Hazard Ranking System Issue Analysis: Classification of Hazardous Substances for Potential to Accumulate in the Food Chain

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ABSTRACT

This report, prepared for the Office of Emergency and Remedial Response (OERR) of the Environmental Protection Agency, contains an option for rating the relative potential of hazardous substances to bioaccumulate. This rating scheme is intended as a component of a human food chain exposure methodology which is being separately developed for possible inclusion in the EPA Hazard Ranking System (HRS). This rating scheme makes use of available data on bioconcentration factors, n-octanol-water partition coefficients, and water solubility. In addition, the rating scheme makes use of available information on potential biomagnification of hazardous substances. The system makes use of data in order of its reliability and its availability, as well as on its ability to describe, quantitatively, the potential of a substance to bioconcentrate.

Suggested Keywords: Superfund, Hazard ranking, Hazardous waste, Bioconcentration, Bioconcentration factor surrogates.

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1.0 INTRODUCTION

1.1 Background

The Comprehensive Environmental Response, Compensation, and Liability Act of 1980 (CERCLA) (PL 96-510) requires the President to identify national priorities for remedial action among releases or threatened releases of hazardous substances. These releases are to be identified based on criteria promulgated in the National Contingency Plan (NCP). On July 16, 1982, EPA promulgated the Hazard Ranking System (HRS) as Appendix A to the NCP (40 CFR 300; 47 FR 31180). The HRS comprises the criteria required under CERCLA and is used by EPA to estimate the relative potential hazard posed by releases or threatened releases of hazardous substances.

The HRS is a means for applying uniform technical judgment regarding the potential hazards presented by a release relative to other releases. The HRS is used in identifying releases as national priorities for further investigation and possible remedial action by assigning numerical values (according to prescribed guidelines) to factors that characterize the potential of any given release to cause harm. The values are manipulated mathematically to yield a single score that is designed to indicate the potential hazard posed by each release relative to other releases. This score is one of the criteria used by EPA in determining whether the release should be placed on the National Priorities List (NPL).

During the original NCP rulemaking process and the subsequent application of the HRS to specific releases, a number of technical issues have been raised regarding the HRS. These issues concern the desire for modifications to the HRS to further improve its capability to estimate the relative potential hazard of releases. The issues include:

- Review of other existing ranking systems suitable for ranking hazardous waste sites for the NPL.
- Feasibility of considering ground water flow direction and distance, as well as defining "aquifer of concern," in determining potentially affected targets.
- Development of a human food chain exposure evaluation methodology.
- Development of a potential for air release factor category in the HRS air pathway.
- Review of the adequacy of the target distance specified in the air pathway.
- Feasibility of considering the accumulation of hazardous substances in indoor environments.
- Feasibility of developing factors to account for environmental attenuation of hazardous substances in ground and surface water.
- Feasibility of developing a more discriminating toxicity factor.
- Refinement of the definition of "significance" as it relates to observed releases.
- Suitability of the current HRS default value for an unknown waste quantity.
- Feasibility of determining and using hazardous substance concentration data.

- Feasibility of evaluating waste quantity on a hazardous constituent basis.
- Review of the adequacy of the target distance specified in the surface water pathway.
- Development of a sensitive environment evaluation methodology.
- Feasibility of revising the containment factors to increase discrimination among facilities.
- Review of the potential for future changes in laboratory detection limits to affect the types of sites considered for the NPL.

Each technical issue is the subject of one or more separate but related reports. These reports, although providing background, analysis, conclusions and recommendations regarding the technical issue, will not directly affect the HRS. Rather, these reports will be used by an EPA working group that will assess and integrate the results and prepare recommendations to EPA management regarding future changes to the HRS. Any changes will then be proposed in Federal notice and comment rulemaking as formal changes to the NCP. The following section describes the specific issue that is the subject of this report.

1.2 Issue Description

The U.S. Congress, EPA personnel, and the public have expressed the concern that public health and welfare are potentially threatened by exposure through the human food chain to hazardous substances released from CERCLA sites, and that this route of exposure is not adequately considered in the HRS. In order to

evaluate the potential exposure of humans to hazardous substances through the food chain, it is necessary to evaluate those substances that have the capability to accumulate in parts of the food chain at levels substantially higher than in the surrounding environment. This capability, often referred to as bioaccumulation, has been demonstrated most clearly in the aquatic food chain, although there is reason to believe it also exists in the terrestrial food chain. This paper addresses the issue of how to evaluate those substances which may pose a substantial danger due to their capability to concentrate in the food chain.

1.3 Scope

This paper presents a methodology for classifying substances in order to identify those of primary concern should they enter the human food chain. Specifically, the paper presents a classification scheme based on the potential of the substances to accumulate in the human food chain. This paper is restricted to consideration of the accumulation of hazardous substances in the human food chain; it does not address the relative toxicity of these substances. DeSesso et al. (1986) addresses the toxicity of these substances.

The likely availability (and cost) of the required data was a major consideration in the development of this classification methodology. The methodology presented here is based on the

assumption that the level of data available will continue to be those data obtained during a CERCLA site inspection. This paper is restricted to the potential of substances to accumulate in the food chain. It is not intended to be used to establish a comprehensive human food chain rating methodology for the HRS. Saari (1986) addresses the broader questions of developing a comprehensive human food chain rating methodology for use in the HRS.

In addition, the focus of this paper is primarily on the accumulation of hazardous substances in the surface water pathway component of the food chain. This focus is largely a function of available data. Although a review of the research reported in the literature revealed that aquatic and terrestrial ecosystems both exhibit bioconcentration and, in some cases, biomagnification, there are many references to the potential threat to humans through the aquatic food chain, but none indicating a serious threat via the terrestrial food chain. As a result, it was possible to more readily identify aquatic human food chain impacts, and, therefore, the scope of this paper was largely restricted to the surface water pathway.

In this paper, common definitions are used for processes related to the uptake of hazardous substances (Appendix E contains a comprehensive glossary for all terms in this report). The following four definitions are particularly important:

- Bioconcentration: The process whereby chemical substances enter aquatic organisms through the gills or epithelial tissue directly from water, and are accumulated at levels that exceed the concentration of the substance in the surrounding environment.

- Bioaccumulation: A broader term referring to a process which includes bioconcentration but also any uptake of chemical residues from dietary sources.

