Background Report Reference

AP-42 Section Number:	9.2.2
Background Chapter:	4
Reference Number:	22
Title:	"Critical Review of Henry's Law Constants fro Pesticides" in Reviews of Environmental Contamination and Toxicology

L.R. Suntio

1988

AP-42 Section 9.2.2
Reference
Report Sect. 4
Reference 22

Critical Review of Henry's Law Constants for Pesticides

L.R. Suntio,* W.Y. Shiu,* D. Mackay,* J.N. Seiber,**
and D. Glotfelty***

Contents

I. Introduction

Pesticides play an important role in maintaining agricultural productivity, but they may also be causes of contamination of air, water, soil, and food, with possible adverse effects on human and animal health. The proper use of pesticide chemicals must be based on an understanding of the behavior of the chemicals as they interact with air, water, soil, and biota, react or degrade, and migrate. This behavior is strongly influenced by the chemicals' physical-chemical properties of solubility in water, vapor pressure or volatility, and tendency to sorb to organic and mineral matter in the soil.

Reviews of such physical-chemical properties have been compiled by Kenaga (1980), Kenaga and Goring (1980), Briggs (1981), and Bowman and Sans (1983) for aqueous solubility, octanol–water partition coefficient, bioaccumulation, and soil sorption; Spencer and Cliath (1970, 1973, 1983), and Spencer (1976) for vapor pressure and volatilization from soil.

In this chapter we compile and discuss data for Henry's Law constant H (which is the ratio of solute partial pressure in the air to the equilibrium water concentration and thus has units of Pa m^3/mol) or the air–water partition

---

* Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto, Ontario, M5S 1A4, Canada.
** Department of Environmental Toxicology, University of California, Davis, CA 95616, USA.
*** Soil Nitrogen and Environmental Chemistry Laboratory, Agricultural Environmental Quality Institute, US Department of Agriculture, Beltsville, MD 20705, USA.

Reviews of Environmental Contamination and Toxicology, Vol. 103.

coefficient K_{AW} which is the dimensionless ratio of air and water concentrations. Both H and K_{AW} are used to describe air–water partitioning of the solutes including pesticides (Mackay and Shiu, 1981).

The Henry's Law constant (HLC) is important in several respects. As is discussed more fully later, the tendency of a chemical to volatilize from water solution to air is largely determined by the HLC, a high value favouring volatilization. Chemicals of low HLC may persist in soil, surface, or groundwaters. If the HLC is large, the chemical may be analyzed by head space analysis or gas stripping. Samples of water containing chemicals of large HLC must be handled carefully to avoid vapor loss. Aquatic bioassays and other tests involving these chemicals must be carefully designed and controlled to avoid loss of chemical. Air–water partitioning is also important in studies of pesticide associations with rain, cloudwater, fogwater, dew, and in the alveoli of the human and other animal lungs.

It is noteworthy that air and water are the ubiquitous, fluid, mobile components of the environment. Many pesticides (and other man-made chemicals) are known to move, as vapor, between the atmosphere and soil, plant, and water surfaces. The direction of this transfer is dictated by the fugacity of each component of the system, which in turn is controlled by the HLC. Thus, pesticides volatilize from treated soil and plant surfaces and their vapors are transported away, often to distant locations by atmospheric movement. Once outside the treated area the vapors may be readsorbed by "dry deposition." "Wet deposition" also occurs when the atmospheric vapors partition into, and are brought to the soil surface by rain. The processes of wet deposition, dry deposition, and volatilization are all influenced in rate by the HLC.

Pesticide volatilization from soil has been extensively studied. Transport upward through the soil to the soil–atmosphere interface occurs by either gaseous diffusion through the air-filled volume of the soil, or by the upward flow of soil solution induced by water evaporation. In either case, the concentration in soil–air at the surface will be governed by soil water–air equilibrium, i.e., by Henry's Law, and such partitioning is a major determinant of the rate of pesticide volatilization from soil.

When attempting to model this process it is commonly assumed that a thin boundary layer of near-stagnant air exists between the atmosphere and the soil surface, across which transport occurs by molecular diffusion. Thus, no matter how the chemical migrates upwards to the soil surface, the pesticide flux to the atmosphere will be essentially determined by the product of the diffusion coefficient and the concentration gradient across the laminar layer. Model calculations predict that this boundary layer resistance may lead to the accumulation of compounds with very low HLCs at the soil surface, because these compounds can establish only very low concentrations in the soil air and thus very slow fluxes across the boundary layer (Jury et al., 1984).

An analogous modelin
ization from water surfac
model (Liss and Slater, 1
connected by two thin b
water phase, across wh
Transport through one o
step in volatilization or a
the magnitude of the HL
As described earlier,
atmospheric pesticides at
dependent upon the HLC
atmosphere. In this proce
surface with the precipita
from the atmosphere to t

where C_A is the total vapo
rate (m/hr), and W_g is
$(g/m^3)_{air}$]. If the pesticide
W_g is the reciprocal of t
equals $1/K_{AW}$. If washou
Equation 1 that the half-
directly proportional to t
Atmospheric washout
that W_g contains contribu
the relationship between
Ligocki et al. (1985) foun
vided the temperature de
and Christensen (1979),
DDT were much greater
of attachment and wash
recently measured the w
five orders of magnitude
quantitative predictor of
et al. (1986).
There are problems wi
determined. Air concentr
compared to concentrati
sphere. This raises questi
and if indeed the air and
air. Glotfelty et al. (1987
distribution of pesticides
attained, and the water an

ss ratio of air and water concentra-
cribe air–water partitioning of the
Shiu, 1981).
important in several respects. As is
f a chemical to volatilize from water
the HLC, a high value favouring
y persist in soil, surface, or ground-
al may be analyzed by head space
r containing chemicals of large HLC
r loss. Aquatic bioassays and other
arefully designed and controlled to
ning is also important in studies of
er, fogwater, dew, and in the alveoli

are the ubiquitous, fluid, mobile
pesticides (and other man-made
, between the atmosphere and soil,
of this transfer is dictated by the
, which in turn is controlled by the
ted soil and plant surfaces and their
ant locations by atmospheric move-
vapors may be readsorbed by "dry
urs when the atmospheric vapors
surface by rain. The processes of wet
tion are all influenced in rate by the

een extensively studied. Transport
osphere interface occurs by either
lume of the soil, or by the upward
poration. In either case, the concen-
overned by soil water–air equilib-
titioning is a major determinant of
il.
it is commonly assumed that a thin
ts between the atmosphere and the
rs by molecular diffusion. Thus, no
ds to the soil surface, the pesticide
determined by the product of the
n gradient across the laminar layer.
ndary layer resistance may lead to
ery low HLCs at the soil surface,
nly very low concentrations in the
e boundary layer (Jury et al., 1984).

An analogous modeling approach may be used for calculations of volatilization from water surfaces. The conventional "two resistance" or "two film" model (Liss and Slater, 1974) assumes that the well-mixed bulk phases are connected by two thin boundary layers, one in the air phase and one in the water phase, across which transport only occurs by molecular diffusion. Transport through one or both of these two films is thus the rate controlling step in volatilization or adsorption. The relative resistances are controlled by the magnitude of the HLC.

As described earlier, the so-called "dry deposition," or adsorption of atmospheric pesticides at soil and water surfaces, is a process that is largely dependent upon the HLC. Wet deposition also removes pesticides from the atmosphere. In this process, pesticides dissolve in rain and are brought to the surface with the precipitation. The flux N (g/m^2 hr) of a vapor-phase pesticide from the atmosphere to the surface with rain is given by

$$N = W_g C_A K_P \tag{1}$$

where C_A is the total vapor-phase concentration (g/m^3), K_P is the precipitation rate (m/hr), and W_g is the vapor-phase washout coefficient, $[(\text{g/m}^3)_{\text{rain}}/(\text{g/m}^3)_{\text{air}}]$. If the pesticide forms an ideal dilute solution in the raindrop, then W_g is the reciprocal of the air–water partition coefficient or HLC, i.e. W_g equals $1/K_{AW}$. If washout is a first-order process, then it can be shown from Equation 1 that the half-life of a pesticide in the atmosphere during rain is directly proportional to the HLC.

Atmospheric washout coefficients have been extensively studied. It is clear that W_g contains contributions from both particle and vapor scavenging; thus the relationship between W_g and K_{AW} is variable and not entirely predictable. Ligocki et al. (1985) found excellent agreement between K_{AW}^{-1} and W_g provided the temperature dependence of K_{AW} was taken into account. Bidleman and Christensen (1979), on the other hand, found that W_g for PCBs and DDT were much greater than K_{AW}^{-1}, which they interpreted as evidence of attachment and washout upon atmospheric particles. Williams (1986) recently measured the washout of a group of pesticides whose H spanned five orders of magnitude. He found that K_{AW}^{-1} was at best only a semiquantitative predictor of W_g. This issue has also been discussed by Mackay et al. (1986).

There are problems with the way in which these washout coefficients are determined. Air concentrations are normally measured at ground level and compared to concentrations in rain that forms at some height in the atmosphere. This raises questions about the extent to which equilibrium is attained and if indeed the air and rain samples are representative of the same mass of air. Glotfelty et al. (1987) recently reported measurements of the air–water distribution of pesticides in fog, a situation in which equilibrium should be attained, and the water and air samples are undoubtedly taken from the same mass of air. They found that the HLC was a poor predictor of the air–water distribution. Volatile, hydrophobic pesticides were enriched in the aqueous phase as much as several thousand times greater than predicted by *H*. It appears that, in the case of fog, the assumption of ideal dilute solution properties is invalid.

In summary, the HLC plays a critical role in determining the environmental dynamics of chemicals in general and pesticides in particular. Although in certain areas the role of the HLC remains obscure, it is clear that elucidating the nature of these roles requires accurate values of this parameter. Accordingly, in this chapter we examine first the thermodynamic background to HLCs, discuss methods of experimental determinations, then present a compilation of data.

II. Thermodynamic Basis

A fairly complete account of the thermodynamic basis has been presented by Mackay and Shiu (1981) and only a brief review of the salient points is given here.

A chemical achieves equilibrium between air and water when its chemical potential or fugacity (f) is equal in each phase. Applying the conventional Raoult's Law expression (Prausnitz, 1969) gives

$$f = y\varnothing P_T = x\gamma P_L^s \tag{2}$$

where f is fugacity (Pa), y is mole fraction in vapor phase, $\varnothing$ is the fugacity coefficient (which is usually unity for nonassociating chemicals at low pressure), P_T is total (atmospheric) pressure (e.g., 101,325 Pa), x is mole fraction in the liquid phase, γ is the activity coefficient in the liquid phase (on a Raoult's Law basis such that γ is 1.0 when x is 1.0), and P_L^s is the vapor pressure (Pa) of the pure chemical in the liquid (or subcooled liquid) state. The group yP_T is P the partial pressure of the chemical (Pa). The concentration in the air phase C_A is yP_T/RT where R is the gas constant (8.314 Pa m^3/mol K) and T is absolute temperature (K). The concentration in the water phase C_W is x/v where v is the molar volume (m^3/mol) of the solution. In dilute solution v approaches that of water, i.e., 18×10^{-6} m^3/mol.

