 5–6, such as DDT and DDE, direct experimental determination of S_w and K_{ow} can be problematic. This situation has spurred development of estimation techniques that rely either on correlations of S_w or K_{ow} with other known and/or measurable properties (for example, molecular

connectivity indices, liquid chromatography capacity factors) or calculation of S_w and K_{ow} using group contribution, fragment constant, molecular, or atomistic approaches (*6,10*). The various techniques depend on many different assumptions and they produce results that are not always of comparable accuracy.

Much of the impetus for determining S_w and K_{ow} comes from the fact that these parameters can be used to estimate or predict other properties of more immediate environmental and ecotoxicological interest. Often the latter are too difficult or costly to determine directly. For this reason, a primary focus of research in the last 20 years has been development of linear regression equations in which S_w and K_{ow} (or more accurately, their logarithms) are correlated with parameters such as the organic carbon-normalized partition coefficient (K_{oc}; for example, *11–15*), bioconcentration and bioaccumulation factors (BCF, BAF; for example, *16-23*), and indices of biodegradability (*24,25*) or toxicity (*26–29*). Ultimately, these correlations can be incorporated into models that attempt to characterize the equilibrium distribution and transport rates of organic contaminants among environmental media (for example, *30–32*) or to predict impacts on indigenous biota (*21,27,29*). The results of such models have taken on greater immediacy in the last decade with the recognition that certain persistent organic pollutants (POPs), such as DDT and DDE, are globally distributed (*33*). Another important application is analysis of field data, where S_w and K_{ow} are used to identify factors controlling the phase distribution and composition of complex mixtures of organic contaminants (*34–36*) as well as the toxic effects, if any, they exert (*37*). Here, systematic differences in the physico-chemical properties of homologous series and similarities of these properties between isomers can be exploited for purposes of identifying the effects of natural processes on contaminant fate (*38–40*). Finally, sediment quality criteria proposed by the U.S. Environmental Protection Agency [EPA] (*41*) rely, in part, on estimates of contaminant bioavailability. These, in turn, are based on equilibrium partitioning of hydrophobic organic chemicals. Because K_{ow} is used to estimate K_{oc}, it has become a key parameter for the regulation and management of contaminated sediments.

The authors' interest in the octanol-water partition coefficients and aqueous solubilities of DDT and DDE arose in the context of research on the behavior and fate of these compounds in heavily contaminated sediments of the Palos Verdes Shelf (*42,43*). At the

outset it was expected that studies reporting S_w and K_{ow} values for *p,p'*-DDT and its primary metabolite, *p,p'*-DDE, would be well documented because DDT has a very long history (*44*), and its widespread application and biological effects are well known (*45,46*). DDT is among the most studied of all synthetic organic chemicals. However, the results of this preliminary search were unsatisfactory due to a large spread in the data values. Therefore, an exhaustive review of the scientific literature was performed to identify all measured and estimated values of S_w and K_{ow} for these compounds. Although the intent was to determine what the 'true' S_w and K_{ow} values of DDT and DDE were, a number of serious problems were encountered that severely limited use of the database. These problems include the following: 1) the literature is characterized by errors in reporting data and references, 2) review articles and data compilations, intended to summarize and evaluate available data, are incomplete and often serve to perpetuate these errors, 3) the original data span 2 - 4 orders of magnitude, and 4) there are few sources of original data that can be considered reliable by objective standards; the majority are of poor or unevaluatable quality. Whereas some of these conclusions have been reached previously (*1,47–50*), this study is the first to provide quantitative documentation of these problems for specific compounds. The authors are unaware of any class of synthetic chemicals for which a more comprehensive search of S_w and K_{ow} data has been made. To the extent that the DDT/DDE database may be representative of data for many other hydrophobic organic contaminants of interest, it is important to draw attention to these issues. The purpose of this report is to demonstrate the scope of the problems in quantitative terms and to stimulate interest in correcting them.

METHODOLOGY

The authors obtained and reviewed commonly available databases (*51–54*), handbooks (*1,5,47,55–66*), review articles (*48,49,67–72*), and bibliographies (*73,74*) for data, methodological details and pertinent literature citations. The initial survey was augmented by a computerized search of the scientific literature utilizing the Chemical Abstracts Search Service Index (CASSI) database. The CASSI search employed multiple limiting parameters (DDT, *p,p'*-DDT, DDE, *p,p'*-DDE, respective Chemical Abstracts Service [CAS] numbers, K_{ow}, log K_{ow}, octanol-water partition coefficient, aqueous solubility, aqueous soly) identified in title, abstract and keyword fields. Parameters for a specific compound (for example, DDT <u>or</u> *p,p'*-DDT <u>or</u> CAS number 50-29-3) were crossed with those corresponding to a physico-chemical property (for example, K_{ow} <u>or</u> octanol-water partition coefficient) for publications in all languages. The search encompassed articles abstracted from January 1960 to February 2001 and resulted in 107 hits. A general search of the World Wide Web also was performed using the same limiting parameters and a variety of Internet search-engines (*75*). Several hundred potential articles of interest were generated by these surveys. Each article was retrieved and scrutinized for applicable data, methodology and citation content. Additional relevant leads were identified from the reference lists in these publications, and they underwent a similar investigation process. The search progressed in stepwise fashion until no further leads could be identified. Finally, up-to-date information (as of March 2000) on the S_w and K_{ow} values contained in the AQUASOL (*76*) and MedChem databases (*77*) was obtained. In the course of assembling the current data compilation and reviewing the development of S_w and K_{ow} determination methodologies, approximately 700 publications were examined from the fields of medicinal chemistry, toxicology, chromatography, pesticide chemistry, molecular design, and the environmental sciences.

Throughout this report, the term "data" includes values for S_w or K_{ow} that were obtained by direct experimental determination (for example, generator

column method), indirect experimental determination (for example, the reversed phase-high performance liquid chromatography [RP-HPLC] method) and calculation-based estimation (for example, CLOGP method, see reference *78*). In cases where data were published without a source citation, the suspect data have been classified as being of 'uncertain origin' (see further discussion below). Also, many authors have reported data for DDT or DDE without specifying the positions of chlorine atom substitution. For purposes of the present study it was assumed that such references were intended to mean *p,p'*-substitution because this is the dominant isomer in technical DDT. The term, **DDT**, is hereafter used to designate data reported in the literature as either DDT or *p,p'*-DDT, whereas **DDE** will be used to designate data reported as either DDE or *p,p'*-DDE.

Although a goal of this study has been to identify all published DDT/DDE S_w and K_{ow} data, some results may have inadvertently been overlooked due to inattention, the incompleteness of databases employed, and/or the fact that computerized searches are not foolproof. The authors would greatly appreciate learning of any data that are missing from this compilation.

LITERATURE ERRORS

Types

Because the purpose of our search (data location and verification) differed from that of many bibliometric studies, a distinct error classification scheme was used. Three error types were commonly observed in the DDT/DDE S_w and K_{ow} literature: 1) multi-level referencing, 2) citation errors, and 3) data errors. *Multi-level referencing* is the practice of attributing data to a source other than the original published work. A non-original source publication may correctly reference the original published work (in which case, it would be considered a secondary source) or it may reference another publication that may or may not reference the original published work (in which case, it would be considered a tertiary or higher source). Thus, secondary or higher sources can mistakenly be cited as original sources of data, and multiple levels of referencing can result. It is not uncommon for the original citation to be lost entirely after several cycles of multi-level referencing (*79*). This type of error is the result of author inattention; original data sources are either over-looked or simply not verified. Aside from the loss of credit experienced by the originator(s) of the data, multi-level referencing results in misleading inflation of the database because the same data are attributed to several publications rather than the original source. The danger of this type of error is that users may assume that such data have greater validity because they appear to have been produced by different research groups. Moreover, the practice of averaging data sets that include multi-level references can result in bias of unknown sign and magnitude. These problems are discussed in more detail below.

Examination of the DDT/DDE S_w and K_{ow} literature indicates that multi-level referencing is a common problem. For example, despite the fact that Kenaga and Goring (*13*) only present data previously published by other investigators (that is, no original data are given), their paper has been cited at least 32 times as an original source of data. The ease with which multi-level referencing can proliferate is illustrated in figure 1. Here, citations of the DDT/DDE log K_{ow} data published by O'Brien (*80*) are depicted in a reference tree. [It must be emphasized that additional references to the O'Brien (*80*) data, not shown on this figure, may exist.] There are two types of sources secondary to the original O'Brien (*80*) data: those that correctly cite O'Brien (*14,18,71,81–85*; indicated by a solid arrow) and those for which the data are presumed to derive from O'Brien (*31,47,62,86–103*; indicated by a thick dashed arrow). In the latter case, data given in the secondary sources are identical to the O'Brien (*80*) data, but no reference to O'Brien was provided in those publications. At the same time, no other source for these values is known to exist in the literature, suggesting that O'Brien (*80*) was the source. Immediately below the secondary sources are publications (*64,68,69,78,87,104–117*) that report the O'Brien data but incorrectly attribute them to secondary sources. These are tertiary sources. Two more levels can be seen below the tertiary sources (*64,118*). In this example, only 14 percent (8 of 58) of the citations of O'Brien's DDT/DDE log K_{ow} data were properly referenced to the original publication. One paper (*64*), exemplifying an extreme case of the pitfalls involved in multi-level referencing, attributes O'Brien (*80*) data to 10 other publications.
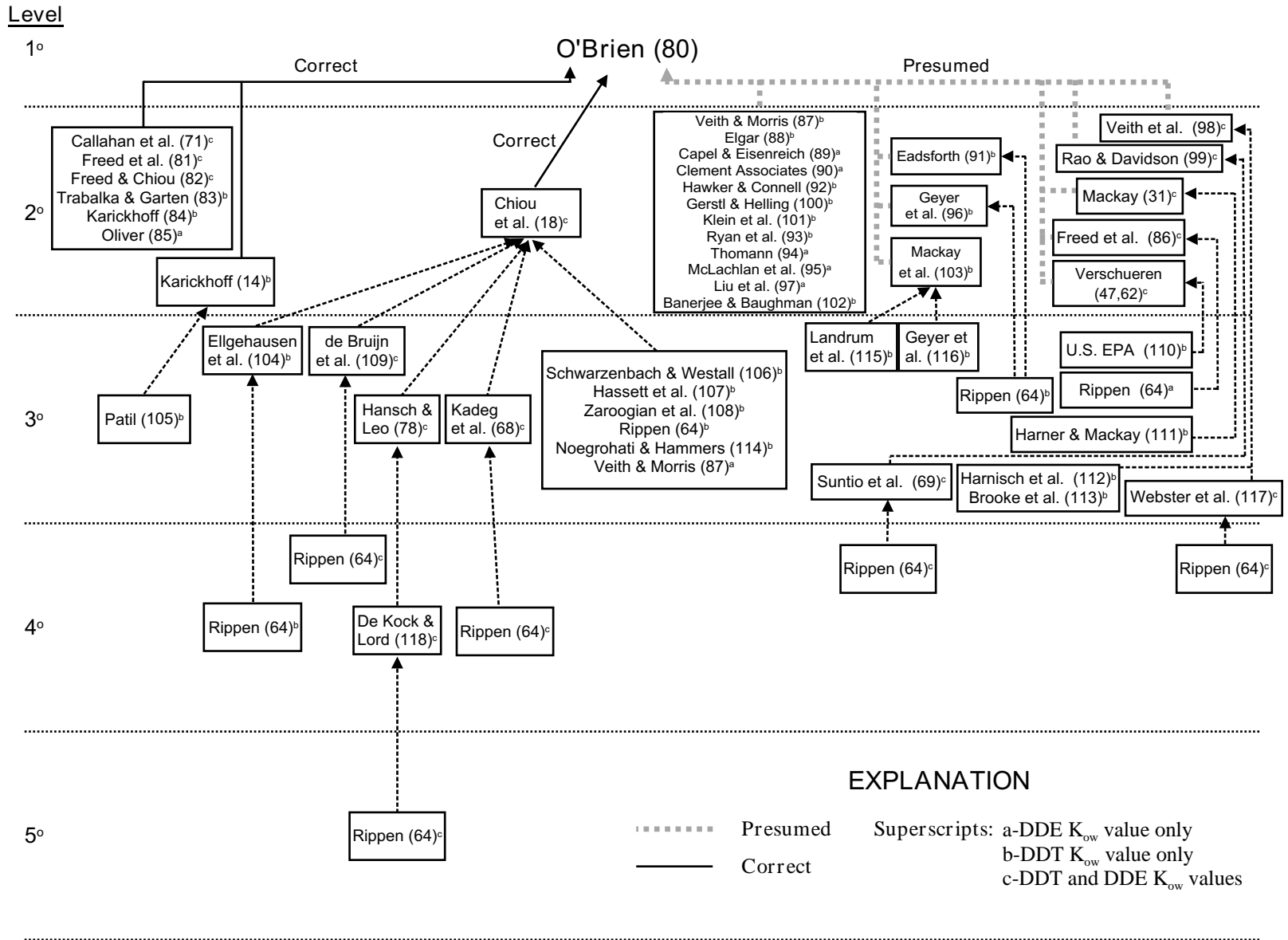
Figure 1. Reference tree showing original O'Brien (*80*) publication and secondary, tertiary and higher references as an example of multi-level referencing.
[Note: Non-USGS symbols and abbreviations are employed in this figure due to space limitations ("&" for "and"; "et al." for "and others").]

Citation errors include incorrect references, non-existent references, and missing references. 'Incorrect references' are the most common type of citation error. They result from mistakes that occur during transcription of the author's name, the publication date, volume number, pagination, and/or title of the article or journal. A commonly encountered incorrect reference in the DDT/DDE literature involves the work of "Kenaga and Goring, 1980" (*13*), which is often referred to as "Kenaga and Goring, 1978." In this case, authors mistakenly cite the earlier conference date rather than the actual publication date of the conference proceedings volume. Such mistakes may seem minor, but they often result in lengthier article retrieval times or computer search failures. In some instances, the article cannot be recovered at all on the basis of the citation given. An example of a recurring 'non-existent reference' in the literature is that of "Triggan *et al.* (*119*)", an erroneous reference to the work of Biggar and others (*120*). At least five publications (*48,69,121–123*) have included the erroneous "Triggan *et al.* (*119*)" citation in their bibliographies. A review paper (*121*) apparently initiated the error, which was repeated by other authors who did not verify the reference. 'Missing references' are instances where an abbreviated citation (either number or name) given in the text, tables or figures of a publication does not correspond to any of that publication's bibliographic entries.

Data errors include numerically and parametrically garbled data, unreferenced data, and data erroneously attributed to unrelated publications. 'Numerically garbled data' include numbers with juxtaposed digits or numbers that are similar, but not identical, to the original data (for example, an original log K_{ow} value of 5.75 given as 5.57 or 5.76). This error is primarily the result of faulty transcription, and it commonly occurs in compilations where large amounts of data are being manipulated. 'Parametrically garbled data' (for example, DDD data given as DDT data, K_{oc} data given as K_{ow} data, data for systems other than octanol-water given as K_{ow} data, *o,p'* data instead of *p,p'* data) also result from inattention during data compilation. 'Unreferenced data,' or the practice of not providing a reference to the source of data, is often found in compilations such as the *Merck Index* (*55*) and *Lange's Handbook of Chemistry* (*124*). However, it also occurs frequently in journal articles as shown in figure 1 [see references depicted as 'presumed' to originate from O'Brien (*80*)]. Unreferenced data and data associated with nonexistent references and missing references may be termed 'data of uncertain origin' for which only a provisional identification (based on numerical similarity and a comparison of the respective publication dates) is possible. Data that are unpub-

lished or appear in the literature as personal communications should also be included in this classification. Data of uncertain origin are of no value because their reliability is indeterminate.