- Biomagnification: A process by which the tissue concentrations of bioaccumulated chemical residues increase as these materials run up through the food chain through two or more trophic levels. Historically implicit in the use of this term is the connotation that residue concentrations at successively higher trophic levels increase by integral multiples (e.g., by factors of 3, 4, 5, etc.).

- n-Octanol-Water Partition Coefficient: A measure of the preferential partitioning of a substance between n-octanol and water.

- Solubility: A property of a substance by virtue of which it forms chemically and physically homogeneous mixtures with other substances.

1.4 Approach

In brief, the approach taken to examine the question of which hazardous substances are of most concern in the human food chain incorporated four steps. These steps were: (1) a literature search for indicators which could be used to identify substances with the potential to accumulate in the human food chain, (2) a review of those methods found in the literature search for classifying hazardous substances as to their potential to accumulate in the food chain, (3) the development of a classification scheme suitable for hazardous substances found at waste sites, and (4) the application of the scheme to illustrate the classification of several substances typically found at NPL facilities.

As a result of the literature search and the review of other methods of ranking hazardous substances, several measures were identified as indicators of the potential for a substance to accumulate in food chain organisms. The most important of these are:

- Biomagnification factor
- Bioconcentration factor
- n-octanol-water partition coefficient
- Solubility

As mentioned in Section 2, the occurrence of biomagnification far in excess of reported bioconcentration levels has been documented in the literature for a few substances (e.g., methylmercury, DDT, PCBs). For other substances, however, there is some evidence that the process of biomagnification of chemical residues in the aquatic food chain is quantitatively insignificant when compared to the process of bioconcentration (Macek, 1979).

Bioconcentration factors (BCF) are well documented in the literature for a number of substances. The U.S. Environmental Protection Agency, for example, reports BCFs (when available) in their water quality criteria documents. Reported BCFs range from less than one up to a million. A BCF of 1,000 or more for a given substance indicates a potential for significant bioaccumulation (Trabalka and Garten, 1982), that could cause substantial human exposure to that substance, even if relatively small amounts of food in which the substance is concentrated are ingested.

Unfortunately, BCFs are not available for all of the hundreds of substances found at CERCLA sites. For those substances for which BCFs are not available, it is necessary to estimate BCFs.

The logarithm of the n-octanol-water partition coefficient (log Pow) has been used as a surrogate measurement for the BCF. While the direct measurement of bioconcentration from the environment is preferred, the log Pow commonly is recommended as a surrogate in evaluating the bioconcentration potential of hazardous substances in the absence of direct measurement (e.g., Van Gestel et al., 1985).

The water solubility of a substance is an important characteristic for establishing that substance's potential environmental movement and distribution. In the absence of log Pow data, it is possible to make use of water solubility data to determine the extent to which a substance is inclined to bioconcentrate in an organism (Verschueren, 1983).

Of these four types of data, data on the biomagnification of substances are the least available; BCFs are more commonly available; and log Pow and/or water solubility data are most readily available for a majority of the hazardous substances of concern under CERCLA. A classification scheme using all four types of data is proposed in this report. The scheme uses a hierarchy based on data reliability and availability. Using this hierarchy of data, selected hazardous substances are classified for their potential to bioaccumulate.

Results presented in this report have been used in developing a proposed methodology for incorporating the potential for exposure to hazardous substances via the human food chain in the HRS (Saari, 1986).

1.5 Organization of Report

This report presents a proposed scheme developed to classify the bioaccumulation potential of hazardous substances. The scientific basis of the proposed method is documented and the results of applying the scheme to selected hazardous substances are presented.

The concepts of biomagnification and bioconcentration factors are discussed in Section 2. Examples from field and laboratory studies are provided to support the use of these factors in the classification scheme.

A classification scheme which could be used in the HRS is presented in Section 3. The scheme incorporates a decision tree based on the availability of biomagnification, BCF, log Pow, or solubility data. Using this decision tree, several substances were classified; the results are reported in Appendix A.

Section 4 contains a bibliography of references.

Appendix B provides, for several hundred substances, BCF and log Pow data obtained from the literature and other available data bases.

Appendices C and D provide background material applicable to the proposed ranking scheme. These appendices provide an

explanation for why the reported BCF data have such wide variations. Ecological factors which affect bioaccumulation are explained in Appendix C and chemical factors are explained in Appendix D.

Appendix E is a glossary of ecological terms, acronyms, and other technical terms used in this paper.

Appendix F contains a summary description of other existing methods used to rank hazardous substances and which were reviewed in preparing this report.

2.0 MEASURES OF BIOACCUMULATION POTENTIAL

Many hazardous substances may be concentrated in the aquatic food chain from low ambient levels in water to much higher levels in various species of fish.* For example, fish and shellfish are able to bioaccumulate some organic compounds to levels thousands of times greater than the concentration in the water in which they live. Thus, even substances with very low solubility in water have the potential to achieve high concentrations in aquatic organisms.

The process of bioaccumulation is an especially important consideration in evaluating whether a fish population has accumulated a substance in concentrations which might pose a health hazard to humans eating the fish.

Unfortunately, data providing direct measurement of the ability of a given substance to bioaccumulate in a given species of fish are very limited. Indeed, the very large number of fish species, coupled with the extremely large number of potentially hazardous substances, makes any comprehensive compilation of such measurements impractical. As a result, scientists have developed several methods for estimating the potential of hazardous substances to bioaccumulate in aquatic life. While these methods have their inadequacies, they do provide an indication of the relative hazard

*The term fish as used throughout this report includes fish, shellfish and other aquatic human food chain organisms.

posed by the potential bioaccumulation of hazardous substances, based on data which are readily available.

This section provides information on the processes and chemical characteristics which can be used to describe, in a quantitative manner, the potential for bioaccumulation. These are biomagnification, bioconcentration, the n-octanol-water partition coefficient, and solubility. This section provides technical definitions for each of these, and illustrates how data on each could be used in a hazardous substance food chain impact classification scheme.

Several studies were reviewed to determine possible approaches to estimating bioaccumulation potential. Summary discussions of these studies may be found in Wolfinger and Haus (1986).