Three expressions for HLC are commonly used,

$$P = HC_W \tag{3}$$

$$P = \bar{H}x \tag{4}$$

$$\text{or } C_A = K_{AW}C_W \tag{5}$$

H has units of Pa/(mol/m^3) or Pa m^3/mol, $\bar{H}$ has units of Pa, and K_{AW} is dimensionless and is often referred to as the air–water partition coefficient.

These HLCs are thus defined as follows

$$H = P/C_W = yP_T/(x/v) = v\gamma P_L^s \tag{6}$$

$$\bar{H} = P/x = yP_T/x = \gamma P_L^s \tag{7}$$

$$K_{AW} = C_A/C_W = (yP_T/RT)/(x/v) = v\gamma P_L^s/RT \tag{8}$$

Clearly H is $\bar{H}v$ and K_{AW} is H/RT. In principle the required data are thus v, γ, and P_L^s. In practice the usually available data are water solubility and vapor pressure.

For a liquid chemical, if the solubility of water in the liquid is negligible then at saturation the fugacity is P_L^s and the product $x\gamma$ must be unity, or γ is $1/x^s$ where x^s is the mole fraction solubility. Alternatively γ is $1/vC_W^s$ where C_W^s is the solubility in units of mol/m^3 and v is the molar volume of the saturated aqueous solution. If water is appreciably soluble in the chemical this expression becomes invalid, because the water-saturated chemical exerts a different (and probably lower) fugacity than the pure liquid chemical. A better estimate of this fugacity is $P_L^s(1 - x_w)$ where x_w is the mole fraction solubility of water in the chemical. The expression for γ then becomes $(1 - x_w)/vC_W^s$.

For a solid chemical the fugacity is that of the solid P_S^s which is less than that of the liquid. An estimate of the ratio of solid/liquid vapor pressure (or fugacity ratio F) can be obtained from

$$F = P_S^s/P_L^s = \exp[-\Delta S((T_M/T) - 1)/R] = \exp[-0.023(T_M - 298)] \tag{9}$$

where ΔS is the entropy of fusion. Some ΔS measurements are available for pesticides determined by differential scanning calorimetry (e.g., Plato and Glasgow 1969; Plato 1972). When no experimental value is available an estimate of 56 J/mol K is generally adopted, but it should be recognized that ΔS can vary substantially from this figure (Yalkowsky, 1979). It follows that

$$\gamma = F/x^s = F/C_S^s v \tag{10}$$

The use of solubility as a source of information on γ results in the following expressions for H

$$\text{liquids } H = v\gamma P_L^s = P_L^s/C_L^s \text{ or } P_L^s(1 - x_w)/C_L^s \tag{11}$$

$$\text{solids } H = v\gamma P_L^s = FP_L^s/C_S^s = P_S^s/C_S^s = P_L^s/C_L^s \tag{12}$$

because FP_L^s equals P_S^s the solid vapor pressure, i.e., F equals both P_S^s/P_L^s and C_S^s/C_L^s.

The Henry's Law constant is thus conveniently calculated as the ratio of the liquid vapor pressure and solubility, or the solid vapor pressure and solubility. It is a mistake to mix a solid and a liquid property. The use of this ratio is equivalent to assuming that a plot of partial pressure versus concentration is linear extending from the origin to the saturation point P^s, C^s which may be either of the liquid or solid. Implicit in this are the assumptions:

i. The solubility of water in the chemical is so small that it negligibly affects the vapor pressure;
ii. The activity coefficient γ does not vary appreciably with concentration.

These assumptions break down when water is appreciably (e.g., >5% mol) soluble in the chemical or when the chemical is appreciably (e.g., >5% mol) soluble in water.

This approach breaks down completely for chemicals which are miscible with water and thus have no reported solubility (e.g., ethanol). In such cases H or γ must be determined by another method, such as direct measurement of HLC or by estimating γ from other measurable quantity or from correlations or predictive procedures.

In summary, for solid or liquid chemicals which display little mutual miscibility with water, H is conveniently estimated as P_s^s/C_s^s or P_L^s/C_L^s, or it can be measured as P/C. For appreciably water miscible systems it is best to measure H as P/C, although an estimate of H can be made as $P_L^s(1 - x_w)/C_L^s$. For water miscible systems H can only be estimated as P/C or as $v\gamma P_L^s$ provided that data for γ can be located.

A rigorous procedure is to measure P^s, C^s, and H and perform a consistency check. Obviously the data must be at the same temperature since all three quantities are temperature dependent, especially P^s and H.

III. Experimental Determination

A. From Solubility and Vapor Pressure

As discussed earlier, if the mutual miscibility of water and the chemical is less than a few mole percent, H can be estimated from experimentally determined solubilities and vapor pressures. The preferred methods involve flow of air or water through "generator columns," as described by May et al. (1978a,b) for water and Spencer and Cliath (1969, 1983) for air. Gas chromatographic methods can also be used for determining vapor pressure (Bidleman, 1984).

B. From Equilibrium Closed Conditions

Lincoff and Gossett (1984), and Gossett (1987) have developed a "Equilibrium Partitioning in Closed System" (EPICS) method that is very suitable for chemicals of high HLC, i.e., H is >100 Pa m^3/mol. Essentially it involves measurement of gas headspace concentration ratio from pairs of sealed bottles containing differing liquid volumes after equilibrium is reached.

C. From Equilibrium Flow Conditions

Mackay et al. (1979) devised a flow system in which the concentration of the chemical in water is measured as a function of time as it is stripped with a

---

steady stream of gas. Thi
Millicic (1985), and Yin
which is suitable for mea

A very simple, approxim
the chemical in water, p
mental temperature cond
and in the liquid can be
the chemical, which can
concentration of the che
depleted in the liquid) the
is the vapor pressure of w
i.e., 55,000 mol/m^3), an
potential for volatilizatio

Table 1 gives the chemic
pesticides. Molar volum
et al., 1979) which is a
culated with equation 9 u
(Yalkowsky, 1979).

Table 2 gives the aque
water partition coefficien
given and then converted
fugacity ratio when the
log C_L versus molar volu
volume increase in a line
(1984), Shiu and Mackay

Table 3 gives the vap
As discussed by Spencer a
exhibit wide discrepancie
dieldrin at 20° varies fror
(Atkins and Eggleton, 19
chosen from data on the
column (Hamilton 1980; 1
1984; Kim et al. 1984) wi
known reliable vapor pr
subcooled liquid vapor p
mentally determined He
Table 3. Therefore, Henr
C_L's and P_L's. Table 4 giv
properties of 96 pesticide

to the saturation point P^s, C^s which
icit in this are the assumptions:
l is so small that it negligibly affects
appreciably with concentration.
vater is appreciably (e.g., $>5\%$ mol)
ical is appreciably (e.g., $>5\%$ mol)

ly for chemicals which are miscible
lubility (e.g., ethanol). In such cases
ethod, such as direct measurement
easurable quantity or from correla-

micals which display little mutual
estimated as P_s^s/C_s^s or P_L^s/C_L^s, or it
water miscible systems it is best to
of H can be made as $P_L^s(1 - x_w)/C_L^s$.
estimated as P/C or as $v\gamma P_L^s$ provided

C^s, and H and perform a consistency
e same temperature since all three
pecially P^s and H.

Determination

d Vapor Pressure

lity of water and the chemical is less
ed from experimentally determined
erred methods involve flow of air or
escribed by May et al. (1978a,b) for
983) for air. Gas chromatographic
vapor pressure (Bidleman, 1984).

losed Conditions

(1987) have developed a "Equilib-
CS) method that is very suitable for
Pa m^3/mol. Essentially it involves
ration ratio from pairs of sealed
s after equilibrium is reached.

low Conditions

in which the concentration of the
on of time as it is stripped with a

---

steady stream of gas. This avoids the need for gas phase analysis. Hassett and Millicic (1985), and Yin and Hassett (1986) have developed a similar system which is suitable for measuring the HLCs in natural waters.

D. Distillation

A very simple, approximate method of estimating H is to distill a solution of the chemical in water, possibly under reduced pressure to obtain environmental temperature conditions. The ratio of water to chemical in the vapor and in the liquid can be used to estimate the relative volatility of water and the chemical, which can be shown to be the ratio of their HLCs. If the concentration of the chemical is enhanced in the vapor or distillate (and depleted in the liquid) the HLC of the chemical exceeds that of water (which is the vapor pressure of water divided by the concentration of water in water i.e., 55,000 mol/m^3), and vice versa. This is useful as a simple screen of potential for volatilization loss.

IV. Data Analysis

Table 1 gives the chemical name, synonym, and other physical data for 96 pesticides. Molar volume was calculated using the Le Bas method (Reid et al., 1979) which is a group additive method. Fugacity ratio was calculated with equation 9 using an average entropy of fusion $\Delta S = 56$ J/mol K (Yalkowsky, 1979).

Table 2 gives the aqueous solubility at specific temperature and octanol/water partition coefficient ($\log K_{OW}$). The selected value of solubility is also given and then converted to subcooled liquid solubility C_L (mol/m^3) with the fugacity ratio when the chemical is a solid at room temperature. A plot of $\log C_L$ versus molar volume (Fig. 1) shows a decrease in solubility as molar volume increase in a linear relationship as reported earlier by Miller et al. (1984), Shiu and Mackay (1986) for aromatic hydrocarbons and PCBs.

Table 3 gives the vapor pressures and their methods of determination. As discussed by Spencer and Cliath (1983), the reported vapor pressures often exhibit wide discrepancies between different authors, e.g., vapor pressure of dieldrin at 20° varies from 2.37×10^{-5} Pa (Martin, 1971) to 3.87×10^{-4} Pa (Atkins and Eggleton, 1971). The selected vapor pressure value was usually chosen from data on the gas chromatographic retention time on a nonpolar column (Hamilton 1980; Ripley 1983; Westcott and Bidleman 1981; Bidleman 1984; Kim et al. 1984) with respect to a structurally similar compound with known reliable vapor pressure. All vapor pressures were also converted to subcooled liquid vapor pressures P_L (Pa). There are very few reported experimentally determined Henry's law constants for pesticides as indicated in Table 3. Therefore, Henry's law constants were calculated from the selected C_L's and P_L's. Table 4 gives complete summarized selected physical-chemical properties of 96 pesticides.

