

AGROCHEMICALS

Desk Reference

2nd EDITION

John H. Montgomery



LEWIS PUBLISHERS

Boca Raton New York

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Product Manager: *Karen Feinstein*
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PREFACE

The use of pesticides, herbicides, fungicides and other agricultural chemicals has increased significantly over the last several decades. These "agrochemicals" have varying degrees of stability in the environment. Despite their degradation in the environment by a variety of mechanisms, the parent compounds and their degradates persist long enough to adversely impact soils and/or groundwater. As a consequence, the contamination of soil and groundwater by agrochemicals has gained considerable attention. The sources of agrochemicals adversely impacting the groundwater environment include, but are not limited to, hazardous waste sites, municipal landfills, forested land areas, agricultural operations (e.g., farmlands and pesticide-treated forests), domestic practices (e.g., fertilizers, herbicides, etc.) and non-point source areas.

The protection of groundwater from agrochemicals and other pollutants requires that regulators plus public and private interests cooperate. In addition, understanding the fate and transport of these chemicals is required to assess the exposure to humans, wildlife, and biota. To this end, professionals ranging from environmental consultants to the local health officials need reliable, accurate, and readily accessible data to accomplish these tasks. Unfortunately, the necessary data are scattered throughout many reference books, papers, and journals. *Agrochemicals Desk Reference, 2nd Edition* was published to bring all this necessary information together in one publication. Now this desk reference is included in the CD-ROM *Agrochemical and Pesticide Profile Desk Reference CRCnet-BASE*. It is based on more than 1700 references. Most of the citations reviewed from the document literature pertain to the fate and transport of agrochemicals in various environmental compartments (e.g., air, soil, groundwater, and surface water).

Every effort has been made to select the most accurate information and present it factually and accurately. The publisher and authors would appreciate hearing from readers regarding corrections and suggestions for material that might be included for use in future versions of the CD-ROM.

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INTRODUCTION

The compounds profiled include those herbicides, insecticides and fumigants most commonly found in the groundwater environment. The number of compounds included in this book was narrowed down based on information available in the documented literature. Compounds profiled in this book include pesticides having the potential for contaminating groundwater in New Jersey (Murphy and Fenske, 1987), compounds for which physicochemical data are available from the U.S. Department of Agriculture (1990) and those compounds which have been identified as organic Priority Pollutants promulgated by the U.S. Environmental Protection Agency (U.S. EPA) under the Clean Water Act of 1977 (40 CFR 136, 1977).

The compound headings are those commonly used by the U.S. EPA and many agricultural organizations. Positional and/or structural prefixes set in italic type are not an integral part of the chemical name and are disregarded in alphabetizing. These include *asym-*, *sym-*, *n-*, *sec-*, *cis-*, *trans-*, α -, β -, γ -, *o-*, *m-*, *p-*, *N-*, etc.

Synonyms: These are listed alphabetically following the convention used for the compound headings. Compounds in boldface type are the Chemical Abstracts Service (CAS) names listed in the eighth or ninth Collective Index. If no synonym appears in boldface type, then the compound heading is the CAS assigned name. Synonyms include chemical names, common or generic names, trade names, registered trademarks, government codes and acronyms. All synonyms found in the literature are listed.

Although synonyms were retrieved from several references, most of them were retrieved from the Registry of Toxic Effects of Chemical Substances (RTECS, 1985).

Structure: This is given for every compound regardless of its complexity. The structural formula is a graphic representation of atoms or group(s) of atoms relative to each other. Clearly, the limitation of structural formulas is that they depict these relationships in two dimensions.

DESIGNATIONS

Chemical Abstracts Service (CAS) Registry Number: This is a unique identifier assigned by the American Chemical Society to chemicals recorded in the CAS Registry System. This number is used to access various chemical databases such as the Hazardous Substances Data Bank (HSDB), CAS Online, Chemical Substances Information Network and many others. This entry is also useful to conclusively identify a substance regardless of the assigned name.

Department of Transportation (DOT) Designation: This is a four-digit number assigned by the U.S. Department of Transportation (DOT) for hazardous materials and is identical to the United Nations identification number (which is preceded by the letters UN). This number is required on shipping papers, on placards or orange panels on tanks and on a label or package containing the material. These numbers are widely used for personnel responding to emergency situations, e.g., overturned tractor trailers, in which the identification of the transported material is quickly and easily determined. Additional informa-

tion may be obtained through the U.S. Department of Transportation, Research and Special Programs Administration, Materials Transportation Bureau, Washington, DC 20590.

Molecular Formula (mf): This is arranged by carbon, hydrogen and remaining elements in alphabetical order in accordance with the system developed by Hill (1900). Molecular formulas are useful in identifying isomers (i.e., compounds with identical molecular formulas) and are required if one wishes to calculate the formula weight of a substance.