2.1 Biomagnification

2.1.1 Definition

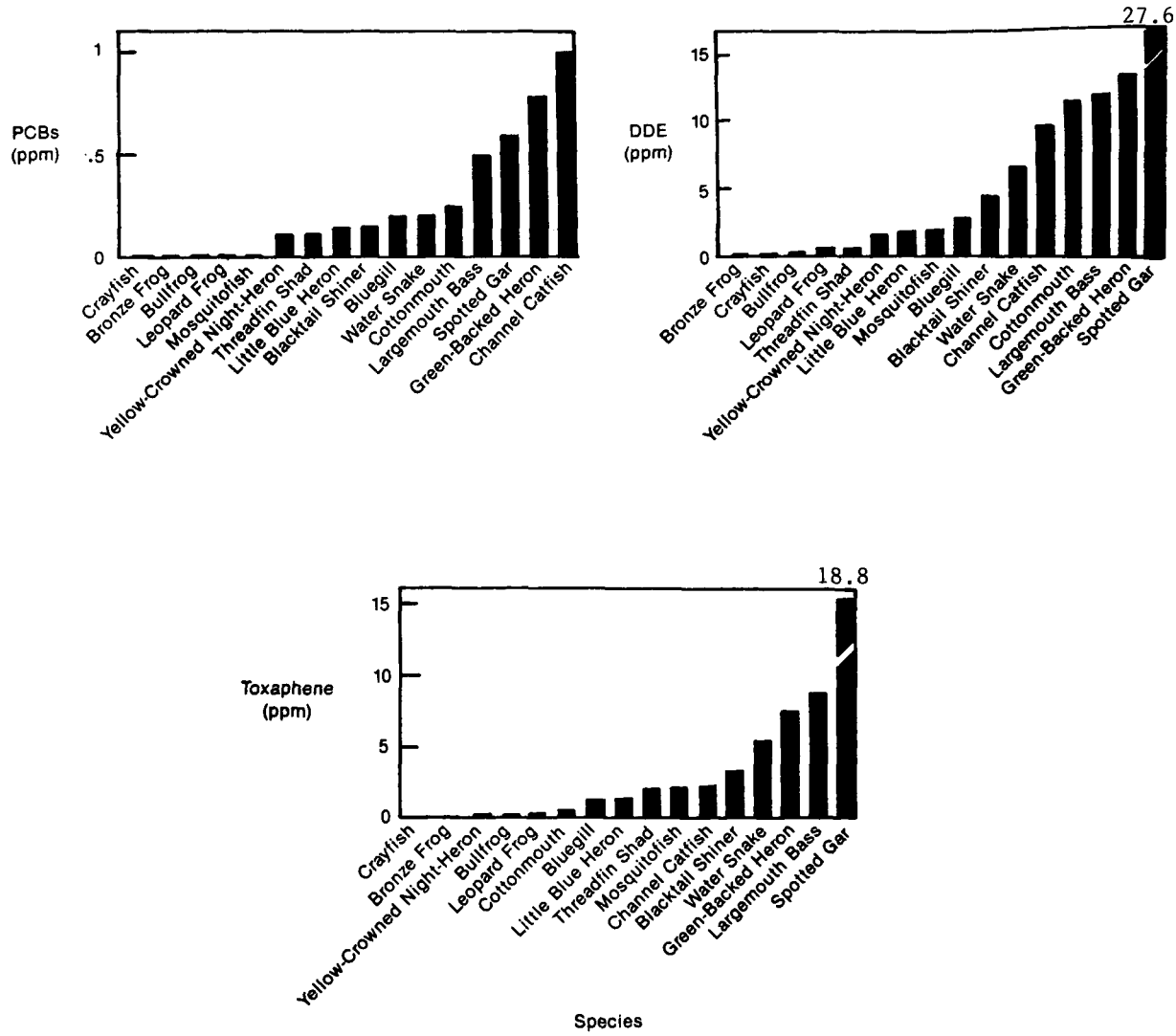
Biomagnification is a biological process whereby a substance becomes increasingly more concentrated in the tissue of different species as the substance moves up the food chain through two or more trophic levels. For example, the environment (e.g., a specific body of water) may have a very low concentration of a substance, but aquatic insects living in it have higher concentrations. The small fish that eat those insects may concentrate the substance even further. Near the top of the food chain, large predator fish may have very high concentrations of that substance.

Figure 1 (from Niethammer et al., 1984) illustrates the classic biomagnification process as it occurs in freshwater lakes of Louisiana. The vertical axes represent the concentrations (in parts per million) of DDE, PCBs, and toxaphene. The horizontal axes, reading from left to right, represent the trophic levels of the animals sampled. For example, on the left are lower order crayfish and frogs which show very low residues. In the middle are small consumers such as bluegills and shiners, which have low concentrations. As one moves up the food chain (to the right), predatory fish, such as the gar and largemouth bass, have higher concentrations of these residues.

2.1.2 Discussion

There are a number of studies (see Appendix B) which report biomagnification of substances in the aquatic ecosystem. It is not so clear that this process occurs in terrestrial ecosystems (Garten and Trabalka, 1983; Walton and Edwards, 1986). In those cases where there is some indication of biomagnification in the terrestrial ecosystem (e.g., the biomagnification of pesticides in birds of prey), very often the top predator is a fish eater.

Measurement of a hazardous substance in all parts of the ecosystem and at all trophic levels of the food chain is both difficult and expensive. While not all research results agree, it is clear that some substances do biomagnify. For example, published