$K_{AW} = \frac{H}{RT}$ $RT = 2.437 \times 10^3$ Pa m³/mol

Table 4. Summary of selected values of pesticides

20°C K_{AW}	Name	MW	mp, °C	Molar volume LeBas method cm³/mol	Fugacity ratio F at 20°C	Vapor pressure $P^s_L = P^s_S/F$ Pa	Solubility $C^s_L = C^s_S/F$ mol/m³	$\log K_{OW}$	H, Pa m³/mol calc'd from at 20°C
3.2×10^{-3}	Acrolein (H)	56.06	−88	66.6	1	28700	3710.31	−0.1	7.74
2.5×10^{-6}	Alachlor (H)	269.77	41	240.7	0.62	0.0048	0.78	2.8	0.0062
1.3×10^{-7}	Aldicarb (I)	190.25	99–100	224.3	0.16	0.063	197.11	1.1	0.00032
3.7×10^{-2}	Aldrin (I)	364.93	104	316.8	0.14	0.036	0.00039	3.0	91.23
4.9×10^{-8}	Ametryn (H)	227.35	84–85	277.5	0.22	0.00045	3.70		0.00012
1.2×10^{-7}	Atrazine (H)	214.68	174	250.6	0.028	0.0014	4.99	2.4	0.00029
1.3×10^{-6}	Azinphosmethyl (I)	317.34	73–74	270.4	0.29	0.0010	0.33	2.7	0.0032
5.5×10^{-4}	Benefin	335.30	65–66.5	295.9	0.34	0.012	0.0088		1.34
7.8×10^{-7}	Bromacil (H)	261.11	158–159	193.1	0.04	0.125	64.15	2.0	0.0019
2.3×10^{-4}	Butylate (H)	217.37	Liquid	280.9	1	0.10	0.18		0.56
2.5×10^{-4}	Captan (F)	300.60	178	250.5	0.026	0.038	0.064	1.8	0.60
5.3×10^{-7}	Carbaryl (I)	201.22	142	218.7	0.059	0.0034	2.70	2.3	0.0013
2.1×10^{-7}	Carbofuran (I)	221.30	150–152	240.8	0.048	0.031	61.19	1.6	0.00051
1.9×10^{-5}	Carbophenothion (I)	342.85	Liquid	323.2	1	0.000040	0.00088	5.1	0.046
3.7×10^{-3}	Chlordane (I)	409.80	103–105	336.5	0.14	0.0079	0.00087	3.0	9.02
1.1×10^{-7}	Chlorfenvinphos (I)	359.56	−19	321.4	1	0.00010	0.36	3.1	0.00028
8.1×10^{-2}	Chloropicrin (I, F)	164.39	−64	105.2	1	2400	12.17		197.27
8.6×10^{-7}	Chlorpropham (H)	213.68	40.7–41.1	232.4	0.63	0.0016	0.74	3.1	0.0021
7.2×10^{-4}	Chlorpyrifos (I)	350.57	41–42	298.8	0.6	0.0025	0.0014	5.0	1.75
2.2×10^{-4}	2,4-D (H)	221.04	135–138	209.8	0.036	27.78	50.27		0.55
2.6×10^{-4}	*o,p'*-DDD (I)	320.00	112	312.6	0.12	0.0017	0.0026	6.1	0.64
2.6×10^{-4}	*p,p'*-DDD (I)	320.00	112	312.6	0.12	0.00083	0.0013	5.5	0.64
1.0×10^{-3}	*o,p'*-DDE (I)	318.00	88–90	305.2	0.2	0.0040	0.0016	5.8	2.54
3.3×10^{-3}	*p,p'*-DDE (I)	318.00	88–90	305.2	0.2	0.0050	0.00063	5.7	7.95
9.7×10^{-4}	DDT (I)	354.50	108.5–109	333.5	0.13	0.00015	0.000065	6.0	2.36
	Demeton (I)	258.34	Liquid	264.8	1	0.030	0.23		0.13
	Dialifor (I)	393.84	67–69	350.8	0.33	0.00020	0.0014	4.7	0.14
	Diallate (H)	270.24	25–30	305.1	0.83	0.016	0.062		0.25
	Diazinon (I)	304.36	Liquid	320.2	1	0.0080	0.12	3.3	0.067
	Dicamba (H)	221.04	114–116	207.9	0.11	0.027	230.32	0.5	0.00012
	Dicapthon (I)	297.68	62–53	228.4	0.47	0.0011	0.045	3.6	0.024
	Dichlobenil (H)	172.02	144–145	148.9	0.055	1.27	1.90	2.9	0.67
	Dichlofenthion (I)	315.17	Liquid	281.1	1	25.00	0.00079	5.1	31645.57
	Dichlorvos (I)	220.98	Liquid	167.5	1	7.00	36.2	1.5	0.19
	Dieldrin (I)	380.93	176–177	318.2	0.026	0.019	0.017	3.7	1.12

Carbofuran (I)	221.30	150–152	240.8	0.048	0.031	61.19	1.6	0.00051
Carbophenothion (I)	342.85	Liquid	323.2	1	0.000040	0.00088	5.1	0.046
Chlordane (I)	409.80	103–105	336.5	0.14	0.0079	0.00087	3.0	9.02
Chlorfenvinphos (I)	359.56	−19	321.4	1	0.00010	0.36	3.1	0.00028
Chloropicrin (I, F)	164.39	−64	105.2	1	2400	12.17		197.27
Chlorpropham (H)	213.68	40.7–41.1	232.4	0.63	0.0016	0.74	3.1	0.0021
Chlorpyrifos (I)	350.57	41–42	298.8	0.6	0.0025	0.0014	5.0	1.75
2,4-D (H)	221.04	135–138	209.8	0.036	27.78	50.27		0.55
o,p′-DDD (I)	320.00	112	312.6	0.12	0.0017	0.0026	6.1	0.64
p,p′-DDD (I)	320.00	112	312.6	0.12	0.00083	0.0013	5.5	0.64
o,p′-DDE (I)	318.00	88–90	305.2	0.2	0.0040	0.0016	5.8	2.54
p,p′-DDE (I)	318.00	88–90	305.2	0.2	0.0050	0.00063	5.7	7.95
DDT (I)	354.50	108.5–109	333.5	0.13	0.00015	0.000065	6.0	2.36

K_{aw}									
5.3×10^{-5}	Demeton (I)	258.34	Liquid	264.8	1	0.030	0.23		0.13
5.7×10^{-5}	Dialifor (I)	393.84	67–69	350.8	0.33	0.00020	0.0014	4.7	0.14
$1,0\times10^{-4}$	Diallate (H)	270.24	25–30	305.1	0.83	0.016	0.062		0.25
$2,7\times10^{-5}$	Diazinon (I)	304.36	Liquid	320.2	1	0.0080	0.12	3.3	0.067
4.9×10^{-8}	Dicamba (H)	221.04	114–116	207.9	0.11	0.027	230.32	0.5	0.00012
$9,8\times10^{-6}$	Dicapthon (I)	297.68	62–53	228.4	0.47	0.0011	0.045	3.6	0.024
2.7×10^{-4}	Dichlobenil (H)	172.02	144–145	148.9	0.055	1.27	1.90	2.9	0.67
13.0	Dichlofenthion (I)	315.17	Liquid	281.1	1	25.00	0.00079	5.1	31645.57
$7,7\times10^{-5}$	Dichlorvos (I)	220.98	Liquid	167.5	1	7.00	36.2	1.5	0.19
$4,6\times10^{-4}$	Dieldrin (I)	380.93	176–177	318.2	0.026	0.019	0.017	3.7	1.12
4.5×10^{-8}	Dimethoate (I)	229.28	52–52.5	205.6	0.48	0.021	181.73	0.8	0.00011
6.6×10^{-5}	Dinitramine	322.20	98–99	265.7	0.16	0.0025	0.016		0.16
$2,1\times10^{-2}$	Dinoseb (H, I)	240.22	38–42	218.0	0.63	15.87	0.31		51.11
$9,0\times10^{-5}$	Disulfoton (I)	274.38	108	282.1	0.13	0.15	0.70	4.0	0.22
4.9×10^{-7}	Diuron (H)	233.10	158–159	223.8	0.04	0.0050	4.29	2.6	0.0012
$4,5\times10^{-6}$	DNOC	148.10	86	147.7	0.22	0.050	4.60		0.011
$1,2\times10^{-3}$	Endosulfan	406.95	70–100	312.8	0.22	0.0050	0.0017	3.6	2.98
$1,4\times10^{-5}$	Endrin (I)	380.93	208–210	318.2	0.013	0.0015	0.046	3.2	0.033
$4,2\times10^{-4}$	EPTC (H)	189.31	Liquid	236.5	1	2.00	1.95		1.02
$1,3\times10^{-5}$	Ethion (I)	384.48	−12	350.2	1	0.00015	0.0047	5.1	0.032
$1,5\times10^{-6}$	Fenitrothion (I)	277.25	Liquid	229.7	1	0.00040	0.11	3.4	0.0036
$9,0\times10^{-6}$	Fenthion (I)	278.34	Liquid	264.6	1	0.0040	0.18	4.1	0.022
$1,1\times10^{-7}$	Fenuron (H)	164.20	131–133	182.0	0.075	0.067	243.61	0.5	0.00027
4.6×10^{-2}	Heptachlor (I)	373.35	95–96	308.2	0.17	0.18	0.0016	3.9	112.01
2.9×10^{-3}	Hexachlorobenzene	284.80	231	221.4	0.0075	0.13	0.0190	6.0	7.12
—	Hexachlorocyclohexane	291.00							
3.6×10^{-4}	α-BHC	291.00	157–160	243.6	0.041	0.073	0.084	3.8	0.87
4.9×10^{-5}	*β*-BHC	291.00	309–310	243.6	0.0012	0.033	0.29	3.8	0.12
$3,0\times10^{-5}$	*δ*-BHC	291.00	138–139	243.6	0.064	0.031	0.43	4.1	0.073
2.4×10^{-4}	Isophorone	138.20	−8	177.4	1	50	86.83	1.7	0.58

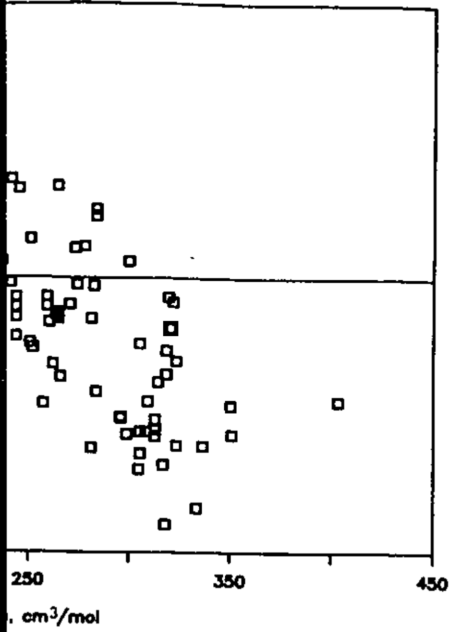
Table 4 (*continued*)

