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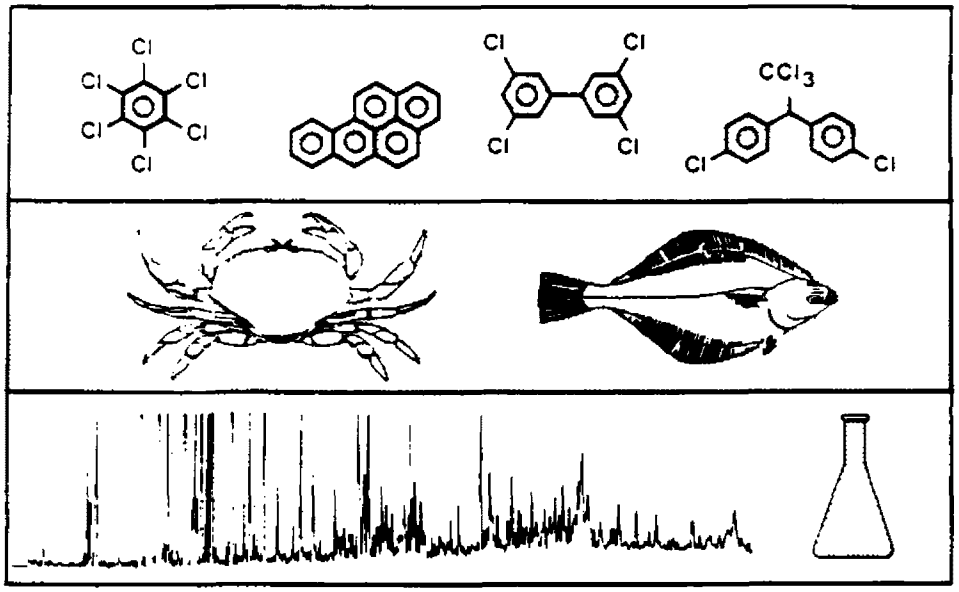
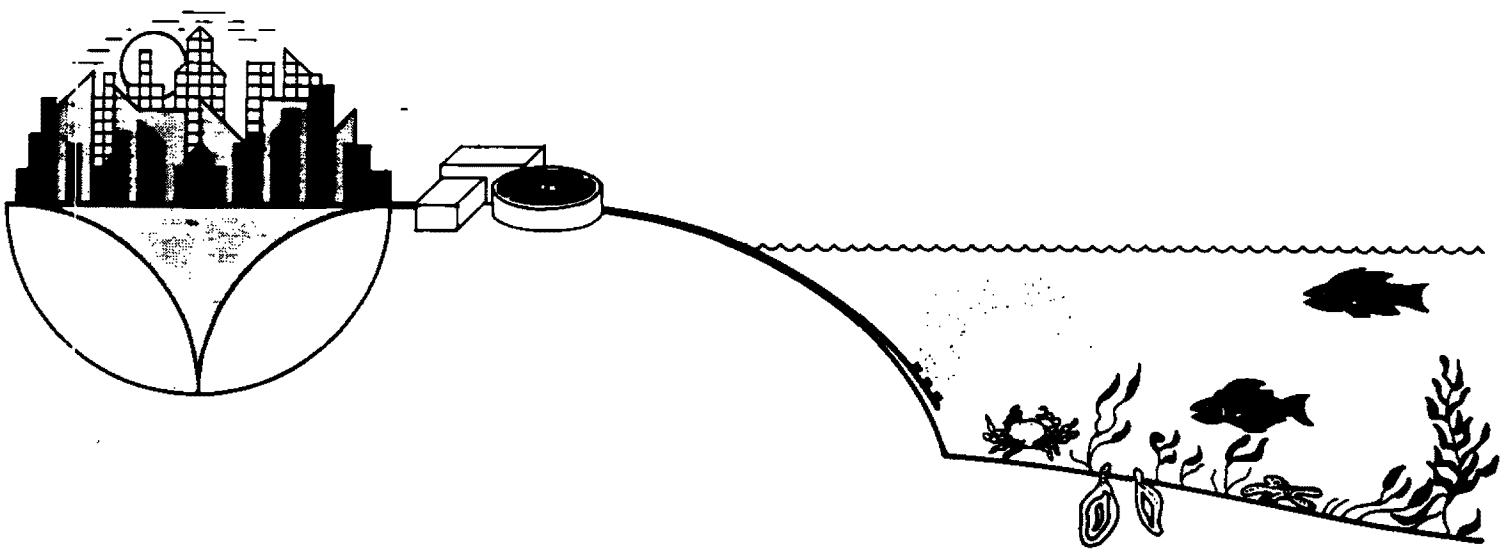
BIOACCUMULATION MONITORING GUIDANCE:

1. ESTIMATING THE POTENTIAL FOR BIOACCUMULATION OF PRIORITY POLLUTANTS AND 301(h) PESTICIDES DISCHARGED INTO MARINE AND ESTUARINE WATERS





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ESTIMATING THE POTENTIAL FOR BIOACCUMULATION OF PRIORITY POLLUTANTS AND 301(h) PESTICIDES DISCHARGED INTO MARINE AND ESTUARINE WATERS

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PREFACE

This report is one element of the Bioaccumulation Monitoring Guidance Series. The purpose of this series is to provide guidance for monitoring of priority pollutant residues in tissues of resident marine organisms. These guidance documents were prepared for the 301(h) sewage discharge permit program under the U.S. EPA Office of Marine and Estuarine Protection, Marine Operations Division. Two kinds of monitoring guidance are provided in this series: recommendations for sampling and analysis designs, and aids for interpretation of monitoring data.

Some basic assumptions were made in developing the guidance presented in these documents: 1) each bioaccumulation monitoring program will be designed to meet the requirements of the 301(h) regulations, 2) tissue samples will be collected from appropriate locations near the sewage discharge and from an unpolluted reference site, 3) the initial chemicals of concern are the U.S. EPA priority pollutants and 301(h) pesticides, and 4) the monitoring data should be suitable for a meaningful evaluation of the potential hazards to living marine resources as well as human health. It should be recognized that the design of a monitoring program reflects the site-specific characteristics of the pollutant discharge and the receiving environment. Thus, site-specific considerations may lead to a modification of the generic recommendations herein. Finally, although these guidance documents were prepared specifically for monitoring of sewage discharges under the 301(h) program, their potential use extends to assessment and monitoring of bioaccumulation resulting from other kinds of pollutant discharges into marine and estuarine environments.

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ACKNOWLEDGEMENTS

This document has been reviewed by the 301(h) Task Force of the Environmental Protection Agency, which includes representatives from the Water Management Divisions of U.S. EPA Regions I, II, III, IV, IX, and X; the Office of Research and Development - Environmental Research Laboratory - Narragansett (located in Narragansett, RI and Newport, OR), and the Marine Operations Division in the Office of Marine and Estuarine Protection, Office of Water.

This technical guidance document was produced for the U.S. Environmental Protection Agency under the 301(h) post-decision technical support contract No. 68-01-6938, Allison J. Duryee, Project Officer. This report was prepared by Tetra Tech, Inc., under the direction of Dr. Thomas C. Ginn. The primary authors were Dr. Leslie G. Williams and Dr. Robert A. Pastorok. Ms. Marcy B. Brooks-McAuliffe performed technical editing and supervised report production.

INTRODUCTION

The accumulation of toxic substances in marine organisms that may lead to adverse biological effects or affect commercial or recreational fishes is one of the major concerns in evaluating the effects of sewage discharges into marine and estuarine waters (Tetra Tech 1982). Accumulation of chemical contaminants in marine and estuarine organisms may: 1) cause significant mortality in susceptible organisms, 2) produce either a lethal or chronic toxic response at later stages of the life cycle or under conditions of stress, or 3) be tolerated but result in transfer of toxic pollutants to higher trophic level organisms, including humans (Davies and Dobbs 1984). The 301(h) regulations state that "biological monitoring shall include to the extent practicable: periodic determinations of the accumulation of toxic pollutants and pesticides..." [40 CFR 125.62(b)(1)(ii)]. Therefore, characterization of toxic substances in tissues of marine organisms will be an important feature in many 301(h) monitoring programs.

The objectives of this report are to:

- Provide an overview of important environmental, biological, and chemical processes that affect bioaccumulation of chemical contaminants in marine and estuarine animals

- Review predictive and empirical approaches used to determine the bioaccumulation potential of toxic chemicals

- Develop a method for ranking U.S. EPA priority pollutants and 301(h) pesticides in terms of bioaccumulation potential

- Provide guidance for selection of pollutants to analyze in 301(h) monitoring programs.

Functional relationships between bioaccumulation and various environmental and chemical variables are shown in the studies reviewed in this document. The quantitative relationships between contaminant concentrations in various exposure media and bioaccumulation in animal tissues are emphasized. Where

appropriate, the limitations and uncertainties of the available data are noted and discussed with respect to their implications for 301(h) monitoring programs. A quantitative index is provided for ranking the bioaccumulation potential of contaminants that may be present in sewage effluent.

The review and monitoring guidance recommendations are based on the best available bioaccumulation data, regardless of target organ or tissue type. The liver in fishes and the hepatopancreas in invertebrates are fatty tissues in which most hydrophobic organic contaminants are concentrated, stored, and transformed metabolically. Thus, liver concentrations of contaminants are highly relevant to determining bioaccumulation potential, and many of the bioaccumulation studies reviewed in this report focus on liver tissues. In general, lipid content of muscle tissue is less than that of liver tissue. Therefore, as indicated in this report, the concentrations of lipophilic organic contaminants in muscle tissue tend to be less than those in liver tissue. Nevertheless, selection of muscle tissue (i.e., the edible portion of seafood) as a target tissue for monitoring programs may be important for human exposure assessments and quantitative health risk determinations. As indicated below, lipid normalization of tissue contaminant concentrations eliminates much of the variation in bioaccumulation data due to tissue type and should be incorporated in 301(h) monitoring.

The guidance provided for evaluation of bioaccumulation potential of 301(h) priority pollutants and pesticides is expected to result in well-designed monitoring studies that generate useful information needed to safeguard enviornmental and public health. This monitoring program information should also dispel many of the uncertainties and limitations noted above and provide a quantitative basis for re-evaluation of generalizations and guidelines provided herein.

BIOACCUMULATION OVERVIEW

Bioaccumulation is the overall process of biological uptake and retention of chemical contaminants obtained from food, water, contact with sediments, or any combination of exposure pathways. Factors important in determining bioaccumulation potential of a substance are environmental influences on

its bioavailability, physiological mechanisms of uptake and elimination, and chemical properties of the substance.

Processes of dispersion, sedimentation, physicochemical transformation, and biodegradation interact to render toxic substances more, or less, bioavailable than when first discharged. Toxic substances introduced into the marine environment through sewage outfalls are partitioned among water, suspended particulates, sediments, and biota. The effect of this partitioning is to provide numerous routes of exposure to benthic and pelagic organisms (Figure 1). Most organic and trace metal contaminants are associated primarily with the particulate phase of sewage effluent and are rapidly incorporated into sediments in the vicinity of the discharge (Morel and Schiff 1983). Therefore, benthic organisms (e.g., benthic infauna and demersal fishes) are most likely to accumulate contaminants because they are directly associated with the sediments.

Biological processes affecting contaminant bioaccumulation are membrane permeability and absorption, translocation from absorption sites to other tissues and organs, enzymatic transformations to metabolic daughter compounds, and excretion of either the untransformed contaminant or its metabolites. Once the contaminant is absorbed, the degree of contaminant bioaccumulation is largely determined by the efficiency of metabolic and excretory processes which may vary considerably among species. Because some contaminants are easily metabolized by certain species (e.g., PAH in fish), they do not usually accumulate in tissues of those species. However, rapidly metabolized substances may result in the bioactivation of highly toxic daughter compounds. Consequently, low body burden of easily metabolized substances does not necessarily indicate low potential hazard to either marine fauna or humans. Some metabolized substances (e.g., trace metals) may be sequestered in the organism because their solubility or ionization characteristics preclude active excretion. Finally, contaminants that are not easily metabolized (e.g., high molecular weight chlorinated compounds) tend to bioaccumlate in most species. In summary, bioaccumulation is a consequence of the physiological limitations inherent in an organism's ability to transform and excrete invading chemical substances. These limitations are often a direct reflection of the chemical properties of the accumulated substances.

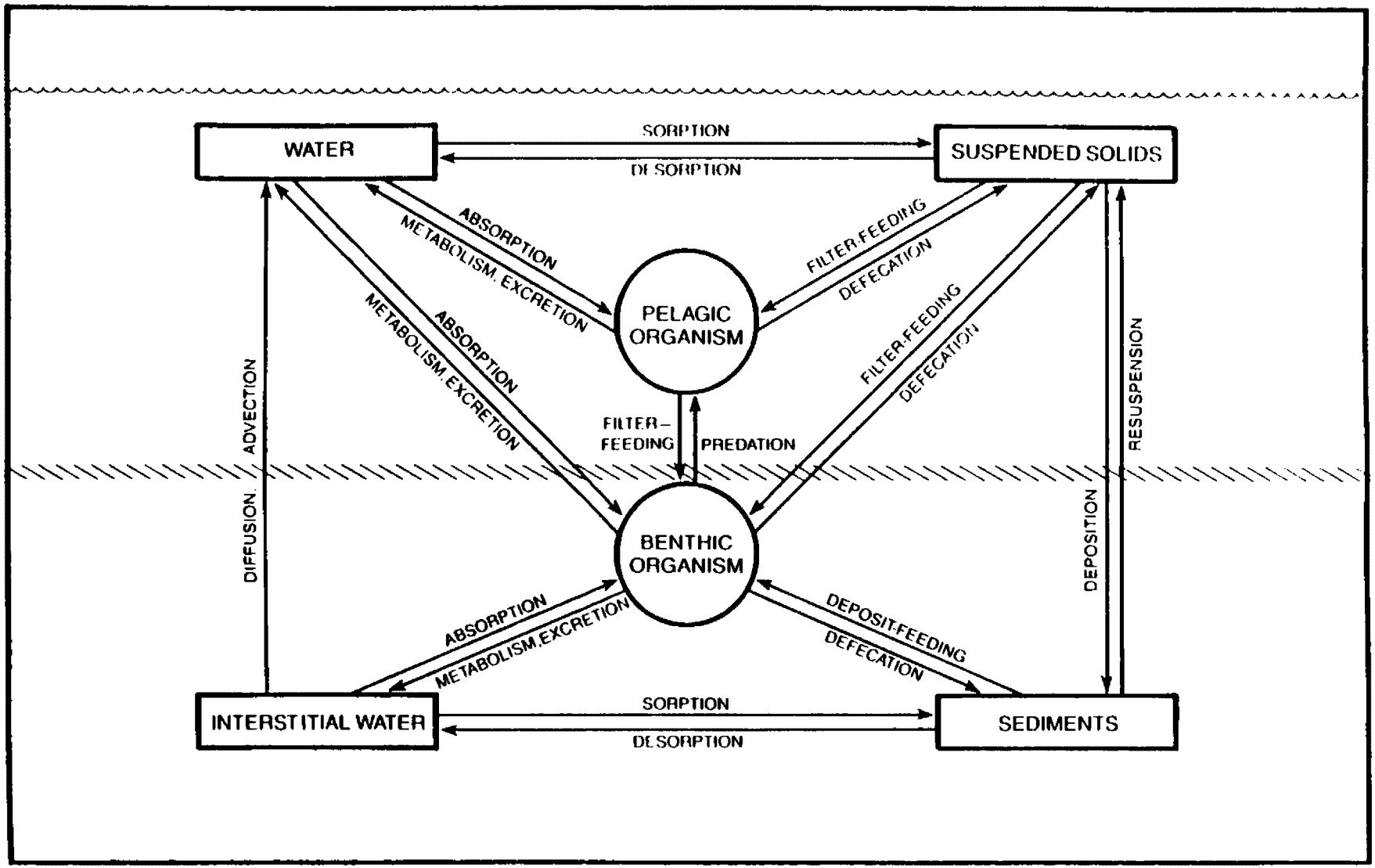


Figure 1. Environmental partitioning of chemical contaminants, and pathways of exposure for pelagic and benthic organisms.

Important chemical properties that affect both bioavailability and bioaccumulation of contaminants are hydrophobicity (i.e., lipophilicity), chemical structure (e.g., molecular size, steric configuration, degree and nature of chlorination), and ionization state (i.e., pK_a) at physiological and environmental pH. In general, non-ionized, hydrophobic substances are readily absorbed since they are relatively nonpolar and membrane-permeable. Hydrophobicity is also a key factor in determining soil sorption and sediment partitioning behavior of chemical contaminants. Thus, properties describing hydrophobicity and ionization state of chemical contaminants have often been used to develop predictive relationships between contaminant concentrations in various environmental media and their bioaccumulation in exposed organisms.