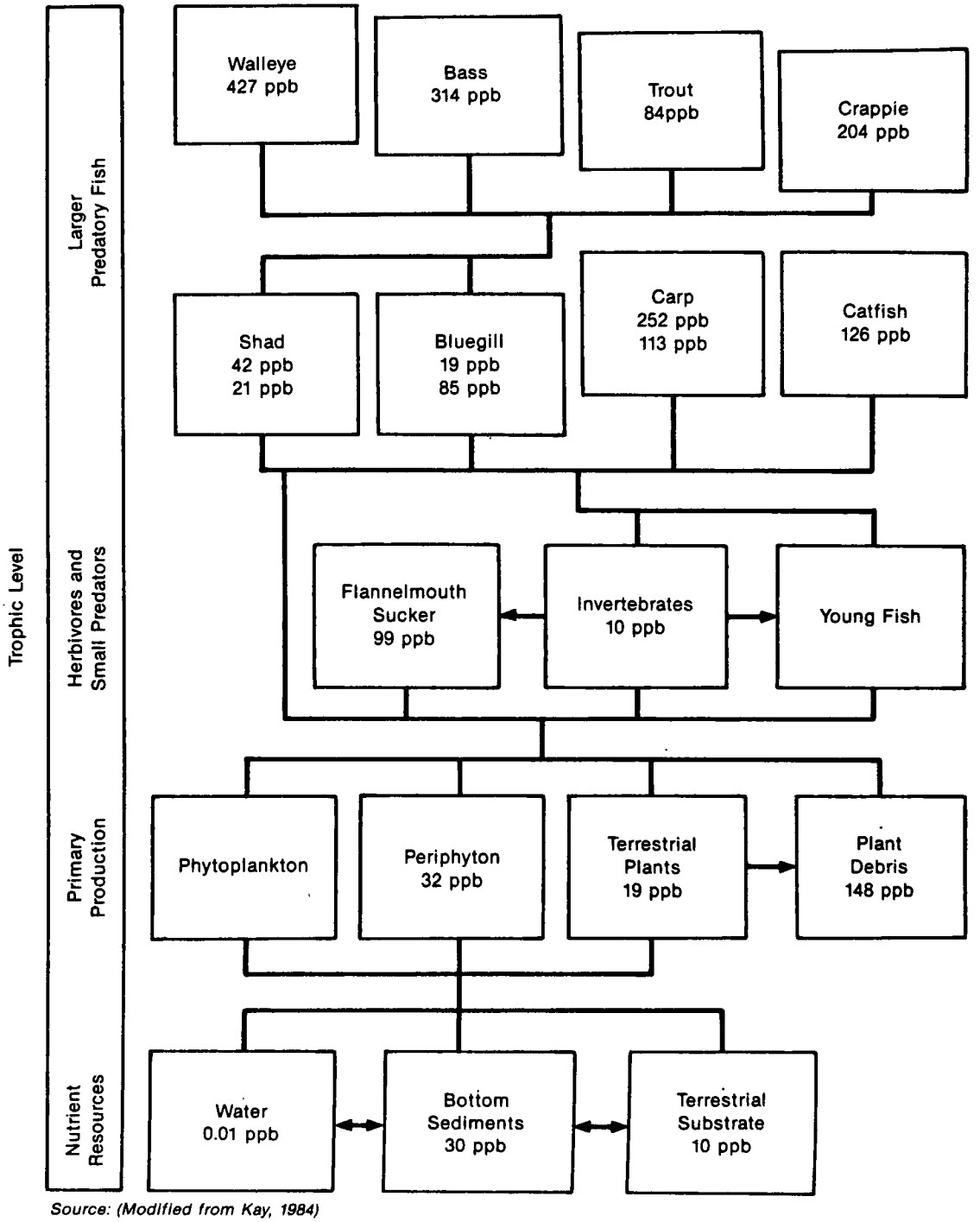
Source: Niethammer et al., 1984.

FIGURE 1
BIOMAGNIFICATION OF DDE, PCBs
AND TOXAPHENE IN LAKE PROVIDENCE, LOUISIANA

research almost universally supports the concept of biomagnification of DDT and its metabolites, PCBs, and mercury. Numerous studies show that DDT biomagnifies in the food chain (Carey et al., 1973; Daly, 1984; Domsch, 1984; Hatfull, 1983; Keene, 1983; Kenaga, 1980; Kodric-Smit et al., 1980; Niethammer et al., 1984; Niewiadowska and Sosyniak, 1983; Ofstad and Martinsen, 1983; U.S. Environmental Protection Agency, 1983). However, Kay (1984) concludes that while there appears to be biomagnification potential for PCBs, methylmercury, kepone, mirex, benzo-a-pyrene, and naphthalenes, "compounds which probably do not biomagnify include DDT and its derivatives."

Kay (1984) describes the biomagnification (Figure 2) of mercury in Lake Powell, Arizona (from Potter et al., 1975). In this case, the water and sediments had relatively low concentrations; small consumers and producers (plants) had slightly higher levels, and the top predator fish (walleye and bass) had the highest concentrations. In countries where fish are a major diet component, methylmercury poisoning of human populations is possible (Ditri and Ditri, 1976).

PCBs have also been demonstrated to biomagnify, especially in large predatory fish (Ray et al., 1984). O'Connor (1984) reports that while fish can take PCBs directly from water (bioconcentration), for striped bass at least, diet appears to be the most significant source of PCBs. Both Larsson (1984) and Rubenstein et al. (1984) conducted laboratory experiments with fish and found food uptake of



Source: (Modified from Kay, 1984)

FIGURE 2
LAKE POWELL, ARIZONA TROPHIC LEVELS
WITH MEAN PARTS PER BILLION MERCURY

PCBs to be the most important route of exposure. In the example of PCB bioaccumulation at the top of the food chain (e.g., lake trout), the older and larger individuals usually have the greatest concentrations of the substance (Thomann and Connolly, 1984). Black (1983) compared the human consumption rates for drinking water and eating fish from the Great Lakes, and he concluded "the relative importance of the fish versus drinking water in this situation can be a little better appreciated if one considers that given a fish contaminated with PCB at 5 ppm, a human would have to drink Great Lakes water for about 1,000 years in order to equal the amount of PCB that you get in a single one pound serving of these contaminated fish."

2.2 Bioconcentration

2.2.1 Definition

Bioconcentration refers to a process through which an organism accumulates a substance to levels that exceed the concentration of the substance in its environment (U.S. Environmental Protection Agency, 1982b). This can also be regarded as the first step in biomagnification. Bioconcentration is most often expressed in terms of a bioconcentration factor (BCF), the ratio of the concentration of the substance in an organism, for example in fish tissue, to the concentration of the same substance in the ambient water. Another, less common measure of bioconcentration is the ratio of the concentration of a substance in plant tissue to its concentration in

the soil the plant grows in. A little used measure of bioconcentration is the ratio of the concentration in animal tissue (e.g., beef) to the concentration in feed.