K_{AW}	Name	MW	mp, °C	Molar volume LeBas method cm^3/mol	Fugacity ratio F at 20°C	Vapor pressure $P_L^s = P_S^s/F$ Pa	Solubility $C_L^s = C_S^s/F$ mol/m^3	log K_{OW}	H, Pa m^3/mol calc'd from at 20°C
1.0×10^{-4}	Leptophos (I)	412.06	55–67	317.8	0.38	0.0000079	0.000032	5.9	0.25
5.3×10^{-5}	Lindane (γ-BHC)	290.85	112.5	243.6	0.12	0.025	0.19	3.8	0.13
2.2×10^{-6}	Linuron (H)	249.11	93–94	232.9	0.18	0.0078	1.45	2.2	0.0054
9.4×10^{-7}	Malathion	330.36	2.9	319.1	1	0.0010	0.44	2.8	0.0023
2.7×10^{-8}	Methomyl (I)	162.20	78–79	179.9	0.26	0.015	237.12	0.2	0.000065
1.4×10^{-4}	Methylchlorpyrifos	322.55	44.5–45.5	261.8	0.56	0.0089	0.026	4.3	0.34
8.7×10^{-6}	Methylparathion (I)	263.23	37–38	207.5	0.66	0.0030	0.14	3.0	0.0211
0.34	Mirex (I)	545.59	485	403.2	0.000021	4.76	0.0057	6.9	839.37
1.2×10^{-6}	Monuron (H)	198.65	176–177	202.9	0.026	0.12	38.72	1.8	0.0030
5.7×10^{-2}	Nitralin (H)	345.37	150–151	323.1	0.048	4.17	0.030		138.15
1.1×10^{-7}	Oxamyl (I)	219.25	100–102	212.4	0.15	0.20	760.17		0.00026
0.11	Paradichlorobenzene	147.00	53	137.8	0.47	265.96	1.01	2.4	262.5
4.9×10^{-6}	Parathion (I)	291.27	6	251.9	1	0.00060	0.051	3.8	0.012
1.8×10^{-5}	PCP (F)	266.35	190–191	207.9	0.019	0.11	2.37	4.2	0.044
4.8×10^{-3}	Pebulate (H)	203.36	Liquid	258.7	1	3.5	0.30		11.67
2.7×10^{-8}	Phenylmercuryacetate	336.75	149	151.4	0.05	0.016	237.56		0.000067
2.7×10^{-4}	Phorate (I)	260.40	−43	259.9	1	0.10	0.15	3.8	0.65
3.9×10^{-7}	Phosmet (I)	317.32	71.9	263.3	0.3	0.00020	0.21	2.8	0.00095
1.5×10^{-4}	Phosphamidon (I)	299.69	−45	283.5	1	0.0030	0.0083		0.36
1.4×10^{-8}	Picloram (H)	241.48	218–219	204.2	0.01	0.0060	178.07	0.3	0.000034
1.3×10^{-7}	Pirimor (I)	238.29	90.5	264.0	0.2	0.015	46.16		0.00032
1.6×10^{-2}	Profluralin (H)	347.30	33–36	304.7	0.71	0.013	0.00032		39.07
3.7×10^{-8}	Prometone	225.30	91–92	283.2	0.19	0.0016	17.52		0.000090
2.1×10^{-7}	Prometryn (H)	241.37	118–120	299.7	0.1	0.0010	1.99		0.00050
	Propachlor (H)	211.69	67–76	231.6	0.3	0.10	9.45	1.6	0.011
	Propanil (H)	218.09	91–93	220.1	0.19	0.026	7.24	2.0	0.0036
	Propazine (H)	230.09	213	272.8	0.011	0.00035	3.40		0.00010
	Propoxur (I)	209.24	91.5	244.7	0.19	5.26	40.25	1.5	0.13

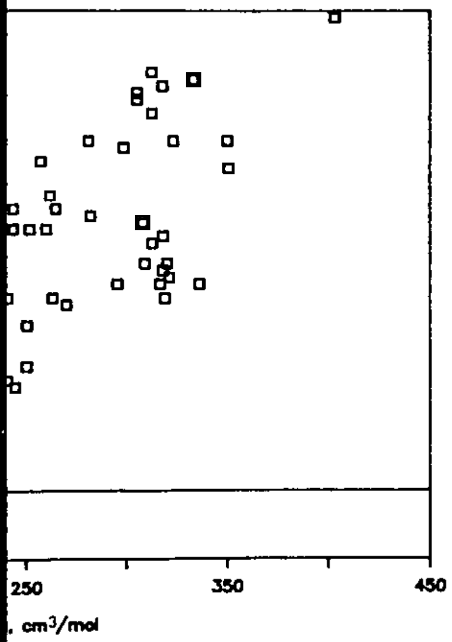
Parathion (I)	291.27	6	251.9	1	0.00060	0.051	3.8	0.012
PCP (F)	266.35	190–191	207.9	0.019	0.11	2.37	4.2	0.044
Pebulate (H)	203.36	Liquid	258.7	1	3.5	0.30		11.67
Phenylmercuryacetate	336.75	149	151.4	0.05	0.016	237.56		0.000067
Phorate (I)	260.40	−43	259.9	1	0.10	0.15	3.8	0.65
Phosmet (I)	317.32	71.9	263.3	0.3	0.00020	0.21	2.8	0.00095
Phosphamidon (I)	299.69	−45	283.5	1	0.0030	0.0083		0.36
Picloram (H)	241.48	218–219	204.2	0.01	0.0060	178.07	0.3	0.000034
Pirimor (I)	238.29	90.5	264.0	0.2	0.015	46.16		0.00032
Profluralin (H)	347.30	33–36	304.7	0.71	0.013	0.00032		39.07
Prometone	225.30	91–92	283.2	0.19	0.0016	17.52		0.000090
Prometryn (H)	241.37	118–120	299.7	0.1	0.0010	1.99		0.00050

Kaw									
4.5×10^{-6}	Propachlor (H)	211.69	67–76	231.6	0.3	0.10	9.45	1.6	0.011
1.5×10^{-6}	Propanil (H)	218.09	91–93	220.1	0.19	0.026	7.24	2.0	0.0036
4.1×10^{-8}	Propazine (H)	230.09	213	272.8	0.011	0.00035	3.40		0.00010
5.3×10^{-5}	Propoxur (I)	209.24	91.5	244.7	0.19	5.26	40.25	1.5	0.13
1.8×10^{-3}	Pyrazon	221.60	207	205.7	0.013	538.46	124.97		4.31
1.3×10^{-3}	Ronnel (I)	321.57	41	257.3	0.62	0.016	0.0050	4.8	3.22
1.4×10^{-7}	Secbumeton	225.00	86–88	283.2	0.21	0.0046	13.12		0.00035
1.4×10^{-7}	Simazine (H)	201.67	225–227	228.4	0.0085	0.0010	2.92	1.9	0.00034
2.4×10^{-6}	2,4,5-T (H)	255.49	153	226.1	0.046	0.11	18.72	0.8	0.0058
7.4×10^{-9}	Terbacil (H)	216.65	175–177	217.7	0.027	0.0019	102.57	1.9	0.000018
1.4×10^{-10}	TCA	163.40	59	121.8	0.41	0.0034	9702.36		0.00000035
5.3×10^{-7}	Terbutryn	241.40	104	273.8	0.14	0.00093	0.74		0.0013
1.7×10^{-4}	Toxaphene (I)	414.00	65–90	358.2	0.26	0.0019	0.0046	3.3	0.42
4.2×10^{-4}	Triallate	304.70	29–30	314.0	0.79	0.013	0.012		1.02
7.0×10^{-10}	Trichlorfon (I)	257.45	83–84	194.9	0.23	0.0043	2600.76	0.4	0.0000017
1.6×10^{-3}	Trifluralin (H)	335.29	46–47	295.9	0.54	0.011	0.0028	3.0	4.02
8.4×10^{-4}	Vernolate (H)	203.35	Liquid	258.7	1	0.90	0.44		2.05
3.4×10^{-5}	Zinophos (I)	248.20	−1.69	233.2	1	0.30	3.63		0.083

F, fungicide; H, herbicide; I, insecticide



vs. molar volume.



$_W$ vs. molar volume.

The user is cautioned that while every effort has been made to avoid errors in tabulating and processing the data, there is an ever-present possibility that the data may contain error of experimental determination, temperature adjustment, change of units or transcription. The primary reference should be consulted to verify values.

The Figures are included to convey an impression of the dependence of these properties on molar volume. As expected, increases in molar volume generally cause a decrease in solubility (Fig. 1), an increase in K_{OW} (Fig. 2), a decrease in vapor pressure (Fig. 3), and no trend in HLC (Fig. 4). There is a tendency for the "pseudosolubility" of liquid chemical in octanol, Q, i.e., the product of K_{OW} and C_L^s, to fall (Miller et al. 1985, Shiu and Mackay, 1986) with increase in molar volume, but the effect is slight (Fig. 5). Most Q values fall between 10^2 and 10^4. Finally, Fig. 6 shows the often reported inverse relationship between octanol–water partition coefficient and subcooled liquid solubility.

When a water solubility in excess of 10000 g/m^3 (i.e., 1%) is used to calculate the HLC the value should be treated with caution for reasons discussed earlier.

V. Discussion

It is convenient to group these chemicals into several classes depending on the values of H. For the eight chemicals for which H exceeds 100 Pa m^3/mol or K_{AW} exceeds 0.04, the chemical is highly volatile and is expected to be lost rapidly to the atmosphere under normal environmental conditions. The rate of volatilization will normally be controlled by diffusional resistances in the water phase. Analysis by head space techniques is satisfactory.

For another 8 chemicals H lies in the range 25–100 Pa m^3/mol (K_{AW} is 0.01–0.04) volatilization will be appreciable but slower, some gas phase resistance occurring. Head space analysis is still possible but prolonged purging may be required.

In the range 1–25 Pa m^3/mol, volatilization is slower still and may or may not be significant depending on the rates of competitive processes. Head space analysis is rarely feasible. Below 1 Pa m^3/mol the chemical (and this includes most pesticides) is only slightly volatile and the rate of evaporation falls as H decreases. At this HLC the equilibrium concentration in air is only approximately 1/2500 of that of water. Volatilization from water can often be ignored as a significant environmental process except where there is the potential to expose a small volume of water (e.g., a thin layer on flooded soil) to a large volume of air.

When using these data care must be taken to note the following:

i. HLCs are very temperature sensitive, thus values change diurnally and seasonally. A rule of thumb of a factor of 2 increase for an 8°C temperature rise gives the order of magnitude variation.

ii. Only the dissolved chemical exerts a partial pressure, thus if the water containing organic or mineral matter which appreciably sorbs or binds the chemical, the "apparent" HLC will be lower if the total concentration in water, rather than the truly dissolved concentration is used.

iii. The presence of dissolved electrolytes, organic matter, detergent and emulsified materials will affect the "solubility" of the chemical in water (or more strictly γ) and thus alter the HLC.