Extent

In order to evaluate the state of the literature, an analysis of citations reported in 11 compilations (*1,48,49,63,64,67–72*) and four databases (*51,52,76,77*) was conducted. These represent all of the known compilations and databases that contain a significant amount of data on the aqueous solubility and octanol-water partition coefficients for DDT and DDE. One compilation (*66*) and one database (*54*) were not included in this analysis due to the small number of data citations they contained (n ≤ 2 for each compound-property pair). [It is important to recognize that the objectives and procedures of these compilations and databases vary. In this case, three of the compilations (*1,49,72*) attempted exhaustive data collections, two (*63,70*) screened data prior to inclusion in their reports, and the other six (*48,64,67–69,71*) did not specify their literature review procedures. In the case of the databases, all used screened data; in two instances (*52,77*), the screened data were evaluated in order to arrive at a "suggested value."] The purpose of the present study was to determine what fraction of the citations reported in these compilations and databases were original data sources. In addition, it was of interest to know the fraction of original data (extant at the time of publication) reported in the compilation or database.

The distribution of citations to DDT/DDE S_w and log K_{ow} data are plotted by date of publication in figure 2. The data for DDT and DDE were combined in order to simplify the visualization of trends. There were two instances where compilations were published in the same year (1988–*69,72*; 1997–*1,70*). In these cases, citation category statistics were combined and are presented for that year as a single group. Also shown is information for databases (indicated by the letter "D" above the uppermost symbol for the date the database was published or made available). Citations to data reported in compilations and databases are categorized as: 1) original data sources, 2) multi-level references (including secondary sources), 3) citation errors, and 4) data errors as discussed above. The total number of citations associated with the DDE and DDT data for a specified date is given as a fraction (that is, # DDE data points reported/# DDT data points reported) near the uppermost symbol for that year.

Aqueous solubility, S_w

Octanol-water partition coefficient, Log K_{ow}
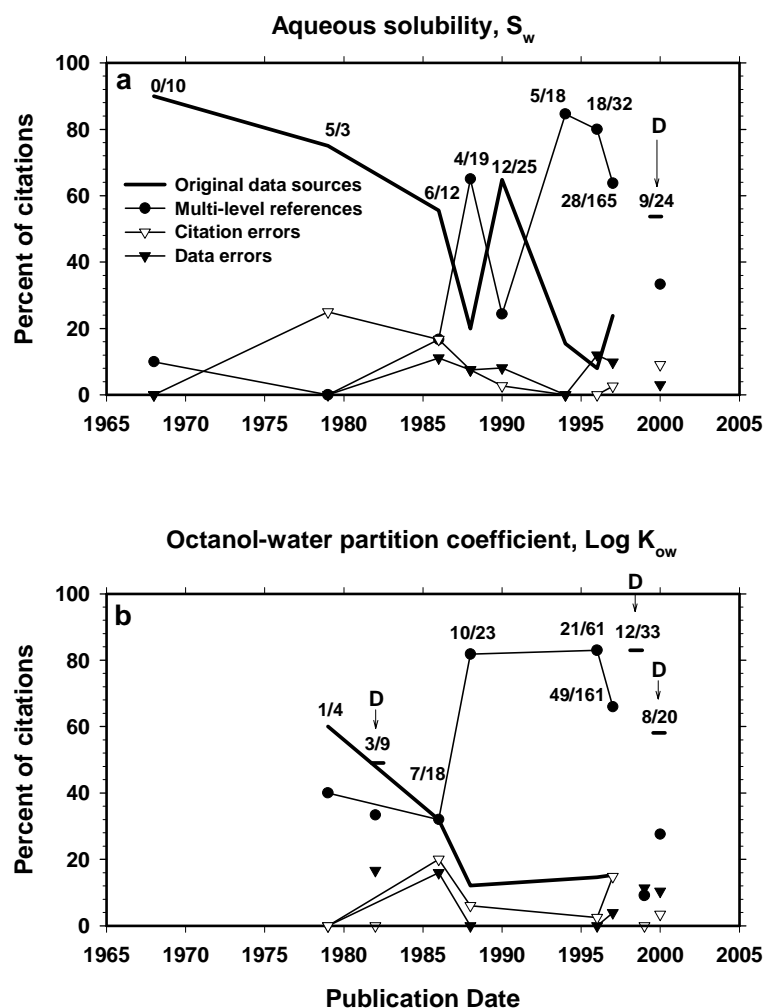
Figure 2. Plots of percent of citations in compilation articles and databases that are original data sources, multi-level references, citation errors or data errors by date of publication/acquisition: a) aqueous solubility (S_w), b) log octanol-water partition coefficient (log K_{ow}). Fractions above data points reflect number of data for DDE and DDT given in compilation/database (n/m = number of data points for DDE/number of data points for DDT). "D" above data points indicates data given in databases. See text for sources of data.

Over the last three decades, DDT/DDE S_w compilations have become less reliable with time (fig. 2a). This result is evidenced by a general decline in the percentage of correctly cited original data sources. [The only exception to this trend is a compilation published in 1990 (*48*), which contains 65 percent original data sources.] The most recent compilations (*1,63,64,67*) are composed of 6–23 percent original data sources. The remaining 'data' citations consist primarily of numerically redundant multi-level references (86 percent of the non-original data source citations). By comparison, the AQUASOL database (indicated by the "D" on fig. 2a; *76*) appears to have a higher proportion (55 percent) of original data sources than the most recent compilations.

Compilations of DDT/DDE log K_{ow} data are fewer in number and span a shorter time period (fig.

2b), but the trends are similar. Fourteen to twenty-six percent of the data reported in the most recent compilations (*1,64,70*) are correctly attributed to original data sources. The rest consist primarily of numerically redundant multi-level references (83 percent of the non-original data source citations). In general, the DDT/DDE log K_{ow} databases (*51,52,77*; indicated by the "D" on fig. 2b) have higher proportions (50–80 percent) of original data sources than recent compilations. The percentages of citation errors and data errors for both S_w and K_{ow} in compilations have remained relatively constant with time, whereas the proportions of original data sources and multi-level references have assumed an inverse relation with a sizable growth in reporting of the latter since about 1985. This pattern highlights a key feature of multi-level referencing; it tends to proliferate with time.

Despite similarities in the S_w and K_{ow} compilation trends, it cannot be assumed that the distribution of data citations among compilations is uniform (figs. 3a–d). For purpose of illustration, four compilations were selected that reflect the range of data-citation practices. [The reader should keep in mind that differences shown here might result, in part, from differences in the objectives and procedures of the respective studies.] Some compilations are heavily dominated by multi-level references (figs. 3c,d), whereas others show a more even distribution of citation types (fig. 3b) or are dominated by data errors (fig. 3a). When the data for all 11 compilations were pooled, citations associated with multi-level references, citation errors and data errors outnumbered those for original data sources by a factor of 3. Clearly, the database is of limited use when correctly cited original data sources are only a minor component of published compilations.

A second issue concerning compilations and databases is their completeness. What proportion of the existing published original data do they report? The three most recent databases (*52,76,77*) and the most recent compilation (*1*) were examined, comparing the original data reported therein with original data that were available 1 year prior to the time the compilation/databases became available. The AQUASOL database (*76*) was found to contain 29 percent of the existing published original DDT/DDE S_w data, whereas the compilation (*1*) reported 68 percent. In the case of DDT/DDE K_{ow} data, the figures were lower [databases (*52,77*): 17–40 percent, compilation (*1*): 30 percent]. The lower percentages observed for the databases result, in part, from intentional screening of published data. However, the compilation did not screen data prior to publication.

Figure 3. Plots of citation categories for four compilation articles with S_w (unfilled bars) and K_{ow} (filled bars) data. n = number of citations; M-L-references = multi-level references.

Effects

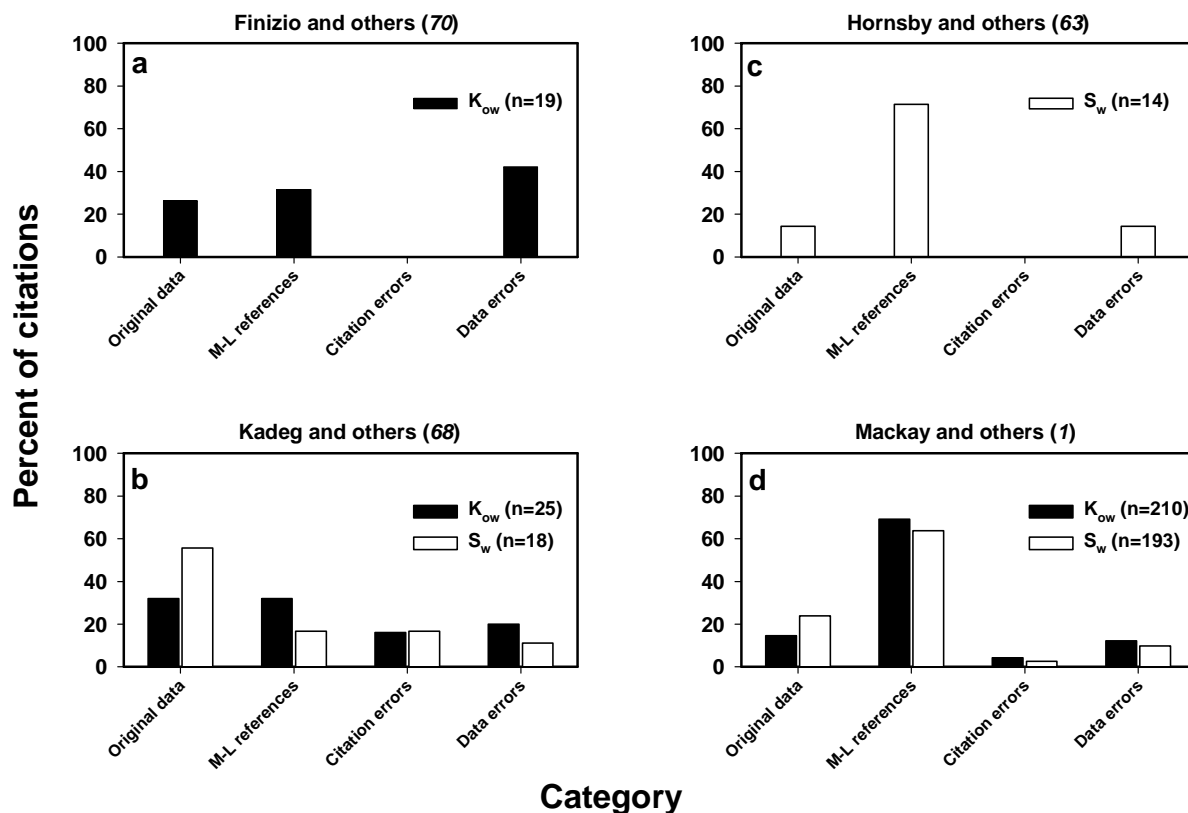The cumulative effect of the aforementioned errors has been to obscure the extent and reliability of the original database. Plots of correctly cited 'original data' and 'erroneous data' from Mackay and others (*1*) for DDT/DDE S_w and log K_{ow} illustrate this point. 'Erroneous data' refers to published data that are derived from one of the three types of reference errors discussed previously (that is, multi-level references, citation errors, data errors). As noted earlier, original data are a minority of the total data presented. When reported solubilities or log K_{ow} values are plotted by date of publication (figs. 4a–d), a data point can develop into what appears as a linear sequence of erroneous data points (that is, an erroneous data string) with time. This pattern is due to multi-level referencing. It is important to note that whenever two or more secondary or higher sources report the same data and are published in the same year, the data points are superposed. [For example, the erroneous data string corresponding to a log K_{ow} value for DDT of 6.19 (fig. 4b) has 32 data points. Sixteen of these points are not visible in the figure due to superimposition of data points.] Thus, some points in the erroneous data strings depicted in figure 4 cannot be seen. In most cases, the *originating* data point is original data (for example, fig. 4b: DDT log K_{ow} value of 6.19) or erroneous data (for example, fig. 4b: DDT log K_{ow} value of 5.98). However, the publication of "selected" or "recommended" values has, at times, resulted in a similar effect, creating erroneous data strings that cannot be traced back to an original data point (for example, fig. 4d: DDE log K_{ow} value of 6.51). These effects are further examined in table 1 where the numbers, types, and sizes of erroneous data strings are given and in table 2 where the contribution of erroneous data strings to the overall database is shown. It is clear from data given in table 1 that long strings can arise from originating data points that are erroneous (for example, DDT K_{ow} data = 6.00) and that "selected" or "recommended" values occasionally result in strings of considerable size (for example, DDT S_w data = 0.003 mg/L). As shown in table 2, strings of erroneous data compose as much as 41–73 percent of the total data. [Recall that this does not include erroneous data resulting from citation errors or data errors but is caused only by multi-level referencing.] In all cases, erroneous data are generated predominantly from originating data points that are original data (see *Number of Erroneous Points in Strings* columns, table 2).

The effects of erroneous data on the database can also be examined statistically (table 3). The erroneous DDT/DDE S_w data has a noticeable effect on the statistics of the 'all data' set. Mean values of the DDT/DDE S_w 'all data' sets are 23 - 65 percent lower than those for the original data alone. The redundant nature of the erroneous data results in artificially lower standard deviations and 95-percent confidence limits in the 'all data' sets as compared with the original data sets. The inclusion of erroneous log K_{ow} data apparently has slightly less effect on the mean values of the 'all data' set (log $K_{ow\text{-}DDT}$ = 6.04-'all data' as opposed to 6.24-'original data', log $K_{ow\text{-}DDE}$ = 5.99-'all data' as opposed to 6.23-'original data'). Mean K_{ow} values for 'all data' sets are 37–42 percent lower than those for the original data alone. Again, inclusion of erroneous log K_{ow} data in the 'all data' set leads to artificially lower standard deviations and 95-percent confidence limits when compared with the original data. Given the amount of scatter in the original data and the confusing overlay of erroneous data, deducing a reliable S_w or K_{ow} value would be difficult for most users of the data compilation. Although the Mackay and others (*1*) compilation was used for purposes of illustration here, the literature reviewed in the present study indicates that such problems are the rule, not the exception.