2.2.2 Bioconcentration Factor

There is a large volume of scientific literature in which the BCFs for a number of substances are reported. Data have been reported on bioconcentration of radionuclides since the 1950s, of pesticides since the 1960s, and of heavy metals since the 1970s. More recently, in the 1980s, ecologists have been reporting measurements of complex organics in food chains. The reports on complex organics include uptake rates and modes of transfer from the environment to biota via food, and directly from water or air.

Research results are available from controlled laboratory experiments as well as from measurements of biota in the field. While some food chain studies may report on only a single segment of the food chain (e.g., uptake from sediment by worms), others report on the entire food chain from producers to consumers, to first order predators, and finally to top predators. Some studies show uptake of residues in a matter of days, while others report uptake only after a year or more of exposure. In some instances where actual measured concentrations in the field or laboratory are unavailable, it may be possible to calculate the BCF by one of several methods described in Moriarty (1983).

Table B-1 of Appendix B summarizes bioconcentration factor data from EPA criteria documents and the peer reviewed literature for over 130 substances reported to be present at NPL sites. Most of these data are reported for aquatic ecosystems, and the BCF values were calculated as the ratio of the concentration of the chemical in fish tissue to the concentration of the chemical in the aquatic habitat of the fish. In many cases, different authors report different BCF values for the same substance (even for the same species), and opinions vary as to the specific value which should be used for the bioconcentration factor.

The wide range in BCFs reported in the literature (see Appendix B) can be explained by a number of ecological and chemical factors. They include:

- Mobility and availability of a particular compound
- Species role or niche in the environment
- Physiological differences among species
- Testing and measurement protocols

These factors are discussed in more detail in Appendices C and D.

2.2.3 Potential Surrogates for Bioconcentration Factor

A number of different factors which might indicate the potential of a substance to bioconcentrate have been considered as surrogates for the BCF. These factors have included the n-octanol-water partition coefficient, solubility, and the soil adsorption coefficient. Each of these has been found to correlate with the bioconcentration factor and

may, therefore, be useful as surrogates when direct bioconcentration measurements are not available (Geyer et al., 1984; Lyman et al., 1982; Veith et al., 1980). For the purposes of classifying bioconcentration potential in the HRS, the n-octanol-water partition coefficient (Pow) and solubility factors have been included in the ranking scheme as surrogates for the BCF for reasons discussed below. The soil adsorption coefficient has not been used for reasons also discussed below. Appendix D discusses other potential surrogates that were considered and rejected because they have not been found to correlate with bioconcentration.

2.2.3.1 n-Octanol-Water Partition Coefficient. When n-octanol, water, and an organic substance are mixed together until equilibrium has been reached, and then allowed to stand, the n-octanol and water will separate into two distinct phases, each of which contains some of the organic substance. The n-octanol-water partition coefficient (Pow) is the ratio of the concentration of the organic substance in the n-octanol to its concentration in water when the system is in equilibrium. In addition to the direct measurement of the Pow, a method of calculating the Pow from information on the chemical structure of a substance has been developed by Lyman et al. (1982).

In general, higher values of the logarithm of the Pow for a substance correlate with higher values of its BCF in fish, and consequently, its bioaccumulation potential. For example, compounds such as DDT and some PCBs which have high BCF values in fish have log

Pow values above 5. Compounds such as monochlorobenzene and tetrachloroethylene which have low BCFs also have log Pow values of less than 3. Garten and Trabalka (1983) suggested that for screening purposes, substances with a log Pow of 3.5 or more should be considered as having the potential to bioaccumulate in mammals or birds.

Many researchers have stated that the logarithm of the Pow has a statistically significant linear correlation with the logarithm of the bioconcentration factor of organic chemical compounds (e.g., Chiou, 1985; Geyer et al., 1984; Lyman et al., 1982; Veith et al., 1980). This relationship is illustrated in Figure 3. Table 1 presents a range of values which various researchers have presented as indicators of this relationship.

This linear relationship occurs because many organic substances bioconcentrate by incorporation into fatty tissue, and the n-octanol-water partition coefficient provides a measure of the preferential partitioning of substances between water and organic or fatty tissue. Based on these relationships and the correlations indicated above, many researchers (e.g., Trabalka and Garten, 1982) have concluded that the log Pow is a highly satisfactory indication of bioaccumulation potential in aquatic systems.

The log Pow cannot, however, be used as a predictor of bioconcentration for inorganic substances, because the mechanism by which inorganic substances accumulate in food chain organisms is different from that for organic substances. Where metals are involved,