REVIEW OF PAST APPROACHES

Several approaches that have been used to estimate the bioaccumulation potential of toxic substances are evaluated in the sections below. Past approaches can be categorized as:

- Empirical measures of bioaccumulation and bioconcentration
- Structure-activity relationships
- Equilibrium-partitioning models
- Metabolic half-life and detoxification models.

The approaches vary in experimental sophistication and are not necessarily independent of one another. For example, understanding of metabolic half-life and detoxification is useful in determining bioconcentration factors (discussed below), particularly when contaminant concentrations in tissues have not reached equilibrium with exposure concentrations. Also structure-activity relationships are useful in predicting bioconcentration factors for some substances.

Empirical Measures of Bioaccumulation and Bioconcentration

Approaches to measure bioaccumulation of chemical substances may be categorized as simple laboratory two-compartment systems, laboratory multi-compartment systems, or field observations. All three approaches require direct measurement of tissue residues, but vary in the extent to which contaminant concentrations are measured in other environmental media. Tissue residue alone is not a convenient index of bioaccumulation potential because the effects of exposure concentration and metabolic efficiency are not considered. Marine and estuarine organisms can sequester, transform, mobilize, and eliminate many chemical contaminants. Effective transformation and elimination are homeostatically controlled, and will lead toward steady-state concentrations of toxic substances in tissues, assuming equilibrium in the partitioning of the substance among aqueous, particulate, and biotic phases (discussed in detail below). The physiological mechanisms necessary to achieve steady-state are described for many substances in simple two-compartment systems and have led to the development of bioconcentration factors (BCFs). Bioconcentration refers to steady-state bioaccumulation of chemicals from a specific medium, usually water (cf., Brungs and Mount 1978; Macek et al. 1979; U.S. EPA 1980; and Taylor 1983).

Two-Compartment Systems and Bioconcentration--

In two-compartment systems, a single species is exposed to a toxic substance dissolved in water at concentrations less than those that produce a chronic toxic effect. Under such conditions, many substances show first-order uptake and depuration kinetics such that tissue concentrations increase to a maximum over time and remain constant thereafter (i.e., are at steady-state). At steady-state, the relationship between tissue and water concentrations can be expressed according to the following equation (cf., Esser and Moser 1982; Connell and Miller 1984):

$$K_1 C_w = K_2 C_t$$

and

$$BCF = C_t/C_w = K_1/K_2 \quad (1)$$

where:

BCF = bioconcentration factor
K_1 = uptake rate from the surrounding medium
K_2 = depuration rate from exposed organism
C_w = contaminant concentration in water
C_t = tissue contaminant concentration in the exposed organism.

Equation (1) states that the bioconcentration factor (BCF) can be determined either from the ratio of contaminant concentration in tissue to that in water, or from the ratio of contaminant uptake rate to depuration rate. Determination of BCFs from steady-state tissue and water concentrations is the traditional approach to estimating bioaccumulation potential and was recommended by the U.S. EPA (1980) in development of water quality criteria.

The foremost limitation to this approach is the assumption of steady-state or equilibrium partitioning of contaminants. Because some bioaccumulated substances are not easily transformed or eliminated, their tissue concentrations may increase during exposure without ever reaching steady-state. In the past, the U.S. EPA (1980) indicated that BCFs may be calculated from tissue and water residues existing at the end of a 28-day exposure period if steady-state conditions were not met. Although this approach leads to consistent definitions of bioaccumulation potential for problematic substances, enormous variability in the accuracy of steady-state BCFs estimated by this approach may be encountered. In such circumstances, BCFs should be determined by measuring the kinetics of both uptake and depuration (Veith et al. 1979b, 1980; Bishop and Maki 1980; Kosian et al. 1981; Banerjee et al. 1984). However, this approach may prove experimentally difficult where substances equilibrate slowly or where the depuration rate is much smaller than the uptake rate. In the latter case, curvilinear models used in calculations of BCFs cannot be fit with any confidence (Kosian et al. 1981). In addition,

depuration may follow second-order rather than first-order kinetics, and causing slight variations in derived bioconcentration factors (Ellgehausen et al. 1980; Esser and Moser 1982). Inconsistency among methods of exposure (e.g., static equilibrium, flow-through equilibrium, kinetic, and pharmacokinetic methods) and calculation of results may also affect accuracy of BCFs. For instance, Kosian et al. (1981) found that numerous methods of measuring BCFs offered reasonable precision (i.e., were reproducible), but that different methods of calculating the final bioconcentration factor produced results differing by as much as a factor of three.

Multicompartment and Field Estimated-BCFs--

Methods to determine BCFs as an index of bioaccumulation potential have been extended to more complex multicompartment laboratory studies and field studies. However, there are many technical and interpretive difficulties associated with BCFs estimated from these kinds of studies. Hence, BCFs generated in multicompartment and field studies will be qualified as "estimated-BCFs" to distinguish them from those measured in more tightly controlled, and more theoretically tractable, two-compartment experimental systems.

In multicompartment systems, one or more species is exposed to one or more contaminants in sediments, water, or food (e.g., Augenfeld et al. 1982; Rubinstein et al. 1983). Multiple species exposures (e.g., Rubinstein et al. 1983) are designed to assess the bioavailability of contaminants partitioned among water, sediments, and several trophic levels of biota. In field studies, estimated BCFs are determined from measurements of contaminant concentrations in tissues of natural or caged populations of organisms and ambient contaminant concentrations in all environmental media of water, sediments, and food (Mackay 1982; U.S. EPA 1980). The two major problems encountered in deriving estimated BCFs from these types of studies are 1) satisfying assumptions of steady-state and equilibrium partitioning and 2) integrating the relative contributions of various exposure media (i.e., food, water, and sediments) to total body burden.

Steady-state conditions in laboratory multicompartment systems may be verified empirically as they are in the two-compartment systems. Steady-state conditions for field-collected specimens are difficult to quantify. When field observations or field experiments are used to determine estimated BCFs, it is assumed that the concentration of the contaminant is constant over both time and the range of the organism. However, spatial gradients in contaminant concentrations are typical of discharges and these assumptions are difficult to verify, except perhaps in massively contaminated areas or for caging experiments. An additional assumption is that steady-state concentrations of tissue residues may be approximated for the relatively short time intervals over which a bioaccumulation study is conducted (U.S. EPA 1980). Again, this assumption is difficult to verify and may be valid for only those species that are either sedentary (e.g., bivalves) or show extreme diel and seasonal stability in migratory behavior.

Assuming that steady-state conditions are reasonably approximated in multicompartment and field studies, determination of bioaccumulation potential from estimated-BCFs remains problematic. Estimated-BCFs determined from the ratio of contaminant concentration in tissues to that in water vary considerably from those determined in simple laboratory two-compartment systems. For a given contaminant concentration in water, tissue residues derived from all media in field studies may be higher than those derived from water alone in laboratory studies (cf., Thomann and Connolly 1984). Although water may be the dominant route of exposure for some organisms in nature, additional uncertainty exists regarding bioavailability of contaminants partitioned among microparticulate, colloidal, and aquaeous phases of natural waters (cf., Carter and Suffet 1982; Chiou et al. 1984; Gschwemd and Wu 1985).

Although multicompartment and field estimated-BCFs present certain technical and interpretive difficulties in comparison with two compartment systems, they nevertheless provide meaningful information regarding bioaccumulation potential of chemical contaminants. In two-compartment experiments, the principal exposure route is through the integument or respiratory surfaces, and not through ingestion of food or contact with sediments. However, many studies indicate the relative importance of uptake from sediments

or food in the field (Karickhoff et al. 1979; Genest and Hatch 1981; Morel and Schiff 1983; McFarland 1983). Multicompartment systems offer a means to assess the relative contributions of various exposure pathways. However, they are experimentally complex and not conducted routinely to estimate bioconcentration of individual substances. Multicompartment systems containing more than one contaminant are further limited because synergism and antagonism of the test substances are difficult to document and may therefore confound attempts to develop indices of bioaccumulation potential (cf., Brown et al. 1984c,d). Thus, in development of guidelines for water quality criteria, the U.S. EPA (1980) recommended discarding bioaccumulation data that were based on exposure to "formulated" mixtures.

Estimated-BCFs derived from field studies require extensive spatial and temporal characterization of contaminated organisms and the habitat from which they are collected. Therefore, field-estimated BCFs are more time-consuming and less controlled than are those derived from laboratory experiments. They require monitoring or historical documentation of the type and extent of contamination, and may be confounded by the presence of interacting and possibly synergistic substances. Nevertheless, properly conducted field studies provide a more realistic assessment of actual bioaccumulation of contaminants because they integrate the effects of environmental partitioning and multiple routes of exposure. Schnoor (1982) found that field estimated-BCFs for five priority pollutants and their metabolites (aldrin and dieldrin; DDT, DDE, DDD; PCBs; chlordane; and heptachlor) measured in lipids of freshwater fishes exceeded the laboratory BCFs for the same substances by a factor of 1-4. When estimated-BCF values from field experiments are consistently higher or lower than those from laboratory studies, U.S. EPA (1980) recommended that only field-derived values be used in the development of water quality criteria.

Summary--

In summary, there are three principal approaches to empirical determination of bioaccumulation potential. The approaches vary in experimental complexity from controlled two-compartment laboratory systems to highly variable field studies. Bioconcentration factors as an indices of bioaccumulation potential

may be estimated from data generated in each type of approach. However, experimental complexities, uncertainties regarding actual exposure concentrations, and difficulties in verifying steady-state tissue residues indicate that estimated-BCFs generated in multicompartment and field studies may vary considerably in comparison with BCFs generated in well-controlled, two-compartment studies. Although estimated-BCFs in field studies may exceed laboratory values by a factor of 4, they integrate the effects of numerous routes of exposure and provide a realistic assessment of bioaccumulation potential. A final major limitation to empirical measurements of bioaccumulation is the time required to determine bioconcentration factors for thousands of potential chemical contaminants. Therefore, most laboratory investigations of bioaccumulation potential focus on predictive relationships between bioconcentration factors and the chemical properties of various classes of contaminants.

Structure-Activity Relationships

In structure-activity relationships, bioconcentration and toxic effects are predicted from the physicochemical properties of organic substances (Hopfinger et al. 1981), particularly their electronic, steric, and hydrophobic properties (Hansch and Leo 1979). Hydrophobicity is perhaps the most important property with respect to biological uptake and concentration of substances, but not necessarily with respect to specific toxic activity. A practical model system measuring hydrophobic partitioning of a substance between octanol and water was developed to quantitatively predict partitioning among polar and nonpolar (i.e., principally lipids) biological compartments (Leo 1981). The model predicts that equilibrial partitioning of nonionic organic contaminants between biota and water will be proportional to the octanol-water partition coefficient, which is defined as:

$$K_{ow} = C_o/C_w$$

where:

K_{ow} = the partition coefficient
C_o = chemical concentration in n-octanol
C_w = chemical concentration in water.

There are many limitations to use of the octanol-water partitioning model for predicting bioaccumulation of organic compounds. First, the octanol-water partition coefficient (K_{ow}) measures only the hydrophobicity of a chemical compound and therefore ignores other properties that may affect bioaccumulation of a substance (e.g., latent heat of solution, hydrolysis, ionization, and vapor pressure). Also, there are numerous techniques (e.g., shake flask, HPLC, TLC, solubility) for measurement of K_{ow}, each of which has its particular set of advantages, problems, and limitations (Esser and Moser 1982). Measured K_{ow} values may be affected by impurities, temperature, pH, low solubility, volatility, and degree of ionization. However, log K_{ow} can be closely approximated from chemical properties of the molecule (Hansch and Leo 1979).

Application of the log K_{ow} model to partitioning of chemical contaminants between the aquatic environment and fish tissues was initially described by Neely et al. (1974), further developed by Veith et al. (1979b, 1980), and embellished by Mackay (1982). Veith et al. (1980) showed that the log of the bioconcentration factor for 84 organic compounds in three species of freshwater fishes is a linear function of log K_{ow}, as approximated by the regression function:

$$\log BCF = 0.76 \log K_{ow} - 0.23 \quad (R=0.907, P<0.001, N=84) \qquad (2)$$

This relationship agrees with Veith et al.'s (1979b) earlier equation, which was used by the U.S. EPA (1980) to predict BCFs for which there were no empirical values.

Although the log K_{ow} vs. log BCF model as developed by Veith et al. (1980) is based on 84 substances representing 18 classes of priority pollutants, there are several limitations. First, the model is based on a two-compartment

experimental approach, which limits assessment to organic substances dissolved in water. Second, the model assumes that bioconcentration of organic substances is dependent on tissue lipid content, although other nonpolar molecular components may affect uptake. It is widely recognized that lipid content of experimental organisms affects bioconcentration of organic substances. However, the regression function described above uses empirically determined bioconcentration factors that are not normalized to percent lipids. Schnoor (1982) showed that lipid normalization eliminated 60 to 90 percent of the variance of of estimated-BCFs measured in four species of freshwater fishes. In practice, lipid content of tissues is rarely measured in conjunction with determination of BCFs, although it is often estimated from values reported in the literature. Furthermore, qualitative differences in lipid content among organisms may affect bioaccumulation but are not well studied (Varanassi and Malins 1977; Phillips 1980; Brown et al. 1982, 1983). Nevertheless, properly designed bioaccumulation studies should measure both organic contaminant tissue residues and tissue lipid concentrations and should express data in units of contaminant concentration per gram of lipid.

For unknown reasons, some substances such as hexachloropentadiene may have low bioconcentration factors despite comparatively large K_{ow} values (Veith et al. 1979b). Log K_{ow} estimated BCFs for polycyclic aromatic hydrocarbons (PAH) may also be overestimated because they are partitioned almost exclusively into the particulate phase, require an extremely long time to reach steady-state with biological tissues, and are rapidly metabolized by many aquatic organisms. Also, cell membranes may be relatively impermeable to high molecular weight PAH (Mackay 1982; Connell and Miller 1984). Similarly, PCB-1260 has a high log K_{ow} (6.91) that may overestimate log BCF because of poor membrane permeability brought about by its steric configuration (Connell and Miller 1984; Shaw and Connell 1984). Other substances such as 301(h) organophosphate pesticides have K_{ow} values that range from 1.93 to 3.81, but have a low bioaccumulation potential because they are rapidly degraded and easily metabolized (Brown 1978). Finally, field estimated BCFs based on lipid normalized data may be four times greater than those predicted by log K_{ow} values when the principal route of exposure is through the food rather than water (Thomann and Conolly 1984).

In summary, log K_{ow} values provide an order of magnitude estimate of bioaccumulation potential of organic substances. Numerous factors contribute to this range of variation, including: properties of chemical contaminants, analytical methods, experimental conditions, and biological variability of experimental organisms (Esser and Moser 1982).

Equilibrium Partitioning Models

Kenaga and Goring (1980) attempted to quantify the effects of environmental partitioning of organic substances on bioavailability in order to arrive at a more realistic assessment of bioaccumulation potential. They examined the relationships among water solubility, soil sorption, octanol-water partitioning, and concentrations of chemicals in biota. Data summarized from the literature for 170 chemicals showed significant correlations among the logarithms of water solubility, K_{ow}, BCFs, and soil sorption coefficients normalized to percent organic carbon (K_{oc}), principally for freshwater fishes. Note that K_{oc} values may be derived empirically in the same fashion as K_{ow}:

$$K_{oc} = C_{soc}/C_w$$

where:

K_{oc} = The organic carbon soil sorption partition coefficient
C_{soc} = Equilibrial contaminant concentration in sediment organic carbon
C_w = Equilibrial contaminant concentration in water.

Soil sorption coefficients and K_{oc} values can also be derived theroetically from the chemical potential (i.e., fugacity) of nonideal solutes at thermodynamic equlibrium (cf., Mackay 1982; Karickhoff 1984; Connell and Miller 1984 for detailed discussion of this approach).

In general log BCF, log K_{ow}, and log K_{oc} are inversely proportional to the log of water solubility, whereas log BCF and log K_{oc} are directly proportional to log K_{ow}. Kenaga and Goring (1980) concluded that K_{oc} seemed

to be the best predictor of the other parameters, and that BCF and K_{ow} are key indicators for the behavior of chemicals in the environment. However, recent advances in measurement, calculation, and development of a computerized database of octanol-water partition coefficients make K_{ow} useful in predicting both K_{oc} and bioaccumulation potential (Hansch and Leo 1979; Veith et al. 1979a; Leo, A., 20 November 1984, personal communication).