PUBLISHED ORIGINAL DATA

All verifiable, published original DDT/DDE S_w and K_{ow} data produced by direct experimental determination, indirect experimental determination, and computational methods for the period 1944–2001 are presented in tables 4 and 5. These uncensored data, consisting of 62 S_w values (45 DDT, 17 DDE) and 100 log K_{ow} values (64 DDT, 36 DDE), are tabulated in groups according to method of determination/estimation. The data sources are widely dispersed throughout the literature (32 journals, 2 books, 1 symposium proceedings, 6 government reports). For example, only *Chemosphere* and *Environmental Science & Technology* have published data for a given compound/property pair more than twice. Although the vast majority of the solubility data are for determinations made within 18–25°C, data exist over a temperature range of 2–45°C. Tables of S_w and log K_{ow} data for which no published source was cited (that is, 'data of uncertain origin') are available in appendix A. The data of uncertain origin comprise at least 42 S_w values (30 DDT, 12 DDE) and 71 log K_{ow} values (45 DDT, 26 DDE). Such a large number of unverifiable data is further evidence of the poor quality of the DDT/DDE S_w and K_{ow} literature.
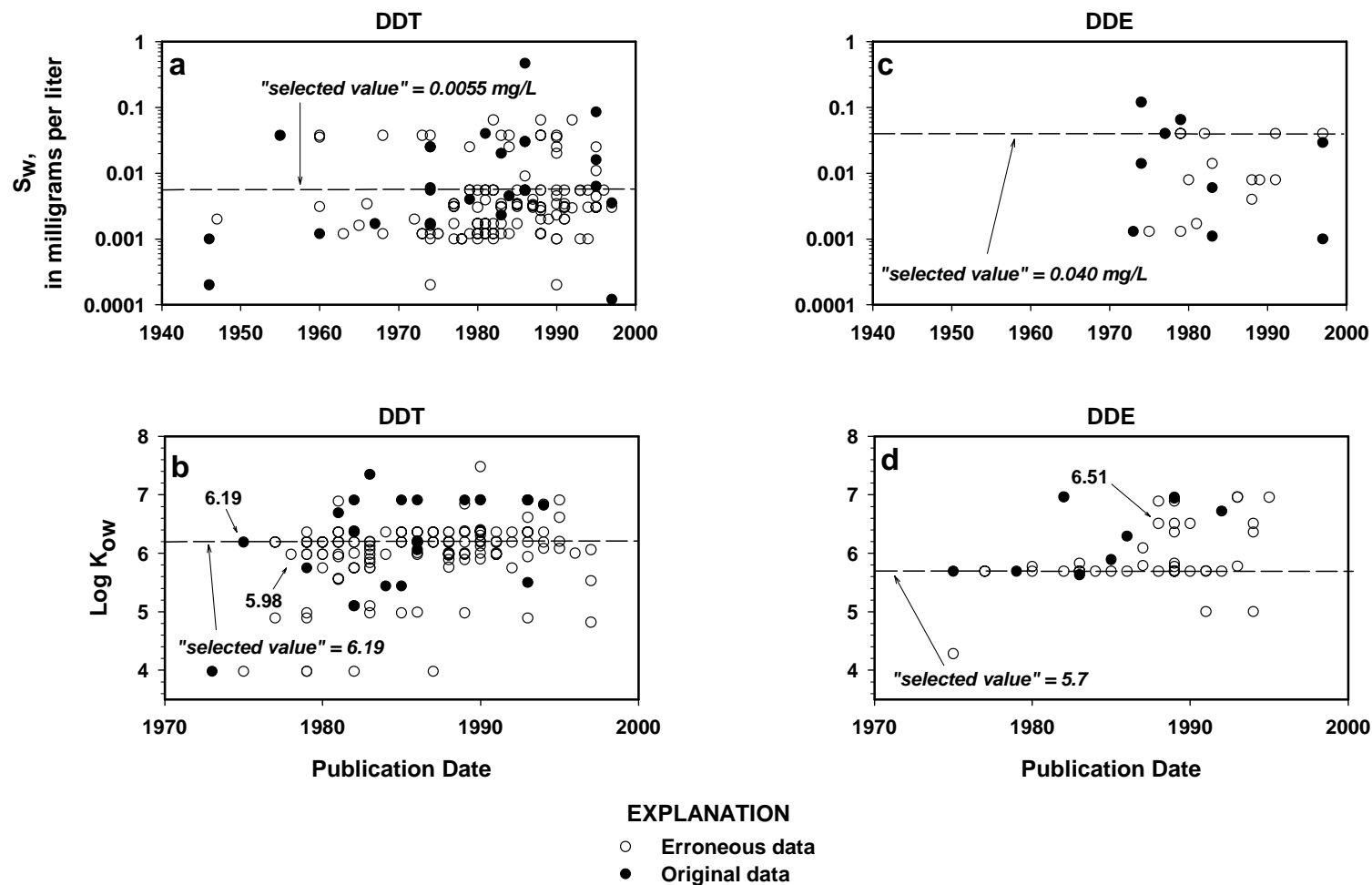
Figure 4. Plots of aqueous solubility (S$_w$) and log octanol-water partition coefficient (log K$_{ow}$) data for DDT and DDE in references reported by Mackay and others (*1*). a) DDT/S$_w$, b) DDT/log K$_{ow}$, c) DDE/S$_w$, d) DDE/log K$_{ow}$. See text for explanation of data points for which values are shown. "Selected values" are those identified in summary table of Mackay and others (*1*). Note: S$_w$ data shown are for 18 - 25°C only.

Table 1. Numbers, Types and Sizes of Erroneous Data Strings Reported in Compilation of Mackay and others (*1*)

Originating Data Point	Type of Originating Data Point[a]	Number of Data Points in String[b]	Originating Data Point	Type of Originating Data Point[a]	Number of Data Points in String[b]
DDT S_w Data[c]			**DDT log K_{ow} Data[d]**		
0.0002	original	2	3.98	original	5
0.001	original	10	4.89	erroneous/de	2
0.0012	original	26	4.98	erroneous/de	3
0.0016	erroneous/de	1	5.10	original	2
0.0017	original	11	5.75	original	7
0.002	erroneous/de	5	5.98	selected/ recommended	12
0.0023	original	1	6.00	erroneous/de	7
0.003	selected/ recommended	12	6.083	erroneous/de	1
0.0031	erroneous/de	6	6.12	selected/ recommended	1
0.0034	erroneous/ce	7	6.19	original	32
0.004	original	1	6.20	erroneous/de	4
0.0045	original	1	6.36	original	21
0.0055	original	17	6.36	erroneous/de	6
0.02	original	1	6.613	erroneous/de	1
0.025	original	4	6.84	erroneous/de	1
0.035	erroneous/ce	1	6.91	original	3
0.0374	original	9			
0.0645	erroneous/de	2			
DDE S_w Data[c]			**DDE log K_{ow} Data[d]**		
0.0013	original	2	5.00	selected/ recommended	1
0.0079	erroneous/de	3	5.69	original	17
0.014	original	1	6.36	erroneous/de	1
0.040	original	5	6.51	selected/ recommended	3
			6.89	erroneous/de	1
			6.956/6.96	original	3

[a] Originating data point types: original=original data, erroneous/de=erroneous data/data error, erroneous/ce=erroneous data/citation error, selected/recommended=data value selected or recommended by author(s). [b] Does not include originating data point. [c] S_w = aqueous solubility in units of milligrams per liter. [d] K_{ow} = octanol-water partition coefficient.

Table 2. Contribution of Erroneous Data to Overall Database in Compilation of Mackay and others (*1*)

Data Type[b]	Total[a]			Erroneous Originating Point			Originating Point-Original Data		
	Number of Data Strings	Number of Erroneous Points in Strings[c]	Percentage of Total Data[d]	Number of Data Strings	Number of Erroneous Points in Strings[c]	Percentage of Total Data[d]	Number of Data Strings	Number of Erroneous Points in Strings[c]	Percentage of Total Data[d]
DDT S_w	18	117	72.7	7	34	21.1	11	83	51.6
DDT K_{ow}	16	108	65.5	10	38	23.0	6	70	42.4
DDE S_w	4	11	40.7	1	3	11.1	3	8	29.6
DDE K_{ow}	6	26	53.1	4	6	12.2	2	20	40.8

[a] Total = Erroneous data strings resulting from erroneous originating data points and originating data points that are original data (see text for explanation). [b] S_w = aqueous solubility; K_{ow} = octanol-water partition coefficient. [c] Does not include originating data point. [d] Erroneous data points as a percentage of total data points.

Table 3. Statistical Comparison of S_w and log K_{ow} Data Reported in Compilation of Mackay and others ([1])

| | Aqueous solubility, S_w (milligrams per liter) | | | | | |
| | DDT | | | DDE | | |
Statistic	Original Data[a]	Erroneous Data[b]	All Data[c]	Original Data[a]	Erroneous Data[b]	All Data[c]
Mean	0.034	0.008	0.012	0.031	0.020	0.024
Standard Deviation	0.094	0.013	0.040	0.040	0.018	0.028
95-percent Confidence Limit	0.035	0.002	0.006	0.025	0.009	0.011
	Log octanol-water partition coefficient, log K_{ow}					
Mean	6.24	6.02	6.04	6.23	5.94	5.99
Standard Deviation	0.83	0.57	0.61	0.58	0.58	0.58
95-percent Confidence Limit	0.38	0.09	0.09	0.55	0.16	0.16

[a] Obtained from original data source. [b] Multi-level references + citation errors + data errors. [c] Original data + erroneous data.

The S_w and K_{ow} data-generation histories for DDT and DDE are illustrated in figure 5. These curves are based on the verified original data given in tables 4 and 5. Also shown is a timeline of key events in the history of DDT. The DDT and DDE S_w data curves exhibit much flatter profiles than the corresponding K_{ow} curves, and the DDT S_w curve begins approximately 30 years before the DDE S_w and DDT/DDE K_{ow} curves. The earlier interest in the aqueous solubility of DDT corresponds to its use as an insecticide starting in 1942 and numerous laboratory studies undertaken during the 1940s to determine the basis for DDT's acute toxicological effects, as well as the cause of insect resistance to it. Data on the aqueous solubility of DDE first appeared in the literature in the early 1970s. This is about the time DDT was banned by the EPA (1972), and it probably reflects growing concern for the environmental fate of this highly persistent DDT metabolite. DDT/DDE K_{ow} data production began about 1973, rising rapidly until the mid-1980s when data accumulation slowed. This trend may be related to the general increase in K_{ow} data for anthropogenic contaminants during this period when it was realized that K_{ow} could serve as a predictor of sorption and bioconcentration. Not surprisingly, the timing also corresponds to the advent of modern methods for estimation and experimental determination of K_{ow} for a wide range of organic contaminants ([6]).
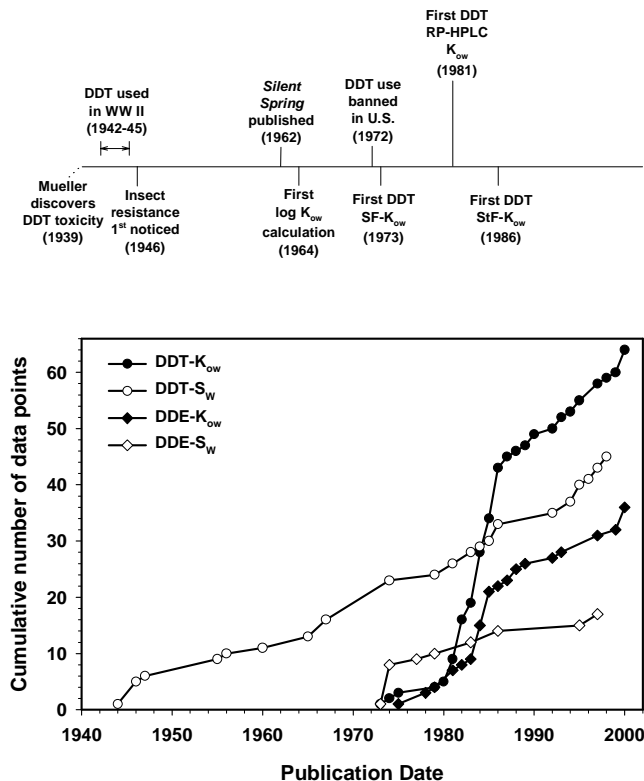
Figure 5. DDT and DDE S_w and K_{ow} original data generation plots as a function of publication date along with a timeline of important historical events.

Table 4. Published Original DDT S_w and log K_{ow} Data

S_w or log K_{ow}[a]	Compound Designation	Method[b]	Temp (°C)	# Rep[c]	Precision	Reference
			Aqueous solubility, S_w			
1	DDT	nr	nr	nr	nr	125
< 1	DDT	nr	nr	nr	nr	126
0.016, 0.040	DDT	nr	ambient	nr	nr	127
0.0002-0.001	DDT	SF	nr	nr	nr	128
0.0034, 0.002, 0.0017	*p,p*'-DDT	SF/GC	25	>1	± 0.00017, nr ± 0.00017	120
0.017	*p,p*'-DDT	SF/GC	15	≥3	nr	129
0.0017, 0.006, 0.025	*p,p*'-DDT	SF/GC	25	≥3	nr	129
0.037	*p,p*'-DDT	SF/GC	35	≥3	nr	129
0.045	*p,p*'-DDT	SF/GC	45	≥3	nr	129
0.0054	*p,p*'-DDT	SF/GC	24	>1	nr	130
0.0059	DDT	SF/RA	2	10	± 0.0004	131
0.0374	DDT	SF/RA	25	10	± 0.0005	131
0.045	DDT	SF/RA	37.5	10	± 0.001	131
≤ 0.0012	DDT	SF/RA	25	>1	nr	132
0.0045	DDT	SF/RA	25	3	nr	133
0.01-0.1	*p,p*'-DDT	TOX$_{est}$	22	nr	nr	134
0.04	*p,p*'-DDT	Turbidity	20	nr	nr	135
0.004	*p,p*'-DDT	Turbidity/N	24	nr	± 0.0002	136
0.1	DDT	Turbidity/N	18	nr	nr	137
0.0055	DDT	GnC	25	>1	nr	138
0.0023	DDT	GnC	25	nr	nr	139
0.0077	*p,p*'-DDT	GnC	20	nr	nr	117
0.0053	*p,p*'-DDT	GnC	24	3	± 0.0009	140
0.0051	*p,p*'-DDT	GnC/SPME/GC	25	5	± 0.00011	123
0.020	DDT	RP-HPLC	25	nr	nr	139
0.0302	*p,p*'-DDT	RP-HPLC	nr	nr	nr	141
0.467	*p,p*'-DDT	PPR	nr	nr	nr	141
0.085	DDT	PPR	25	na	na	142
0.00012, 0.00346	*p,p*'-DDT	PPR	25	na	na	143
0.00132	*p,p*'-DDT	SPR	nr	na	na	105
0.0039	DDT	SPR	nr	na	na	144
6.22	DDT	Top/ANN	na	na	na	145
0.00175, 0.00355	DDT	G-C	nr	na	na	25
0.0063	DDT	G-C	25	na	na	146
0.0158	DDT	G-C/AQUAFAC-3	25	na	na	142
0.0013	*p,p*'-DDT	G-C	na	na	na	147
			Log K_{ow}			
3.98	DDT	SF	nr	nr	nr	24
6.36	*p,p*'-DDT	SF/GC	20	nr	nr	148
6.33	*p,p*'-DDT	SF/GC	24	--[d]	--[d]	148
5.1	DDT	SF/RA	20-25	7	± 0.1	149
5.44	DDT	SF/RA	25	3	nr	133
6.17, 6.16, 6.22, 6.24	*p,p*'-DDT	StF	nr	nr	nr	150
6.914	*p,p*'-DDT	StF	25	10	± 0.030	109
6.307	*p,p*'-DDT	StF	25	>1	± 0.045	113
5.73	DDT	'StF'[e]	ambient	--[f]	--[f]	140
6.00	*p,p*'-DDT	StF-SPME	25	4	± 0.05	123
5.94	*p,p*'-DDT	S_{oct}/S_w	20	nr	nr	135

Table 4. Published Original DDT S_w and log K_{ow} Data—Continued

S_w or log K_{ow}[a]	Compound Designation	Method[b]	Temp (°C)	# Rep[c]	Precision	Reference
		Log K_{ow}				
5.74	DDT	CPE[g]	25	--[h]	--[h]	140
5.75	*p,p'*-DDT	RP-HPLC	na	nr	nr	151
6.38	*p,p'*-DDT	RP-HPLC	na	nr	nr	152
6.06, 5.84	*p,p'*-DDT	RP-HPLC	na	3-5	nr	112
6.40	DDT	RP-HPLC	na	>1	± 0.11	153
5.13	*p,p'*-DDT	RP-HPLC	na	10	nr	154
5.56, 5.65, 5.51, 5.49, 5.45, 5.44	*p,p'*-DDT	RP-HPLC	na	nr	nr	155
5.44	*p,p'*-DDT	RP-HPLC	na	nr	nr	156
5.53, 5.65	*p,p'*-DDT	RP-HPLC	na	nr	nr	117
5.27, 5.87	*p,p'*-DDT	RP-HPLC	na	nr	nr	157
5.3, 6.4	*p,p'*-DDT	RP-HPLC	na	nr	nr	150
6.06	*p,p'*-DDT	RP-HPLC	na	nr	nr	141
6.21	*p,p'*-DDT	RP-HPLC	na	2	nr	91
5.63	*p,p'*-DDT	RP-HPLC	na	nr	nr	118
6.51	DDT	RP-HPLC	na	nr	nr	158
5.50	DDT	RP-HPLC	na	3	nr	159
7.48	*p,p'*-DDT	PPR	nr	na	na	103
6.69	DDT	PPR	nr	na	na	160
5.60	*p,p'*-DDT	PPR	nr	na	na	83
7.7	*p,p'*-DDT	PPR	nr	nr	nr	150
6.06	*p,p'*-DDT	PPR	nr	na	na	70
7.92	*p,p'*-DDT	PPR	25	na	na	161
6.50	*p,p'*-DDT	PPR	25	na	na	162
6.82	*p,p'*-DDT	SPR	nr	na	na	105
6.89	DDT	SPR	nr	na	na	144
6.84	*p,p'*-DDT	SPR	na	na	na	163
5.76	DDT	FC-H&L	na	na	na	164
6.91	DDT	FC-H&L	na	na	na	165
5.76	*p,p'*-DDT	FC-H&L	na	na	na	83
6.91	*p,p'*-DDT	FC-H&L	na	na	na	156
6.763	*p,p'*-DDT	FC-H&L	na	na	na	77
6.91	*p,p'*-DDT	FC-H&L	na	na	na	91
6.91	*p,p'*-DDT	FC-H&L	na	na	na	166
6.76	*p,p'*-DDT	FC-H&L	Temp	na	na	70
7.35	*p,p'*-DDT	FC-R	na	na	na	112
7.51	*p,p'*-DDT	FC-R	na	na	na	114
6.79	*p,p'*-DDT	FC-M&H	na	na	na	167
6.92	DDT	G-C	na	na	na	168
6.19	*p,p'*-DDT	SC	na	na	na	80
6.91	*p,p'*-DDT	'QSAR'	na	na	na	169
7.05	*p,p'*-DDT	SPARC	na	na	na	170

[a] S_w = aqueous solubility in units of milligrams per liter; K_{ow} = octanol-water partition coefficient. [b] Method acronyms as follows : SF=shake-flask, GC=gas chromatography, RA=radiometric analysis, TOX_est=estimated from toxic response, StF=stir-flask, GnC=generator column, N=nephelometry, SPME=solid phase microextraction, CPE=continuous phase equilibration, S_{oct}/S_w= solubility in *n*-octanol/aqueous solubility, RP-HPLC=reversed phase-high performance liquid chromatography, PPR=property-property relationship, SPR=structure-property relationship, Top/ANN=topological indices/artificial neural network, FC-H&L=fragment constant-Hansch and Leo (*78*), FC-R=fragment constant-Rekker (*171*), FC-M&H=fragment constant-Meylan and Howard (*172*), G-C=Group contribution, SC=substituent constant, 'QSAR'=quantitative structure activity relationship-based chemical modeling and information system, SPARC=SPARC Performs Automated Reasoning in Chemistry (*173*). [c] Number of replicates reported. [d] Data were generated based on ten separate experimental determinations at different nominal DDT saturation levels (50-90%). Number of replicates and precision are, therefore, not reported here. [e] Method involves 'stir flask-like' technique-see reference for details. [f] Precision is not reported here because twelve experiments were conducted with addition of octanoic acid at seven different concentrations. [g] Methodology involves unique closed loop phase equilibration-see reference for details. [h] Precision is not reported here because eight experiments were conducted at five different solute concentrations. nr-not reported, na-not applicable.