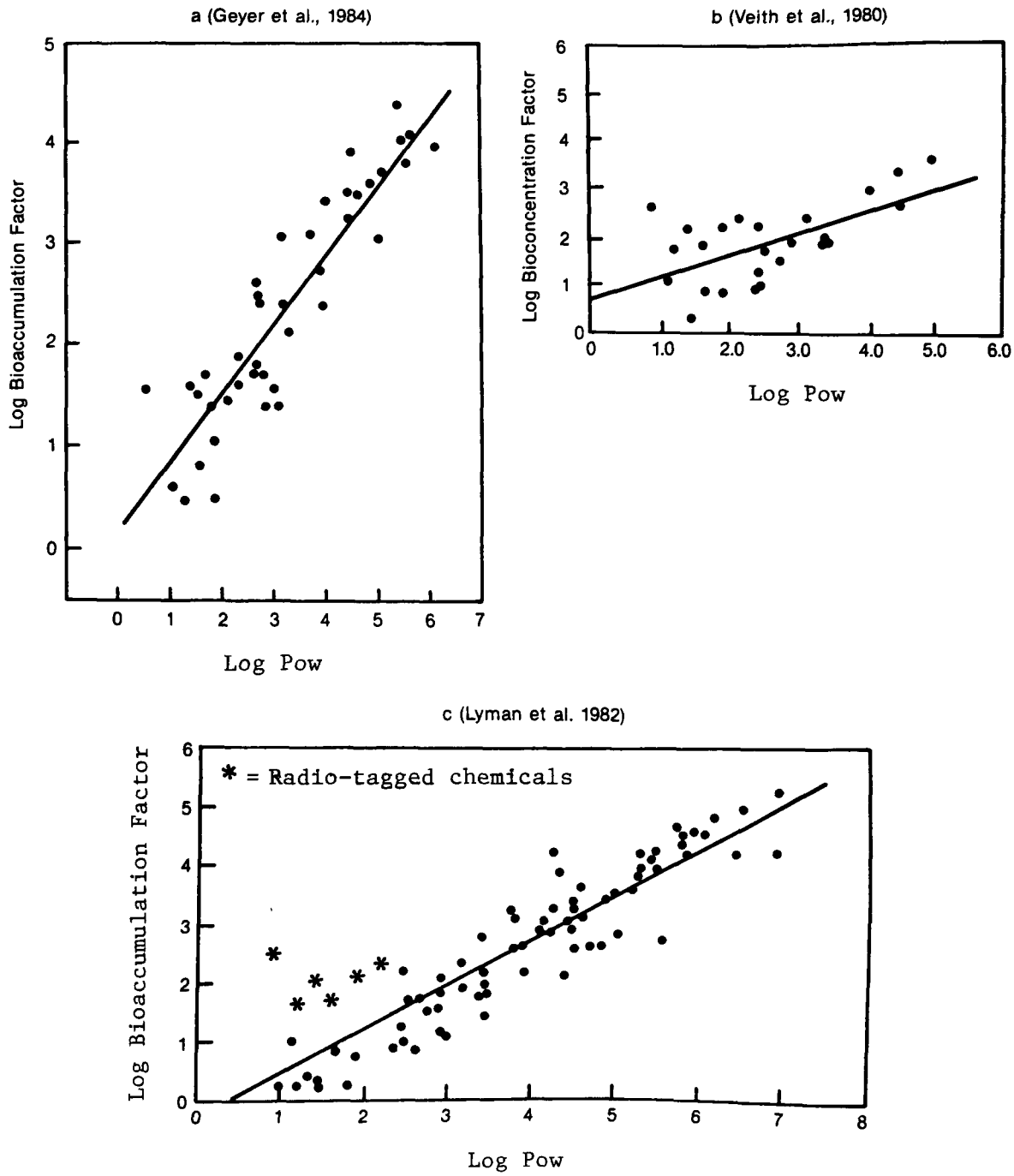


FIGURE 3
EXAMPLE CORRELATIONS OF LOG BCF VERSUS LOG P FOR BIOACCUMULATION

TABLE 1

SUMMARY OF VALUES FOUND IN THE LITERATURE
FOR THE CONSTANTS a AND b IN THE
EQUATION log BCF = a log P_{oct} + b

Value of a	Value of b	r	n	Reference
0.76	-0.23	0.907	84	Veith et al., 1980
0.85	-0.70	0.947	59	Veith et al. 1979
0.858	-0.808	0,955	16	Geyer et al. 1982
0.542	0.124	0.948	8	Neeley et al., 1974
1.1587	-0.7504	0.9771	9	Metcalf et al., 1975
0.6335	0.7285	0.7879	11	Lu and Metcalf, 1975
0.935	-1.495	0.87	26	Kenaga and Goring, 1980
1.53	-3.03	0.843	15	Kanazawa, 1981
1.022	-0.632	0.993	11	Oliver and Niimi, 1983
0.997	-0.869	0.993	11	Oliver amd Niimi, 1983
0.84	-0.057	0.976	12	Oliver and Niimi, 1983
0.86	-0.333	0.984	12	Oliver and Niimi, 1983
0.79	-0.40	0.928	122	Veith and Kosian, 1983

Note: BCF is based on wet weight concentrations.
r = correlation coefficient; n = number of chemicals tested.

Source: van Gestal et al., 1985.

the BCF typically is available from direct measurements (Hildebrand and Cushman, 1976).

For a variety of reasons discussed in Appendices C and D, the relationships indicated in Table 1 do not always provide reliable estimates of the BCF. In addition to being inapplicable for metallic substances, log Pow is generally considered a poor indicator of BCF in those instances where it is greater than 6 (Hawker and Connell, 1985). The table illustrates that different authors have developed different regression equations relating BCF to the Pow. Figure 3 illustrates the potential for outliers. The number of substances used to develop the correlation, the biological organism used, and the accuracy of the measurement technique appear to contribute to the differences in results.

As a result of these and other difficulties, many researchers have warned against indiscriminate use of the Pow. Several authors (e.g., Chiou, 1985; Garten and Trabalka, 1982) have noted, for example, that the bioaccumulation of organic substances that bind to proteins (e.g., methylmercury) is not adequately predicted by generalized relationships based on chemical characteristics such as the Pow. Some substances with a low log Pow (e.g., organometallic compounds), will, in fact, have a high BCF, while other substances with a high log Pow may not show much evidence of bioaccumulation, either because they are not absorbed by the organism, are present in an unavailable form, or are readily metabolized and excreted. These

possibilities are graphically illustrated by the fact that about 25 percent of 68 substances studied by Garten and Trabalka (1983) were classified on the basis of their log Pow values as having a higher bioconcentration potential than their actual measured bioconcentration factors. Additional considerations are generally necessary to establish the potential for bioaccumulation of a substance in the food chain. Only chronic feeding tests can adequately predict the bioaccumulation of a substance. Such tests, however, are both time-consuming and expensive.

As a result, although problems remain in using the n-octanol-water partition coefficient to predict bioconcentration (most notably, log Pow is not applicable for inorganics), it is widely used to rapidly screen organic substances to identify those with potential for bioconcentration.

2.2.3.2 Other Chemical Parameters. Besides the n-octanol-water partition coefficient, water solubility and soil adsorption coefficients are the properties most commonly used to predict the bioconcentration of organic compounds in food chain organisms. Substances with low water solubility are likely to bioconcentrate. Substances with high soil adsorption are also likely to bioconcentrate. Both measures have been used to predict BCFs in a manner similar to the Pow. Both are well correlated with log Pow; however, because solubility data are more readily available than soil adsorption coefficients, the solubility data have been adopted for use in this classification scheme.

The measurement of water solubility does not usually impose particularly complicated demands on standard chemical techniques, although measurement for some barely soluble substances can require specialized equipment. However, since the design of many chemical and environmental tests requires precise information on water solubility, these tests are standard for the chemical industry, and data are widely available.

Unfortunately, there are many variables which can affect the solubility of a substance in water, including other chemicals in the water, the temperature, and the molecular structure of a substance and the associated purity of the substance. In addition, there are some difficulties in conducting measurements of low solubility substances. As a result of these factors, specific values reported for water solubility may be suspect (Verschueren, 1983).