Kenaga and Goring's (1980) review has provided the impetus for recent research into estimating bioaccumulation potential of chemicals present in sediments. The hypothesis is that bioconcentration of hydrophobic chemicals from sediments into organisms can be predicted on the basis of equilibrium partitioning among sediments, water, and biota. The major assumptions (McFarland 1983; Karickhoff, S., 20 November 1984, personal communication) to this approach are that:

- Maximum bioconcentration potential is reached when all three compartments are at thermodynamic equilibrium
- The solubilities of organic contaminants in organic carbon of sediments are about equal to their solubilities in organic carbon or lipid of tissues
- Equilibrium concentrations in sediments and tissues will be approximately equal if normalized to organic carbon or lipid content
- Concentrations in the water phase affect rates of uptake but are unnecessary to determine partitioning of substances between sediments and tissues under equilibrium conditions.

The obvious limitation to this approach is that equilibrium conditions are unlikely in natural environments because of the dynamics of both physical and biological processes. For instance, Connor (1983) has shown that the ratio of the PCB concentration in fish tissues to that in marine sediments from a number of locations is proportional to flushing time. Also, rates

of uptake from sediments may be profoundly affected by ingestion of sediments or sediment-associated prey by benthic or bottom-feeding organisms.

Other biological factors that may affect the equilibrium partitioning approach include:

- Improbable routes of exposure (e.g., exposure of pelagic fishes to contaminated sediments)
- Limited time of exposure due to the mobility of exposed organisms
- Metabolic pathways that quickly mobilize and eliminate contaminants
- Growth and age of exposed organisms (e.g., weight-specific uptake of contaminated food may be much less for older individuals than for younger faster-growing individuals within a species)
- Unusual periods of lipid utilization and consequent concentration of toxic substances in the remaining lipid pool (Karickhoff, S., 20 November 1984, personal communication).

In summary, equilibrium partitioning of nonionic chemical substances among water, sediments, and biota at thermodynamic equilibrium may provide an indication of maximum bioaccumulation potential (McFarland 1983). However, this approach is highly theoretical at present and requires empirical substantiation (Karickhoff, S., 20 November 1984, personal communication). Nevertheless, it provides a framework for unifying environmental partitioning, biological uptake, and chemical variables that affect bioaccumulation of nonionic organic contaminants. It also indicates the importance of normalizing tissue residue data to lipid content and of normalizing sediment residue data to organic carbon content.

Metabolism and Detoxification Models

Two approaches have been used to assess the role of metabolism in bioconcentration of organic and trace metal contaminants. The first is an index of depuration of a substance, which measures declining tissue concentrations of a contaminant following removal of the exposed organisms to a clean, contaminant-free environment. The metabolic half-life, the amount of time required for tissue burdens of a parent compound to decline by 50 percent, is calculated from experimental data in order to arrive at a measure of biological persistence of the parent compound. This approach is subject to many of the same limitations as the kinetic approach for calculating bioconcentration factors. Calculation of metabolic half-life may be further hampered by a multiphasic decline in tissue concentrations (Bryan 1976; Hardy and Roesijadi 1982). In addition, the half-life approach does not consider toxic potential and persistence of daughter compounds of organic contaminants, or of various bound forms of trace metals. The rates of accumulation, the metabolic conversion of accumulated substances, and the relative proportions of intermediate metabolites can vary among closely related species (Frazier and George 1983; Reichert et al. 1985). Furthermore, there is a great deal of variation in the capacity of marine organisms to produce mixed function oxidases (MFOs) required to metabolize organic contaminants. Malins et al. (1979) reviewed metabolism of aromatic hydrocarbons in marine organisms and reported a 600-fold variation in enzymatic activity among various species of teleosts. Finally, determination of metabolic half-life may be subject to enormous variation because of the variety of metabolic compartments involved in storage and elimination of contaminants and their relative importance under different exposure conditions (George 1982).

Despite such limitations, metabolic half-life has been used as an index of depuration for both organic substances and trace metals. Veith et al. (1980) reported tissue half-life for 25 organic contaminants in bluegill sunfish (Lepomis macrochirus). Half-lives ranged from less than 1 day for 15 of the compounds to more than 7 days for acrolein. In general, metals appeared to be more persistent than organic contaminants. Bryan (1976) reviewed biological half-lives of some radio-labelled trace metals

[mercury(II), methylmercury, mercury-protein complex, zinc, and manganese] in a variety of marine and estuarine organisms. Half-lives ranged from 11 days for manganese in the lobster Homarus gammarus to 1,200 days for methyl-mercury in the flounder Platichthys flesus.

The second approach to assessing the role of metabolism in bioaccumulation is to measure saturation of detoxification pathways for both organic and trace metal contaminants. Brown et al. (1984a) proposed that partitioning of contaminants between intracellular sites of detoxification and toxic action could provide an index of the accumulative capacity of an organism. Both metals and organic contaminants were measured in the high molecular weight (>20,000 daltons) enzyme-containing, medium molecular weight (3,000-20,000 daltons) metallothionein-containing, and low molecular weight (<3,000 daltons) glutathione fractions of cytosol obtained from a variety of marine fishes and invertebrates. Appearance of organic contaminants in either the enzyme-containing or metallothionein fractions indicates that bioaccumulation has exceeded normal metabolic capabilities of the MFO-glutathione system (Brown et al. 1984a,b,c). Similarly, appearance of trace metal contaminants in either the enzyme-containing or glutathione fraction indicates that bioaccumulation has exceeded normal metabolic capabilities of the metallothionein and lysosomal-vacuolar systems (George 1982; Jenkins et al. 1982; Brown et al. 1984a,b,c). Using this approach, Brown et al. (1984a) indicated that Dover sole (Microstomus pacificus) with fin erosion contained a greater proportion of oxygenated metabolites of DDT in enzyme-containing and metallothionein pools than did conspecifics without fin erosion. According to Brown et al. (1984a), these results suggest that high concentrations of DDT metabolites in cytosolic pools other than the low molecular weight glutathione fraction are related to toxic pathological effects such as fin erosion lesions in fishes. Other studies of the cytosol distribution of organic and trace metal contaminants have shown that high levels of exposure to organic contaminants may interfere with normal trace metal metabolism (Brown et al. 1984d; in press).

The approach of Brown et al. (1984c) may not be as widely applicable to marine organisms as originally hypothesized. Frazier and George (1983) reported a wide range in concentrations of cadmium-induced metallothionein-

like protein in two species of oysters (Crassostrea gigas and Ostrea edulis). Also, induction of the metallothionein-like protein in O. edulis was dependent on geographic location of the sample population. A further limitation to this recent approach is that it has not been assessed for the wide range of compounds needed to develop predictive relationships.

EMPIRICAL BCF VS. K_{ow} MODEL FOR MARINE ORGANISMS

The foregoing review of past approaches to assessing the bioaccumulation potential of chemical contaminants indicates that log K_{ow} values may provide a quantitative index for determining the rank order of bioaccumulation potential of organic contaminants in marine and estuarine organisms. However, previous workers have developed log K_{ow} (octanol-water partition coefficent) vs. log BCF (bioconcentration factor) models primarily for freshwater and marine species combined or for freshwater species only. Davies and Dobbs (1984) suggested that empirically derived BCFs for saltwater species are lower than those for freshwater species. Thus, previous models (e.g., Veith et al. 1979b, 1980) may not be applicable to the marine environment. In this section, empirical relationships between log K_{ow} and log BCF are examined for marine and estuarine organisms.

The U.S. EPA (1980) collected, reviewed, and screened available data on bioconcentration factors for priority pollutants. Both freshwater and saltwater organisms were used in development of U.S. EPA's (1980) Water Quality Criteria. For the purposes of this review, empirical bioconcentration factors for saltwater organisms that met U.S. EPA's screening criteria were tabulated for four major animal taxa: polychaetes, molluscs, crustaceans, and fishes. A computer search of Oceanic Abstracts, NTIS, BIOSIS, and Enviroline abstracting services was then conducted for additional new information concerning bioconcentration factors published since 1979. The data characteristics used to select recently published BCF values were adapted from the procedures established in the Water Quality Criteria Guidelines (U.S. EPA 1980). Data were rejected according to the following guidelines:

- Species were not resident in marine or estuarine waters of North America

- Inappropriate taxa: Only BCFs for polychaetes, molluscs, crustaceans, and fishes were accepted

- Unpublished report: Data in letters, memos, or personal communications were unacceptable

- Inadequate controls were used in either field studies or lab experiments

- Signs of stress, disease, or mortality in experimental organisms were apparent

- Chemical substances examined were formulated mixtures or emulsifiable concentrates

- Steady-state was not obtained, experiment was shorter than 28 days, or inappropriate kinetic model was used to determine bioconcentration factor.

Results of this review show that empirically determined BCFs for marine and estuarine organisms are available for 14 organic substances and 9 trace metals on the priority pollutant list (Appendix A). These data are based on 24 studies of 44 species of polychaetes, molluscs, crustaceans, and fishes (Table 1). Most of the U.S. EPA (1980) Water Quality Criteria for marine and estuarine organisms are based on extrapolation from BCF measurements on freshwater organisms or on structure-activity models that are based primarily on freshwater studies. Note that the existing model used by U.S. EPA to predict bioconcentration factors from octanol-water partition coefficients is based on carefully controlled studies of freshwater fishes conducted by a single investigator (Veith et al. 1979a,b; 1980) and on a wide range of contaminants, many of which are not priority pollutants.

To derive a K_{ow}-BCF model for marine and estuarine organisms, the geometric mean of the log BCF values for each of the 14 priority pollutant compounds summarized in Appendix A was plotted against the log K_{ow} value

TABLE 1. SUMMARY OF INFORMATION ON BIOCONCENTRATION FACTORS FOR PRIORITY POLLUTANTS IN MARINE AND ESTUARINE ORGANISMS AS MODIFIED FROM U.S. EPA (1980) WATER QUALITY CRITERIA DOCUMENTS AND ADDITIONAL INFORMATION PUBLISHED FROM JANUARY, 1980, TO AUGUST, 1984

Structural Compound Class	PP#	Pollutant	Number of Species Tested (studies) Polychaetes	Crustaceans	Molluscs	Fishes	Total
Substituted Phenols	64	pentachlorophenol	1 (1)	0	2 (3)	1 (2)	4 (6)
Low Molecular Weight Aromatic Hydrocarbons	55	naphthalene	0	1 (1)	0	0	1 (1)
High Molecular Weight PAH	73	benzo(a)pyrene	0	0	1 (4)	0	1 (4)
Chlorinated Aromatic Hydrocarbons	8	1,2,4-trichlorobenzene	0	0	1 (1)	0	1 (1)
	9	hexachlorobenzene	0	0	0	2 (2)	2 (2)
PCBs	107	PCB-1254	2 (2)	2 (3)	2 (3)	2 (2)	8 (10)
	112	PCB-1016	0	0	1 (1)	2 (5)	3 (5)
Pesticides	90	dieldrin	0	1 (1)	1 (1)	2 (2)	4 (4)
	91	chlordane	0	0	0	1 (2)	1 (2)
	92	DDT (a)	0	2 (3)	2 (3)	9 (17)	13 (23)
	95	endosulfan (b)	0	0	0	2 (3)	2 (3)
	98	endrin	0	1 (2)	1 (1)	2 (4)	4 (7)
	100	heptachlor	0	0	0	2 (3)	2 (3)
	113	toxaphene	0	0	1 (1)	2 (6)	3 (7)
Metals	115	arsenic	0	0	1 (1)	0	1 (1)
	118	cadmium	1 (1)	5 (7)	6 (9)	0	12 (17)
	119	chromium	1 (1)	0	3 (5)	0	4 (4)
	120	copper	5 (5)	1 (1)	6 (11)	0	12 (17)
	122	lead	0	0	4 (10)	0	4 (10)
	123	mercury	1 (1)	1 (1)	2 (5)	0	4 (7)
	124	nickel	0	0	3 (5)	0	3 (5)
	127	thallium	0	0	2 (2)	0	2 (2)
	128	zinc	1 (1)	1 (1)	4 (7)	0	6 (9)
		Summary (c)	9 (7)	10 (10)	8 (19)	17 (11)	44 (24)

a Includes DDT, DDD, and DDE.

b Includes alpha-endosulfan, beta-endosulfan, and endosulfan sulfate.

c Number of species (number of substances).

derived from the literature (Table 2). Correlation analysis indicated a poor fit of the linear regression model to these data ($R=0.243$, $P>0.05$, $N=14$). Part of the reason for the poor correlation may be that the data collected were biased towards high log K_{ow} values, in the range of 3.25 to 6.5. Also, it should be noted that empirically derived BCFs for 4 of the 14 substances deviated by more than an order of magnitude from those predicted by Veith et al. (1980) (Figure 2). Bioconcentration of naphthalene and toxaphene were much higher than predicted, whereas bioconcentration of pentachlorophenol and benzo(a)pyrene were much lower than predicted. Plots of log BCF vs. log K_{ow} for two of the major taxa (fishes and molluscs) considered individually indicated a similar lack of agreement, with correlation coefficients less than 0.5 in each case. However, BCFs for fish correlated with those for molluscs ($R=0.89$, $P<0.05$, $N=7$). In contrast to these results, Zaroogian et al. (1985) found that freshwater models of the log K_{ow} vs. log BCF relationship provide a reasonable order-of-magnitude estimate of bioconcentration factors in marine species. Their review focused on laboratory studies of marine fishes [the sheepshead minnow (Cyprinodon variegatus) and the pinfish (Lagodon rhomboides)] and two species of bivalves [mussels (Mytilus edulis) and oysters (Crassostrea virginica)], and considered a range of 15 priority pollutant and 6 non-priority pollutant compounds. The fact that the present review includes BCFs derived from a greater diversity of organisms (molluscs, crustaceans, polychaetes, and fishes) that were studied under field as well as laboratory conditions may explain conflicting results between the present analyses and those of Zaroogian et al. (1985). These discrepancies indicate the need for a single study to characterize bioaccumulation of a range of priority pollutants in marine organisms under natural conditions. Consequently, remaining sections of this report focus on recent field studies that quantify the relationship between log K_{ow} and bioaccumulation of organic contaminants in marine and estuarine fauna.

ESTIMATION OF BIOACCUMULATION POTENTIAL FROM FIELD STUDIES

The Palos Verdes Shelf in southern California is perhaps one of the best studied systems with respect to compartmental characterization of chemical contaminants in the vicinity of a sewage discharge into marine waters. Gossett et al. (1983b) measured contaminant concentrations in

TABLE 2. OCTANOL-WATER PARTITION COEFFICIENTS (K_{OW}) FOR PRIORITY POLLUTANTS AND 301(h) PESTICIDES AS MODIFIED FROM CALLAHAN ET AL. (1979)

PP#	Pollutant	log(Kow)
	Phenols	
65	phenol	1.46 a
34	2,4-dimethylphenol	2.42 b
	Substituted Phenols	
21	2,4,6-trichlorophenol	3.69 c
22	para-chloro-meta cresol	1.10 a
24	2-chlorophenol	2.16 b
31	2,4-dichlorophenol	3.08 a
57	2-nitrophenol	1.77
58	4-nitrophenol	2.91 d
59	2,4-dinitrophenol	1.53
60	4,6-dinitro-o-cresol	2.85
64	pentachlorophenol	5.00 d
	Organonitrogen Compounds	
5	benzidine	1.81 g
28	3,3'-dichlorobenzidine	3.02
35	2,4-dinitrotoluene	2.00
36	2,6-dinitrotoluene	2.00
37	1,2-diphenylhydrazine	2.94 g
56	nitrobenzene	1.83 b
61	N-nitrosodimethylamine	-0.58 g
62	N-nitrosodiphenylamine	3.13 b
63	N-nitrosodipropylamine	1.31
	Low Molecular Weight Aromatic Hydrocarbons	
1	acenaphthene	3.92 b
55	naphthalene	3.59 d
77	acenaphthylene	4.08
78	anthracene	4.34 d
81	phenanthrene	4.46 d
80	fluorene	4.38 d
	High Molecular Weight PAH	
39	fluoranthene	5.53
74	benzo(a)anthracene	5.61 d
73	benzo(a)pyrene	6.00
74	benzo(b)fluoranthene	6.60
75	benzo(k)fluoranthene	6.85
76	chrysene	5.60
79	benzo(ghi)perylene	7.00
82	dibenzo(a,h)anthracene	6.00
83	indeno(1,2,3-cd)pyrene	7.70
84	pyrene	4.88 e
	Chlorinated Aromatic Hydrocarbons	
8	1,2,4-trichlorobenzene	4.23 d
9	hexachlorobenzene	5.23 d
2[illegible]	2-chloronaphthalene	4.72 g
25	1,2-dichlorobenzene	3.40 b
26	1,3-dichlorobenzene	3.44 b
27	1,4-dichlorobenzene	3.53 d