Finally, it should be emphasized that the volatilization of these chemicals from water or their air–water partitioning is controlled by H. It is only indirectly influenced by vapor pressure in combination with solubility. A low vapor pressure is no guarantee of a low HLC and thus of a low volatilizing tendency. Chemicals such as DDT which have very low vapor pressures also have very low solubility, thus they maintain appreciable HLCs and are subject to evaporative loss. The critical determinant of volatilization is thus H.

VI. List of Symbols

C_A	concentration in air, mol/m^3
C_W	solute concentration in water, mol/m^3
C_W^s	solubility in water, mol/m^3
C_S^s	solid solute solubility in water, mol/m^3
C_L^s	subcooled liquid solubility in water, mol/m^3
F	fugacity ratio
H	Henry's Law constant, Pa m^3/mol
$\bar{H}$	Henry's Law constant, Pa
K_{AW}	dimensionless Henry's Law constant or the air/water partition coefficient
K_{OW}	octanol/water partition coefficient
K_P	precipitation rate, mm/hr
N	flux g/m^2/hr
P	partial pressure of solute, Pa
P_T	total pressure, i.e., 101,325 Pa
P_s^s	solid vapor pressure, Pa
P_L^s	subcooled liquid vapor pressure, Pa
Q	"pseudosolubility" of liquid chemical in octanol ($K_{OW} \cdot C_L$), mol/m^3
R	gas constant, 8.314 Pa m^3/mol K
ΔS	entropy of fusion, J/mol K
T	system temperature, K
T_M	melting point, K
v	molar volume of the solution, m^3/mol
W_g	vapor phase washout coefficient, $(g/m^3)_{rain}/(g/m^3)_{air}$
x	solute mole fraction in the liquid phase
x_w	mole fraction solubility of water in solute
x^s	mole fraction solubility of solute in water
y	solute mole fraction in vapor phase

γ	activity coefficient in t
$\varnothing$	fugacity coefficient

The authors are grateful to
for financial support, an
valuable contributions.

Addison JB (1981) Measure
Chemosphere 10:355–36
Ali S (1978) Degradation anc
fan sulfate in mouse, inse
Illinois. 101 pp. Univ. Mi
Abstr Int B 1978, 39(5):2
Ashton FM, Crafts AS (197
New York.
Atkins DHF, Eggleton AEJ (
γ-BHC, dieldrin and p,p'
Tech Environ Pollut, pp 5
Atlas E, Foster R, Giam C
pollutants: laboratory stu
Balson EW (1947) Studies i
manometer sensitive to 5
and other slightly volatile
Baur JR, Bovey RW (1974) U
Contam Toxicol 2:275–2
Benchmark Pesticides (1975)
Surveys of Benchmark Pes
Draft dated October 30, 1
Best R (1975) Stamford (Am
Data provided by W.F. S
Bidleman TF (1984) Estimati
by capillary gas chromato
Bidleman TF, Christensen E (
weight organochlorines. J
Biggar JW, Riggs IR (1974) A
at various temperature. H
Bobra A, Shiu WY, Mackay
for the acute toxicity of chi
4:297–305.
Bowery TG (1964) Heptachl
Regulators, and Food Add
p 245.

partial pressure, thus if the water
which appreciably sorbs or binds the
e lower if the total concentration in
concentration is used.
es, organic matter, detergent and
olubility" of the chemical in water
HLC.

the volatilization of these chemicals
ing is controlled by *H*. It is only
combination with solubility. A low
HLC and thus of a low volatilizing
have very low vapor pressures also
in appreciable HLCs and are subject
ant of volatilization is thus *H*.

ymbols

^{3}

ol/m^3

r the air/water partition coefficient

in octanol ($K_{OW} \cdot C_L$), mol/m^3

$)_{rain}/(g/m^3)_{air}$
e
ute
ter

γ	activity coefficient in the liquid phase
$\varnothing$	fugacity coefficient

Acknowledgements

The authors are grateful to NSERC and the Ontario Ministry of Environment for financial support, and to T.S. Bidleman and W.S. Spencer for their valuable contributions.

References

Addison JB (1981) Measurement of vapor pressures of fenitrothion and matacil. Chemosphere 10:355–364.

Ali S (1978) Degradation and environmental fate of endosulfan isomers and endosulfan sulfate in mouse, insect and laboratory model ecosystem. Ph.D. Thesis. Univ. Illinois. 101 pp. Univ. Microfilms, Ann Arbor, Mich., Order No. 7820891 (Diss Abstr Int B 1978, 39(5):2117).

Ashton FM, Crafts AS (1973) Mode of Action of Herbicides. John Wiley and Sons, New York.

Atkins DHF, Eggleton AEJ (1971) Studies of atmospheric washout and deposition of γ-BHC, dieldrin and *p,p'*-DDT using radio-labelled pesticides. Proc Symp Nucl Tech Environ Pollut, pp 521–533. Intl Atomic Energy Agency, Vienna.

Atlas E, Foster R, Giam CS (1981) Air–sea exchange of high molecular weight pollutants: laboratory studies. Environ Sci Technol 16:283–286.

Balson EW (1947) Studies in vapour pressure measurement. Part III. An effusion manometer sensitive to 5×10^{-6} millimetres of mercury: vapour pressure of DDT and other slightly volatile substances. Trans Faraday Soc 43:54–60.

Baur JR, Bovey RW (1974) Ultraviolet and volatility loss of herbicides. Arch Environ Contam Toxicol 2:275–288.

Benchmark Pesticides (1975) Draft report of Preliminary Summaries of Literature Surveys of Benchmark Pesticides. George Washington University Medical Center. Draft dated October 30, 1975.

Best R (1975) Stamford (American Cyanamid Co. Research Report) 4:11051–11019. Data provided by W.F. Spencer.

Bidleman TF (1984) Estimation of vapor pressures for nonpolar organic compounds by capillary gas chromatography. Anal Chem 56:2490–2496.

Bidleman TF, Christensen E (1979) Atmospheric removal processes for high molecular weight organochlorines. J Geophys Res 84(C12):857–862.

Biggar JW, Riggs IR (1974) Apparent solubility of organochlorine insecticides in water at various temperature. Hilgardia 42:10:383–391.

Bobra A, Shiu WY, Mackay D (1985) Quantitative structure-activity relationships for the acute toxicity of chlorobenzenes to *Daphnia magna*. Environ Toxicol Chem 4:297–305.

Bowery TG (1964) Heptachlor. In: Analytical Methods for Pesticides Plant Growth Regulators, and Food Additives. Vol. II. Zweig, G (ed) Academic Press, New York, p 245.

Bowman BT, Sans WW (1982) Adsorption, desorption, soil mobility, aqueous persistence and octanol–water partitioning coefficients of terbufos, terbufos sulfoxide and terbufos sulfone. J Environ Sci Health B17:447–462.

Bowman BT, Sans WW (1983) Determination of octanol–water partitioning coefficient (K_{OW}) of 61 organophosphorous and carbamate insecticides and their relationship to respective water solubility (S) values. J. Environ Sci Health B18:6:667–683.

Bowman MC, Acree F, Jr., Corbett MK (1960) Solubility of carbon-14 DDT in water. J Agric Food Chem 8:5:406–408.

Briggs GG (1969) Molecular structure of herbicides and their sorption by soils. Nature 223:1288.

Briggs GG (1981) Theoretical and experimental relationships between soil adsorption, octanol–water partition coefficients, water solubilities, bioconcentration factors, and the Parachor. J Agric Food Chem 29:1050–1059.

Briggs GG, Bromilow RM, Evans AA (1982) Relationship between lipophilicity and root uptake and translocation of non-ionised chemical by barly. Pestic Sci 13:495–504.

Bright NFH, Cuthill JC, Woodbury NH (1950) Vapor pressure of parathion and related compounds. J Sci Food Agric 1:344–348.

Brooks GT (1974) Chlorinated Insecticides: Volume I: Technology and applications. CRC Press, Cleveland, OH.

Brust HF (1966) A Summary of chemical and physical properties of Dursban. Down to Earth 22:3:21–22.

Callahan MA, Slimak MW, Gabel NW, May IP, Fowler CF, Freed JR, Jennings P, Durfee RL, Whitmore FC, Maestri B, Mabey WR, Holt BR, Gould C (1979) Water-related environmental fate of 129 priority pollutants, Vol. I, EPA Report No. 440/4-79-029a. Versar, Inc., Springfield, VA.

Chiou C, Freed D, Schmedding D, Kohnert R (1977) Partition coefficient and bioaccumulation of selected organic chemicals. Environ Sci Technol 11:5:475–478.

Cook RF (1973) Carbofuran. In: Analytical Methods for Pesticides and Plant Growth Regulators, Vol. III. Academic Press, New York, pp 187–210.

Demozay D, Marechal G (1972) Physical and chemical properties of lindane: monograph of an insecticide. E Ulmann, K Schiller, Freiburg im Breisgau pp 15–21.

Dickenson W (1956) The vapour pressure of 1:1:*p*:*p*′-dichlorodiphenyl trichloroethane (D.D.T.) Trans Faraday Soc 52:31–35.

Dobbs AJ, Cull MR (1982) Volatilisation of chemicals-relative loss rates and the estimation of vapour pressures. Environ Pollut (Series B) 3:289–298.

Edwards CA (1966) Insecticide residues in soils. Residue Reviews 13:83–132.

Eichler W (Ed.) (1965) Handbuch der Insektizidkunde. Veb Verlag Volk Gesundheit, Berlin, pp 1–84.

Elgar KE (1983) Pesticide residues in water—an appraisal. In: International Union of Pure and Applied Chemistry. Pesticide Chemistry: Human welfare and the environment. Vol. 4. Miyamoto J, Kearney, PC (eds). Pergamon Press, Oxford, England, p 34.

Farmer WJ, Yang MS, Letey J, Spencer WF (1980) Hexachlorobenzene: its vapor pressure and vapor phase diffusion in soil. Soil Sci Soc Am J 44:676–680.