Chiou et al. (1977) and others have noted nonetheless that there is a good correlation between the logarithm of water solubility of organic compounds and the logarithm of their n-octanol-water partition coefficient. Furthermore, this correlation has been extended to determine a correlation between the BCF and the solubility of a substance. Overall, while there are a variety of factors which make the correlation between solubility and BCF less certain than the correlation between log Pow and BCF, the correlation is quite strong (R^2 greater than .66), and these solubility values can be used effectively when Pow data are not available.

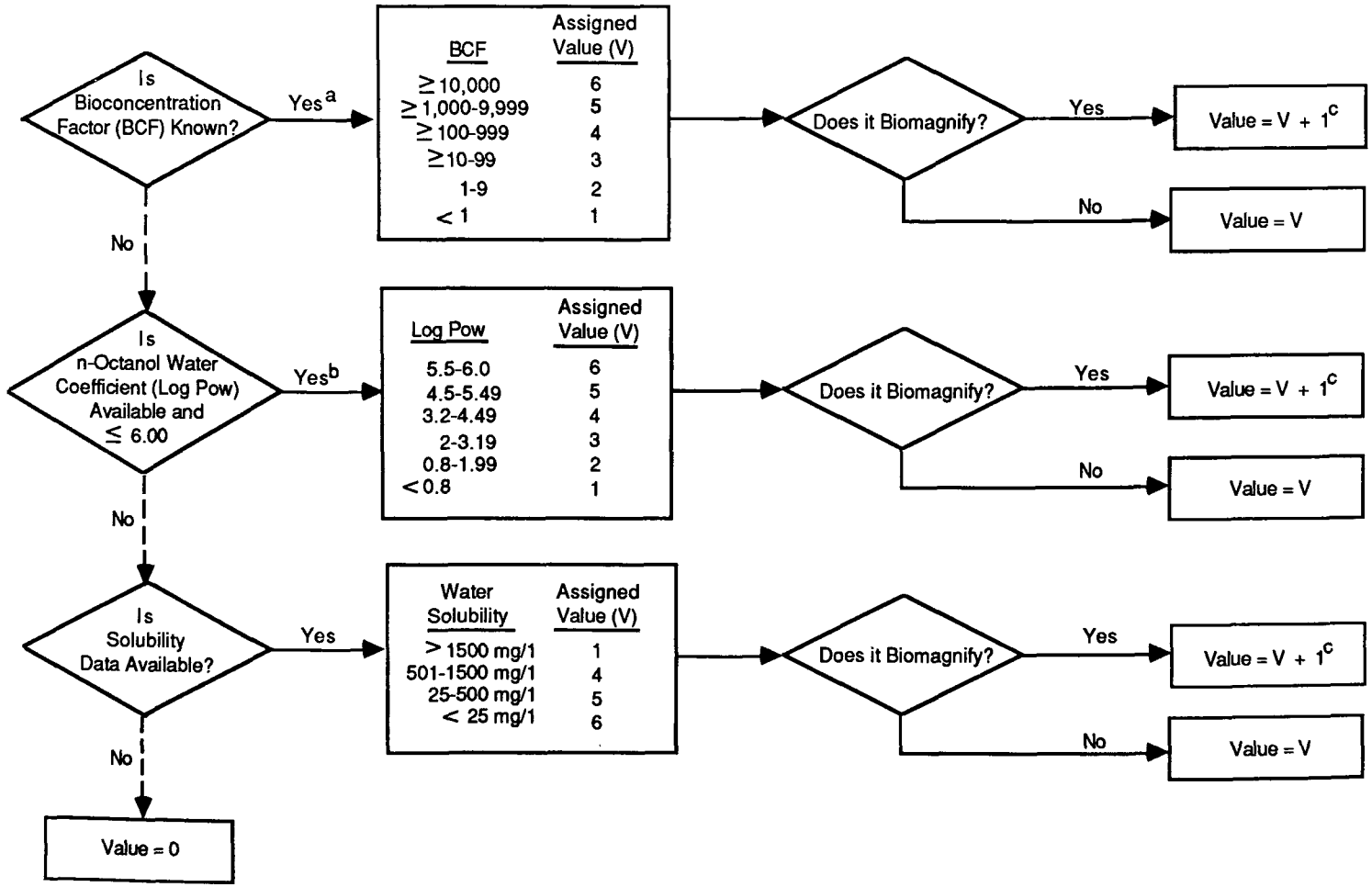
3.0 THE PROPOSED RANKING SCHEME

This chapter contains a scheme for classifying the potential of substances to bioaccumulate in the food chain. The proposed methodology meets the following conditions:

- Supported by published scientific literature.
- Uses readily available data.
- Able to differentiate among different levels of potential bioaccumulation.
- Easily calculable by, or available to, a nonchemist.
- Easily applied to a large number of substances.

3.1 Overview of the Ranking Scheme

The proposed scheme is illustrated as a decision tree in Figure 4. The guiding principle of this scheme is that it is adaptable to the data available for a substance. Within this context, data obtained from direct measurements of bioconcentration factors are considered to be most reliable, and should be used first. Within this category, field measurements should be used before laboratory measurements. If BCF data are not available, data on n-octanol-water partition coefficient should be used, if these data are not available information on solubility should be used. Although information on biomagnification is considered somewhat controversial, available data on this process are included in the scoring system to slightly elevate the rating for those substances which may biomagnify. If none of these data are available, the substance is given a score of zero. If available data show that the substance is not found in food or biota,



[a] Use EPA bioconcentration values provided in EPA Water Quality Criteria documents if available, otherwise use maximum value found in literature.
[b] Either as reported from published literature; or calculated by Leo's Fragment Constant Method; or from Log P Data Base.
[c] If V = 6, then final score is 6, regardless of biomagnification.

FIGURE 4
DECISION TREE FOR RANKING SUBSTANCES FOR POTENTIAL TO BIOACCUMULATE IN THE FOOD CHAIN

the substance is assumed to not bioaccumulate, and is assigned a score of one in the evaluation scheme.