PP#	Pollutant	log(Kow)
	Chlorinated Aliphatic Hydrocarbons	
52	hexachlorobutadiene	4.78 f
12	hexachloroethane	3.93 b
53	hexachlorocyclopentadiene	5.31 d
	Haloyenated Ethers	
18	bis(2-chloroethyl)ether	1.12 b
40	4-chlorophenyl phenyl ether	4.92 g
41	4-bromophenyl phenyl ether	5.08 g
42	bis(2-chloroisopropyl)ether	2.58 g
43	bis(2-chloroethoxy)methane	1.26 g
	Phthalates	
66	bis(2-ethylhexyl)phthalate	4.20 d
67	butyl benzyl phthalate	4.05 b
68	di-n-butyl phthalate	5.15 a
69	di-n-octyl phthalate	9.20
70	diethyl phthalate	1.40 b
71	dimethyl phthalate	1.61 b
	PCB's	
106	PCB-1242	6.00 a
107	PCB-1254	6.48 a
108	PCB-1221	4.00
109	PCB-1232	4.48
110	PCB-1248	6.11 d
111	PCB-1260	6.91 d
112	PCB-1016	5.88 d
	Miscellaneous Oxyyenated Compounds	
129	TCDD (dioxin)	6.10 i
54	isophorone	1.67 b
	Pesticides	
89	aldrin	3.00 c
90	dieldrin	5.48 d
91	chlordane	6.00 d
92	4,4'-DDT	5.75 d
93	4,4'-DDE	5.69 d
94	4,4'-DDD	6.00 d
95	alpha-endosulfan	3.60
96	beta-endosulfan	3.60
97	endosulfan sulfate	3.60
98	endrin	4.56 d
99	endrin aldehyde	5.60
100	heptachlor	5.45 d
101	heptachlor epoxide	5.40 d
102	alpha-hexachlorocyclohexane	3.85 h
103	beta-hexachlorocyclohexane	3.85 h
104	delta-hexachlorocyclohexane	3.85 h
105	gamma-hexachlorocyclohexane	3.85 d

TABLE 2. (Continued)

PP#	Pollutant	log(Kow)
	Pesticides continued	
113	toxaphene	3.30
--j	mirex	6.89 b
--j	methoxychlor	4.30 b
--k	parathion	3.81 e
--k	malathion	2.89 e
--k	guthion	2.18
--k	demeton	1.93
	Volatile Halogenated Alkanes	
6	tetrachloromethane	2.64 d
10	1,2-dichloroethane	1.45 b
11	1,1,1-trichloroethane	2.47 b
13	1,1-dichloroethane	1.78
14	1,1,2-trichloroethane	2.18
15	1,1,2,2-tetrachloroethane	2.39 b
16	chloroethane	1.54
23	chloroform	1.90 b
32	1,2-dichloropropane	2.28
44	dichloromethane	1.30
45	chloromethane	0.90
46	bromomethane	1.00
47	bromoform	2.30
48	dichlorobromomethane	1.88
51	chlorodibromomethane	2.08
49	fluorotrichloromethane (Removed)	3.53 c
50	dichlorodiflouromethane (Removed)	2.16 c
	Volatile Halogenated Alkenes	
29	1,1-dichloroethylene	1.48
30	1,2-trans-dichloroethylene	1.97 c
33	trans-1,3-dichloropropene	1.98
	cis-1,3-dichloropropene	1.98
85	tetrachloroethene	2.88 d
87	trichloroethene	2.42 b
88	vinyl chloride	0.60
	Volatile Aromatic Hydrocarbons	
4	benzene	2.11 d
38	ethylbenzene	3.15
86	toluene	2.21 b
	Volatile Chlorinated Aromatic Hydrocarbons	
7	chlorobenzene	3.79 c
	Volatile Unsaturated Carbonyl Compounds	
2	acrolein	0.90 b
3	acrylonitrile	1.23 b
	Volatile Ethers	
19	2-chloroethylvinylether	1.28 g
	Metals	
114	antimony	NA
115	arsenic	NA
117	beryllium	NA
118	cadmium	NA
119	chromium (trivalent)	NA
119	chromium (hexavalent)	NA
120	copper	NA
122	lead	NA
123	mercury	NA
123	methylmercury	NA
123	phenylmercury	NA
123	mercuric acetate	NA
124	nickel	NA
125	selenium	NA
126	silver	NA
127	thallium	NA
128	zinc	NA
	Miscellaneous	
121	cyanide	NA
116	asbestos	NA

a Veith et al. 1979a.

b Veith et al. 1980.

c Gossett et al. 1983.

d Veith et al. 1979b.

e Kenaga and Goring 1980.

f Leo, A., 20 November 1984, personal communication.

g U.S. EPA (1980).

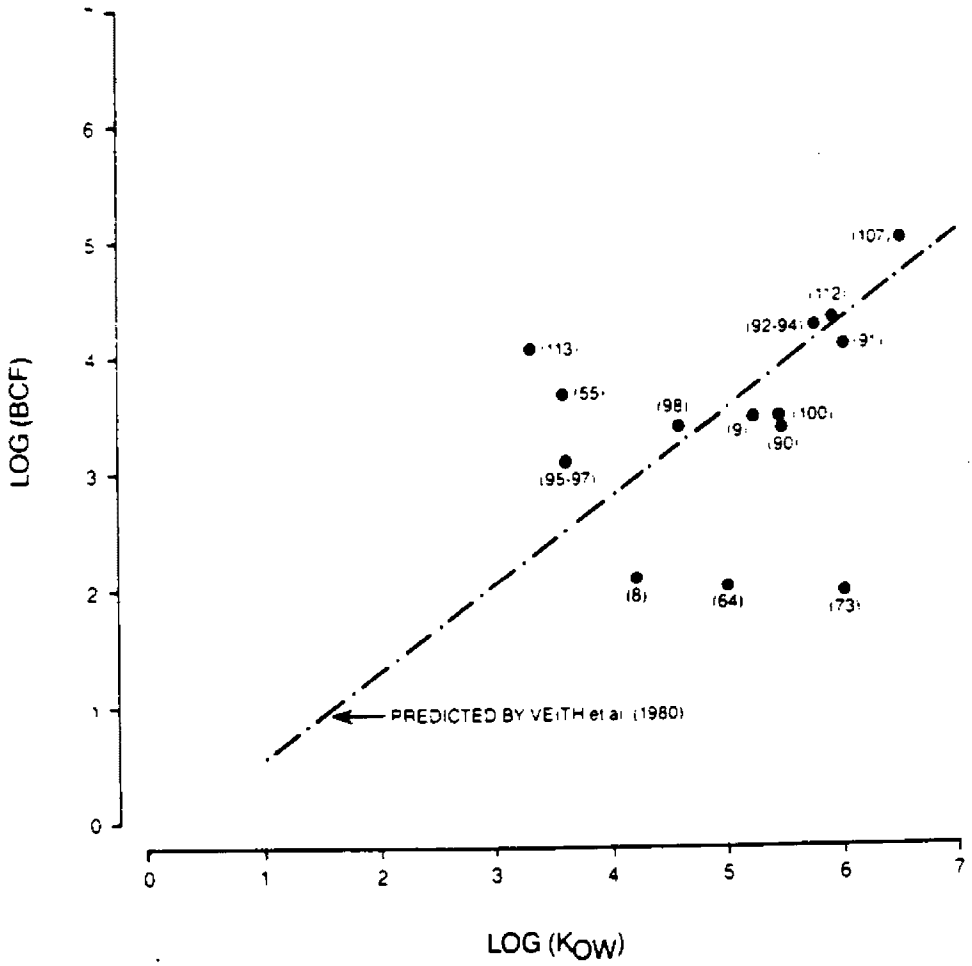
h Solubilities of the various isomers of HCH indicate that they will have similar log(Kow) values.

i Estimated according to the procedure described by Chiou et al. (1982).

j Chlorinated 301(h) pesticides that are not on the priority pollutant list.

k Organophosphorus 301(h) pesticides that are not on the priority pollutant list.

NA = not applicable.



Note: Priority pollutant number in parenthesis. See Appendix B for a key to priority pollutant numbers.

Figure 2. Bioconcentration factors for priority pollutants in marine and estuarine organisms vs. octanol-water partition coefficients.

sewage effluent, fish liver tissues, and sediments. Data from this study were used in this review to develop a predictive relationship between field bioaccumulation and octanol-water partition coefficients for the following reasons:

- The study was conducted on samples collected in the vicinity of a marine discharge and therefore circumvented possible artifacts inherent in the octanol-water model developed for freshwater fishes in the laboratory.

- Concentrations of contaminants in effluent are based on both the aqueous and particulate phases of the sample. Therefore, liver-effluent estimated-BCFs represent the three major compartments of water, particulates, and biota discussed in the equilibrium partitioning approach to bioaccumulation.

- The study has an extensive database, with 27 contaminants (22 of which are priority pollutants) analyzed in effluent, sediment, and tissue samples collected concurrently.

- The investigation was conducted in an area about 6 km (3.7 mi) northwest of the Whites Point outfall, where the level of contamination of surficial sediments in recent years appears to have been relatively constant both temporally and spatially (Tetra Tech 1984; Gossett, R.W., 24 September 1984, personal communication).

- Lipid content of liver tissues was measured and thereby permits lipid normalization of calculated bioconcentration factors.

- The study focused on demersal or benthic-feeding fishes: California halibut (Paralichthys californicus), Pacific sanddab (Citharichthys xanthostigma), Dover sole (Microstomus pacificus), scorpionfish (Scorpaena guttata), and white croaker (Genyonemus lineatus) (Allen 1982).

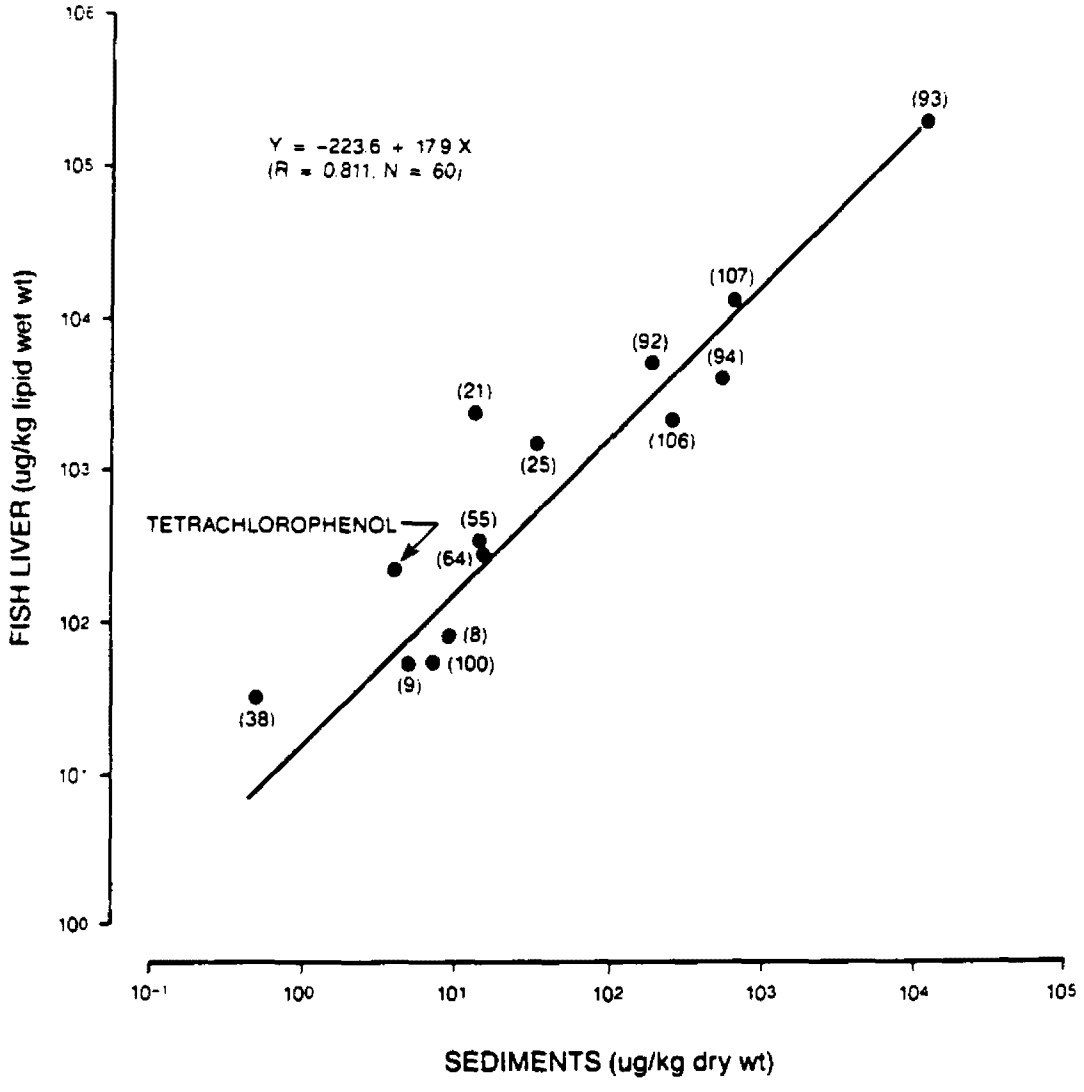
- Finally, the metabolic toxification and detoxification capabilities of the test organisms are well-studied (Jenkins et al. 1982; Brown et al. 1982, 1983, 1984a,b,c,d).

Gossett et al. (1983b) established significant ($P<0.05$) positive rank correlations between sediment concentration and tissue concentration (Rho = 0.77 to 0.95), log K_{ow} and tissue concentration (Rho = 0.63 to 0.75), and log K_{ow} and sediment concentration (Rho = 0.74) for the various compounds studied. However, effluent concentration was negatively correlated with sediment (Rho = -0.55) and tissue (Rho = -0.4 to -0.69) concentrations.

Inspection of Gossett et al.'s (1983b) data showed that, depending on species of fish examined, 4-12 of the compounds that were analyzed (principally the volatiles) were below analytical detection limits. However, the detection limits of these compounds were included in the original rank correlation analysis (Gossett, R.W., 24 September 1984, personal communication). In the present reanalysis of Gossett et al.'s (1983b) data, values that were below detection limits were discarded, and tissue concentrations of contaminants were normalized to lipid fraction (lipid fraction = percent lipids/100). Reanalysis of the reduced data set showed highly positive Pearson product-moment correlations ($R>0.99$) between sediment and lipid-normalized liver concentrations of the various contaminants for each of the five species of fish studied (Figure 3). However, log K_{ow} was not significantly correlated ($P>0.05$, $N=60$) with the log of fish liver-sediment estimated-BCFs. The field-derived BCF in this case was calculated as the ratio of lipid normalized contaminant concentration in fish liver to the concentration in sediments.

A much better correlation was apparent between the ratio of liver tissue concentration to effluent concentration of contaminant and the corresponding K_{ow} value (Figure 4):

$$\log (C_l/C_e) = -2.568 + 1.123 \log K_{ow} \quad (R=0.837,\ P<0.001,\ N=76) \qquad (4)$$



Note: Priority pollutant number in parenthesis. See Appendix B for a key to priority pollutant numbers.

Regression function based on individual values for each species of fish.

Figure 3. Mean contaminant concentration in fish-liver lipids vs. concentration in sediments for five species of fish. Data from Gossett et al. (1983b).