Felsot A, Dahm PA (1979)
ticides by soil. J Agric F
Freed VH (1966) Chemistr
and Water. Breth SA (ed
Freed VH, Chiou CT, Hag
chemicals in the enviro
Health Perspect 20:55.
Freed VH, Schmedding D,
of several organophosph
behavior. Pestic Biochem
Gaines TB (1969) Acute tox
Glotfelty DE, Seiber JN, Li
Gossett JM (1987) Measure
hydrocarbons. Environ S
Grover R, Spencer WF, Fa
volatilization from glass
Gückel W, Synnatschke G,
of active ingredients used
Gückel W, Ritting FR, Synn
of active ingredients used
Pestic Sci 5:393.
Günther FA, Westlake WE,
chemicals in water. Resid
Hamaker JW, Kerlinger H
86:39–54.
Hamilton DJ (1980) Gas c
esters. J Chromatog 195:
Hartley GS (1969) Evaporat
Gould, R.F. (ed), Am Ch
Hartley GS, Graham-Bryce
Dynamics of Applied Pest
Response, Vol. 2, Acaden
Hassett JP, Millicic E (1985
binding of a polychlorin
Environ Sci Technol 19:6
Herbicide Handbook of the
Inc., Geneva, NY, 1st Ed.
Herbicide Handbook (1974)
Ed.
Jacob F, Neumann S (1983)
mobility and criteria of th
of Pure and Applied Ch
Environment. Vol. I. Mi
England, p 362.
Jaber HM, Smith JH, Cwir
to Measure Vapor pressu
Menlo Park, CA.

sorption, soil mobility, aqueous persis-
ficients of terbufos, terbufos sulfoxide
B17:447–462.
on of octanol–water partitioning co-
and carbamate insecticides and their
y (*S*) values. J. Environ Sci Health
) Solubility of carbon-14 DDT in water.
cides and their sorption by soils. Nature
l relationships between soil adsorption,
solubilities, bioconcentration factors,
1050–1059.
Relationship between lipophilicity and
ised chemical by barly. Pestic Sci 13:
950) Vapor pressure of parathion and
4–348.
olume I: Technology and applications.
physical properties of Dursban. Down
IP, Fowler CF, Freed JR, Jennings P,
labey WR, Holt BR, Gould C (1979)
riority pollutants, Vol. I, EPA Report
d, VA.
R (1977) Partition coefficient and bio-
als. Environ Sci Technol 11:5:475–
ethods for Pesticides and Plant Growth
York, pp 187–210.
chemical properties of lindane: mono-
ller, Freiburg im Breisgau pp 15–21.
f 1:1:*p*:*p*'-dichlorodiphenyl trichloro-
–35.
f chemicals-relative loss rates and the
ollut (Series B) 3:289–298.
ls. Residue Reviews 13:83–132.
idkunde. Veb Verlag Volk Gesundheit,
–an appraisal. In: International Union
e Chemistry: Human welfare and the
ey, PC (eds). Pergamon Press, Oxford,
(1980) Hexachlorobenzene: its vapor
Soil Sci Soc Am J 44:676–680.

Felsot A, Dahm PA (1979) Sorption of organophosphorous and carbamate insecticides by soil. J Agric Food Chem 27:557–563.

Freed VH (1966) Chemistry of herbicides. In: Pesticides and Their Effects on Soils and Water. Breth SA (ed), Soil Science Society of America, Inc., pp 28–39.

Freed VH, Chiou CT, Hague R (1977) Chemodynamics: Transport and behavior of chemicals in the environment—A problem in environmental health. Environ Health Perspect 20:55.

Freed VH, Schmedding D, Kohnert R, Hague R (1979) Physical chemical properties of several organophosphates: Some implication in environmental and biological behavior. Pestic Biochem Physiol 10:203–211.

Gaines TB (1969) Acute toxicity of pesticides. Toxicol Appl Pharmacol 14:515.

Glotfelty DE, Seiber JN, Liljedahl LA (1987) Pesticides in fog. Nature 325:602–605.

Gossett JM (1987) Measurement of Henry's law constants for C_1 and C_2 chlorinated hydrocarbons. Environ Sci Technol 21:202–208.

Grover R, Spencer WF, Farmer WJ, Shoup TD (1978) Triallate vapor pressure and volatilization from glass surfaces. Weed Sci 26:505–508.

Gückel W, Synnatschke G, Rittig R (1973) A method for determining the volatility of active ingredients used in plant protection. Pestic Sci 4:137–147.

Gückel W, Ritting FR, Synnatschke G (1974) A method for determining the volatility of active ingredients used in plant protection. II Application to formulated products Pestic Sci 5:393.

Günther FA, Westlake WE, Jaglan PS (1968) Reported solubilities of 738 pesticide chemicals in water. Residue Reviews 20:1–148.

Hamaker JW, Kerlinger HO (1969) Vapor pressure of pesticides. Adv Chem Ser 86:39–54.

Hamilton DJ (1980) Gas chromatographic measurement of volatility of herbicide esters. J Chromatog 195:75–83.

Hartley GS (1969) Evaporation of Pesticides. In: Pesticidal Formulations Research. Gould, R.F. (ed), Am Chem Soc, Washington, DC, p 132.

Hartley GS, Graham-Bryce IJ (1980) Physical Principles of Pesticide Behaviour, the Dynamics of Applied Pesticides in the Local Environment in Relation to Biological Response, Vol. 2, Academic Press, London, pp 892–925.

Hassett JP, Millicic E (1985) Determination of equilibrium and rate constants for binding of a polychlorinated biphenyl congener by dissolved humic substances. Environ Sci Technol 19:638–643.

Herbicide Handbook of the Weed Society of America (1967) W.F. Humphrey Press Inc., Geneva, NY, 1st Ed.

Herbicide Handbook (1974) Weed Science Society of America, Champaign, IL, 3rd Ed.

Jacob F, Neumann S (1983) Quantitative determination of mobility of xenobiotics of mobility and criteria of their phloem and xylem mobility. In: International Union of Pure and Applied Chemistry. Pesticide Chemistry: Human Welfare and the Environment. Vol. I. Miyamoto J, Kearney PC (eds), Pergamon Press, Oxford, England, p 362.

Jaber HM, Smith JH, Cwirla AN (1982) Evaluation of Gas Saturation Methods to Measure Vapor pressure (EPA Contract No. 68-01-5117). SRI International, Menlo Park, CA.

Johnson H (1978) Calculation of the estimated partition coefficient for isophorone. Chemist., Biorganic Chem Lab. SRI-International.

Jury WA, Farmer WJ, Spencer WF (1984) Behavior assessment model for trace organics in soil. II. Chemical classification and parameter sensitivity. J Environ Qual 13:567–572.

Kanazawa J (1981) Japan Pestic Info No 39:12–16.

Kapoor IP, Metcalf RL, Hirwe AS, Coats JR, Khaisa MS (1973) Structure activity correlations of biodegradability of DDT analogs. J Agric Food Chem 21:2: 310–315.

Kavanaugh MC, Trussel RR (1980) Design of aeration towers to strip volatile contaminants from drinking water. J Am Water Works Assoc 72:684–692.

Kenaga EE (1980a) Predicted bioconcentration factors and soil sorption coefficients of pesticides and other chemicals. Ecotoxicol Environ Safety 4:26–38.

Kenaga EE (1980b) Correlation of bioconcentration factors of chemicals in aquatic and terrestrial organisms with their physical and chemical properties. Environ Sci Technol 14:553–556.

Kenaga EE, Goring CAI (1980) In: Aquatic Toxicology. Eaton JG, Parrish PR, Hendricks AC (eds), Am Soc for Testing and Materials, STP 707, pp 78–115.

Khan UK (1980) Pesticides in the Soil Environment. *Elsevier, Amsterdam, Holland.*

Kim YH, Woodrow JE, Seiber JN (1984) Evaluation of a gas chromatographic method for calculating vapor pressures with organophosphorus pesticides. J Chromatog 314:37–53.

Kim Y-H (1985) Evaluation of a Gas Chromatographic Method for Estimating Vapor Pressures with Organic Pollutants. Ph.D. Thesis, University of California, Davis.

Kuhn W, Massini P (1949) *Temperatur-abhängigkeit des Dampfdrucks sowie der* Verdampfungsgeschwindigkeit von Dichlordiphenyltrichloräthan. Helv Chim Acta 32:1530–42.

Kurihara NMU, Fujita T, Nakajima M (1973) Studies on BHC isomers and related compounds V. Some physicochemical properties of BHC isomers. Pestic Biochem Physiol 2(4):383–390.

Leo A, Hansch C, Elkins D (1971) Partition coefficients and their uses. Chem Rev 71:525–616.

Ligocki MP, Leuenberger C, Pankow JF (1985) Trace organic compounds in rain. II. Gas scavenging of neutral organic compounds. Atmos Environ 19:1609–1617.

Lincoff AH, Gossett JM (1984) The determination of Henry's law constant for volatile organics by equilibrium partitioning in closed systems. In: Gas Transfer at Water Surfaces; Brusasert W, Jirka GH, (eds) Reidel: Dordrecht, Holland, pp 17–25.

Liss PS, Slater PG (1974) Flux of gases across the air-sea interface. Nature 247:181–184.

Loos MA (1975) Phenoxyalkanoic acids. In: Herbicides. Chemistry, degradation and mode of action. Kearney PC, Kaufmann DD (eds), Marcel Dekker, Vol. 1, 2nd Ed p 3.

Lu P-Y, Metcalf R (1975) Environmental fate and biodegradability of benzene derivatives as studied in a model aquatic ecosystem. Environ Health Perspect 10:269.

Lyman WJ, Reehl WF, Rosenblatt DH (1982) Handbook of Chemical Property Estimation Methods, McGraw-Hill, New York.

Mabey W, Smith JH, Podo
Partridge I, Jaber H, V
Priority Pollutants. EPA
MacDougall D (1964) Dyl
Regulators, and Food A
p 199.
Mackay D, Leinonen PJ (1
from water to atmosphe
Mackay D, Shiu WY, Suth
constants for hydrophob
Mackay D, Bobra A, Shiu V
solubility and octanol-w
Mackay D, Shiu WY (1981
of environmental interes
Mackay D, Paterson S, Sch
processes of organic che
nol 20:810–816.
Margot A, Stammbach K
Plant Growth Regulatio
Press, New York, pp 11
Marquardt RP (1964) Ron
Regulators, and Food A
p 428.
Martens R (1972) Decompc
Wasser-, Bodden-, Luft
Marti E (1976) Ciba-Geigy
by WF Spencer.
Martin H (1972) Pesticide
cester, England.
May WE, Wasik SP, Free
polynuclear aromatic h
technique. Anal Chem 5
May WE, Wasik SP, Freem
of some polycyclic arom
Melnikov NN (1971) Chem
Menn JJ, Patchett GG, Ba
Plant Growth Regulato
Press, New York, p 546
The Merck Index. An En
Windholz M (ed), Merc
Metcalf R (1971) The ch
Environment. White-St
Metcalf RL (1972) DDT S
Metcalf RL, Kapoor IP, 1
studies of the environm
Perspect 4:35–44.

ted partition coefficient for isophorone.
rnational.
) Behavior assessment model for trace
on and parameter sensitivity. J Environ

12–16.
R, Khaisa MS (1973) Structure activity
T analogs. J Agric Food Chem 21:2:

of aeration towers to strip volatile con-
ter Works Assoc 72:684–692.
ion factors and soil sorption coefficients
col Environ Safety 4:26–38.
ntration factors of chemicals in aquatic
cal and chemical properties. Environ Sci

ic Toxicology. Eaton JG, Parrish PR,
and Materials, STP 707, pp 78–115.
onment. Elsevier, Amsterdam, Holland.
Evaluation of a gas chromatographic
h organophosphorus pesticides. J Chro-

tographic Method for Estimating Vapor
Thesis, University of California, Davis.
hängigkeit des Dampfdrucks sowie der
hlordiphenyltrichloräthan. Helv Chim

3) Studies on BHC isomers and related
perties of BHC isomers. Pestic Biochem

coefficients and their uses. Chem Rev

5) Trace organic compounds in rain. II.
unds. Atmos Environ 19:1609–1617.
tion of Henry's law constant for volatile
osed systems. In: Gas Transfer at Water
eidel: Dordrecht, Holland, pp 17–25.
s the air-sea interface. Nature 247:181–

Herbicides. Chemistry, degradation and
D (eds), Marcel Dekker, Vol. I, 2nd Ed

e and biodegradability of benzene deriv-
stem. Environ Health Perspect 10:269.
982) Handbook of Chemical Property
York.