Formula Weight (fw): This is calculated to the nearest hundredth using the empirical formula and the 1981 Table of Standard Atomic Weights as reported in Weast (1986). Formula weights are required for many calculations, such as converting weight/volume units, e.g., mg/L or g/L, to molar units (mol/L); with density for calculating molar volumes; and for estimating Henry's law constants.

Registry of Toxic Effects of Chemical Substances (RTECS) Number: Many compounds are assigned a unique accession number consisting of two letters followed by seven numerals. This number is needed to quickly and easily locate additional toxicity and health-based data which are cross-referenced in the RTECS (1985). Contact the National Institute for Occupational Safety and Health (NIOSH), U.S. Department of Health and Human Services, 4676 Columbia Parkway, Cincinnati, OH 45226 for additional information.

PHYSICAL AND CHEMICAL PROPERTIES

Appearance and Odor: The appearance, including the physical state (solid, liquid, or gas) of a chemical at room temperature (20–25°C) is provided. If the compound can be detected by the olfactory sense, the odor is noted. Unless noted otherwise, the information provided in this category is for the pure substance and was obtained from many sources (Hawley, 1981; Verschueren, 1983; Windholz et al., 1983; CHRIS Hazardous Chemical Data, 1984; Sax, 1984; Sittig, 1985; Toxic and Hazardous Industrial Chemicals Safety Manual for Handling and Disposal with Toxicity and Hazard Data, 1986; Sax and Lewis, 1987; Hazardous Substances Data Bank, 1989).

Bioconcentration Factor (BCF): The bioconcentration factor is defined as the ratio of the chemical accumulated in tissue to the concentration in water. Generally, high bioconcentration factors tend to be associated with very lipophilic compounds. Conversely, low bioconcentration factors are associated with compounds having high aqueous solubilities.

Bioconcentration factors have been shown to be correlated with the octanol/water partition coefficient in aquatic organisms (Davies and Dobbs, 1984; de Wolf et al., 1992; Isnard and Lambert, 1988) and fish (Davies and Dobbs, 1984; Kenaga, 1980; Isnard and Lambert, 1988; Neely et al., 1974; Ogata et al., 1984; Oliver and Niimi, 1985).

Boiling Point (bp): This is defined as the temperature at which the vapor pressure of a liquid equals the atmospheric pressure. Unless noted otherwise, all boiling points are reported at one atmosphere pressure (760 mmHg). Although not used in environmental assessments, boiling points for aromatic compounds have been found to be linearly correlated with aqueous solubility (Almgren et al., 1979). Boiling points are also useful in assessing entry of toxic substances into the body. Body contact with high-boiling liquids is the most common means of entry into the body, whereas the inhalation route is the most common for low-boiling liquids (Shafer, 1987).

Dissociation Constant (pK_a): In an aqueous solution, an acid (HA) will dissociate into the carboxylate anion (A^-) and hydrogen ion (H^+) and may be represented by the general equation:



At equilibrium, the ratio of the products (ions) to the reactant (non-ionized electrolyte) is related by the equation:

$$K_a = ([H^+][A^-]/[HA]) \quad [2]$$

where K_a is the dissociation constant. This expression shows that K_a increases if there is increased ionization and vice versa. A strong acid (weak base) such as hydrochloric acid ionizes readily and has a large K_a , whereas a weak acid (or stronger base) such as benzoic acid ionizes to a lesser extent and has a lower K_a . The dissociation constants for weak acids are sometimes expressed as K_b , the dissociation constant for the base, and both are related to the dissociation constant for water by the expression:

$$K_w = K_a + K_b \quad [3]$$

where K_w is the dissociation constant for water (10^{-14} at 25°C), K_a is the acid dissociation constant, K_b is the base dissociation constant.

The dissociation constant is usually expressed as $pK_a = -\log_{10}K_a$. Equation [3] becomes:

$$pK_w = pK_a + pK_b \quad [4]$$

When the pH of the solution and the pK_a are equal, 50% of the acid will have dissociated into ions. The percent dissociation of an acid or base can be calculated if the pH of the solution and the pK_a of the compound are known (Guswa et al., 1984):

$$\text{For organic acids:} \quad \alpha_a = [100/(1 + 10^{(pH-pK_a)})] \quad [5]$$

$$\text{For organic bases:} \quad \alpha_b = [100/(1 + 10^{(pK_w-pK_b-pH)})] \quad [6]$$

where α_a is the percent of the organic acid that is nondissociated, α_b is the percent of the organic base that is nondissociated, pK_a is the $-\log_{10}$ dissociation constant for an acid, pK_w is the $-\log_{10}$ dissociation constant for water (14.00 at 25°C), pK_b is the $-\log_{10}$ dissociation constant for base ($pK_b = pK_w - pK_a$) and pH is the $-\log_{10}$ hydrogen ion activity (concentration) of the solution.