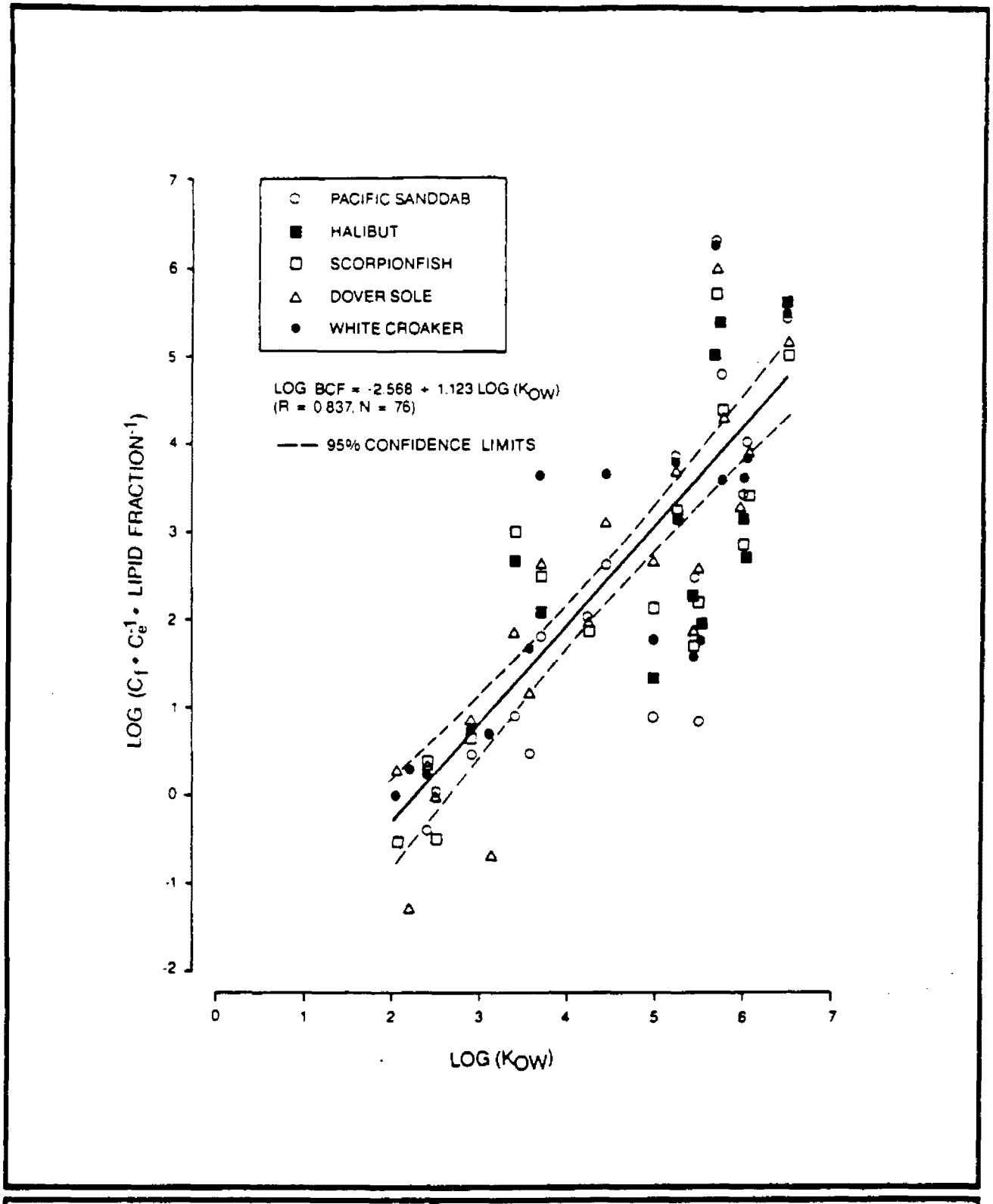


Figure 4. Liver-effluent bioconcentration factors normalized to lipid fraction vs. octanol-water partition coefficients for five species of fishes from the Palos Verdes shelf. Data from Gossett et al. (1983b).

where:

C_l = lipid-normalized liver tissue concentration for each of the five species of fish studied (ug/kg lipid wet wt)

C_e = concentration in effluent (ug/L)

K_{ow} = octanol-water partition coefficient.

This method seems to provide a reasonable estimate of bioconcentration potential in the vicinity of sewage discharges. For instance, Young and Gossett (1980) measured chlorinated benzenes (p-dichlorobenzene, 1,2,4-trichlorobenzene, hexachlorobenzene), PCBs (1242 and 1254), and total DDTs in effluent and in liver tissues of Dover sole collected in the area of the Hyperion 7-mi outfall in Santa Monica Bay and in a reference area. Although not normalized to lipid fraction, their data indicate that the ratio of contaminant concentration in fish liver to that in the effluent is a function of log K_{ow}:

$$\log (C_f/C_e) = -4.255 + 1.223 \log K_{ow} \quad (R=0.859,\ 0.02<P<0.05,\ N=6) \qquad (5)$$

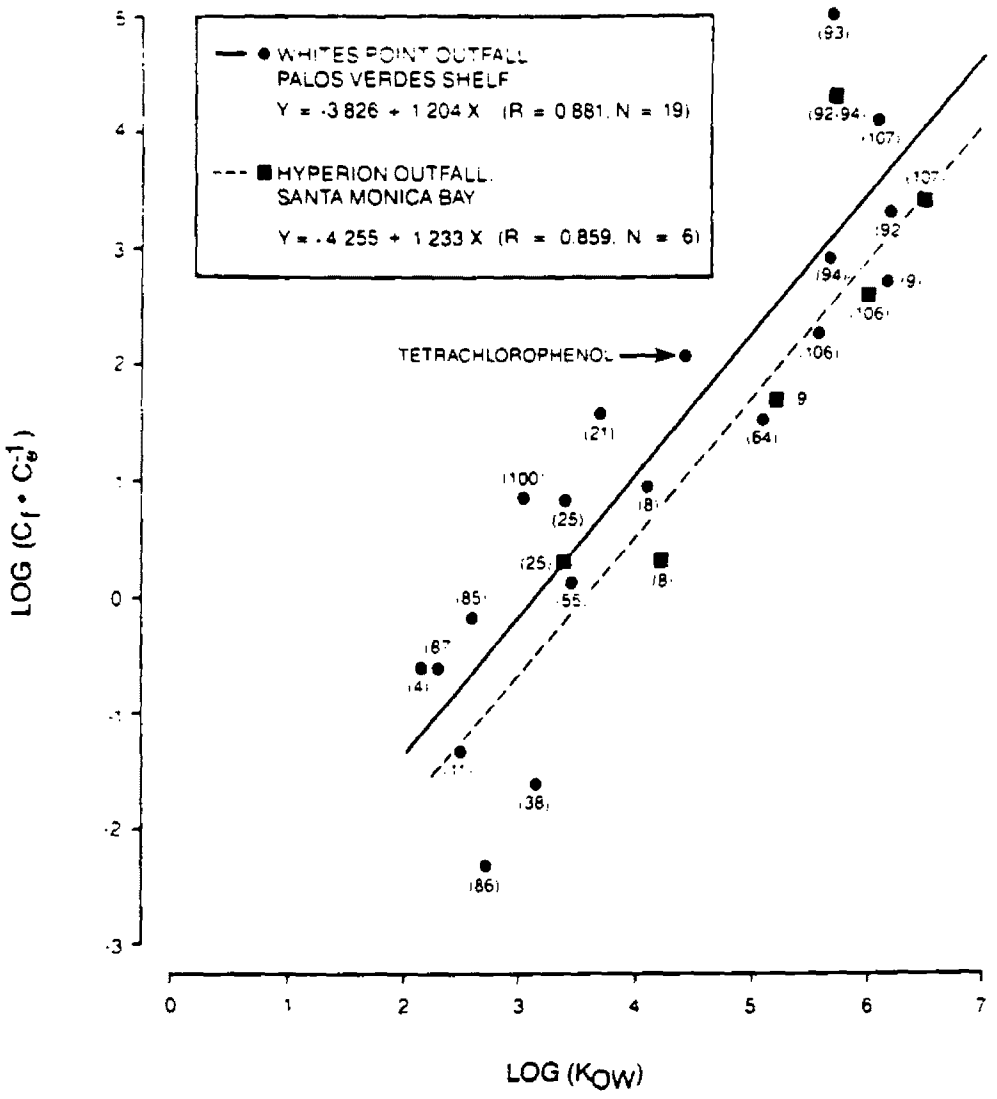
where:

C_f = concentration in fish liver corrected for concentration in tissues from the reference sample (ug/kg wet wt)

C_e = concentration in the effluent (ug/L).

The estimated-BCFs based on these data are generally within an order of magnitude of the corresponding BCFs calculated without lipid-normalization from data collected by Gossett et al. (1983b) for Dover sole in the area of the Whites Point discharge (Figure 5). Note that higher-than-predicted BCFs for DDT in both Gossett et al.'s (1983b) and Young and Gossett's (1980) studies may be due to environmental persistence of DDT in sediments and associated biological uptake while effluent concentration of DDT declined.

In conclusion, analysis of two independent data sets (Gossett et al. 1983b; Young and Gossett 1980) shows that bioaccumulation potential of organic contaminants in fish-liver lipids may be predicted from the octanol-water



Note: Priority pollutant number in parenthesis. See Appendix B for a key to priority pollutant numbers.

Figure 5. Ratio of contaminant concentration in Dover sole liver to effluent concentration as a function of the octanol-water partition coefficient. Data from Gossett et al. (1983b) and Young and Gossett (1980).

partition coefficient (Figures 4 and 5). Furthermore, the extent of tissue contamination will be proportional to the contaminant concentration in sediments (Figure 3; Connor 1983). Finally, it should be recognized that these data are highly site-specific and may only be applicable to the Southern California Bight. Thus, quantitative predictions of contaminant tissue residues for other discharges and other regions are not possible. However, these studies indicate that log K_{ow} is a reasonable index for determining the rank order of bioaccumulation potential of organic contaminants discharged through marine sewage outfalls.

PROPOSED RANKING OF BIOACCUMULATION POTENTIAL

The results of the foregoing review indicate that the octanol-water partition coefficient provides the best available index for potential bioaccumulation of organic contaminants in marine and estuarine organisms because:

- It can provide an order-of-magnitude estimate of the bioconcentration of discharged substances in fish liver (Figure 4)
- It is a reasonable model for partitioning between water and biological tissues
- It is useful for predicting soil sorption coefficients and is thereby implicated in equilibrium partitioning among sediments, water, and biota.

A list of organic priority pollutants and 301(h) pesticides and their proposed ranking of bioaccumulation potential based on the octanol-water partition coefficient is given in Table 3. A list of trace metals and their proposed ranking of bioaccumulation potential based on empirically determined BCFs is given in Table 4. Trace metals are ranked separately from organic contaminants because chemical indices, such as log K_{ow}, that predict bioaccumulation potential have not yet been developed for trace metals.

Calculation of fish liver-effluent estimated-BCFs from K_{ow} is proposed as a second element in this ranking procedure because it provides a basis

TABLE 3. RANK ORDER OF ORGANIC PRIORITY POLLUTANTS AND 301(h) PESTICIDES BASED ON EMPIRICAL BCFs FOR WATER AND SEWAGE EFFLUENT, AND ON OCTANOL-WATER PARTITION COEFFICIENTS (K_{OW})

PP#	Pollutant	Empirical Geometric Mean BCFs: Tissue-water log BCF a	Rank	Liver-effluent log BCF b	Rank	Octanol-water Partition Coefficients: log Kow	log BCF c	Rank
69	di-n-octyl phthalate	ND	--	ND	--	9.20	7.764	1
83	indeno(1,2,3-cd)pyrene	ND	--	ND	--	7.70	6.079	2
79	benzo(ghi)perylene	ND	--	ND	--	7.00	5.293	3
111	PCB-1260	ND	--	ND	--	6.91	5.192	4
--	mirex d	ND	--	ND	--	6.89	5.169	5
75	benzo(k)fluoranthene	ND	--	ND	--	6.85	5.125	6
74	benzo(b)fluoranthene	4.481	1	5.340	2	6.60	4.844	7
107	PCB-1254	ND	--	ND	--	6.48	4.709	8
110	PCB-1248	ND	--	ND	--	6.11	4.294	9
129	TCDD (dioxin)	2.423	13	ND	--	6.10	4.282	10
73	benzo(a)pyrene	4.104	4	3.255	6	6.00	4.170	11
91	chlordane	ND	--	3.576	4	6.00	4.170	12
106	PCB-1242	ND	--	ND	--	6.00	4.170	13
94	4,4'-DDD	ND	--	ND	--	6.00	4.170	14
82	dibenzo(a,h)anthracene	4.322	2	4.463	3	6.00	4.170	15
112	PCB-1016	4.286 e	3	5.853	1	6.00	4.035	16
92	4,4'-DDT	ND	--	ND	--	5.88	3.889	17
93	4,4'-DDE	ND	--	ND	--	5.75	3.822	18
72	benzo(a)anthracene	ND	--	ND	--	5.69	3.732	19
76	chrysene	ND	--	ND	--	5.61	3.721	20
99	endrin aldehyde	ND	--	ND	--	5.60	3.721	21
39	fluoranthene	ND	--	ND	--	5.60	3.642	22
53	hexachlorocyclopentadiene	3.388	11	ND	--	5.53	3.620	23
90	dieldrin	3.441	8	ND	--	5.51	3.586	24
100	heptachlor	ND	--	3.531	5	5.48	3.552	25
101	heptachlor epoxide	3.480	7	ND	--	5.45	3.496	26
9	hexachlorobenzene	ND	--	ND	--	5.40	3.305	27
68	di-n-butyl phthalate	ND	--	1.718	10	5.23	3.215	28
41	4-bromophenyl phenyl ether	2.037	15	ND	--	5.15	3.137	29
64	pentachlorophenol	ND	--	ND	--	5.08	3.047	30
40	4-chlorophenyl phenyl ether	ND	--	ND	--	5.00	2.957	31
84	pyrene	ND	--	ND	--	4.92	2.912	32
20	2-chloronaphthalene	3.396	10	ND	--	4.88	2.733	33
98	endrin	ND	--	ND	--	4.72	2.553	34
109	PCB-1232	ND	--	ND	--	4.56	2.463	35
81	phenanthrene	ND	--	ND	--	4.48	2.441	36
80	fluorene	ND	--	ND	--	4.46	2.351	37
78	anthracene	ND	--	ND	--	4.38	2.306	38
--	methoxychlor d	ND	--	1.976	9	4.34	2.261	39
52	hexachlorobutadiene	2.114	14	ND	--	4.30	2.238	40
8	1,2,4-trichlorobenzene	ND	--	ND	--	4.28	2.182	41
66	bis(2-ethylhexyl)phthalate	ND	--	ND	--	4.23	2.149	42
77	acenaphthylene	ND	--	ND	--	4.20	2.014	43
67	butyl benzyl phthalate	ND	--	ND	--	4.08	1.980	44
108	PCB-1221	ND	--	ND	--	4.05	1.924	45
12	hexachloroethane					4.00	1.845	46
						3.93		

TABLE 3. (Continued)

PP#	Pollutant	Empirical Geometric Mean BCFs: Tissue-water log BCF a	Rank	Liver-effluent log BCF b	Rank	Octanol-water Partition Coefficients: log Kow	log BCF c	Rank
1	acenaphthene	ND	--	ND	--	3.92	1.834	47
102	alpha-hexachlorocyclohexane	ND	--	ND	--	3.85	1.756	48
104	delta-hexachlorocyclohexane	ND	--	ND	--	3.85	1.756	49
103	beta-hexachlorocyclohexane	ND	--	ND	--	3.85	1.756	50
105	gamma-hexachlorocyclohexane	ND	--	ND	--	3.85	1.756	51
--	parathion d	ND	--	ND	--	3.81	1.711	52
7	chlorobenzene	ND	--	ND	--	3.79	1.688	53
21	2,4,6-trichlorophenol	ND	--	2.512	7	3.69	1.576	54
96	beta-endosulfan	ND	--	ND	--	3.60	1.475	55
97	endosulfan sulfate	3.415	9	ND	--	3.60	1.475	56
95	alpha-endosulfan	2.516 f	12	ND	--	3.60	1.475	57
55	napnthalene	3.699	6	1.104	11	3.59	1.464	58
49	fluorotrichloromethane (Removed)	ND	--	ND	--	3.53	1.396	59
27	1,4-dichlorobenzene	ND	--	ND	--	3.53	1.396	60
26	1,3-dichlorobenzene	ND	--	ND	--	3.44	1.295	61
25	1,2-dichlorobenzene	ND	--	2.094	8	3.40	1.250	62
113	toxaphene	4.082	5	ND	--	3.30	1.138	63
38	ethylbenzene	ND	--	0.012	14	3.15	0.969	64
62	N-nitrosodiphenylamine	ND	--	ND	--	3.13	0.947	65
22	para-chloro-meta cresol	ND	--	ND	--	3.10	0.913	66
31	2,4-dichlorophenol	ND	--	ND	--	3.08	0.891	67
28	3,3'-dichlorobenzidine	ND	--	ND	--	3.02	0.823	68
89	aldrin	ND	--	ND	--	3.00	0.801	69
37	1,2-diphenylhydrazine	ND	--	ND	--	2.94	0.734	70
58	4-nitrophenol	ND	--	ND	--	2.91	0.700	71
--	malathion d	ND	--	ND	--	2.89	0.677	72
85	tetrachloroethene	ND	--	0.672	12	2.88	0.666	73
60	4,6-dinitro-o-cresol	ND	--	ND	--	2.85	0.633	74
6	tetrachloromethane	ND	--	ND	--	2.64	0.397	75
42	bis(2-chloroisopropyl)ether	ND	--	ND	--	2.58	0.329	76
11	1,1,1-trichloroethane	ND	--	-0.322	16	2.47	0.206	77
87	trichloroethene	ND	--	0.115	13	2.42	0.150	78
34	2,4-dimethylphenol	ND	--	ND	--	2.42	0.150	79
15	1,1,2,2-tetrachloroethane	ND	--	ND	--	2.39	0.116	80
47	bromoform	ND	--	ND	--	2.30	0.015	81
32	1,2-dichloropropane	ND	--	ND	--	2.28	-0.008	82
86	toluene	ND	--	-0.505	17	2.21	-0.086	83
14	1,1,2-trichloroethane	ND	--	ND	--	2.18	-0.120	84
--	guthion d	ND	--	ND	--	2.18	-0.120	85
50	dichlorodiflouromethane (Removed)	ND	--	ND	--	2.16	-0.142	86
24	2-chlorophenol	ND	--	ND	--	2.16	-0.142	87
4	benzene	ND	--	-0.011	15	2.11	-0.198	88
51	chlorodibromomethane	ND	--	ND	--	2.08	-0.232	89
35	2,4-dinitrotoluene	ND	--	ND	--	2.00	-0.322	90
36	2,6-dinitrotoluene	ND	--	ND	--	2.00	-0.322	91
33	trans-1,3-dichloropropene	ND	--	ND	--	1.98	-0.344	92
33	cis-1,3-dichloropropene	ND	--	ND	--	1.98	-0.344	93
30	1,2-trans-dichloroethylene	ND	--	ND	--	1.97	-0.356	94
--	demeton d	ND	--	ND	--	1.93	-0.401	95
23	chloroform	ND	--	ND	--	1.90	-0.434	96
48	dichlorobromomethane	ND	--	ND	--	1.88	-0.457	97
56	nitrobenzene	ND	--	ND	--	1.83	-0.513	98
5	benzidine	ND	--	ND	--	1.81	-0.535	99