Mabey W, Smith JH, Podoll RT, Johnson HL, Mill T, Chou TW, Gate J, Waight Partridge I, Jaber H, Vandenberg D. (1982) Aquatic Fate Process for Organic Priority Pollutants. EPA Report No. 440/4-81-014.

MacDougall D (1964) Dylox. In: Analytical Methods for Pesticides, Plant Growth Regulators, and Food Additives. Vol. II. Zweig G (ed), Academic Press, New York p 199.

Mackay D, Leinonen PJ (1975) Rate of evaporation of low-solubility contaminants from water to atmosphere. Environ Sci Technol 7:1178–1180.

Mackay D, Shiu WY, Sutherland RP (1979) Determination of air-water Henry's law constants for hydrophobic pollutants. Environ Sci Technol 13:333–337.

Mackay D, Bobra A, Shiu WY, Yalkowsky SH (1980) Relationships between aqueous solubility and octanol-water partition coefficient. Chemosphere 9:701–711.

Mackay D, Shiu WY (1981) A critical review of Henry's law constants for chemicals of environmental interest. J Phys Chem Ref Data 10:1175–1199.

Mackay D, Paterson S, Schroeder WH (1986) Model describing the rates of transfer processes of organic chemicals between atmosphere and water. Environ Sci Technol 20:810–816.

Margot A, Stammbach K (1964) Diazinon. In: Analytical Methods for Pesticides, Plant Growth Regulations, and Food Additives, Vol II. Zweig G (ed), Academic Press, New York, pp 110.

Marquardt RP (1964) Ronnel. In: Analytical Methods for Pesticides, Plant Growth Regulators, and Food Additives, Vol. II. Zweig G (ed), Academic Press, New York, p 428.

Martens R (1972) Decomposition of endosulfan by soil microorganisms. Schrifter Ver Wasser-, Bodden-, Lufthg, Berlin-Dahlem 37:167–173.

Marti E (1976) Ciba-Geigy Research Report. Basel, West Germany. Data provided by WF Spencer.

Martin H (1972) Pesticide Manual, 3rd Ed., British Crop Protection Council, Worcester, England.

May WE, Wasik SP, Freeman DH (1978a) Determination of aqueous solubility of polynuclear aromatic hydrocarbons by a coupled column liquid chromatographic technique. Anal Chem 50:175–179.

May WE, Wasik SP, Freeman DH (1978b) Determination of the solubility behaviour of some polycyclic aromatic hydrocarbons in water. Anal Chem 50:997–1000.

Melnikov NN (1971) Chemistry of Pesticides. Springer-Verlag, New York.

Menn JJ, Patchett GG, Batchelder GH (1964) In: Analytical Methods for Pesticides, Plant Growth Regulators, and Food Additives. Vol. II. Zweig G (ed), Academic Press, New York, p 546.

The Merck Index. An Encyclopedia of Chemicals, Drugs and Biologicals (1983). Windholz M (ed), Merck and Co., Inc., Rahway, NJ, 10th Ed.

Metcalf R (1971) The chemistry and biology of pesticides. In: Pesticides in the Environment. White-Stevens J (ed), Part I, Vol 1, Marcel Dekker, New York, p 50.

Metcalf RL (1972) DDT Substitutes. Crit Rev Environ Control 3(1):25–59.

Metcalf RL, Kapoor IP, Lu PY, Schuth CK, Sherman P (1973) Model ecosystem studies of the environmental fate of six organochlorine pesticides. Environ Health Perspect 4:35–44.

Metcalfe CD, Mcleese DW, Zitko V (1980) Rate of volatilization of fenitrothion from fresh water. Chemosphere 9:151–155.

Miller MM, Ghodbane S, Wasik SP, Tewari YB, Martire DE (1984) Aqueous solubilities, octanol/water partition coefficients and entropies of melting of chlorinated benzenes and biphenuls. J Chem Engr Data 29:184–190.

Miller MM, Wasik SP, Huang GL, Shiu WY, Mackay D (1985) Relationships between octanol–water partition coefficient and aqueous solubility. Environ Sci Technol 19:522–529.

Miskus R (1964) DDT. In: Analytical Methods for Pesticides Plant Growth Regulators, and Food Additives. Vol. II. Zweig G (ed), Academic Press, New York, p 97.

Montgomery JM, Consulting Engineering, Inc. (1986) Private communication.

Murphy TJ, Mullin MD, Meyer JA (1987) Equilibration of polychlorinated biphenyls and toxaphene with air and water. Environ Sci Technol 21:2:155–162.

Neely WB, Branson DR, Blau GE (1974) Partition coefficient to measure bioconcentration potential of organic chemicals in fish. Environ Sci Technol 8:13:1113–1115.

O'Brien RD (1974) Nonenzymic effects of pesticides on membranes. In: Environmental dynamics of pesticides. Haque R, Freed VH (eds), Plenum Press, New York, pp 331–342.

OECD (1981) OECD Guidelines for Testing of Chemicals. Organisation for Economic Co-Operation and Development. (OECD), Paris 104.

Paris DF, Lewis DL, Barnett JT (1977) Bioconcentration of toxaphene by microorganisms. Bull Environ Contam Toxicol 17:5:564–572.

Park KS, Bruce WN (1968) The determination of the water solubility of aldrin, dieldrin, heptachlor and heptachlor epoxide. J Econ Entomol 61:3:770–774.

Patchett GG, Batchelder GH, Menn JJ (1964) Eptam. In: Analytical Methods for Pesticides Plant Growth Regulators, and Food Additives. Vol. IV. Zweig G (ed), Academic Press, New York, p 118.

Patchett GG, Batchelder GH (1967a) Vernam. In: Analytical Methods for Pesticides, Plant Growth Regulators, and Food Additives. Vol. V. Zweig, G. (ed), Academic Press, New York, p 538.

Patchett GG, Batchelder GH (1967b) Ordram. In: Analytical Methods for Pesticides Plant Growth Regulators, and Food Additives. Vol. V. Zweig G (ed), Academic Press, New York, p 470.

Patchett GG, Batchelder GH (1967c) Ro-Neet. In: Analytical Methods for Pesticides, Plant Growth Regulators, and Food Additives. Vol. V. Zweig G (ed), Academic Press, New York, p 492.

Philips FT (1971) Persistence of organochlorine insecticides on different substrates under different environmental conditions. I. The rates of loss of dieldrin and aldrin by volatilisation from glass surfaces. Pestic Sci 2:255–266.

Phillips WEJ (1975) [Publ.] Endosulfan. Its effects on environmental quality. Nat Res Counc Can, Environ Secr, 14098, 100 pp.

Plato C, Glasgow AR, Jr (1969) Differential scanning calorimetry as a general method for determining the purity and heat of fusion of high-purity organic chemicals. Application to 95 compounds. Anal Chem 41:330–336.

Plato C (1972) Differential scanning calorimetry as a general method for determining purity and heat of fusion of high-purity organic chemicals. Application to 64

---

compounds. Anal Chem

Porter PE (1964) Dieldrin
Regulators, and Food A
pp 143–163.

Prausnitz JM (1969) Mole
Hall, Englewood Cliffs,

Probst GW, Golab T, Wri
Degradation and Mode
Dekker, Inc., NY, p 45

Quellette RP, King JA (197
New York.

Radding SB, Liu DH, Joh
of Selected Chemicals.

Rao PSC, Davidson JM (1
parameters required in
Impact of Nonpoint S
Arbor Science Publishe

Raw GR (ed) (1970) CIPA
Pesticides. Collaborativ

Reid RC, Prausnitz JM, S
3rd Ed McGraw Hill,

Ripley BD, Braun HE (1
chlorine, organophosp
column and applicatio
analysis. J Assoc Offic

Rothman AM (1980) Lo
piration method. J Agri

von Rümker Horay F. (1
ticide Manual Part II.

Sanborn JR, Metcalf WN
terrestrial-aquatic mod

Sears GW, Hopke ER (19
chlorobenzene in a low

Seiber JN, Woodrow JE,
of pesticides from gass c
Soc Meeting, New Yor

Shell Development Compa
Pesticides and Plant Gr
New York, p 298.

Shiu WY, Mackay D (198
Henry's law constant
chlorinated biphenyls.

Sittig M (1977) Pesticides

Slade RE (1945) The γ-iso
pp 314–319.

Slater RM, Spedding DJ
Environ Contam Toxic

l.
f volatilization of fenitrothion from
Martire DE (1984) Aqueous solu-
entropies of melting of chlorinated
: 184–190.
kay D (1985) Relationships between
us solubility. Environ Sci Technol
or Pesticides Plant Growth Regula-
), Academic Press, New York, p 97.
986) Private communication.
ration of polychlorinated biphenyls
Technol 21:2:155–162.
ion coefficient to measure biocon-
fish. Environ Sci Technol 8:13:
ides on membranes. In: Environ-
VH (eds), Plenum Press, New York,
emicals. Organisation for Economic
ris 104.
centration of toxaphene by micro-
:564–572.
of the water solubility of aldrin,
Econ Entomol 61:3:770–774.
eptam. In: Analytical Methods for
Additives. Vol. IV. Zweig G (ed),
Analytical Methods for Pesticides,
. Vol. V. Zweig, G. (ed), Academic
: Analytical Methods for Pesticides
s. Vol. V. Zweig G (ed), Academic
Analytical Methods for Pesticides,
s. Vol. V. Zweig G (ed), Academic
insecticides on different substrates
e rates of loss of dieldrin and aldrin
2:255–266.
on environmental quality. Nat Res
ing calorimetry as a general method
of high-purity organic chemicals.
330–336.
s a general method for determining
anic chemicals. Application to 64

compounds. Anal Chem 44:1531–1534.

Porter PE (1964) Dieldrin. In: Analytical Methods for Pesticides, Plant Growth Regulators, and Food Additives, Vol. II, Zweig G (ed), Academic Press, New York, pp 143–163.

Prausnitz JM (1969) Molecular Thermodynamics of Fluid-Phase Equilibria. Prentic Hall, Englewood Cliffs, NJ.