Table 5. Published Original DDE S_W and log K_{ow} Data

S_w or log K_{ow}[a]	Compound Designation	Method[b]	Temp (°C)	# Rep[c]	Precision	Reference
		Aqueous solubility, S_W				
0.055	*p,p*'-DDE	SF/GC	15	≥ 3	nr	129
0.01, 0.04, 0.120	*p,p*'-DDE	SF/GC	25	≥ 3	nr	129
0.235	*p,p*'-DDE	SF/GC	35	≥ 3	nr	129
0.450	*p,p*'-DDE	SF/GC	45	≥ 3	nr	129
0.0013	DDE	SF/RA	25	nr	nr	174
0.040	*p,p*'-DDE	StF/GC	20	nr	nr	18
0.014	*p,p*'-DDE	GnC	25	>1	nr	138
0.0011	DDE	GnC	25	nr	nr	139
0.065	*p,p*'-DDE	Turbidity/N	24	nr	± 0.003	136
0.006	DDE	RP-HPLC	25	nr	nr	139
0.0236	*p,p*'-DDE	RP-HPLC	nr	nr	nr	141
1.24	*p,p*'-DDE	PPR	nr	na	na	141
0.001, 0.029	*p,p*'-DDE	PPR	25	na	na	143
0.0152	DDE	G-C	25	na	na	146
		Log K_{ow}				
6.956	*p,p*'-DDE	StF	25	>2	± 0.011	109
5.83	*p,p*'-DDE	RP-HPLC	na	nr	nr	87
5.69	*p,p*'-DDE	RP-HPLC	na	nr	nr	151
5.89	*p,p*'-DDE	RP-HPLC	na	nr	nr	175
5.63	DDE	RP-HPLC	na	nr	nr	139
6.02, 6.12, 6.02, 6.00, 5.96, 5.94	*p,p*'-DDE	RP-HPLC	na	nr	nr	155
5.89	*p,p*'-DDE	RP-HPLC	na	nr	nr	156
5.99, 6.11	*p,p*'-DDE	RP-HPLC	na	nr	nr	117
5.85, 6.51	*p,p*'-DDE	RP-HPLC	na	nr	nr	157
6.29	*p,p*'-DDE	RP-HPLC	na	nr	nr	141
6.09	*p,p*'-DDE	RP-HPLC	na	nr	nr	118
7.14	DDE	RP-HPLC	na	nr	nr	158
5.78	DDE	RP-HPLC	na	3	nr	159
5.74	*p,p*'-DDE	PPR	nr	na	na	70
7.67	*p,p*'-DDE	PPR	25	na	na	161
5.50	*p,p*'-DDE	PPR	25	na	na	162
6.78	*p,p*'-DDE	SPR	Tema	na	na	163
4.88	*p,p*'-DDE	FC-H&L	na	na	na	175
6.96	DDE	FC-H&L	na	na	na	165
6.94	*p,p*'-DDE	FC-H&L	na	na	na	156
6.94	*p,p*'-DDE	FC-H&L	na	na	na	166
6.736	*p,p*'-DDE	FC-H&L	na	na	na	77
6.94	*p,p*'-DDE	FC-H&L	na	na	na	70
6.00	*p,p*'-DDE	FC-M&H	na	na	na	167
5.01	*p,p*'-DDE	FC-R	na	na	na	175
6.72	*p,p*'-DDE	FC-R	na	na	na	114
7.2	*p,p*'-DDE	G-C	na	na	na	176
5.69	*p,p*'-DDE	SC	na	na	na	80
6.63	*p,p*'-DDE	SPARC	na	na	na	170

[a] S_w = aqueous solubility in units of milligrams per liter; K_{ow} = octanol-water partition coefficient.　[b] Method acronyms as follows: SF=shake-flask, GC=gas chromatography, RA=radiometric analysis, StF=stir-flask, GnC=generator column, N=nephelometry, RP-HPLC=reversed phase-high performance liquid chromatography, PPR=property-property relationship, FC-H&L=fragment constant-Hansch and Leo (*78*), FC-R=fragment constant-Rekker (*171*), FC-M&H=fragment constant-Meylan and Howard (*172*), G-C=Group contribution, SC=substituent constant, SPARC= SPARC Performs Automated Reasoning in Chemistry (*173*).　[c] Number of replicates reported. nr-not reported, na-not applicable.

Uncensored DDT and DDE S_w measurements/estimates (from tables 4 and 5) plotted as a function of date of publication for the period 1944–1998 are shown in figure 6. Only those direct experimental solubilities determined within a temperature range of 18–25°C are plotted here. For purposes of this figure it was assumed (but cannot be confirmed) that solubilities reported as having been determined at "ambient temperatures" and those for which temperatures were not reported also fall within the 18–25°C range. Data published as a range of solubilities (for example, *128,134*) are depicted in figure 6 by double-headed arrows connecting data points, whereas data published as maximum solubilities (for example, *126,132*) are shown as downward-pointing arrows originating at the respective data points. Finally, it was assumed that the solubilities estimated by indirect experimental determination and computational methods, as given in tables 4 and 5, reflect aqueous solubilities for DDT and DDE within 18–25°C.

An examination of the published original data demonstrates that, for nearly 55 years, the range in reported DDT S_w values (fig. 6a) has spanned three to more than four orders of magnitude. Moreover, S_w values developed over the last decade show as much scatter as early measurements made in the 1940s. In the case of the DDE S_w data (fig. 6b), there are fewer measurements/estimates, but the overall range is approximately three orders of magnitude. Given the scatter exhibited by these uncensored data, a user would be hard pressed to select appropriate values for the aqueous solubility of DDT or DDE without further information on data quality. This issue is addressed below.

EXPLANATION

↕ Depicts range of solubilities reported

↓ Depicts solubility reported below a given value

Figure 6. Original S_w data for a) DDT and b) DDE plotted as a function of publication date. Data are taken from tables 4 and 5. See text for explanation.

Uncensored DDT and DDE log K_{ow} values (from tables 4 and 5) plotted as a function of date of publication for the period 1973–2000 are shown in figure 7. As in the case of the solubility data, the range in DDT and DDE log K_{ow} values is large (3.7 and 2.3 log units, respectively), and there is no apparent reduction in the amount of scatter with time. The uncensored S_w and K_{ow} data for DDT and DDE exhibit bimodal or trimodal distributions, and in all cases, the variance appears to exceed the mean values (table 6). The cause(s) for the large variation in S_w and log K_{ow} values is not immediately apparent. However, direct comparison of the standard deviations listed in table 6 with the few reported estimates of experimental reproducibility given in tables 4 and 5, suggest that (within-investigation) methodological problems or between-investigation differences are likely involved. Trends in S_w and log K_{ow} measurements and the relationship between reported data and the methods of determina-

tion/estimation that have been used are examined in a later section (see Effect of Methodology).

The observation that published literature on physico-chemical parameters contains a considerable amount of conflicting data, with reported values differing by several orders of magnitude, is not a new one (*1,47–49*). The pesticide solubility literature was singled out for its unreliability in the late 1960s (*49*). Nevertheless, there has been no subsequent improvement in the database, and the original criticisms remain valid. Moreover, such problems may not be limited to hydrophobic organic compounds with very low aqueous solubilities because marked discrepancies have been found for even moderately soluble pesticides (*177*). Based on these previous reports and the present authors' observations, the common practice of using physico-chemical data without first carefully assessing its reliability is inappropriate.
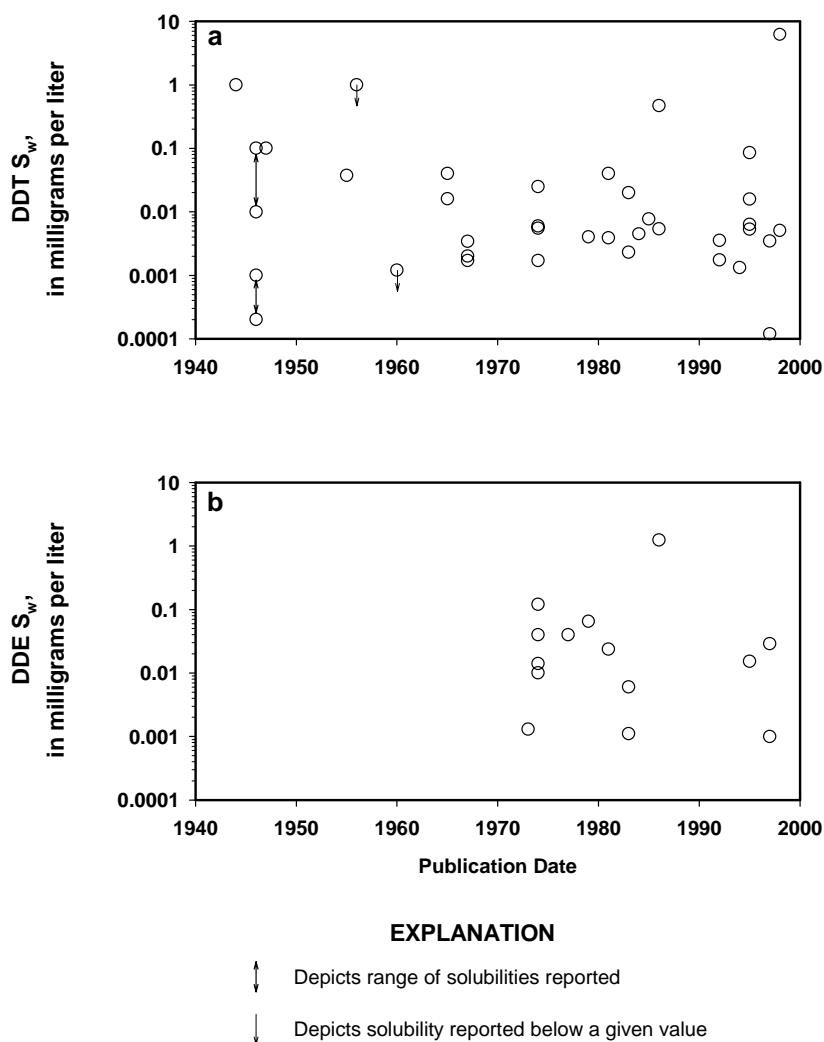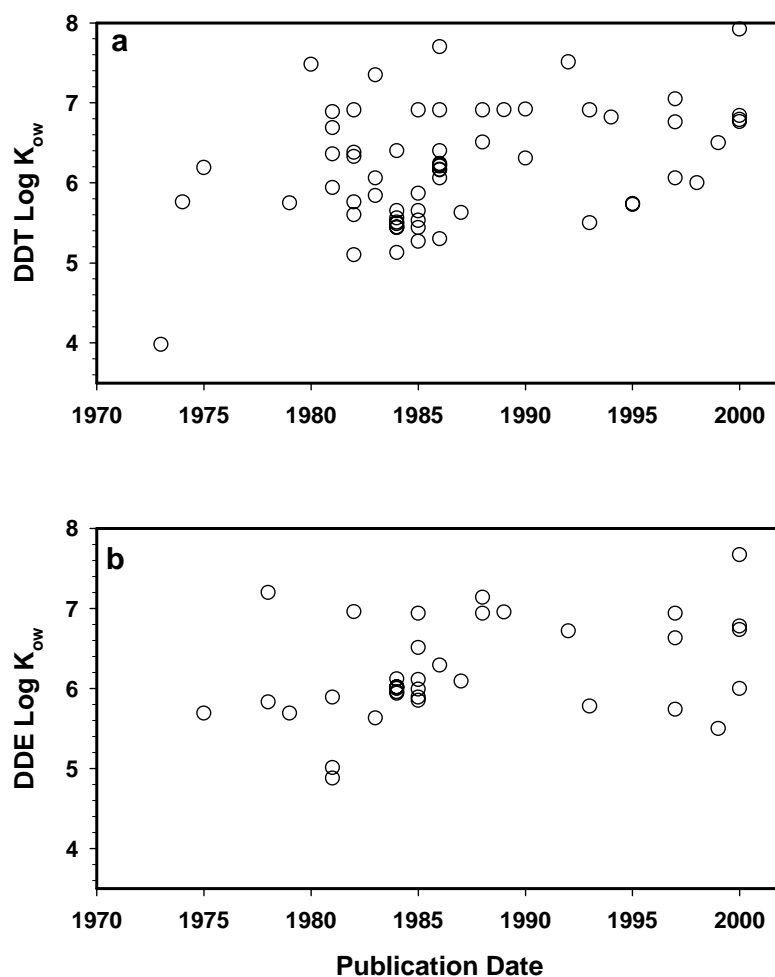

Figure 7. Original log K_{ow} data for a) DDT and b) DDE plotted as a function of publication date. Data are taken from tables 4 and 5.

Data Quality

Data quality is a crucial, though frequently underemphasized, issue in scientific research (*178*). The quality of published physico-chemical property data usually is unknown, and it is common practice for users to accept the data rather than conduct a time-consuming evaluation. Such issues are especially difficult to address for indirect experimental (for example, RP-HPLC) and computational methods that rely upon correlation analysis because information on the underlying data (assumed to be accurate) may not be readily available. A recent study of S_w data for 6 pesticides (not including DDT and DDE) demonstrated that the variation in published data was considerably greater than the expected measurement errors (*178*). Because the data quality was poor or unknown in all cases, the entire data set was judged to be "less than credible." The scarcity of detailed information on the accuracy of reported S_w and log K_{ow} values has been noted (*123*), and the situation for estimates of experimental precision is similar. The DDT/DDE literature appears to be of equally poor quality. For example, of 46 experimental DDT/DDE S_w values reported (tables 4 and 5), only 9 (20 percent) have associated estimates of precision, and of 59 experimental DDT/DDE log K_{ow} values reported, only 6 (10 percent) have associated estimates of precision. When the literature is characterized by numerous inconsistencies and errors, the need for a comprehensive data quality evaluation is obvious.