TABLE 3. (Continued)

PP#	Pollutant	Empirical Geometric Mean BCFs: Tissue-water log BCF a	Rank	Liver-effluent log BCF b	Rank	Octanol-water Partition Coefficients: log Kow	log BCF c	Rank
13	1,1-dichloroethane	ND	--	ND	--	1.78	-0.569	100
57	2-nitrophenol	ND	--	ND	--	1.77	-0.580	101
54	isophorone	ND	--	ND	--	1.67	-0.693	102
71	dimethyl phthalate	ND	--	ND	--	1.61	-0.760	103
15	chloroethane	ND	--	ND	--	1.54	-0.839	104
59	2,4-dinitrophenol	ND	--	ND	--	1.53	-0.850	105
29	1,1-dichloroethylene	ND	--	ND	--	1.48	-0.906	106
65	phenol	ND	--	ND	--	1.46	-0.928	107
10	1,2-dichloroethane	ND	--	ND	--	1.45	-0.940	108
70	diethyl phthalate	ND	--	ND	--	1.40	-0.996	109
63	N-nitrosodipropylamine	ND	--	ND	--	1.31	-1.097	110
44	dichloromethane	ND	--	ND	--	1.30	-1.108	111
19	2-chloroethylvinylether	ND	--	ND	--	1.28	-1.131	112
43	bis(2-chloroethoxy)methane	ND	--	ND	--	1.26	-1.153	113
3	acrylonitrile	ND	--	ND	--	1.20	-1.220	114
18	bis(2-chloroethyl)ether	ND	--	ND	--	1.12	-1.310	115
46	bromomethane	ND	--	ND	--	1.00	-1.445	116
2	acrolein	ND	--	ND	--	0.90	-1.557	117
45	chloromethane	ND	--	ND	--	0.90	-1.557	118
86	vinyl chloride	ND	--	ND	--	0.60	-1.894	119
61	N-nitrosodimethylamine	ND	--	ND	--	-0.58	-3.219	120

a U.S. EPA Water Quality Criteria and new data from Appendix A.

b Data from Gossett et al. (1983).

c BCFs normalized to lipid fraction predicted from Gossett et al.'s (1983) data (see Figure 4).

d 301(h) pesticides not on the priority pollutant list.

e Includes DDT, DDE, and DDD.

f Both alpha and beta isomers.

NA = not applicable.

ND = no data.

TABLE 4. RANK ORDER OF TRACE METAL PRIORITY POLLUTANTS BASED ON EMPIRICAL GEOMETRIC MEAN BCFs

PP#	Pollutant	log BCF a	Rank
123	methylmercury	4.602	1
123	phenylmercury	4.602	2
123	mercuric acetate	3.447	3
120	copper	3.073	4
128	zinc	2.762	5
115	arsenic	2.544	6
118	cadmium	2.513	7
122	lead	2.253	8
119	chromium IV	2.190	9
119	chromium III	2.104	10
123	mercury	2.000	11
124	nickel	1.699	12
127	thallium	1.176	13
114	antimony	ND b	--
121	cyanide	ND	--
116	asbestos	ND	--
126	silver	ND	--
125	selenium	ND	--
117	beryllium	ND	--

a U.S. EPA Water Quality Criteria and new data from Appendix A.

b ND = no data.

for comparison of organic and trace metal contaminants, provided that trace metals and organic substances are measured in comparable fashions (i.e., measured in tissues and in effluent). For example, recent studies of metal accumulation in mussels (Mytilus californianus) conducted within the Zone of Initial Dilution (ZID) and in farfield areas of the Whites Point and Point Loma effluent discharges in the Southern California Bight indicate that such comparisons are feasible (Martin et al. 1984). However, calculation of mussel-effluent ratios for trace metals is not presently possible because trace metals were not measured in the effluent at the time of the study (Norton, J., 27 September 1984, personal communication).

Justification of the proposed ranking procedure for organic substances can be obtained by comparing the different rankings based on the three potential indices of bioaccumulation: octanol-water partition coefficients (Table 3), empirical BCFs obtained in laboratory and field studies (Appendix A), and fish liver effluent estimated-BCFs calculated from the data of Gossett et al. (1983b) (Table 3). There are seven organic priority pollutants with sufficient data for application of all three approaches: PCB 1254, DDTs (including DDD and DDE), heptachlor, HCB, pentachlorophenol, 1,2,4-trichlorobenzene, and naphthalene (Table 5). Friedman's nonparametric analyses of variance by ranks shows that the rank order of bioaccumulation is not the same for all three indices ($P<0.001$). Furthermore, individual two-way comparisons using Spearman's rank correlation procedure showed that correlations of the empirical BCFs obtained from the literature with either K_{ow} or liver-effluent BCFs were not significant ($P>0.05$). However,a significant ($0.01<P<0.02$) correlation between the rank order of K_{ow} and the liver-effluent bioconcentration factor was found.

RECOMMENDATIONS FOR SITE-SPECIFIC MONITORING

The purpose of this section is to determine the extent to which structure-activity models of log K_{ow} vs. estimated-BCFs may be used to select priority pollutants and 301(h) pesticides for monitoring and to provide guidance for development of bioaccumulation studies. As indicated above, structure-activity models have not yet reached the level of sophistication needed to make quantitative predictions of organic contaminant tissue residues

TABLE 5. RANK ORDER OF OCTANOL-WATER PARTITION COEFFICIENT (K_{ow}), EMPIRICAL BCFs, AND FISH LIVER-EFFLUENT BIOCONCENTRATION FACTORS (C_l/C_e) FOR SEVEN PRIORITY POLLUTANTS

Substance	K_{ow}[a]	Rank BCF	C_l/C_e
PCB 1254	1	1	1
DDTs[b]	2	2	2
Heptachlor	3	5	4
HCB	4	4	3
Pentachlorophenol	5	7	6
1,2,4-trichlorobenzene	6	6	5
Naphthalene	7	3	7

[a] Spearman's Rho=0.929 ($0.01<P<0.02$) for K_{ow} vs. C_l/C_e. Remaining comparisons are not signficant ($P>0.05$).

[b] DDT, DDE, DDD.

Reference: Table 3.

in indigenous organisms exposed to sewage effluent. However, log K_{ow} vs. BCF models indicate structural compound classes comprising compounds with a high bioaccumulation potential. Estimated BCFs greater than 1.0 indicate that contaminant concentrations in tissues are greater than those in the exposure medium. As seen in equation 4 and Figure 4, organic substances with log K_{ow} values greater than 2.3 have predicted liver-effluent BCFs (normalized by lipid fraction in liver) greater than 1.0 (i.e., log BCF>0). As shown in Tables 2 and 3, structural compound classes in which all priority pollutants have log K_{ow} values greater than 2.3 are:

- Low molecular weight aromatic hydrocarbons
- High molecular weight polycyclic aromatic hydrocarbons
- Chlorinated aromatic hydrocarbons
- Chlorinated aliphatic hydrocarbons
- Volatile chlorinated aromatic hydrocarbons
- PCBs
- Priority pollutant pesticides.

The priority pollutants with log K_{ow} values less than 2.3 are in the following structural compound classes:

- Phenols (1 substance)
- Substituted phenols (3 substances)
- Organonitrogen compounds (6 substances)
- Halogenated ethers (2 substances)
- Phthalates (2 substances)

- Miscellaneous oxygenated compounds (1 substance)
- 301(h) pesticides (2 organophosphates)
- Volatile halogenated alkanes (12 substances)
- Volatile halogenated alkenes (4 substances)
- Volatile aromatic hydrocarbons (2 substances)
- Volatile unsaturated carbonyl compounds (2 substances)
- Volatile ethers (1 substance).

Eighteen of the twenty structural compound classes identified in Table 2 contain at least one substance with a relatively high bioaccumulation potential (i.e., log K_{ow} > 2.3). The only two compound classes with consistently low bioaccumulation potential are unsaturated carbonyl compounds and volatile ethers. These two compound groups are extracted and analyzed with other volatile compounds that have a higher bioaccumulation potential. Since analytical methods encompass a wide range of compounds that generally fall within a structural compound class, it is not practical at this time to eliminate any of the organic 301(h) priority pollutants or pesticides from monitoring based on their low bioaccumulation potential (i.e., log K_{ow} values less than 2.3).

Our analysis also indicates that all trace metals detected in sewage effluent should be monitored routinely. There are several reasons for recommending this approach. There is a wealth of information concerning bioaccumulation and bioconcentration of trace metals, particularly in bivalve molluscs. However, there is not yet a good predictive relationship between physicochemical characteristics and bioaccumulation potential of trace metals comparable to the octanol-water partition coefficient and BCF model for organic substances. Second, some trace metals are not easily metabolized, do not reach steady-state in tissues, and are slow to depurate. Thus,

empirical BCFs for trace metals such as mercury are nominal values and may be greatly exceeded under conditions of prolonged exposure. Third, a maximum of 10 or 12 trace metals would require monitoring. With the exception of mercury, which requires separate sample preparation, trace metal analyses can be performed on aliquots of a single sample using the same analytical procedure. Therefore, given the analytical sophistication available, the relatively low cost compared to organic analyses, and the potential for bioaccumulation, any reduction in the monitoring of trace metals is not recommended.

Although structure-activity models of bioaccumulation potential cannot be used a priori to eliminate structural compound classes from 301(h) monitoring programs, they provide information useful in designing and managing such monitoring programs. Monitoring the bioaccumulation of toxic pollutants in natural and caged populations of indigenous organisms can be considered as a means of integrating water quality conditions over longer periods of time than can be accurately predicted from one-time or short-term (e.g., one day) composited effluent samples. For example, priority pollutants and 301(h) pesticides may be present in the effluent below current detection limits, but may still bioaccumulate in marine organisms. Thus, compliance with the requirement for monitoring bioaccumulation of priority pollutants and 301(h) pesticides may dispel uncertainties concerning effluent contaminant concentrations and possible biological impacts. Site-specific bioaccumulation data that demonstrates the absence of contaminants in effluent, tissues, and sediments may provide justification for eliminating entire structural compound classes from the monitoring program. For example, most volatile compounds have log K_{ow} values less than 2.3. This group could be eliminated if there is no evidence of their occurrence in effluent or accumulation in sediments or tissues. In general, the volatile compound classes are relatively soluble, are degraded by a variety of environmental processes, and have a low potential for bioaccumulation (Edwards 1977; Morley 1977; Callahan et al. 1979; Connell and Miller 1984). Toxic organic contaminants other than the priority pollutants and 301(h) pesticides may occur in sewage effluent and bioaccumulate in marine organisms. These substances may be identified and quantified from the GC/MS data generated during analysis of priority pollutants and 301(h) pesticides in effluent, tissue, and sediment

samples. Therefore, it is recommended that non-priority pollutants and pesticides be incorporated into 301(h) monitoring programs when they occur in sewage effluent and sediments, and are shown to bioaccumulate in marine organisms. Typically, such analyses would include tentative identification and quantification of a limited number (e.g., 5-10) of the highest GC/MS reconstructed ion chromatogram peaks.

It is recognized that these guidelines need to be tempered by other considerations such as volume of the discharge, receiving water characteristics, history of biological impacts on sensitive communities (e.g., benthic infauna), specific knowledge of the behavior, toxicity of chemical contaminants, and requirements in selection of target organisms, sampling methods and analytical detection limits. Many of these details are discussed in other volumes of the Bioaccumulation Monitoring Guidance Report series (Tetra Tech 1985a,b).

In conclusion, review of the bioaccumulation potential of toxic contaminants indicates that all priority pollutants and 301(h) pesticides should be included in design of 301(h) biological and water quality monitoring programs. However, well designed bioaccumulation studies should provide site-specific information useful in program management and evaluation, and may result in eliminating some compound groups from continued monitoring.

SUMMARY

1. Toxic substances introduced into the marine environment through sewage outfalls are partitioned among environmental compartments of water, suspended particulates, sediments, and biota. Most organic and trace metal contaminants are associated with the particulate phase of sewage effluent and are therefore rapidly incorporated into sediments in the vicinity of the discharge.

2. Approaches used in the past to evaluate bioaccumulation potential of toxic substances are empirical bioconcentration factors (BCFs), structure-activity relationsnips, equilibrium partitioning models, and indices based on metabolism.

3. Based on U.S. EPA's (1980) Water Quality Guidelines, empirically determined BCFs for four major classes of marine and estuarine organisms (polychaetes, molluscs, crustaceans, and fishes) exist for only 14 organic substances and 9 trace metals on the priority pollutant list.

4. Although the relationship between the octanol-water partition coefficient (K_{ow}) and BCF is a reasonable predictor of BCFs in laboratory studies of fishes and bivalves, existing data are too limited to apply the model directly to marine and estuarine organisms in nature.

5. A structure-activity model for bioaccumulation potential was developed from compartmental characterization of chemical contaminants in fish liver, effluent, and sediments in the vicinity of a large sewage discharge into waters of the Palos Verdes Shelf in southern California. The data show that bioaccumulation potential of organic contaminants was correlated with the octanol-water partition coefficient and that the extent of biological contamination was proportional to contaminant concentration in the sediments.

6. Studies conducted since 1980 indicate that tissue concentrations of organic contaminants should be normalized to percent lipids to aid in the interpretation of bioaccumulation data. Therefore, data on lipid concentrations should be included to the extent practicable in bioaccumulation monitoring programs.

7. The proposed ranking of bioaccumulation potential of organic contaminants is based on log K_{ow}. The proposed ranking of bioaccumulation potential of trace metals is based on empirically determined tissue-water BCFs (Table 4).

8. Tissue-effluent BCFs may provide a basis for comparing relative bioaccumulation potentials of organic and trace metal contaminants when more comprehensive data become available. Also, further development of tissue-effluent BCF vs. K_{ow} models should incorporate the effects of distance of the sampling site from the discharge site.

9. Review of the bioaccumulation potential of toxic contaminants indicates that all priority pollutants and 301(h) pesticides should be included in design of 301(h) biological and water quality monitoring programs.

10. Site-specific bioaccumulation data will be useful in management and evaluation of monitoring programs. The failure to detect related contaminants in effluent, tissue, and sediments may provide justification for eliminating entire structural compound classes from the monitoring program.