Probst GW, Golab T, Wright WL (1975) Dinitroanilines. In: Herbicides, Chemistry Degradation and Mode of Action. Vol. 1. Kearney PC, Kaufman DD (eds), Marcel Dekker, Inc., NY, p 457.

Quellette RP, King JA (1977) Chemical Week. Pesticides Register, McGraw-Hill Inc., New York.

Radding SB, Liu DH, Johnson HL, Mill T (1977) Review of the Environmental Fate of Selected Chemicals. USEPA Report No. EPA-560/5-77-003.

Rao PSC, Davidson JM (1980) Estimation of pesticide retention and transformation parameters required in nonpoint source Pollution Models. In: Environmental Impact of Nonpoint Source Pollution. Overcash MR, Davidson JM (eds), Ann Arbor Science Publishers Inc., Ann Arbor, MI.

Raw GR (ed) (1970) CIPAC Handbook. Vol. I. Analysis of Technical and Formulated Pesticides. Collaborative International Pesticides Analytical Council.

Reid RC, Prausnitz JM, Sherwood TK (1977) The Properties of Gases and Liquids, 3rd Ed McGraw Hill, New York.

Ripley BD, Braun HE (1983) Pesticide Residues. Retention time data for organochlorine, organophosphorus, and organonitrogen pesticides on SE-30 capillary column and application of capillary gas chromatography to pesticide residue analysis. J Assoc Offic Anal Chem 66:5:1084–1095.

Rothman AM (1980) Low vapor pressure determination by the radiotracer transpiration method. J Agric Food Chem 28:1225–1228.

von Rümker Horay F. (1972) Information on Thirty-five Pesticide Chemicals. Pesticide Manual Part II. US Agency for International Development.

Sanborn JR, Metcalf WNB, Lu PY (1976) The fate of chlordane and toxaphene in a terrestrial-aquatic model ecosystem. Environ Entomol 5:3:533–538.

Sears GW, Hopke ER (1949) Vapor pressures of naphthalene, anthracene and hexachlorobenzene in a low pressure region. J Am Chem Soc 71:1632–1634.

Seiber JN, Woodrow JE, Sanders PF (1981) Estimation of ambient vapor pressures of pesticides from gass chromatographic retention data. Abstract, 182nd Am Chem Soc Meeting, New York.

Shell Development Company (1973) Gardona Insecticide. In: Analytical Methods for Pesticides and Plant Growth Regulators. Vol. VII. Zweig G (ed), Academic Press, New York, p 298.

Shiu WY, Mackay D (1986) A critical review of aqueous solubilities, vapor pressures, Henry's law constants and octanol-water partition coefficients of the polychlorinated biphenyls. J Phys Chem Data 15:911–929.

Sittig M (1977) Pesticides Process Encyclopedia. Noyes Data, Park Ridge, NJ.

Slade RE (1945) The γ-isomer of hexachlorocychlohexane (Gammexane). Chem Ind pp 314–319.

Slater RM, Spedding DJ (1981) Transport of dieldrin between air and water. Arch Environ Contam Toxicol 10:25–33.

Smith CW (ed) (1962) Acrolein. John Wiley and Sons Inc., New York.

Smith JH, Mabey WR, Bahonos N, Holt BR, Lee SS, Chou TW, Bomberger DC, Mill T (1978) Environmental Pathways of Selected Chemicals in Freshwater Systems: Part II. Laboratory Studies. Interagency Energy-environment Research and Development Program Report. EPA-600/7-78-074. Environmental Research Laboratory Office of Research and Development. USEPA, Athens, Georgia 30605, p 304.

Spencer EY (1973) Guide to the Chemical used in Crop Protection, 6th Ed, Research Branch, Agriculture Canada.

Spencer EY (ed) (1982) Guide to the Chemicals used in Crop Protection. 7th Ed. Research Branch Agriculture Canada, Ontario, Canada.

Spencer WF, Cliath MM (1968) Vapor density of dieldrin. Environ Sci Technol 3:670–674.

Spencer WF, Cliath MM (1970) Vapor pressure and apparent vapor pressure of lindane. J Agric Food Chem 18:529–530.

Spencer WF, Cliath MM (1970) Desorption of lindane from soil as related to vapor density. Soil Sci Soc Am Proc 34:574–578.

Spencer WF, Cliath MM (1973) Pesticide volatilization. Residue Reviews 49:1–47.

Spencer WF (1975) Movement of DDT and its derivatives in the atmosphere. Residue Reviews 59:91–117.

Spencer WF (1976) Vapor pressure and vapor loss, In: A Literature Survey of Benchmark Pesticides. The George Washington University Medical Center Department of Medical and Public Affairs. Science Communication Division, Washington, DC, pp 72–165.

Spencer WF, Shoup TD, Cliath MM, Farmer WJ, Haque R (1979) Vapor pressures and relative volatility of ethyl and methyl parathion. J Agric Food Chem, 27:273–278.

Spencer WF, Cliath MM (1983) Measurement of pesticide vapor pressures. Residue Reviews 85:57–71.

Stansbury HA Jr, Miskus R (1964) In: Analytical Methods for Pesticides, Plant Growth Regulator, and Food Additives, Vol. II. Zweig G (ed), Academic Press, NY, p 438.

Sundaram A, Leung JW (1986) A simple method to determine relative volatilites of aqueous formulation of pesticides. J Environ Sci Health B21:2:165–190.

Sutherland GL, Miskus R (1964) Parathion. In: Analytical Methods for Pesticides, Plant Growth Regulators, and Food Additives, Vol. II. Zweig G (ed), Academic Press, New York, p 322.

Thibodeaux LJ (1979) Chemodynamics. John Wiley and Sons, p 46.

Triggan JW, Dutt GR, Riggs RL (1967) Predicting and measuring the solubility of *p,p*-DDT in water. Bull Environ Contamin Toxicol 2:90.

Veith GD, Austin NM, Morris RT (1979) A rapid method for estimating log P for organic chemicals. Water Res 13:43–47.

Veith GD, DeFoe DL, Bergstedt BV (1979) Measuring and estimating the bioconcentration factor of chemicals in fish. J Fish Res Board Can 26:1040–1048.

Verschueren K (1977) Handbook of Environmental Data on Organic Chemicals, Van Nostrands Reinhold, New York.

Verschueren K (1983) Hand
Ed, Van Nostrand Rein
Warner H, Cohen JM, Irel
of Selected Priority Poll
Weast RC (1984) Handboo
Weil LG, Quentin KL (19
carbons and polychlori
Abwasser Forsch 7:6:1
Westcott JW, Bidleman TF
pressures by capillary ga
Westcott JW, Simon CG,
biphenyl vapor pressure
Technol 15:1375–1378.
Williams EF (1951). Prop
o,o-diethyl *o,p*-nitrophe
Williams GH (1986) Field M
Maryland. MS Thesis, U
Worthing CR (ed) (1983) Th
British Crop Protection
Yalkowsky SH (1979) Estin
Engr Chem Fund 18:10
Yin C, Hassett JP (1986) Ga
mirex fugacity in water.
Yost J (1975) Stamford (Am
provided by WF Spencer
Zepp RG, Wolfe NL, Azarr
formation of the DDT an
by sunlight. Arch Enviro
Zimmerli B, Marek B (1974
mit Pestiziden via Gasph

ınd Sons Inc., New York.
ł., Lee SS, Chou TW, Bomberger DC,
of Selected Chemicals in Freshwater
ragency Energy-environment Research
600/7-78-074. Environmental Research
pment. USEPA, Athens, Georgia 30605,

:d in Crop Protection, 6th Ed, Research

icals used in Crop Protection. 7th Ed.
tario, Canada.
nsity of dieldrin. Environ Sci Technol

ssure and apparent vapor pressure of

of lindane from soil as related to vapor
3.
latilization. Residue Reviews 49: 1–47.
s derivatives in the atmosphere. Residue

r loss, In: A Literature Survey of Bench-
University Medical Center Department
nmunication Division, Washington, DC,

mer WJ, Haque R (1979) Vapor pres-
methyl parathion. J Agric Food Chem,

nt of pesticide vapor pressures. Residue

nalytical Methods for Pesticides, Plant
Vol. II. Zweig G (ed), Academic Press,

ethod to determine relative volatilites of
iron Sci Health B21: 2: 165–190.
. In: Analytical Methods for Pesticides,
ditives, Vol. II. Zweig G (ed), Academic

n Wiley and Sons, p 46.
edicting and measuring the solubility of
in Toxicol 2: 90.
A rapid method for estimating log P for

79) Measuring and estimating the bio-
J Fish Res Board Can 26: 1040–1048.
nmental Data on Organic Chemicals, Van

Verschueren K (1983) Handbook of Environmental Data on Organic Chemicals, 2nd Ed, Van Nostrand Reinhold, New York.

Warner H, Cohen JM, Ireland JC (1980) Determination of Henry's Law Constants of Selected Priority Pollutants. MERL, ORD, US EPA, Cincinnati, OH.

Weast RC (1984) Handbook of Chemistry and Physics, 64th ed., CRC Press, FL.

Weil LG, Quentin KL (1974) Solubility in water of insecticide chlorinated hydrocarbons and polychlorinated biphenyls in view of water pollution. Z Wasser Abwasser Forsch 7: 6: 169–175.

Westcott JW, Bidleman TF (1981) Determination of polychlorinated biphenyl vapor pressures by capillary gas chromatography. J Chromatog 210: 331–336.

Westcott JW, Simon CG, Bidleman TF (1981) Determination of polychlorinated biphenyl vapor pressures by a semimicro gas saturation method. Environ Sci Technol 15: 1375–1378.

Williams EF (1951). Properties of *o,o*-diethyl *o,p*-nitrophenyl thiophosphate and *o,o*-diethyl *o,p*-nitrophenyl phosphate. Ind Engr Chem 43: 950–954.

Williams GH (1986) Field Measurement of Pesticide Washout in Rain Near Beltsville, Maryland. MS Thesis, University of Maryland, College Park, MD, 20742.

Worthing CR (ed) (1983) The Pesticide Manual (A World Compendium) 7th Ed., The British Crop Protection Council, Cryodon.

Yalkowsky SH (1979) Estimation of entropies of fusion of organic compounds. Ind Engr Chem Fund 18: 108–111.

Yin C, Hassett JP (1986) Gas partitioning approach for laboratory and field studies of mirex fugacity in water. Environ Sci Technol 20: 1213–1217.

Yost J (1975) Stamford (American Cynamid Co. Research Report) 2: 6243–46. Data provided by WF Spencer.

Zepp RG, Wolfe NL, Azarraga RH, Coz RH, Pape CW (1977) Photochemical transformation of the DDT and methoxychlor degradation products, DDE and DMDE, by sunlight. Arch Environ Contam Toxicol 6: 305–314.

Zimmerli B, Marek B (1974) Modellversuche zur Kontamination von Lebensmitteln mit Pestiziden via Gasphase. Mitt Gebiete Lebensm Hyg 65: 55–64.