Various subjective criteria have been used by authors when evaluating the validity of data or for arriving at "recommended" S_w and log K_{ow} values. It is not uncommon for experimental data to be compared in the same publication with a few selected data from the literature in order to demonstrate that there is "good agreement with literature values." Such comparisons are meaningless given the extreme variability of the published original DDT/DDE S_w and K_{ow} data. With DDT S_w and K_{ow} values spanning more than three orders of magnitude, it would be difficult not to find agreement with a subset of the data. As noted earlier, "recommended" or "selected" values are often chosen based on examination of highly erroneous and incomplete data compilations (see "selected values" in fig. 4). Without objective substantiating information, the selection of these values would appear to be purely subjective. Moreover, because of the overriding effect of multi-level references and/or missing original data, such "selected values" may be biased (see table 3, fig. 4). Other authors have used the "reasonable trend" approach to assess the validity of data (that is, does a data point fit into a reasonable trend for a series of structurally similar compounds?). This can be an unreliable method, however, because such trends are not always applicable to isomers (*179*) or compounds, such as DDT and DDE, that have unique structures. Even when objective guidelines for selecting reliable physico-chemical parameters are described in a compilation, the authors may not apply this approach to the data being reported. Users are, thus, left to sift through the data at their own discretion with limited or no guidance as to its reliability.

Table 6. Basic Statistics for Uncensored Original S_w and K_{ow} DDT/DDE Data[a]

	DDT	DDE
Statistic	**Aqueous solubility, S_w (milligrams per liter)**	
Mean	0.23	0.12
Standard Deviation	1.00	0.32
	Octanol-water partition coefficient, K_{ow} [b]	
Mean	5.9×10^6 (6.20)	4.5×10^6 (6.22)
Standard Deviation	1.3×10^7 (0.73)	8.3×10^6 (0.63)

[a] Data given in tables 4 and 5 were used for statistical calculations. For S_w, only data for 18–25°C were used. For K_{ow}, all data were used. In cases where solubilities were reported as being 'less than' a specified concentration in the original source publication, that concentration was used as is for the calculation of mean and standard deviation. In cases where ranges of solubilities were reported, the upper and lower bounds of each solubility range were included in the calculations. [b] Mean, standard deviations of log K_{ow} values are given in parentheses.

Assessment of DDT/DDE S_w and K_{ow} Original Data Sources

As previously noted, physico-chemical data contained in many reports are of uncertain reliability because the documentation of methods is inadequate. Whereas it is generally accepted that a hierarchy of data preference exists (that is, direct experimental determination is preferable to indirect experimental determination which is preferable to calculation/correlation), a criteria-based rating system is required for evaluation of published data sources. Such a rating system should address key questions of methodological soundness, data reporting, replicability, and so forth. In principle, the rating system should be objective, systematic in approach, applicable to all methods, and easy to implement. In practice, all conditions cannot be met at the same time.

Heller and others (*178*) developed an expert system for determining the quality of S_w data. According to their system, experimental methodology and associated data are rated on a five-step descending scale from 1 (highest rating) to U (unevaluatable) based on the answers to a series of questions (U.S. Agricultural Research Service/National Institute of Standards and Testing: ARS/NIST; table 7). A slightly modified version of the ARS/NIST system (see appendix B for details) was used in this study to evaluate published original DDT/DDE S_w data sources. The modifications are minor and consist of an additional preliminary query concerning method acceptability, and new rating endpoints corresponding to cases where 1) the purity of water was not reported, and 2) the temperature of determination was given as "ambient." [It is important to recognize that the purpose of the rating system as described here is to assess a publication's capacity to reflect the quality of the data it reports. Although it is important to distinguish between the quality of the data source and the quality of the reported data, these are often inextricably bound. More importantly, data quality cannot always be inferred from source quality.]

Kollig (*180*) also developed criteria for evaluating the reliability of 12 rate and equilibrium constants, including K_{ow}. Focusing on four categories of information (analytical, experimental, statistical, and corroborative), he proposed a series of 31 general and 10 K_{ow}-specific questions. In order to evaluate published DDT/DDE K_{ow} data sources, critical portions of Kollig's query-based approach were incorporated into a rating scheme modeled after the ARS/NIST system (see appendix B for a full description). In addition, a preliminary query concerning method acceptability was added (as per the S_w scheme), and the query on volatilization/adsorption losses was expanded to include possible demonstration of solute mass balance. For both rating systems (S_w and K_{ow}), the initial determination that a given methodology was acceptable, poor (rating$_{max}$ = 4), or unevaluatable (rating = U) was based on a thorough examination of the S_w and K_{ow} literature for hydrophobic organic compounds. It must be noted that these rating schemes do not include explicit queries regarding the quality-control/quality-assurance procedures and analytical methods that were used to determine solute concentrations. Such information is not ordinarily provided in sufficient detail in the published literature to aid in the evaluation process. However, it is clearly critical to the assessment of physico-chemical data quality.

The original DDT/DDE S_w and K_{ow} data sources identified in tables 4 and 5 were evaluated, and the ratings for the respective publications are given in appendix B (tables B2 and B3). The results of these criteria-based evaluations support the conclusion that the DDT/DDE S_w and K_{ow} database is extremely unreliable. A large majority of the data sources received poor (rating = 4) or unevaluatable (rating = U) ratings [that is, DDT S_w = 100 percent (28 of 28), DDE S_w = 100 percent (9 of 9), DDT K_{ow} = 95 percent (41 of 43), DDE K_{ow} = 96 percent (26 of 27)]. Poor or unevaluatable data source ratings generally resulted from use of methods that are widely considered to be unacceptable for hydrophobic organic compounds or from incomplete reporting of methodology, data and statistics. According to this evaluation, only a small percentage [less than 3 percent (2 of 68)] of the data sources received the highest rating (rating = 1) and none received a good rating (rating = 2). Thus, the number of original data

Table 7. ARS/NIST Ratings System (after Heller and others, *178*)

Rating	Explanation
1	Highest rating: method of high quality with excellent reporting of work performed
2	Good rating: some parts of experimental method below the highest standards
3	Acceptable rating: experimental methods all defined, work performed or reported at minimum scientific level
4	Poor rating: lack of reporting for key or multiple experimental details, studies with outdated or unacceptable methods
U	Unevaluatable: insufficient information on which to base a rating

sources that may be considered reliable as judged by the assigned ratings is very small (table 8). It must be recognized that the data contained in many of the publications for which poor or unevaluatable ratings were assigned may well be of acceptable quality. However, inadequate documentation precluded a higher rating by the modified evaluation scheme of Heller and others (*178*). In these instances, determination of the true quality of the reported data would require unsupported inference. This highlights one of the most serious shortcomings of the published literature: inadequate documentation.

In the case of DDT log K_{ow} data, the only data sources that received the highest rating were publications reporting the results of an inter-laboratory comparison study (*109,113*). The mean log K_{ow} values determined by the two participating laboratories [which used similar (but non-identical) procedures] differed by more than 0.6 log unit. For comparison, previously published "recommended values" (*1,6,47,61,77*) for log K_{ow} span considerably larger ranges: DDT log K_{ow} (4.89–6.914), and DDE log K_{ow} (4.28–6.96). Despite widespread citation and use of these "recommended values," the criteria-based evaluations conducted in this study indicate that the number of reliable data sources upon which "recommended values" might be based is grossly inadequate.

Effect of Methodology

Methods of S_w and K_{ow} determination can be divided into three general categories: direct experimental, indirect experimental (including correlation with other physico-chemical parameters) and computational. Many of these methods have been summarized and evaluated previously (*5,6,181*), and a comprehen-

sive review is beyond the scope of this study. For present purposes, only those methods that have been used in DDT/DDE parameter determinations were considered (tables 4 and 5). At least 10 different methods have been used for DDT/DDE S_w determination (*direct experimental*-generator column, stir-flask, shake-flask, turbidity/nephelometry; *indirect experimental*-RP-HPLC, property-property relations [PPR], structure-property relations [SPR], toxicity, topology/artificial neural network; *computational*-group contribution). At least nine different methods have been used for DDT/DDE K_{ow} determination (*direct experimental*-stir-flask, shake-flask, continuous phase equilibration (*140*); *indirect experimental*-RP-HPLC, S_{oct}/S_w, PPR, SPR; *computational*-substituent constant/group contribution/fragment constant, SPARC/quantitative structure activity relationship models ['QSAR']).

Basic statistics (mean, standard deviation, minimum and maximum) for uncensored original S_w and log K_{ow} data have been tabulated and examined for potential methodologically based differences (table 9). The extreme variability of the S_w values, with standard deviations often exceeding the mean value, precludes any meaningful interpretation of the data set. Underlying some of this variability may be effects due to specific aspects of the protocols used, operator/laboratory differences, and quality control/quality assurance issues. Information relevant to these aspects of the measurement process is rarely provided in the published literature, and in some cases may have been unknown to investigators. Examples include the analytical difficulties associated with measuring K_{ow} of highly hydrophobic organic compounds at infinite dilution (*8,9*), the importance of maintaining temperature control during equilibration (*7,113*), and possible decomposition of DDT in heated gas chromatographic inlets (*182*). Rather than attempting to identify all of the relevant issues here, the existing data were ana-

Table 8. DDT/DDE S_w and log K_{ow} Original Data Sources that Received the Highest Rating (rating = 1) using Criteria-based Data Source Quality Evaluation Schemes[a]

	Source	Value
DDE log K_{ow}		
	de Bruijn and others (*109*)	6.956 ± 0.011
DDT log K_{ow}		
	de Bruijn and others (*109*)	6.914 ± 0.030
	Brooke and others (*113*)	6.307 ± 0.045
DDE S_w		
	---[b]	---[b]
DDT S_w		
	---[b]	---[b]

[a] See text and appendix B for explanation of aqueous solubility (S_w) and octanol-water partition coefficient (K_{ow}) data source evaluation schemes as modified from Heller and others (*178*) and Kollig (*180*).   [b] No original data source met the highest rating criteria for this compound property.

Table 9. Statistical Information on Uncensored Original DDT/DDE S_w and log K_{ow} Data by Method of Determination

Method[a]	Mean	Standard Deviation	Minimum Value	Maximum Value	Number of Data Points	Percentage of Data Points	Percentage of Data Points <1980	Percentage of Data Points 1980-1989	Percentage of Data Points ≥1990
DDT S_w (milligrams per liter)									
Shake-Flask	0.014	0.017	0.0002	0.045	17	37.8	62.5	22.2	0.0
Gen. column	0.005	0.002	0.0023	0.0077	5	11.1	4.2	22.2	16.7
Stir-Flask	--	--	--	--	--	--	--	--	--
PPR/SPR+	0.759	2.053	0.0001	6.22	9	20.0	0.0	44.4	41.7
Calculated	0.006	0.006	0.0013	0.0158	5	11.1	0.0	0.0	41.7
Miscellaneous	0.051	0.047	0.004	0.1	5	11.1	16.7	11.2	0.0
Not reported	0.514	0.561	0.016	1	4	8.9	16.7	0.0	0.0
DDT log K_{ow}									
Shake-Flask	5.44	0.99	3.98	6.36	5	7.8	25.0	9.1	0.0
Stir-Flask	6.22	0.33	5.73	6.914	8	12.5	0.0	11.4	18.8
RP-HPLC	5.75	0.40	5.13	6.51	24	37.5	25.0	52.3	0.0
PPR/SPR	6.85	0.72	5.60	7.92	10	15.6	0.0	11.4	31.3
Calculated	6.76	0.50	5.76	7.51	15	23.4	50.0	13.6	43.8
Miscellaneous	5.84	0.14	5.74	5.94	2	3.1	0.0	2.3	6.3
DDE S_w (milligrams per liter)									
Shake-Flask	0.130	0.162	0.0013	0.450	7	41.2	70.0	0.0	0.0
Gen. column	0.008	0.009	0.0011	0.014	2	11.8	10.0	20.0	0.0
Stir-Flask	0.040	--	0.040	0.040	1	5.9	10.0	0.0	0.0
PPR/SPR+	0.260	0.548	0.001	1.24	5	29.4	0.0	60.0	100.0
Calculated	0.0152	--	0.0152	0.0152	1	5.9	0.0	20.0	0.0
Miscellaneous	0.065	--	0.065	0.065	1	5.9	10.0	0.0	0.0
Not reported	--	--	--	--	--	--	--	--	--
DDE log K_{ow}									
Shake-Flask	--	--	--	--	--	--	--	--	--
Stir-Flask	6.956	--	6.956	6.956	1	2.8	0.0	4.5	0.0
RP-HPLC	6.04	0.33	5.63	7.14	19	52.8	50.0	72.7	10.0
PPR/SPR	6.42	1.00	5.50	7.67	4	11.1	0.0	0.0	40.0
Calculated	6.39	0.80	4.88	7.2	12	33.3	50.0	22.7	50.0
Miscellaneous	--	--	--	--	--	--	--	--	--

[a] For definitions of method acronyms see footnotes, tables 4 and 5. Combined method groups are as follows. S_w: PPR/SPR+ = PPR ± SPR, RP-HPLC ± TOP/ANN; Miscellaneous=N ± TOX$_{est}$ ± turbidity; K_{ow}: Miscellaneous = S$_{oct}$/S$_w$.

lyzed to identify trends. The major observations for S_w (table 9) that can be made are that: 1) more measurements have been made with the shake-flask method than any other (38–41 percent), 2) there has been a clear shift away from experimental determination and toward computational and correlational (that is, PPR/SPR+) methods since the early 1980s, and 3) the generator column method is the only direct experimental method that continues to be utilized.

Although there appears to be some correlation between method type and mean value for DDT/DDE log K_{ow}, the within-method variance is significant. In some instances (stir-flask/DDE K_{ow}), interpretation of between-method differences is hampered by a scarcity of data. For purposes of illustration, the DDT log K_{ow} data have been plotted by method as a function of date of publication (fig. 8a) and irrespective of date of publication (fig. 8b). These data and plots show that: 1) the stir-flask method tends to produce higher DDT K_{ow} values than other experimental methods (for example, shake-flask, RP-HPLC) [Possible explanations

include the fact that gentle stirring appears to avoid formation of solute-enriched emulsions in the octanol-saturated water phase, which can occur with shake-flask methods, and the fact that the RP-HPLC method can be biased as a result of calibration with uncertain K_{ow} data or compounds having lower K_{ow}s (*113,150*).], 2) although little used during the last decade, RP-HPLC accounts for the greatest number of DDT log K_{ow} data points (table 9), 3) mean DDT log K_{ow} values estimated by computational and correlational (that is, PPR/SPR) methods are consistently higher than experimentally determined values [This is likely because these techniques ignore effects due to the mutual solubility of the solvents and complex solute-solvent interactions that are structure-specific (*113*).], and 4) since the early 1990s there has been a clear shift away from experimental determination methods and toward computational and correlational methods. For the DDE log K_{ow} data, only the last three points are applicable; as noted above, interpretations regarding the stir-flask method are unwarranted given the lack of data (n=1).
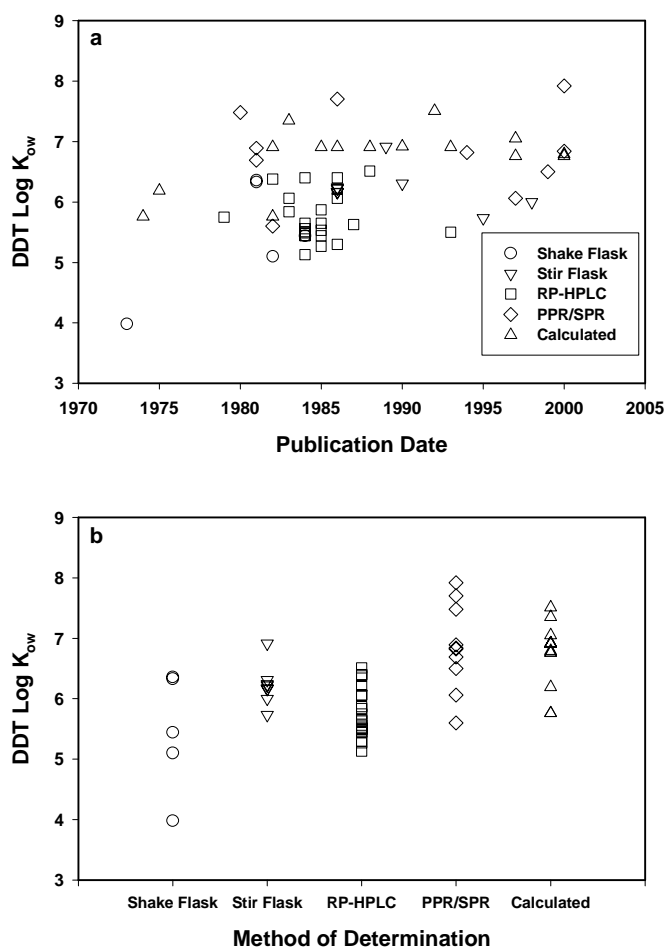

Figure 8. Original DDT log K_{ow} data plotted according to method of determination/estimation a) by date of publication, and b) irrespective of date of publication. Symbols in panel 'b' are as described in legend of panel 'a'. Number of data points: Shake Flask-5, Stir Flask-8, RP-HPLC-24, PPR/SPR-10, Calculated-15.