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APPENDIX A. BIOCONCENTRATION FACTORS FOR PRIORITY POLLUTANTS AND 301(h) PESTICIDES IN MARINE AND ESTUARINE ORGANISMS AS MODIFIED FROM U.S. EPA (1980) WATER QUALITY CRITERIA DOCUMENTS AND ADDITIONAL INFORMATION PUBLISHED FROM JANUARY, 1980, TO AUGUST, 1984

PP#	Pollutant	Higher Taxon	Species	Tissue a	Percent Lipids	BCF	Days of Exposure	Number of Studies	References
	Phenols								
65	phenol								
34	2,4-dimethylphenol								
	Substituted Phenols								
21	2,4,6-trichlorophenol								
22	para-chloro-meta cresol								
24	2-chlorophenol								
31	2,4-dichlorophenol								
57	2-nitrophenol								
58	4-nitrophenol								
59	2,4-dinitrophenol								
60	4,6-dinitro-o-cresol								
64	pentachlorophenol	polychaete	Lanice conchilega	W	--	3,830	8	1	Ernst 1979
64	pentachlorophenol	mollusc	Mytilus edulis	EP	--	335	8	4	Ernst 1979
64	pentachlorophenol	mollusc	Crassostrea virginica	EP	--	56	28 b	2	Schimmel et al. 1978
64	pentachlorophenol	mollusc	Crassostrea virginica	--	0.6 c	53	steady state	1	U.S. EPA 1981
64	pentachlorophenol	fish	Cyprinodon variegatus, juv.	W	--	34	28	1	Parrish et al. 1978
64	pentachlorophenol	fish	Cyprinodon variegatus, adult	W	--	13	151	1	Parrish et al. 1978
64	pentachlorophenol								
	Organonitrogen Compounds								
5	benzidine								
28	3,3'-dichlorobenzidine								
35	2,4-dinitrotoluene								
36	2,6-dinitrotoluene								
37	1,2-diphenylhydrazine								
56	nitrobenzene								
61	N-nitrosodimethylamine								
62	N-nitrosodiphenylamine								
63	N-nitrosodipropylamine								
	Low Molecular Weight Aromatic Hydrocarbons								
1	acenaphthene	crustacean	Eurytemora affinis	W	--	5,000 d	9	1	Harris et al. 1977
55	naphthalene								
77	acenaphthylene								
78	anthracene								
81	phenanthrene								
80	fluorene								

APPENDIX A. (Continued)

PP#	Pollutant	Higher Taxon	Species	Tissue a	Percent Lipids	BCF	Days of Exposure	Number of Studies	References
	High Molecular Weight PAH								
39	fluoranthene								
72	benzo(a)anthracene								
73	benzo(a)pyrene	mollusc	Mytilus edulis	EP	--	265	field data	1	Gossett et al. 1983
74	benzo(b)fluoranthene								
75	benzo(k)fluoranthene								
76	chrysene								
79	benzo(ghi)perylene								
82	dibenzo(a,h)anthracene								
83	indeno(1,2,3-cd)pyrene								
84	pyrene								
	Chlorinated Aromatic Hydrocarbons								
8	1,2,4-trichlorobenzene	mollusc	Crassostrea virginica		0.6 b	130	steady state	1	U.S. EPA 1981
9	hexachlorobenzene	fish	Lagodon rhomboides	EP	--	23,000	42	1	Parrish et al. 1974a
9	hexachlorobenzene	fish	Fundulus similis	EP	--	397	11	1	Giam et al. 1980
20	2-chloronaphthalene								
25	1,2-dichlorobenzene								
26	1,3-dichlorobenzene								
27	1,4-dichlorobenzene								
	Chlorinated Aliphatic Hydrocarbons								
52	hexachlorobutadiene								
12	hexachloroethane								
53	hexachlorocyclopentadiene								
	Halogenated Ethers								
18	bis(2-chloroethyl)ether								
40	4-chlorophenyl ether								
41	4-bromophenyl ether								
42	bis(2-chloroisopropyl)ether								
43	bis(2-chloroethoxy)methane								
	Phthalates								
66	bis(2-ethylhexyl)phthalate								
67	butyl benzyl phthalate								
68	di-n-butyl phthalate								
69	di-n-octyl phthalate								
70	diethyl phthalate								
71	dimethyl phthalate								

APPENDIX A. (Continued)

PP#	Pollutant	Higher Taxon	Species	Tissue a	Percent Lipids	BCF	Days of Exposure	Number of Studies	References
	PCBs								
106	PCB-1242								
107	PCB-1254	polychaete	Nereis virens	W	--	14,870	3-100	1	Rubinstein et al. 1983
107	PCB-1254	mollusc	Crassostrea virginica	EP	--	101,000	245	1	Lowe et al. 1972
107	PCB-1254	mollusc	Crassostrea virginica	EP	--	> 100,000	field data	2	Duke et al. 1970; Nimmo et al. 1975
107	PCB-1254	mollusc	Mercenaria mercenaria	EP	--	140	3-100	1	Rubinstein et al. 1983
107	PCB-1254	crustacean	Palaemonetes pugio	W	--	> 230,000	field data	1	Nimmo et al. 1975
107	PCB-1254	crustacean	Palaemonetes pugio	W	--	5,990	3-100	2	Rubinstein et al. 1983; Nimmo et al. 1974
107	PCB-1254	fish	Leiostomus xanthurus	W	1.1	37,000	28	1	Hansen et al. 1971
107	PCB-1254	fish	Cynoscion nebulosus	W	--	> 670,000	field data	2	Duke et al. 1970; Nimmo et al. 1975
107	PCB-1254	fish	Cyprinodon variegatus	W	3.6	30,000	28	1	Hansen et al. 1975
108	PCB-1221								
109	PCB-1232								
110	PCB-1248								
111	PCB-1260								
112	PCB-1016	mollusc	Crassostrea virginica	EP	--	13,000	84	1	Parrish et al. 1974b
112	PCB-1016	fish	Cyprinodon variegatus, adult	W	3.6	25,000	28	1	Hansen et al. 1975
112	PCB-1016	fish	Cyprinodon variegatus, juv.	W	--	24,910	28	2	Hansen et al. 1975
112	PCB-1016	fish	Lagodon rhomboides	W	--	17,000	21-28	1	Hansen et al. 1974
	Miscellaneous Oxygenated Compounds								
54	Isophorone								
129	TCDD (dioxin)								
	Pesticides								
89	aldrin								
90	dieldrin	mollusc	Crassostrea virginica	EP	--	8,000	392	1	Parrish 1974
90	dieldrin	crustacean	Leptodius floridanus, larva	W	--	400 d	16	1	Epifanio 1973
90	dieldrin	fish	Poecilia latipinna	EP	--	4,870	238	1	Lane & Livingston 1970
90	dieldrin	fish	Leiostomus xanthurus	W	1.1	2,300	35	1	Parrish et al. 1973
91	chlordane	fish	Cyprinodon variegatus, juv.	W	--	10,130	28	3	Parrish et al. 1976, 1978
91	chlordane	fish	Cyprinodon variegatus, adult	W	3.6	16,000	189	1	Parrish et al. 1978
92	4,4'-DDT e	mollusc	Crassostrea virginica		0.6 b	45,530 f	steady state	1	U.S. EPA 1981
92	4,4'-DDT e	mollusc	Crassostrea virginica	W	--	56,880	168-252	2	Lowe et al. 1970
92	4,4'-DDT e	crustacean	Penaeus duorarum	W	--	1,200	56	1	Nimmo et al. 1970
92	4,4'-DDT e	crustacean	Cancer magister	W	1.3	8,230	field	2	Earnest & Benville 1971
92	4,4'-DDT e	fish	Micropogonius undulatus	W	--	16,000	21-35	1	Hansen & Wilson 1970
92	4,4'-DDT e	fish	Cymatogaster aggregata	W	3.4	38,770	field	2	Earnest & Benville 1971
92	4,4'-DDT e	fish	Micrometrus minimus	W	6.4	41,480	field	2	Earnest & Benville 1971
92	4,4'-DDT e	fish	Phanerodon furcatus	W	2.8	25,510	field	2	Earnest & Benville 1971
92	4,4'-DDT e	fish	Raccochilus vacca	W	4.4	29,490	field	2	Earnest & Benville 1971
92	4,4'-DDT e	fish	Leptocottus armatus	W	1.9	19,450	field	2	Earnest & Benville 1971
92	4,4'-DDT e	fish	Citharichthys stigmaeus	W	2.7	13,670	field	2	Earnest & Benville 1971

APPENDIX A. (Continued)

PP#	Pollutant	Higher Taxon	Species	Tissue a	Percent Lipids	BCF	Days of Exposure	Number of Studies	References
92	4,4'-DDT e	fish	Parophrys vetulus	W	2	16,120	field	2	Earnest & Benville 1971
92	4,4'-DDT e	fish	Platichthys stellatus	W	2.5	24,250	field	2	Earnest & Benville 1971
93	4,4'-DDE e								
94	4,4'-DDD e								
95	alpha-endosulfan g	fish	Cyprinodon variegatus	W	3.6	328	28	1	U.S. EPA 1980a
96	beta-endosulfan								
97	endosulfan sulfate	fish	Mugil cephalus	EP	--	2,430	28	1	Schimmel et al. 1977a
97	endosulfan sulfate	fish	Mugil cephalus	W	1	2,755	28	1	Schimmel et al. 1977a
98	endrin	mollusc	Crassostrea virginica	EP	--	2,225	7	1	Mason & Rowe 1976
98	endrin	crustacean	Palaemonetes pugio	EP	--	1,540	10-145	2	Tyler-Schroeder 1979
98	endrin	fish	Leiostomus xanthurus	W	1.1	1,450	5-8 months	1	Lowe 1966
98	endrin	fish	Cyprinodon variegatus	W	3.6	4,000	28-161	2	Hansen et al. 1977
98	endrin	fish	Cyprinodon variegatus-emb.,juv	W	--	4,800	33	1	Schimmel et al. 1975
99	endrin aldehyde								
100	heptachlor	fish	Cyprinodon variegatus, juv.	W	--	3,580	28	1	Goodman et al. 1978
100	heptachlor	fish	Leiostomus xanthurus	EP	--	1,850	24	1	Schimmel et al. 1976
100	heptachlor	fish	Leiostomus xanthurus	W	1.1	3,180	24	1	Schimmel et al. 1976
101	heptachlor epoxide								
102	alpha-hexachlorocyclohexane								
103	beta-hexachlorocyclohexane								
104	delta-hexachlorocyclohexane								
105	gamma-hexachlorocyclohexane								
113	toxaphene	mollusc	Crassostrea virginica	EP	--	32,800	168	1	Lowe et al. 1970
113	toxaphene	fish	Fundulus similis, fry	W	--	27,900	28	1	Schimmel et al. 1977b
113	toxaphene	fish	Fundulus similis, juv.	W	--	29,400	28	1	Schimmel et al. 1977b
113	toxaphene	fish	Fundulus similis, adult	W	--	5,400	32	1	Schimmel et al. 1977b
113	toxaphene	fish	Fundulus similis, ova	W	--	2,170	14-32	2	Schimmel et al. 1977b
113	toxaphene	fish	Cyprinodon variegatus	W	3.6	9,800	28	1	Goodman et al. 1978
--	mirex (h)								
--	methoxychlor (h)								
--	parathion (i)								
--	malathion (i)								
--	guthion (i)								
--	demeton (i)								
	Volatile Halogenated Alkanes								
6	tetrachloromethane								
10	1,2-dichloroethane								
11	1,1,1-trichloroethane								
13	1,1-dichloroethane								
14	1,1,2-trichloroethane								
15	1,1,2,2-tetrachloroethane								
16	chloroethane								
23	chloroform								

APPENDIX A. (Continued)

PP#	Pollutant	Higher Taxon	Species	Tissue a	Percent Lipids	BCF	Days of Exposure	Number of Studies	References
32	1,2-dichloropropane								
44	dichloromethane								
45	chloromethane								
46	bromomethane								
47	bromoform								
48	dichlorobromomethane								
51	chlorodibromomethane								
	fluorotrichloromethane (Removed)								
	dichlorodiflouromethane (Removed)								
	Volatile Halogenated Alkenes								
29	1,1-dichloroethylene								
30	1,2-trans-dichloroethylene								
33	trans-1,3-dichloropropene								
	cis-1,3-dichloropropene								
85	tetrachloroethene								
87	trichloroethene								
88	vinyl chloride								
	Volatile Aromatic Hydrocarbons								
4	benzene								
38	ethylbenzene								
86	toluene								
	Volatile Chlorinated Aromatic Hydrocarbons								
7	chlorobenzene								
	Volatile Unsaturated Carbonyl Compounds								
2	acrolein								
3	acrylonitrile								
	Volatile Ethers								
19	2-chloroethylvinylether								
	bis(chloromethyl)ether (Removed)								

APPENDIX A. (Continued)

PP#	Pollutant	Higher Taxon	Species	Tissue a	Percent Lipids	BCF	Days of Exposure	Number of Studies	References
	Metals								
114	antimony								
115	arsenic	mollusc	Crassostrea virginica	EP	--	350 j	112	1	U.S. EPA 1980b
117	beryllium								
118	cadmium	polychaete	Ophryotrocha diadema	W	--	3,160 k	64	1	Klockner 1979
118	cadmium	mollusc	Crassostrea virginica	EP	--	3,080 k	280	2	Zarooglan 1979; Zarooglan & Cheer 1976
118	cadmium	mollusc	Crassostrea virginica	EP	--	1,220 l	98	1	Shuster & Pringle 1969
118	cadmium	mollusc	Mya arenaria	EP	--	160 l	70	1	Pringle et al. 1968
118	cadmium	mollusc	Mercenaria mercenaria	EP	--	83 l	40	1	Kerfoot & Jacobs 1976
118	cadmium	mollusc	Argopecten irradians	M	--	2,040 k	42	1	Pesch & Stewart 1980
118	cadmium	mollusc	Mytilus edulis	EP	--	185 k	28-35	2	George & Coombs 1977; Phillips 1976
118	cadmium	mollusc	Crassostrea gigas	EP	--	405	28	1	Frazier & George 1983
118	cadmium	crustacean	Penaeus duorarum	W	--	57 k	30	1	Nimmo et al. 1977
118	cadmium	crustacean	Palaemonetes pugio	W	--	69 k	28-42	2	Pesch & Stewart 1980; Nimmo et al. 1977
118	cadmium	crustacean	Palaemonetes vulgaris	W	--	307 k	28	1	Nimmo et al. 1977
118	cadmium	crustacean	Carcinus maenas	M	--	6 k	40-68	2	Wright 1977; Jennings & Rainbow 1979
118	cadmium	crustacean	Pandalus montagui	W	--	2,730	14	1	Ray et al. 1980
119	chromium m	polychaete	Nereis arenaceodentata	W	--	168	158	1	Oshida & Word 1982
119	chromium m	mollusc	Crassostrea virginica	EP	--	116	140	1	Shuster & Pringle 1969
119	chromium m	mollusc	Mya arenaria	EP	--	153 d	168	1	Capuzzo & Sasner 1977
119	chromium m	mollusc	Mytilus edulis	EP	--	86 d	168	1	Capuzzo & Sasner 1977
119	chromium n	mollusc	Crassostrea virginica	EP	--	125	84	1	U.S. EPA 1980c
119	chromium n	mollusc	Mytilus edulis	EP	--	192	84	1	U.S. EPA 1980c
120	copper	polychaete	Cirriformia spirabranchia			250 d	24	1	Milanovich et al. 1976
120	copper	polychaete	Nereis arenaceodentata			2,550 d	28	1	Pesch & Morgan 1978
120	copper	polychaete	Nereis diversicolor			203 d	24	1	Jones et al. 1976
120	copper	polychaete	Phyllodoce maculata			1,750 d	21	1	McLusky & Phillips 1975
120	copper	polychaete	Eudistylia vancouveri	BC	--	9,250	33	1	Young et al. 1981
120	copper	mollusc	Argopecten irradians			3,710	112	2	Zarooglan 1978
120	copper	mollusc	Argopecten irradians	EP	--	1,760 d	56	1	Zarooglan & Johnson 1983
120	copper	mollusc	Crassostrea virginica			24,160	140	2	Shuster & Pringle 1969
120	copper	mollusc	Mercenaria mercenaria			88	70	1	Shuster & Pringle 1968
120	copper	mollusc	Mya arenaria			3,300	35	1	Shuster & Pringle 1968
120	copper	mollusc	Macoma inquinata	EP	--	154 d	30	1	Crecelius et al. 1982
120	copper	mollusc	Mytilus edulis			126	14-112	3	U.S. EPA 1980d; Phillips 1976
120	copper	crustacean	Pandalus danae	W	--	4,820 d	30	1	Crecelius et al. 1982
122	lead	mollusc	Crassostrea virginica	EP	--	371 o	49-140	3	Zarooglan et al. 1979; Pringle et al. 1968; Shuster & Pringle 1969
122	lead	mollusc	Mercenaria mercenaria	EP	--	18 d,o	56	1	Pringle et al. 1968
122	lead	mollusc	Mya arenaria	EP	--	112 o	70	1	Pringle et al. 1968
122	lead	mollusc	Mytilus edulis	EP	--	1,290 d,o	40-130	4	Schulz-Baldes 1972, 1974
122	lead	mollusc	Mytilus edulis	EP	--	200 d,p	37	1	Talbot et al. 1976

APPENDIX A. (Continued)