Since ions tend to remain in solution, the degree of dissociation will affect processes such as volatilization, photolysis, adsorption and bioconcentration (Howard, 1989).

Henry's Law Constant (K_H): Sometimes referred to as the air-water partition coefficient, Henry's law constant is defined as the ratio of the partial pressure of a compound in air to the concentration of the compound in water at a given temperature under equilibrium

conditions. If the vapor pressure and solubility of a compound are known, this parameter can be calculated at 1.0 atm (760 mmHg) as follows:

$$K_H = Pfw/760S \quad [7]$$

where K_H is Henry's law constant ($\text{atm} \cdot \text{m}^3/\text{mol}$), P is the vapor pressure (mmHg), S is the solubility in water (mg/L) and fw is the formula weight (g/mol).

Henry's law constant can also be expressed in dimensionless form and may be calculated using one of the following equations:

$$K_{H'} = K_H/RK \quad \text{or} \quad K_{H'} = S_a/S \quad [8]$$

where $K_{H'}$ is Henry's law constant (dimensionless), R is the ideal gas constant ($8.20575 \times 10^{-5} \text{ atm} \cdot \text{m}^3/\text{mol} \cdot \text{K}$), K is the temperature of water (degrees Kelvin), S_a is the solute concentration in air (mol/L), and S is the aqueous solute concentration (mol/L).

It should be noted that estimating Henry's law constant assumes that the gas obeys the ideal gas law and the aqueous solution behaves as an ideally dilute solution. The solubility and vapor pressure data inputted into the equations are valid only for the pure compound and must be in the same standard state at the same temperature.

The major drawback in estimating Henry's law constant is that both the solubility and the vapor pressure of the compound are needed in equation [7]. If one or both of these parameters is unknown, an empirical equation based on quantitative structure-activity relationships (QSAR) may be used to estimate Henry's law constants (Nirmalakhandan and Speece, 1988). In this QSAR model, only the structure of the compound is needed. From this, connectivity indexes (based on molecular topology), polarizability (based on atomic contributions) and the propensity of the compound to form hydrogen bonds can easily be determined. These parameters, when regressed against known Henry's law constants for 180 organic compounds, yielded an empirical equation that explained more than 98% of the variance in the data set having an average standard error of only 0.262 logarithm units.

Henry's law constant may also be estimated using the bond or group contribution method developed by Hine and Mookerjee (1975). The constants for the bond and group contributions were determined using experimentally determined Henry's law constants for 292 compounds. The authors found that those estimated values significantly deviating from observed values (particularly for compounds containing halogen, nitrogen, oxygen and sulfur substituents) could be explained by "distant polar interactions", i.e., interactions between polar bonds or structural groups.

A more recent study for estimating Henry's law constants using the bond contribution method was provided by Meylan and Howard (1991). In this study, the authors updated and revised the method developed by Hine and Mookerjee (1975) due to new experimental data that have become available since 1975. Bond contribution values were determined for 59 chemical bonds based on known Henry's law constants for 345 organic compounds. A good statistical fit [correlation coefficient (r^2) = 0.94] was obtained when the bond contribution values were regressed against known Henry's law constants for all compounds. For selected chemicals classes, r^2 increased slightly to 0.97.

Russell et al. (1992) conducted a similar study using the same data set from Hine and Mookerjee (1975). They developed a computer-assisted model based on five molecular descriptors which were related to the compound's bulk, lipo-philicity and polarity. They

found that 63 molecular structures were highly correlative with the log of Henry's law constants ($r^2 = 0.96$).

Henry's law constants provided an indication of the relative volatility of a substance. According to Lyman et al. (1982), if $K_H < 10^{-7}$ atm · m³/mol, the substance has a low volatility. If K_H is $> 10^{-7}$ but $< 10^{-5}$ atm · m³/mol, the substance will volatilize slowly. Volatilization becomes an important transfer mechanism in the range $10^{-5} < H < 10^{-3}$ atm · m³/mol. Values of $K_H > 10^{-3}$ atm · m³/mol indicate volatilization will proceed rapidly.

The rate of volatilization will also increase with an increase in temperature. ten Hulscher et al. (1992) studied the temperature dependence of Henry's law constants for three chlorobenzenes, three chlorinated biphenyls and six polynuclear aromatic hydrocarbons. They observed that over the temperature range of 10 to 55°C, Henry's law constant was doubled for every 10°C increase in temperature. This temperature relationship should be considered when assessing the role of chemical volatilization from large surface water bodies whose temperatures are generally higher than those typically observed in ground-water.