The trends and patterns identified in the preceding paragraph have their origin in the natural evolution of methodologies that has taken place in the last 50 years. For example, shake-flask methods for determination of S_w and K_{ow} have been supplanted by techniques (generator column-S_w, stir-flask, generator column-K_{ow}) that are believed to avoid or minimize problems of incomplete phase separation, solute adsorption, and volatilization (*109,181,183*). The observed trend toward correlational and computational methods instead of direct experimental methods has largely grown out of the desire to estimate properties for a diverse array of synthetic compounds, while avoiding the time and cost required of the latter. As problems with application of early experimental methods for determination of S_w and K_{ow} for hydrophobic organic compounds were recognized, reliance on computational methods have tended to increase.

Sangster (*6*) has observed that no general-purpose K_{ow} determination method exists that is "…equally applicable to all kinds of solutes." The same is true for S_w methodologies. Corollary to this is the fact that, in the case of highly hydrophobic organic compounds, all methods require a considerable level of skill on the part of the operator and some methods (such as shake-flask), which are widely perceived as being problematic, can be made to yield acceptable results with sufficient care (*184*). The situation is best exemplified by the lack of uniformity in recommendations concerning preferred S_w and K_{ow} determination methods issued by standards development organizations and regulatory agencies. The EPA has approved the use of the column elution, shake-flask, and generator column methods for S_w determination (*185,186*), whereas the American Society for Testing and Materials (ASTM) recommends the stir-flask method (*187*). The Organisation for Economic Co-operation and Development (OECD) advises use of the shake-flask method for compounds with $S_w > 10^{-2}$ g/L and the column elution method for compounds with $S_w < 10^{-2}$ g/L (*188*). For log K_{ow} determinations in the range, +4 to > +6, EPA has established a hierarchy (most preferred to least preferred) of approved methods: 1) stir-flask or generator column, 2) RP-HPLC with extrapolation to 0 percent solvent, 3) RP-HPLC without extrapolation, 4) shake-flask, and 5) calculation by the Hansch and Leo CLOGP program (*189–191*). ASTM recommends use of the RP-HPLC method (*192*), whereas OECD advises use of the shake-flask method for log K_{ow} values from -2 to +4 and the RP-HPLC method for log

K_{ow} values from 0 to +6 (*101,193*). Computational methods are allowed for quick estimates, as a laboratory data check, and as an experimental substitute in rare cases (*194*). OECD recommendations for S_w and K_{ow} are likely to change in the near future as both parameter guidelines are on the organization's high priority list for revision (*195*). Clearly, the development of improved methods for determination of S_w and K_{ow} and their evaluation by standards and regulatory organizations can be expected to continue; however, improved coordination among these entities would favor generation of more consistent data.

SUMMARY AND CONCLUSIONS

An in-depth examination of the literature on DDT/DDE S_w and K_{ow} has revealed that it is populated by a large amount of multi-level references, citation errors, and data errors. The frequency and repetition of these errors is such that the database has become increasingly unreliable with time. Without corrective action, this trend will likely continue. The collative literature (compilations, review articles, and handbooks) has tended to perpetuate, if not propagate, these problems. Users in search of reliable data have no choice but to search the literature and independently evaluate the applicability of data they wish to use. However, most do not have the time for such an undertaking and simply accept the given recommendations.

The extensive bibliographic inadequacies described in this report indicate that there is a need for improved citation practices. In order to halt the proliferation of these errors, authors, reviewers, and editors will have to make a concerted effort. The only long-term solution is to diligently instruct upcoming generations of researchers on the ethics of acknowledging prior research and the methods of proper referencing. The International Union of Pure and Applied Chemistry (IUPAC) views its uniform, high-quality publications as a major effort to train future generations of scientists on the importance of scientific communication practices. They hope to make authors realize that their work will lack archival value unless it meets IUPAC standards.

Compounding the literature problem is the fact that the original published data span several orders of magnitude, and the true K_{ow} and S_w values for DDT and DDE are unknown. Most published data sources are of poor or unevaluatable quality. This is due, in part, to a lack of information on the performance of

existing methods of K_{ow} and S_w determination for hydrophobic organic compounds. There have been few efforts to conduct interlaboratory comparison exercises using a single method or to carry out systematic evaluations of different determination methodologies in parallel. Thus, whereas some knowledge of the potential methodological pitfalls exists, a basis for assessing the accuracy of various approaches is generally lacking. At the same time, the need for continued development of methods of determining the K_{ow} and S_w for hydrophobic organic compounds is obvious. For new methods to gain credibility, it must be shown that they can be readily implemented and yield accurate and precise data. Otherwise, one can expect continuing use of inappropriate methods and production of unreliable data.

Another issue is the inadequate documentation of methods of determination especially with regard to method applicability, accuracy and reproducibility. Consistent and complete reporting is essential if future data sources are to make a meaningful contribution to a growing database containing reliable data. Presently, the inadequate methodological documentation of the literature makes the systematic evaluation of data quality virtually impossible. A complicating factor here is that physico-chemical property data are published in many journals, reports and books. Consequently, the responsibility for complete reporting falls primarily upon authors.

Despite, or perhaps because of, the data quality problems outlined in this report, an increasing reliance on computational and correlational (as opposed to direct experimental) methods of property estimation has resulted since the early 1990's. Such methods have been developed and validated against data which themselves may be subject to some or all of the problems stated above. The net result has been the creation of an unreliable DDT/DDE S_w and K_{ow} database with little practical value. The derivation of critical environmental parameters (for example, bioconcentration factors, equilibrium partition coefficients) from the current database is inadvisable due to the lack of verifiably reliable data. Use of these data in the past may have resulted in erroneous environmental fate assessments. Given the nature of the literature and the data quality issues observed in the present study, there is little reason to believe that such problems are limited solely to DDT and DDE.

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APPENDIXES

As noted in the main report, 'unreferenced data,' or the practice of customarily not providing a reference to the source of data, is often found in compilations such as the *Merck Index* (Budavari and others, 1996) and *Lange's Handbook of Chemistry* (Dean, 1985). However, this practice also occurs frequently in journal articles. 'Unreferenced data' and data associated with 'nonexistent references' and 'missing references' may be termed 'data of

uncertain origin' for which only a provisional identification (based on numerical similarity and a comparison of the respective publication dates) is possible. Data that are unpublished or appear in the literature as *private communications* are included in this classification. Data of uncertain origin are of no value because their reliability is indeterminate. It should be noted that the following data of uncertain origin (tables A1 and A2) are only from the literature reviewed in this study; other instances undoubtedly exist.

Table A1. DDT S_w and log K_{ow} Data of Uncertain Origin

Reference	Compound Designation	S_w or log K_{ow}	Possible Source
Aqueous solubility, S_w (milligrams per liter)			
Ballschmiter and Wittlinger (1991)	*p,p'*-DDT	0.002	Biggar and others (1967)
Branson (1978)	DDT	0.001	Bowman and others (1960)
Caron and others (1985)	DDT	0.0055	Weil and others (1974)
Chiou and others (1981)	*p,p'*-DDT	0.0050	?
Chiou and others (1986)	*p,p'*-DDT	0.0050	Chiou and others (1981)
Chiou and others (1991)	DDT	0.0055	Weil and others (1974)
Clement Associates (1985)	*p,p'*-DDT	0.0055	Weil and others (1974)
Gerstl and Helling (1987)	DDT	0.0032	?
Headley and others (1998)	*p,p'*-DDT	0.001	Bowman and others (1960)
Isnard and Lambert (1988, 1989)	*p,p'*-DDT	0.002	?
Kenaga (1980)	DDT	0.0017	Biggar and others (1967)
Lipke and Kearns (1960)	DDT	0.035	?
Lu and Metcalf (1975)	DDT	0.0012	Bowman and others (1960)
Mackay (1985)	DDT	0.00329	?
Mackay and Stiver (1991)	DDT	0.003	?
Mackay and others (1986)	*p,p'*-DDT	0.009	?
McCall and others (1981)	DDT	0.0017	Biggar and others (1967)
Melnikov (1971)	DDT	0.001	Bowman and others (1960)
Metcalf (1972)	DDT	0.002	Biggar and others (1967)
Metcalf and Sanborn (1975)	DDT	0.0012	Bowman and others (1960)
Neely (1980)	DDT	0.0012	Bowman and others (1960)
Neely (1982)	DDT	0.0012	Bowman and others (1960)
Paris and others (1977)	DDT	0.001	Bowman and others (1960)
Rippen (1996)	DDT	0.0017	Biggar and others (1967)
Rippen (1996)	DDT	0.0023	Swann and others (1983)
Rippen (1996)	DDT	0.0077	Webster and others (1985)
Verschueren (1983, 1996)	DDT	0.0031	Bowman and others (1960)
Verschueren (1983, 1996)	DDT	0.0034	Bowman and others (1960)
Weber and others (1980)	DDT	0.001	Bowman and others (1960)
Yoshida and others (1983)	*p,p'*-DDT	0.0017	Biggar and others (1967)
Log octanol-water partition coefficient, log K_{ow}			
Banerjee and Baughman (1991)	DDT	6.19	O'Brien (1975)
Brooke and others (1990)	*p,p'*-DDT	6.19	O'Brien (1975)
Burkhard and others (1985)	*p,p'*-DDT	4.98	?
Chiou and Schmedding (1981)	*p,p'*-DDT	6.36	--[a]
Chiou and others (1981)	*p,p'*-DDT	6.36	--[a]
Clement Associates (1985)	DDT	4.98	?
Clement Associates (1985)	*p,p'*-DDT	3.98	Kapoor and others (1973)
Dao and others (1983)	DDT	5.75	Veith, DeFoe and Bergstedt (1979)
DCIS (2000)	DDT	5.76	unpublished results
DCIS (2000)	DDT	6.60	private communication

Table A1. DDT S_w and log K_{ow} Data of Uncertain Origin—Continued

Reference	Compound Designation	S_w or log K_{ow}	Possible Source
Log octanol-water partition coefficient, log K_{ow}			
Devillers and others (1996)	*p,p'*-DDT	6.00	Kenaga and Goring (1980)
Eadsforth (1986)	*p,p'*-DDT	6.19	O'Brien (1975)
Elgar (1983)	DDT	6.2	O'Brien (1975)
Ellgehausen and others (1980)	*p,p'*-DDT	6.19	O'Brien (1975)
Freed and others (1979)	*p,p'*-DDT	6.19	O'Brien (1975)
Gerstl and Helling (1987)	DDT	6.19	O'Brien (1975)
Geyer and others (1984)	*p,p'*-DDT	6.28	?
Geyer and others (1991)	*p,p'*-DDT	6.19	O'Brien (1975)
Harner and Mackay (1995)	*p,p'*-DDT	6.2	O'Brien (1975)
Harnisch and others (1983)	*p,p'*-DDT	6.19	O'Brien (1975)
Hawker and Connell (1986)	DDT	6.19	O'Brien (1975)
Ikemoto and others (1992)	DDT	5.98	Kenaga and Goring (1980)
Isnard and Lambert (1988, 1989)	*p,p'*-DDT	5.98	Kenaga and Goring (1980)
Kenaga (1980)	DDT	5.98	Kenaga and Goring (1980)
Kenaga and Goring (1980)	DDT	5.98	?
Liu and others (1991)	*p,p'*-DDT	5.98	Kenaga and Goring (1980)
Lu and Metcalf (1975)	DDT	3.98	Kapoor and others (1973)
Lyman (1982)	DDT	5.98	Kenaga and Goring (1980)
Mackay and others (1986)	*p,p'*-DDT	6.01	?
Neely (1982)	DDT	6	Kenaga and Goring (1980)
Rao and Davidson (1980)	*p,p'*-DDT	6.19	O'Brien (1975)
Ryan and others (1988)	DDT	5.98	Kenaga and Goring (1980)
Suntio and others (1988)	DDT	5.98	Kenaga and Goring (1980)
Suntio and others (1988)	DDT	6.19	O'Brien (1975)
Thomann (1989)	DDT	5.98	Kenaga and Goring (1980)
Travis and Arms (1988)	DDT	5.76	Trabalka and Garten (1982)
EPA (1986)	DDT	6.19	O'Brien (1975)
EPA (1995)	DDT	6.38	private communication
Veith, Austin and Morris (1979)	*p,p'*-DDT	6.19	O'Brien (1975)
Verschueren (1983, 1996)	DDT	6.19	O'Brien (1975)
Webster and others (1985)	*p,p'*-DDT	5.18	?
Webster and others (1985)	*p,p'*-DDT	5.47	?
Wolfe and others (1977)	DDT	4.89	private communication
Yoshida and others (1983)	*p,p'*-DDT	5.98	Kenaga and Goring (1980)
Yoshioka and others (1986)	DDT	4.99	?

[a] The source of this datum was not provided but is Chiou and others, 1982 (C. Chiou, USGS, personal communication, 7/2000).