PP#	Pollutant	Higher Taxon	Species	Tissue a	Percent Lipids	BCF	Days of Exposure	Number of Studies	References
123	mercury	polychaete	Glycera dibranchiata	W	--	4 q	3	1	Medeiros et al. 1980
123	mercury	mollusc	Crassostrea virginica	EP	--	10,000 q	74	1	Kopfler 1974
123	mercury	mollusc	Crassostrea virginica	EP	--	40,000 r	74	1	Kopfler 1974
123	mercury	mollusc	Crassostrea virginica	EP	--	40,000 s	74	1	Kopfler 1974
123	mercury	mollusc	Crassostrea virginica	EP	--	2,800 t	45	1	Cunningham & Tripp 1973
123	mercury	mollusc	Mytilus edulis	EP	--	8,780	90	1	Roesijadi et al. 1981
123	mercury	crustacean	Homarus americanus	TM	--	129 q	30	1	Thurberg et al. 1977
124	nickel	mollusc	Crassostrea virginica	EP	--	339	84	2	U.S. EPA 1980e
124	nickel	mollusc	Mytilus edulis	EP	--	369	84	2	U.S. EPA 1980e
124	nickel	mollusc	Protothaca staminea	G	--	1 d	2	1	Hardy & Roesijadi 1982
125	selenium								
126	silver								
127	thallium	mollusc	Mya arenaria	EP	--	18	88	1	Zitko & Carson 1975
127	thallium	mollusc	Mytilus edulis	EP	--	12	40	1	Zitko & Carson 1975
128	zinc	polychaete	Nereis diversicolor			20 u	34	1	Bryan & Hummerstone 1973
128	zinc	mollusc	Crassostrea virginica			16,700 v	140	1	Shuster & Pringle 1969
128	zinc	mollusc	Mya arenaria	EP	--	60 v	50-112	2	Pringle et al. 1968; Eisler 1977
128	zinc	mollusc	Mytilus edulis	EP	--	317 v	13-35	3	Pentreath 1973; Phillips 1976, 1977
128	zinc	mollusc	Littorina obtusata			670 v	50	1	Young 1975
128	zinc	crustacean	Carcinus maenas	M	--	8,800 v	22	1	Bryan 1966
	Miscellaneous								
121	cyanide								
116	asbestos								

a W = whole organism, EP = edible portion, M = muscle tissue, BC = branchial crown, TM = tail muscles, G = gills.

b Reached steady state in four days.

c Percent lipid value is a conversion from dry weight to wet weight.

d BCF value is a conversion from dry weight to wet weight.

e DDT and its metabolites (DDE and DDD) unless stated otherwise.

f BCF for 4,4 1-DDE only.

g Data is for technical grade endosulfan, assumed to be both alpha and beta isomers, PP #95, 96.

h Chlorinated 301(h) pesticides that are not on the priority pollutant list.

i Organophosphorus 301(h) pesticides that are not on the priority pollutant list.

j For sodium arsenite.

k For cadmium chloride.

l For cadmium nitrate.

m For trivalent chromium as chromic chloride.

n For hexavalent chromium as sodium dichromate.

o For lead nitrate.

p For lead chloride.

q For mercuric chloride.

r For methylmercuric chloride.

s For phenylmercuric chloride.

t For mercuric acetate.

u For zinc sulfate.

v For zinc chloride.

APPENDIX B. PRIORITY POLLUTANTS AND 301(h) PESTICIDES SORTED BY STRUCTURAL COMPOUND CLASS (TABLE B-1), PRIORITY POLLUTANT NUMBER (TABLE B-2), AND BY ALPHANUMERIC ORDER (TABLE B-3)

TABLE B-1. PRIORITY POLLUTANTS AND 301(h) PESTICIDES LISTED ACCORDING TO STRUCTURAL COMPOUND CLASS

Structural Compound Class	PP#	Pollutant
Phenols	65	phenol
	34	2,4-dimethylphenol
Substituted Phenols	21	2,4,6-trichlorophenol
	22	para-chloro-meta cresol
	24	2-chlorophenol
	31	2,4-dichlorophenol
	57	2-nitrophenol
	58	4-nitrophenol
	59	2,4-dinitrophenol
	60	4,6-dinitro-o-cresol
	64	pentachlorophenol
Organonitrogen Compounds	5	benzidine
	28	3,3'-dichlorobenzidine
	35	2,4-dinitrotoluene
	36	2,6-dinitrotoluene
	37	1,2-diphenylhydrazine
	56	nitrobenzene
	61	N-nitrosodimethylamine
	62	N-nitrosodiphenylamine
	63	N-nitrosodipropylamine
Low Molecular Weight Aromatic Hydrocarbons	1	acenaphthene
	55	naphthalene
	77	acenaphthylene
	78	anthracene
	81	phenanthrene
	80	fluorene
High Molecular Weight PAH	39	fluoranthene
	72	benzo(a)anthracene
	73	benzo(a)pyrene
	74	benzo(b)fluoranthene
	75	benzo(k)fluoranthene
	76	chrysene
	79	benzo(ghi)perylene
	82	dibenzo(a,h)anthracene
	83	indeno(1,2,3-cd)pyrene
	84	pyrene
Chlorinated Aromatic Hydrocarbons	8	1,2,4-trichlorobenzene
	9	hexachlorobenzene
	20	2-chlorbnaphthalene
	25	1,2-dichlorobenzene
	26	1,3-dichlorobenzene
	27	1,4-dichlorobenzene
Chlorinated Aliphatic Hydrocarbons	52	hexachlorobutadiene
	12	hexachloroethane
	53	hexachlorocyclopentadiene
Halogenatec Ethers	18	bis(2-chloroethyl)ether
	40	4-chlorophenyl ether
	41	4-bromophenyl ether
	42	bis(2-chloroisopropyl)ether
	43	bis(2-chloroethoxy)methane

Structural Compound Class	PP#	Pollutant
Phthalates	66	bis(2-ethylhexyl)phthalate
	67	butyl benzyl phthalate
	68	di-n-butyl phthalate
	69	di-n-octyl phthalate
	70	diethyl phthalate
	71	dimethyl phthalate
PCBs	106	PCB-1242
	107	PCB-1254
	108	PCB-1221
	109	PCB-1232
	110	PCB-1248
	111	PCB-1260
	112	PCB-1016
Miscellaneous Oxygenated Compounds	129	TCDD (dioxin)
	54	isophorone
Pesticides	89	aldrin
	90	dieldrin
	91	chlordane
	92	DDT (a)
	95	endosulfan (b)
	98	endrin
	99	endrin aldehyde
	100	heptachlor
	101	heptachlor epoxide
	102	alpha-hexachlorocyclohexane
	103	beta-hexachlorocyclonexane
	104	delta-hexachlorocyclohexane
	105	gamma-hexachlorocyclohexane
	113	toxaphene
	--	mirex (c)
	--	methoxychlor (c)
	--	parathion (d)
	--	malathion (d)
	--	guthion (d)
	--	demeton (d)
Volatile Halogenated Alkanes	6	tetrachloromethane
	10	1,2-dichloroethane
	11	1,1,1-trichloroethane
	13	1,1-dichloroethane
	14	1,1,2-trichloroethane
	15	1,1,2,2-tetrachloroethane
	16	chloroethane
	23	chloroform
	32	1,2-dichloropropane
	44	dichloromethane
	45	chloromethane
	46	bromomethane
	47	bromoform
	48	dichlorobromomethane
	49	fluorotrichloromethane (Removed)
	50	dichlorodifluoromethane (Removed)
	51	chlorodibromomethane

TABLE B-1. (Continued)

Structural Compound Class	PP#	Pollutant
Volatile Halogenated Alkenes	29	1,1-dichloroethylene
	30	1,2-trans-dichloroethylene
	33	trans-1,3-dichloropropene
	33	cis-1,3-dichloropropene
	85	tetrachloroethene
	87	trichloroethene
	88	vinyl chloride
Volatile Aromatic Hydrocarbons	4	benzene
	38	ethylbenzene
	86	toluene
Volatile Chlorinated Aromatic Hydrocarbons	7	chlorobenzene
Volatile Unsaturated Carbonyl Compounds	2	acrolein
	3	acrylonitrile
Volatile Ethers	19	2-chloroethylvinylether
		bis(chloromethyl)ether (Removed)
Metals	114	antimony
	115	arsenic
	117	beryllium
	118	cadmium
	119	chromium
	120	copper
	122	lead
	123	mercury
	124	nickel
	125	selenium
	126	silver
	127	thallium
	128	zinc
Miscellaneous	121	cyanide
	116	asbestos

a Includes DDT, DDD, and DDE.

b Includes alpha-endosulfan, beta-endosulfan, and endosulfan sulfate.

c Chlorinated 301(h) pesticides that are not on the priority pollutant list.

d Organophosphorus 301(h) pesticides that are not on the priority pollutant list.

TABLE B-2. PRIORITY POLLUTANTS AND 301(h) PESTICIDES LISTED BY EPA PRIORITY POLLUTANT NUMBER

PP#	Pollutant	PP#	Pollutant	PP#	Pollutant
1	acenaphthene	46	bromomethane	91	chlordane
2	acrolein	47	bromoform	92	DDT (a)
3	acrylonitrile	48	dichlorobromomethane	95	endosulfan (b)
4	benzene	49	fluorotrichloromethane (Removed)	98	endrin
5	benzidine	50	dichlorodiflouromethane (Removed)	99	endrin aldehyde
6	tetrachloromethane	51	chlorodibromomethane	100	heptachlor
7	chlorobenzene	52	hexachlorobutadiene	101	heptachlor epoxide
8	1,2,4-trichlorobenzene	53	hexachlorocyclopentadiene	102	alpha-hexachlorocyclohexane
9	hexachlorobenzene	54	isophorone	103	beta-hexachlorocyclohexane
10	1,2-dichloroethane	55	naphthalene	104	delta-hexachlorocyclohexane
11	1,1,1-trichloroethane	56	nitrobenzene	105	gamma-hexachlorocyclohexane
12	hexachloroethane	57	2-nitrophenol	106	PCB-1242
13	1,1-dichloroethane	58	4-nitrophenol	107	PCB-1254
14	1,1,2-trichloroethane	59	2,4-dinitrophenol	108	PCB-1221
15	1,1,2,2-tetrachloroethane	60	4,6-dinitro-o-cresol	109	PCB-1232
16	chloroethane	61	N-nitrosodimethylamine	110	PCB-1248
18	bis(2-chloroethyl)ether	62	N-nitrosodiphenylamine	111	PCB-1260
19	bis(chloromethyl)ether (Removed)	63	N-nitrosodipropylamine	112	PCB-1016
19	2-chloroethylvinylether	64	pentachlorophenol	113	toxaphene
20	2-chloronaphthalene	65	phenol	114	antimony
21	2,4,6-trichlorophenol	66	bis(2-ethylhexyl)phthalate	115	arsenic
22	para-chloro-meta cresol	67	butyl benzyl phthalate	116	asbestos
23	chloroform	68	di-n-butyl phthalate	117	beryllium
24	2-chlorophenol	69	di-n-octyl phthalate	118	cadmium
25	1,2-dichlorobenzene	70	diethyl phthalate	119	chromium
26	1,3-dichlorobenzene	71	dimethyl phthalate	120	copper
27	1,4-dichlorobenzene	72	benzo(a)anthracene	121	cyanide
28	3,3'-dichlorobenzidine	73	benzo(a)pyrene	122	lead
29	1,1-dichloroethylene	74	benzo(b)fluoranthene	123	mercury
30	1,2-trans-dichloroethylene	75	benzo(k)fluoranthene	124	nickel
31	2,4-dichlorophenol	76	chrysene	125	selenium
32	1,2-dichloropropane	77	acenaphthylene	126	silver
33	cis-1,3-dichloropropene	78	anthracene	127	thallium
33	trans-1,3-dichloropropene	79	benzo(ghi)perylene	128	zinc
34	2,4-dimethylphenol	80	fluorene	129	TCDD (dioxin)
35	2,4-dinitrotoluene	81	phenanthrene	--	mirex (c)
36	2,6-dinitrotoluene	82	dibenzo(a,h)anthracene	--	methoxychlor (c)
37	1,2-diphenylhydrazine	83	indeno(1,2,3-cd)pyrene	--	parathion (d)
38	ethylbenzene	84	pyrene	--	malathion (d)
39	fluoranthene	85	tetrachloroethene	--	guthion (d)
40	4-chlorophenyl ether	86	toluene	--	demeton (d)
41	4-bromophenyl ether	87	trichloroethene		
42	bis(2-chloroisopropyl)ether	88	vinyl chloride		
43	bis(2-chloroethoxy)methane	89	aldrin		
44	dichloromethane	90	dieldrin		
45	chloromethane				

a Includes DDT, DDD, and DDE.

b Includes alpha-endosulfan, beta-endosulfan, and endosulfan sulfate.

c Chlorinated 301(h) pesticides that are not on the priority pollutant list.

d Organophosphorus 301(h) pesticides that are not on the priority pollutant list.

TABLE B-3. PRIORITY POLLUTANTS AND 301(h) PESTICIDES LISTED IN ALPHANUMERIC ORDER

PP#	Pollutant	PP#	Pollutant	PP#	Pollutant
11	1,1,1-trichloroethane	102	alpha-hexachlorocyclohexane	95	endosulfan (c)
15	1,1,2,2-tetrachloroethane	78	anthracene	98	endrin
14	1,1,2-trichloroethane	114	antimony	99	endrin aldehyde
13	1,1-dichloroethane	115	arsenic	38	ethylbenzene
29	1,1-dichloroethylene	116	asbestos	39	fluoranthene
8	1,2,4-trichlorobenzene	4	benzene	80	fluorene
25	1,2-dichlorobenzene	5	benzidine	49	fluorotrichloromethane (Removed
10	1,2-dichloroethane	72	benzo(a)anthracene	105	gamma-hexachlorocyclohexane
32	1,2-dichloropropane	73	benzo(a)pyrene	--	guthion (b)
37	1,2-diphenylhydrazine	74	benzo(b)fluoranthene	100	heptachlor
30	1,2-trans-dichloroethylene	79	benzo(ghi)perylene	101	heptachlor epoxide
26	1,3-dichlorobenzene	75	benzo(k)fluoranthene	9	hexachlorobenzene
27	1,4-dichlorobenzene	117	beryllium	52	hexachlorobutadiene
21	2,4,6-trichlorophenol	103	beta-hexachlorocyclohexane	53	hexachlorocyclopentadiene
31	2,4-dichlorophenol	43	bis(2-chloroethoxy)methane	12	hexachloroethane
34	2,4-dimethylphenol	18	bis(2-chloroethyl)ether	83	indeno(1,2,3-cd)pyrene
59	2,4-dinitrophenol	42	bis(2-chloroisopropyl)ether	54	isophorone
35	2,4-dinitrotoluene	66	bis(2-ethylhexyl)phthalate	122	lead
36	2,6-dinitrotoluene	19	bis(chloromethyl)ether (Removed)	--	malathion (b)
19	2-chloroethylvinylether	47	bromoform	123	mercury
20	2-chloronaphthalene	46	bromomethane	--	methoxychlor (d)
24	2-chlorophenol	67	butyl benzyl phthalate	--	mirex (d)
57	2-nitrophenol	118	cadmium	55	naphthalene
28	3,3'-dichlorobenzidine	91	chlordane	124	nickel
60	4,6-dinitro-o-cresol	7	chlorobenzene	56	nitrobenzene
41	4-bromophenyl ether	51	chlorodibromomethane	--	parathion (b)
40	4-chlorophenyl ether	16	chloroethane	22	para-chloro-meta cresol
58	4-nitrophenol	23	chloroform	64	pentachlorophenol
92	DDT (a)	45	chloromethane	81	phenanthrene
61	N-nitrosodimethylamine	119	chromium	65	phenol
62	N-nitrosodiphenylamine	76	chrysene	84	pyrene
63	N-nitrosodipropylamine	33	cis-1,3-dichloropropene	125	selenium
112	PCB-1016	120	copper	126	silver
108	PCB-1221	121	cyanide	85	tetrachloroethene
109	PCB-1232	104	delta-hexachlorocyclohexane	6	tetrachloromethane
106	PCB-1242	--	demeton (b)	127	thallium
110	PCB-1248	68	di-n-butyl phthalate	86	toluene
107	PCB-1254	69	di-n-octyl phthalate	113	toxaphene
111	PCB-1260	82	dibenzo(a,h)anthracene	33	trans-1,3-dichloropropene
129	TCDD (dioxin)	48	dichlorobromomethane	87	trichloroethene
1	acenaphthene	50	dichlorodiflouromethane (Removed)	88	vinyl chloride
77	acenaphthylene	44	dichloromethane	128	zinc
2	acrolein	90	dieldrin		
3	acrylonitrile	70	diethyl phthalate		
89	aldrin	71	dimethyl phthalate		

a Includes DDT, DDD, and DDE.

b Organophosphorus 301(h) pesticides that are not on the priority pollutant list.

c Includes alpha-endosulfan, beta-endosulfan, and endosulfan sulfate.

d Chlorinated 301(h) pesticides that are not on the priority pollutant list.