Hydrolysis Half-Life ($H-t_{1/2}$): The hydrolysis half-life of a chemical is the time that it takes to reach one-half or 50% of its original concentration. The rate of chemical hydrolysis is highly dependent upon the compound's solubility, temperature and pH. Since other environmental factors such as photolysis, volatility (i.e., Henry's law constants) and adsorption can affect the rate of hydrolysis, these factors are virtually eliminated by performing hydrolysis experiments under carefully controlled laboratory conditions. The hydrolysis half-lives reported in the literature were calculated using experimentally determined hydrolysis rate constants.

Ionization Potential (IP): The ionization potential of a compound is defined as the energy required to remove a given electron from the molecule's atomic orbit (outermost shell) and is expressed in electron volts (eV). One electron volt is equivalent to 23,053 cal/mol.

Knowing the ionization potential of a contaminant is required in determining the appropriate photoionization lamp for detecting that contaminant or family of contaminants. Photoionization instruments are equipped with a radiation source (ultra-violet lamp), pump, ionization chamber, an amplifier and a recorder (either digital or meter). Generally, compounds with ionization potentials smaller than the radiation source (UV lamp rating) being used will readily ionize and will be detected by the instrument. Conversely, compounds with ionization potentials higher than the lamp rating will not ionize and will not be detected by the instrument.

Soil/Sediment Partition Coefficient (K_{oc}): The soil/sediment partition or sorption coefficient is defined as the ratio of adsorbed chemical per unit weight of organic carbon to the aqueous solute concentration. This value provides an indication of the tendency of a chemical to partition between particles containing organic carbon and water. Compounds that bind strongly to organic carbon have characteristically low solubilities, whereas compounds with low tendencies to adsorb onto organic particles have high solubilities.

Non-ionizable chemicals that sorb onto organic materials in an aquifer (i.e., organic carbon) are retarded in their movement in groundwater. The sorbing solute travels at a linear velocity that is lower than the groundwater flow velocity by a factor of R_d , the retardation factor. If the K_{oc} of a compound is known, the retardation factor may be calculated using the following equation from Freeze and Cherry (1974) for unconsolidated sediments:

$$R_d = V_w/V_c = [1 + (BK_d/n_e)] \quad [9]$$

where R_d is the retardation factor (unitless), V_w is the average linear velocity of groundwater (e.g., ft/day), V_c is the average linear velocity of contaminant (e.g., ft/day), B is the average soil bulk density (g/cm^3), n_e is the effective porosity (unitless), and K_d is the distribution (sorption) coefficient (cm^3/g).

By definition, K_d is defined as the ratio of the concentration of the solute on the solid to the concentration of the solute in solution. This can be represented by the Freundlich equation:

$$K_d = VM_s/MM_L = C_s/C_L^n \quad [10]$$

where V is the volume of the solution (cm^3), M_s is the mass of the sorbed solute (g), M is the mass of the porous medium (g), M_L is the mass of the solute in solution (g), C_s is the concentration of the sorbed solute (g/cm^3), C_L is the concentration of the solute in the solution (g/cm^3) and n is a constant.

Values of n are normally between 0.7 and 1.1 although values of 1.6 have been reported (Lyman et al., 1982). If n is unknown, it is assumed to be unity and a plot of C_s versus C_L will be linear. The distribution coefficient is related to K_{oc} by the equation:

$$K_{oc} = K_d/f_{oc} \quad [11]$$

where f_{oc} is the fraction of naturally occurring organic carbon in soil.

Sometimes K_d is expressed on an organic-matter basis and is defined as:

$$K_{om} = K_d/f_{om} \quad [12]$$

where f_{om} is the fraction of naturally occurring organic matter in soil. The relationship between K_{oc} and K_{om} is defined as:

$$K_{om} = 0.58K_{oc} \quad [13]$$

where the constant 0.58 is assumed to represent the fraction of carbon present in the soil or sediment organic matter (Allison, 1965).

For fractured rock aquifers in which the porosity of the solid mass between fractures is insignificant, Freeze and Cherry (1974) report the retardation equation as:

$$R_d = V_w/V_c = [1 + (2K_A/b)] \quad [14]$$

where K_A is the distribution coefficient (cm) and b is the aperture of fracture (cm).

To calculate the retardation factors for ionizable compounds such as acids and bases, the fraction of un-ionized acid (α_a) or base (α_b) needs to be determined (see **Dissociation Constant**). According to Guswa et al. (1984), if it is assumed only the un-ionized portion of the acid is adsorbed onto the soil, the retardation factor for the acid becomes:

$$R_a = [1 + (\alpha_a BK_d/n_e)] \quad [15]$$