Table A2. DDE S_W and log K_{ow} Data of Uncertain Origin

Reference	Compound Designation	S_W or log K_{ow}	Possible Source
Aqueous solubility, S_W (milligrams per liter)			
Ballschmiter and Wittlinger (1991)	*p,p'*-DDE	0.008	Garten and Trabalka (1983)
Clement Associates (1985)	DDE	0.014	Weil and others (1974)
Freed and others (1977)	*p,p'*-DDE	0.04	Biggar and Riggs (1974) or Chiou and others (1977)
Isnard and Lambert (1988, 1989)	*p,p'*-DDE	0.0079	Garten and Trabalka (1983)
McLachlan and others (1990)	*p,p'*-DDE	0.018	?
Metcalf and Sanborn (1975)	DDE	0.0013	Metcalf and others (1973)
Metcalf and others (1975)	DDE	0.0013	Metcalf and others (1973)
Rippen (1996)	DDE	0.0013	Metcalf and others (1973)
Verschueren (1983, 1996)	*p,p'*-DDE	0.0013	Metcalf and others (1973)
Verschueren (1983, 1996)	*p,p'*-DDE	0.040	Biggar and Riggs (1974) or Chiou and others (1977)
Verschueren (1983, 1996)	*p,p'*-DDE	0.065	Hollifield (1979)
Zepp and others (1977)	DDE	0.0013	Metcalf and others (1973)
Log octanol-water partition coefficient, log K_{ow}			
Burkhard and others (1985)	*p,p'*-DDE	5.69	O'Brien (1975) or Veith, DeFoe and Bergstedt (1979)
Capel and Eisenreich (1990)	*p,p'*-DDE	5.69	O'Brien (1975) or Veith, DeFoe and Bergstedt (1979)
Clement Associates (1985)	DDE	5.69	O'Brien (1975) or Veith, DeFoe and Bergstedt (1979)
Connell and others (1988)	*p,p'*-DDE	6.89	?
Devillers and others (1996)	*p,p'*-DDE	5.83	Veith and Morris (1978)
Ebing and others (1984)	*p,p'*-DDE	5.77	Kenaga and Goring (1980)
Freed and others (1979)	*p,p'*-DDE	5.69	O'Brien (1975) or Veith, DeFoe and Bergstedt (1979)
Isnard and Lambert (1988, 1989)	*p,p'*-DDE	5.69	O'Brien (1975) or Veith, DeFoe and Bergstedt (1979)
Kenaga and Goring (1980)	DDE	5.77	?
Liu and others (1991)	*p,p'*-DDE	5.69	O'Brien (1975) or Veith, DeFoe and Bergstedt (1979)
McLachlan and others (1990)	*p,p'*-DDE	5.7	O'Brien (1975) or Veith, DeFoe and Bergstedt (1979)
Metcalf and others (1975)	DDE	4.28	?
Rao and Davidson (1980)	*p,p'*-DDE	5.69	O'Brien (1975) or Veith, DeFoe and Bergstedt (1979)
Rippen (1996)	DDE	5.77	Kenaga and Goring (1980)
Rippen (1996)	DDE	5.69	O'Brien (1975) or Veith, DeFoe and Bergstedt (1979)
Rippen (1996)	DDE	5.83	Veith and Morris (1978)
Suntio and others (1988)	*p,p'*-DDE	5.69	O'Brien (1975) or Veith, DeFoe and Bergstedt (1979)
Thomann (1989)	*p,p'*-DDE	5.7	O'Brien (1975) or Veith, DeFoe and Bergstedt (1979)
Travis and Arms (1988)	DDE	5.83	Veith and Morris (1978)
EPA (1986)	DDE	7.00	?
EPA (1995)	DDE	6.57	private communication
Veith, Austin and Morris (1979)	*p,p'*-DDE	5.69	O'Brien (1975) or Veith, DeFoe and Bergstedt (1979)
Verschueren (1983, 1996)	*p,p'*-DDE	5.69	O'Brien (1975) or Veith, DeFoe and Bergstedt (1979)
Verschueren (1983, 1996)	*p,p'*-DDE	4.28	Metcalf and others (1975)
Webster and others (1985)	*p,p'*-DDE	5.60	?
Webster and others (1985)	*p,p'*-DDE	5.91	?

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Appendix B: Assessment of DDT/DDE S_w and K_{ow} Original Data Sources using a Criteria-based Rating System

As noted in the main report, physico-chemical data contained in many sources are of uncertain reliability because the documentation of methods is inadequate. Whereas it is generally accepted that a hierarchy of data preference exists (that is, direct experimental determination is preferable to indirect experimental determination which is preferable to calculation/correlation), a criteria-based rating system is required for evaluation of data sources. Such a rating system should address key questions of methodological soundness, data reporting, replicability, and so on. In principle, the rating system should be objective, systematic in approach, applicable to all methods, and easy to implement. In practice, all conditions cannot be met at the same time.

Heller and others (1994) developed a decision tree-type expert system for determining the reliability of S_w data sources. According to their scheme, experimental methodology and associated data are rated on a five-step descending scale from 1 (highest quality) to U (unevaluatable - lowest quality) based on answers to a series of questions (U.S. Agricultural Research Service/National Institute of Standards and Testing: ARS/NIST; table B1). A slightly modified version of the ARS/NIST system was used to assess published original DDT/DDE S_w data sources (fig. B1). The modifications are very minor and consist of an additional preliminary query concerning method acceptability, and new rating endpoints corresponding to cases where 1) the purity of water was not reported, and 2) the temperature of determination was given as 'ambient'. Also an abridged, though unaltered, version of the *Standard Error Table* proposed by Heller and others (1994; level K, range of interest $S_w < 0.1$ mg/L) was used. [Please note that the decision tree shown in figure B1 is labeled with alphanumeric descriptors for each question and rating endpoint. Questions are assigned capital letters (A,B,C…), whereas endpoints for a given question are assigned numbers (1,2,3…). Both letters and numbers appear within circles for ready identification. Alphanumeric codes were created for the endpoints that correspond to a given data source's rating. These codes were designated the 'Ratings Rationale' because they allow the reader to quickly understand how the rating for a given data source was determined. For example, in the case of S_w, if a data source received a rating of U after the question on *Purity of Water* (level C), its endpoint code would be C2.] The reader should note that the response to certain queries may result in a limitation to the maximum rating that a data source can receive (that is, rating$_{max}$). For example, unless dynamic chromatography was used for saturated solution generation in the determination of S_w, a data source will receive a maximum rating of 2 (see fig. B1, query B).
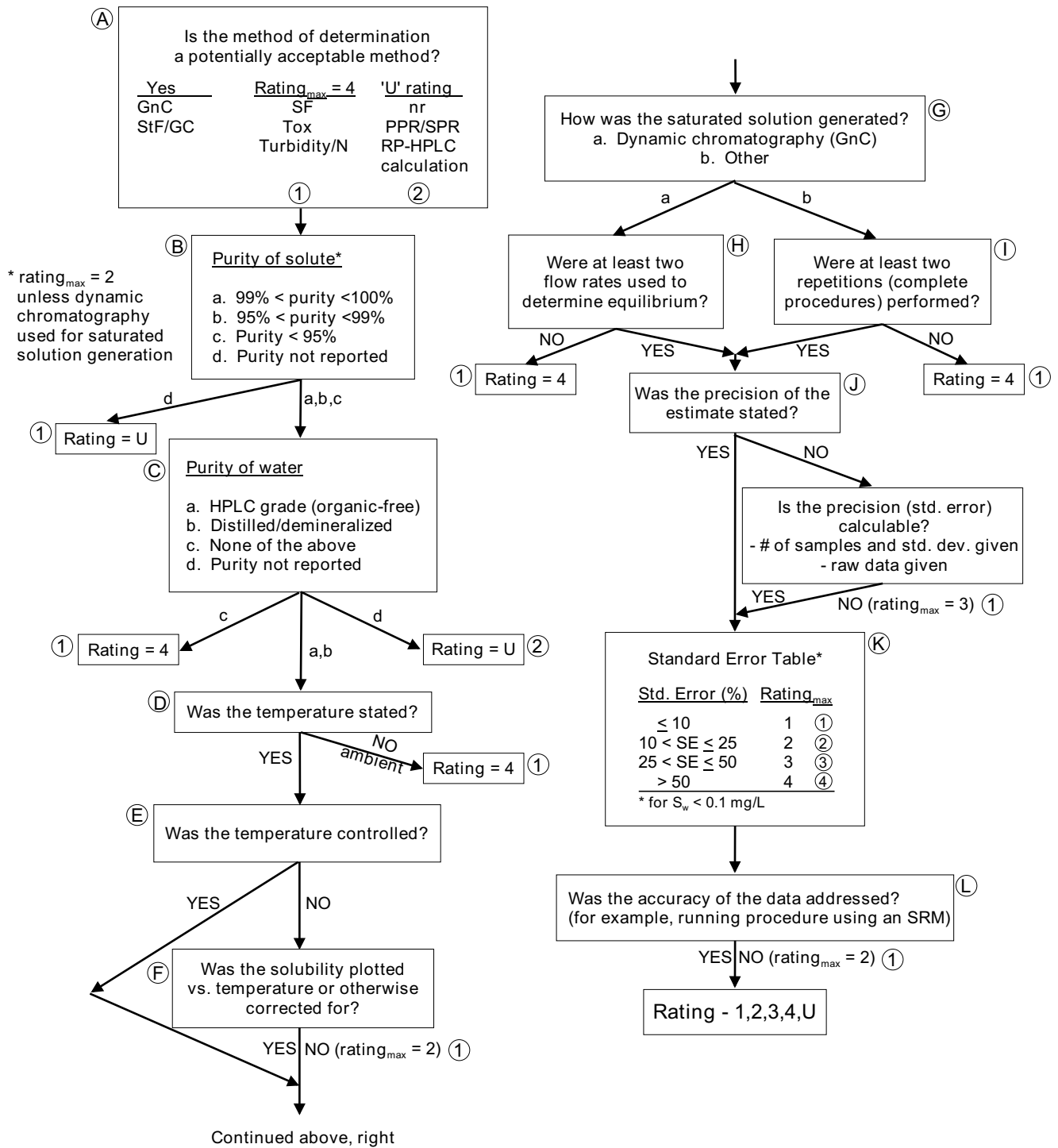
Kollig (1988) also developed criteria for evaluating data sources of 12 rate and equilibrium constants, including K_{ow}. Focusing on four categories of information (analytical, experimental, statistical, and corroborative), Kollig proposed a series of 31 general and 10 K_{ow}-specific questions. In order to evaluate published DDT/DDE K_{ow} data sources, critical portions of Kollig's approach were incorporated into a rating scheme modeled after the ARS/NIST system. A carefully considered subset of Kollig's evaluation questions

(analytical: questions 1, 3, 4, 5; experimental: questions 3, 6, 7, 8, 10, 11, 12, 13; statistical: all questions; corroborative: none; K_{ow}-specific: questions 1, 3, 4, 5, 7, 9) was selected and formed into a decision-tree (fig. B2). A preliminary query concerning method acceptability was added (as per the S_w scheme), and the query on volatilization/adsorption losses was expanded to include possible demonstration of solute mass balance. For both rating systems (S_w and K_{ow}), the initial determination that a given methodology was acceptable, poor (rating$_{max} = 4$), or unevaluatable (rating $= U$) was based on a thorough examination of the S_w and K_{ow} literature. The RP-HPLC method of determining K_{ow}, for example, is known to pose numerous problems (calibration compound selection, the use of questionable K_{ow} data resulting in unreliable calibration curves, and so on) and received a "U" rating at the initial (level A) decision point. It must be noted that these rating schemes do not include explicit queries regarding the quality-control/quality-assurance procedures and analytical methods that were used to determine solute concentrations. Such information is not ordinarily provided in sufficient detail in the published literature to aid in the evaluation process. However, it is clearly critical to the assessment of physico-chemical data quality.

The original DDT/DDE S_w and K_{ow} data sources (tables 4 and 5 in the main report) were evaluated; the ratings and corresponding 'ratings rationale' are given in tables B2 and B3. In instances where a lack of information on solute, solvent or water purity determined the final rating, a *secondary* rating (assuming all purities were satisfactory) was assigned to further characterize the publication's potential quality. The secondary rating is given parenthetically within the 'Data Source Rating' column of tables B2 and B3. The rating rationale corresponding to the secondary rating is given parenthetically within the 'Ratings Rationale' column of tables B2 and B3. The reader is advised that one question not formally included in the K_{ow} ratings scheme was "Was method accuracy validation performed using compounds with known K_{ow}s?" It was decided not to include this question because of the possibility that K_{ow}s of other hydrophobic organic compounds may not be known with certainty for the same reasons that the DDT and DDE K_{ow} database is considered unreliable. Thus, without confirmation of the accuracy of the validating compounds, such a criterion would be of little value. However, this question should be considered in future versions of any rating scheme.

Table B1. ARS/NIST Ratings System (after Heller and others, 1994)

Rating	Explanation
1	Highest rating: method of high quality with excellent reporting of work performed
2	Good quality: some parts of experimental methodology below the highest standards
3	Acceptable quality: experimental methods all defined, work performed or reported at minimum scientific level
4	Poor quality: lack of reporting for key or multiple experimental details, studies with outdated or unacceptable methods
U	Unevaluatable: insufficient information on which to base a rating

(A) Is the method of determination a potentially acceptable method?

Yes	Rating_max = 4	'U' rating
GnC	SF	nr
StF/GC	Tox	PPR/SPR
	Turbidity/N	RP-HPLC
		calculation

(1)   (2)

* rating_max = 2 unless dynamic chromatography used for saturated solution generation

(B) Purity of solute*

a. 99% < purity <100%
b. 95% < purity <99%
c. Purity < 95%
d. Purity not reported

d → (1) Rating = U

a,b,c →

(C) Purity of water

a. HPLC grade (organic-free)
b. Distilled/demineralized
c. None of the above
d. Purity not reported

c → (1) Rating = 4
a,b →
d → Rating = U (2)

(D) Was the temperature stated?

YES →
NO ambient → Rating = 4 (1)

(E) Was the temperature controlled?

YES →
NO →

(F) Was the solubility plotted vs. temperature or otherwise corrected for?

YES | NO (rating_max = 2) (1)

Continued above, right

→ (G) How was the saturated solution generated?
a. Dynamic chromatography (GnC)
b. Other

a →
b →

(H) Were at least two flow rates used to determine equilibrium?

(I) Were at least two repetitions (complete procedures) performed?

NO → (1) Rating = 4

YES → ← YES

NO → Rating = 4 (1)

(J) Was the precision of the estimate stated?

YES →
NO →

Is the precision (std. error) calculable?
- # of samples and std. dev. given
- raw data given

YES →
NO (rating_max = 3) (1)

(K) Standard Error Table*

Std. Error (%)	Rating_max	
≤ 10	1	(1)
10 < SE ≤ 25	2	(2)
25 < SE ≤ 50	3	(3)
> 50	4	(4)

* for S_w < 0.1 mg/L

(L) Was the accuracy of the data addressed?
(for example, running procedure using an SRM)

YES | NO (rating_max = 2) (1)

Rating - 1,2,3,4,U

EXPLANATION
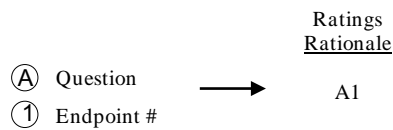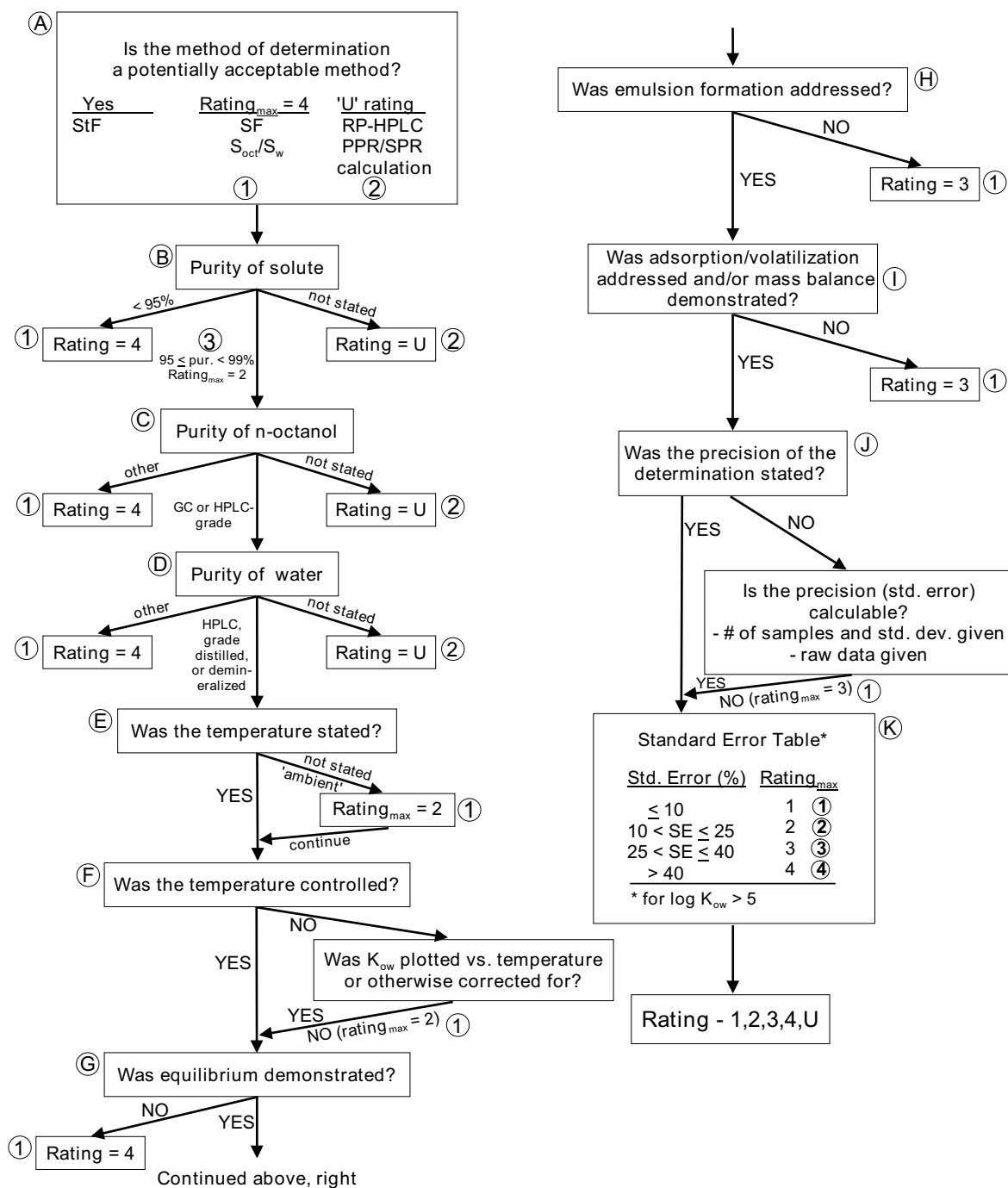
Ratings
Rationale

(A) Question
(1) Endpoint #

→ A1

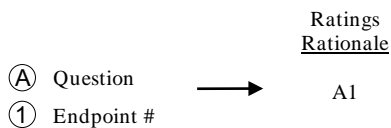**Figure B1.** S_w rating scheme (after Heller and others, 1994)

Figure B2. Log K_{ow} rating scheme (after Heller and others, 1994; Kollig, 1988)

Table B2. DDT S_w and log K_{ow} Original Data Source Ratings

S_w[a]	Method[b]	Reference	Data Source Rating[c]	Ratings Rationale[d]
1	nr	Neal and others, 1944	U	A2
< 1	nr	Sazonov and others, 1956	U	A2
0.016, 0.040	nr	Robeck and others, 1965	U	A2
0.0002-0.001	SF	Richards and Cutkomp, 1946	U (4)	B1 (D1)
0.0034, 0.002, 0.0017	SF/GC	Biggar and others, 1967	4	A1
0.017	SF/GC	Biggar and Riggs, 1974	4	A1
0.0017, 0.006, 0.025	SF/GC	Biggar and Riggs, 1974	4	A1
0.037	SF/GC	Biggar and Riggs, 1974	4	A1
0.045	SF/GC	Biggar and Riggs, 1974	4	A1
0.0054	SF/GC	Chiou and others, 1986	4	I1
0.0059	SF/RA	Babers, 1955	U (4)	B1 (A1)
0.0374	SF/RA	Babers, 1955	U (4)	B1 (A1)
0.045	SF/RA	Babers, 1955	U (4)	B1 (A1)
≤ 0.0012	SF/RA	Bowman and others, 1960	4	I1
0.0045	SF/RA	Gerstl and Mingelgrin, 1984	4	A1
0.01-0.1	TOX$_{est}$	Roeder and Weiant, 1946	U (4)	B1 (I1)
0.04	Turbidity	Ellgehausen and others, 1981	4	A1 (I1)
0.004	Turbidity/N	Hollifield, 1979	4	D1
0.1	Turbidity/N	Gauvadan and Poussel, 1947	U (4)	B1 (I1)
0.0055	GnC	Weil and others, 1974	U (3)	B1 (J1)
0.0023	GnC	Swann and others, 1983	U (4)	B1 (H1)
0.0077	GnC	Webster, Friesen, Sarna and Muir, 1985	U (4)	B1 (H1)
0.0053	GnC	Lodge and others, 1995	U (4)	B1 (H1)
0.0051	GnC/SPME/GC	Paschke and others, 1998	4	H1
0.020	RP-HPLC	Swann and others, 1983	U	A2
0.0302	RP-HPLC	Chin and others, 1986	U	A2
0.467	PPR	Chin and others, 1986	U	A2
0.085	PPR	Myrdal and others, 1995	U	A2
0.00012, 0.00346	PPR	Ruelle and Kesselring, 1997	U	A2
0.00132	SPR	Patil, 1994	U	A2
0.0039	SPR	Briggs, 1981	U	A2
6.22	Top/ANN	Huuskonen and others, 1998	U	A2
0.00175, 0.00355	G-C	Klopman and others, 1992	U	A2
0.0063	G-C	Kühne and others, 1995	U	A2
0.0158	G-C/AQUAFAC-3	Myrdal and others, 1995	U	A2
0.0013	G-C	Kan and Tomson, 1996	U	A2
Log K_{ow}[e]				
3.98	SF	Kapoor and others, 1973	U (4)	B2 (G1)
6.36	SF/GC	Chiou and others, 1982	U (4)	B2 (G1)
6.33	SF/GC	Chiou and others, 1982	U (4)	B2 (G1)
5.1	SF/RA	Platford and others, 1982	U (4)	B2 (G1)
5.44	SF/RA	Gerstl and Mingelgrin, 1984	4	G1
6.17, 6.16, 6.22, 6.24	StF	Brooke and others, 1986	U (3)	B2 (J1)
6.914	StF	de Bruijn and others, 1989	1	---
6.307	StF	Brooke and others, 1990	1	---
5.73	StF	Lodge and others, 1995	U (4)	B2 (G1)
6.00	StF-SPME	Paschke and others, 1998	U (1)	D2 (---)
5.94	S_{oct} / S_w	Ellgehausen and others, 1981	4	G1
5.74	CPE	Lodge and others, 1995	--[f]	--[f]
5.75	RP-HPLC	Veith and others, 1979	U	A2
6.38	RP-HPLC	Hammers and others, 1982	U	A2
6.06, 5.84	RP-HPLC	Harnisch and others, 1983	U	A2
6.40	RP-HPLC	Garst, 1984	U	A2
5.13	RP-HPLC	Rapaport and Eisenreich, 1984	U	A2
5.56, 5.65, 5.51, 5.49, 5.45, 5.44	RP-HPLC	Sarna and others, 1984	U	A2

Table B2. DDT S_w and log K_{ow} Original Data Source Ratings—Continued

LogK$_{ow}$[e]	Method[b]	Reference	Data Source Rating[c]	Ratings Rationale[d]
5.44	RP-HPLC	Burkhard and others, 1985	U	A2
5.53, 5.65	RP-HPLC	Webster, Friesen, Sarna and Muir, 1985	U	A2
5.27, 5.87	RP-HPLC	Webster, Sarna and Muir, 1985	U	A2
5.3, 6.4	RP-HPLC	Brooke and others, 1986	U	A2
6.06	RP-HPLC	Chin and others, 1986	U	A2
6.21	RP-HPLC	Eadsforth, 1986	U	A2
5.63	RP-HPLC	De Kock and Lord, 1987	U	A2
6.51	RP-HPLC	Liu and Qian, 1988	U	A2
5.50	RP-HPLC	Sicbaldi and Finizio, 1993	U	A2
7.48	PPR	Mackay and others, 1980	U	A2
6.69	PPR	Belluck and Felsot, 1981	U	A2
5.60	PPR	Trabalka and Garten, 1982	U	A2
7.7	PPR	Brooke and others, 1986	U	A2
6.06	PPR	Finizio and others, 1997	U	A2
7.92	PPR	Ruelle, 2000	U	A2
6.50	PPR	Paasivirta and others, 1999	U	A2
6.82	SPR	Patil, 1994	U	A2
6.89	SPR	Briggs, 1981	U	A2
6.84	SPR	Dai and others, 2000	U	A2
5.76	FC-H&L	Uchida and others, 1974	U	A2
6.91	FC-H&L	Mabey and others, 1982	U	A2
5.76	FC-H&L	Trabalka and Garten, 1982	U	A2
6.91	FC-H&L	Burkhard and others, 1985	U	A2
6.763	FC-H&L	DCIS, 2000	U	A2
6.91	FC-H&L	Eadsforth, 1986	U	A2
6.91	FC-H&L	Schüürmann and Klein, 1988	U	A2
6.76	FC-H&L	Finizio and others, 1997	U	A2
7.35	FC-R	Harnisch and others, 1983	U	A2
7.51	FC-R	Noegrohati and Hammers, 1992	U	A2
6.79	FC-M&H	SRC, 2000	U	A2
6.92	G-C	Suzuki and Kudo, 1990	U	A2
6.19	SC	O'Brien, 1975	U	A2
6.91	'QSAR'	Kollig, 1993	U	A2
7.05	SPARC	Meador and others, 1997	U	A2

[a] S_w = aqueous solubility in units of milligrams per liter.   [b] Method acronyms as follows: nr=not reported, SF=shake flask, GC=gas chromatography, RA=radiometric analysis, TOX$_{est}$=estimated from toxic response, StF=stir flask, GnC=generator column, N=nephelometry, SPME=solid phase microextraction, CPE=continuous phase equilibration, S_w/S_{oct}=aqueous solubility/solubility in *n*-octanol, RP-HPLC=reversed phase-high performance liquid chromatography, PPR=property-property relationship, SPR=structure-property relationship, Top/ANN=topological indices/artificial neural network, FC-H&L=fragment constant-Hansch and Leo (1979), FC-R=fragment constant-Rekker (1977), FC-M&H=fragment constant-Meylan and Howard (1995), G-C=Group contribution, SC=substituent constant, 'QSAR'=quantitative structure activity relationship-based chemical modeling and information system, SPARC=SPARC Performs Automated Reasoning in Chemistry (Karickhoff and others, 1991).   [c] Data source ratings: S_w-after Heller and others (1994), K_{ow}-after Heller and others (1994) and Kollig (1988). See text for explanation of rating system adaptations. [d] See text for explanation.   [e] Log K_{ow} = log octanol-water partition coefficient.   [f] No rating was possible because methodology was unique to this study.

Table B3. DDE S_w and log K_{ow} Original Data Source Ratings

S_w[a]	Method[b]	Reference	Data Source Rating[c]	Ratings Rationale[d]
0.055	SF/GC	Biggar and Riggs, 1974	4	A1
0.01, 0.04, 0.120	SF/GC	Biggar and Riggs, 1974	4	A1
0.235	SF/GC	Biggar and Riggs, 1974	4	A1
0.450	SF/GC	Biggar and Riggs, 1974	4	A1
0.0013	SF/RA	Metcalf and others, 1973	4	I1
0.040	StF/GC	Chiou and others, 1977	U (4)	B1 (I1)
0.014	GnC	Weil and others, 1974	U (3)	B1 (J1)
0.0011	GnC	Swann and others, 1983	U (4)	B1 (H1)
0.065	Turbidity/N	Hollifield, 1979	4	A1
0.006	RP-HPLC	Swann and others, 1983	U	A2
0.0236	RP-HPLC	Chin and others, 1986	U	A2
1.24	PPR	Chin and others, 1986	U	A2
0.001, 0.029	PPR	Ruelle and Kesselring, 1997	U	A2
0.0152	G-C	Kühne and others, 1995	U	A2
Log K_{ow}[e]				
6.956	StF	de Bruijn and others, 1989	1	---
5.83	RP-HPLC	Veith and Morris, 1978	U	A2
5.69	RP-HPLC	Veith and others, 1979	U	A2
5.89	RP-HPLC	McDuffie, 1981	U	A2
5.63	RP-HPLC	Swann and others, 1983	U	A2
6.02, 6.12, 6.02, 6.00, 5.96, 5.94	RP-HPLC	Sarna and others, 1984	U	A2
5.89	RP-HPLC	Burkhard and others, 1985	U	A2
5.99, 6.11	RP-HPLC	Webster, Friesen, Sarna and Muir, 1985	U	A2
5.85, 6.51	RP-HPLC	Webster, Sarna and Muir, 1985	U	A2
6.29	RP-HPLC	Chin and others, 1986	U	A2
6.09	RP-HPLC	De Kock and Lord, 1987	U	A2
7.14	RP-HPLC	Liu and Qian, 1988	U	A2
5.78	RP-HPLC	Sicbaldi and Finizio, 1993	U	A2
5.74	PPR	Finizio and others, 1997	U	A2
7.67	PPR	Ruelle, 2000	U	A2
5.50	PPR	Paasivirta and others, 1999	U	A2
6.78	SPR	Dai and others, 2000	U	A2
4.88	FC-H&L	McDuffie, 1981	U	A2
6.96	FC-H&L	Mabey and others, 1982	U	A2
6.94	FC-H&L	Burkhard and others, 1985	U	A2
6.94	FC-H&L	Schüürmann and Klein, 1988	U	A2
6.736	FC-H&L	DCIS, 2000	U	A2
6.94	FC-H&L	Finizio and others, 1997	U	A2
6.00	FC-M&H	SRC, 2000	U	A2
5.01	FC-R	McDuffie, 1981	U	A2
6.72	FC-R	Noegrohati and Hammers, 1992	U	A2
7.2	G-C	Tulp and Hutzinger, 1978	U	A2
5.69	SC	O'Brien, 1975	U	A2
6.63	SPARC	Meador and others, 1997	U	A2

[a] S_w = aqueous solubility in units of milligrams per liter. [b] Method acronyms as follows: nr=not reported, SF=shake flask, GC=gas chromatography, RA=radiometric analysis, TOX_{est}=estimated from toxic response, StF=stir flask, GnC=generator column, N=nephelometry, SPME=solid phase microextraction, S_w/S_{oct}=aqueous solubility/solubility in *n*-octanol, RP-HPLC=reversed phase-high performance liquid chromatography, PPR=property-property relationship, SPR=structure-property relationship, Top/ANN=topological indices/artificial neural network, FC-H&L=fragment constant-Hansch and Leo (1979), FC-R=fragment constant-Rekker (1977), FC-M&H=fragment constant-Meylan and Howard (1995), G-C=Group contribution, SC=substituent constant, SPARC=SPARC Performs Automated Reasoning in Chemistry (Karickhoff and others, 1991). [c] Data source ratings: S_w-after Heller and others (1994), K_{ow}-after Heller and others (1994) and Kollig (1988). See text for explanation of rating system adaptations. [d] See text for explanation. [e] Log K_{ow} = log octanol-water partition coefficient.

The results of these criteria-based evaluations support the conclusion that the DDT/DDE S_w and K_{ow} database is extremely unreliable. An overwhelming majority of the data sources received poor (4 rating) or unevaluatable (U rating) ratings (that is, DDT S_w = 100 percent (28 of 28), DDE S_w = 100 percent (9 of 9), DDT K_{ow} = 95 percent (41 of 43), DDE K_{ow} = 96 percent (26 of 27)). Poor and unevaluatable data source ratings resulted from the use of unacceptable or imprecise methods and/or incomplete reporting of methodology, data and statistics. According to our evaluation, only a small percentage ($<$3 percent, 2 of 68) of the data sources received the highest rating (rating = 1) and none received a good rating (rating = 2). Thus, the number of data points that may be considered reliable (as judged by the assigned ratings) is very small (see below).

It must be recognized that the data contained in many of the publications for which poor or unevaluatable ratings were assigned may well be of acceptable quality. However, inadequate documentation precluded a higher rating by the modified evaluation schemes used here. In these instances, determination of the true quality of the reported data would require unsupported inference. This highlights one of the serious shortcomings of the published literature: inadequate documentation.

Original data sources which received highest rating (rating=1):

DDE log K_{ow}
de Bruijn and others (1989)   6.956

DDT log K_{ow}
de Bruijn and others (1989)   6.914
Brooke and others (1990)   6.307

DDE S_w
None

DDT S_w
None

In the case of DDT log K_{ow} data, the only data sources that received a rating of '1' were participants in an interlaboratory comparison study (de Bruijn and others, 1989; Brooke and others, 1990). The mean log K_{ow} values determined by the two laboratories, using similar (but non-identical) procedures differed by more than 0.6 log unit (a factor of four). Previously published "recommended values" (Montgomery, 1997; Verschueren, 1996; Mackay and others, 1997; Sangster, 1997; DCIS, 2000) for log K_{ow} span considerably larger ranges: DDT log K_{ow} (4.89 - 6.914), and DDE log K_{ow} (4.28 - 6.96). Despite widespread citation and use of these "recommended values," the criteria-based evaluations conducted here indicate that the amount of reliable data upon which "recommended values" might be based is grossly inadequate.

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