Within each of the data classes (i.e., BCF, Pow, solubility), evaluation classes of 1 to 6 are used to indicate the relative potential of substances to bioaccumulate. On this relative scale, a value of 1 means that the substance probably does not bioaccumulate in tissues, while a value of 6 indicates a high bioaccumulation potential. A hazardous substance would receive a value of 6 because available data indicates that it has a very high bioconcentration factor. If the literature indicates that a substance may biomagnify, then an enhancement factor of +1 is added to the value obtained from either the BCF, Pow, or solubility data. In no case is a value greater than 6 assigned to a substance. That is, if the BCF of a substance is high enough that the substance is given a score of 6, and the literature indicates that the substance may biomagnify, the final score for the substance under this scheme would be 6.

3.1.1 Classification Based on Bioconcentration Factor

Bioconcentration factors reported in the literature range from less than one (no bioconcentration) to a million. For ranking purposes within the HRS, the scheme presented in this paper uses powers of 10 to create classes, with a BCF of 10,000 set as the upper level (i.e., substances with a BCF of 10,000 or greater receive a score of 6). This ranking reflects the fact that substances such as DDT, dioxin, and PCBs, known to present high risk

to human health, have a BCF of 10,000 or higher. For purposes of ranking in the HRS, an assumption is made that the higher the bioconcentration factor, the greater the potential for humans to ingest, or for seafood to accumulate, significant amounts of a substance, and the greater the potential threat of significant exposure to humans via the food chain.

3.1.2 Classification Based on Logarithm of the n-Octanol-Water Partition Coefficient

If bioconcentration data are not available for a substance, the first choice for a surrogate is log Pow data. While log Pow data allow a good approximation of log BCF, they must be used with care.

For example, Veith (1979) has noted that several researchers have suggested the relationship presented in Section 2 be used with caution for chemicals with a molecular weight greater than 600. Spacie and Hamerlink (1985) have suggested that there are limitations in using log Pow data which are outside the 2-5 range. Hawker and Connell (1985) have suggested that for compounds with log Pow greater than 6, the log BCF/log Pow relationship breaks down due to the lengthy time required to reach equilibrium. Others (e.g., Van Gestal et al., 1985) have suggested that substances with very high values for log Pow (e.g., greater than 6.0) may not tend to bioconcentrate due to their (potentially) large molecular size. In addition to these factors, it has been reported that it is extremely difficult to accurately measure substances with log Pow greater than 6.0 (MacKay, 1982).

Based on these considerations, substances for which log Pow data are available, and whose log Pow is greater than 5.5 and less than 6.0 are assigned a ranking value of 6 (see Figure 4). This practice is consistent with both the Michigan Site Assessment System (1984) and Veith et al. (1980), who use a log Pow of 6.0 as the highest (worst case) score for log Pow. It also is consistent with the assignment of the value of 6 to compounds with a BCF greater than 10,000. Furthermore, this approach will flag those substances whose log Pow values are high enough to suggest that this value may not be a good surrogate for the BCF of a substance. While using a log Pow value of 6.0 may include some substances whose BCF is lower than might be predicted from the log Pow information (Garten and Trabalka, 1982), the value of 6.0 has been selected to make maximum use of available data in the HRS screening process. Substances for which actual BCF data are not available and whose log Pow in greater than 6.0 should be ranked based on solubility data (see below). The remaining assigned values presented in Figure 4 are derived from Veith's (1979) regression equation and the assigned values based on BCF data.

In summary, this scheme would assign the highest rating values (on the 1-6 scale) to those substances with a log Pow from 5.5 to 6.0. The lowest value (1) would be assigned to substances with log Pow less than 0.8. Overall, this ranking scheme matches the six classification categories established using bioconcentration factors and provides a reliable indicator of potential bioaccumulation.

Using the log Pow value for organic substances tends to err on the conservative side; i.e., it may predict an organic substance will bioaccumulate when in fact it does not. For example, as noted earlier, Garten and Trabalka (1983) found that, using log Pow data to predict bioconcentration, 25 percent of the organic compounds reviewed were "false positive" classifications (i.e., overrated with regard to their bioconcentration factor). As a result, use of the log Pow is recommended only when BCF data are not available. It should also be remembered that log Pow data cannot be used for inorganic substances.

3.1.3 Water Solubility

In those instances in which neither BCF nor log Pow data are available (or where log Pow exceed 6.0), data on water solubility (S) can be used as a surrogate for BCF data. In general, water solubility is inversely related to BCF, following the general equation (Garten and Trabalka, 1982):

$$\log BCF = -0.48 \log S + 4.42 \quad R^2 = 0.66$$

Using this relationship, BCF is projected to be less than 100 if S is greater than about 25 mg/liter. Although the constants in the above equation have been subject to some dispute, van Gestal et al. (1985), while recognizing the uncertainty in the regression, have concluded that log Pow would be less than 3 and BCF less than 100, if S is greater than 25 mg/liter.

Similarly, the BCF of a substance is expected to be less than 10 if the solubility of that substance is greater than about 1,500 mg/liter.

Once again, in order to be conservative, in this scheme a rating value of 4 is assigned to those substances with solubility greater than or equal to 25 mg/liter. Again, to provide for a conservative measure, a rating value of 1 is assigned to substances with an S value greater than or equal to 1,500 mg/liter.

Unfortunately, data on the S value for various organic substances does not reliably discriminate among those substances which tend to most strongly bioconcentrate. In order to provide as conservative a screening mechanism as is reasonable in this scheme, a rating value of 6 has been assigned to substances with S values less than 25 mg/liter. The literature does not support further subdivision based on solubility, so none has been attempted. Furthermore, it has been noted that it is extremely difficult to measure S below 10 mg/liter, so concentrations below this level may be suspect. It should be emphasized that under this scheme solubility data would be used only if BCF and log Pow data are not available.

3.2 Decision Procedures for Ranking Hazardous Substances

This section presents the procedures for using the proposed classification methodology. These procedures were used to evaluate

several substances reported present at NPL facilities as an illustration of the classification scheme.

With reference to Figure 4, the first question in the decision tree is to determine whether information on bioconcentration for a specific substance is available. If this data is available, the substance is ranked according to the scheme presented above (e.g., if the BCF is greater than 10,000, the substance is scored as 6).

Similarly, if information on BCF is not available, the substance is ranked on the n-octanol-water partition coefficient, if data for it is available and log Pow is less than 6.0. If data on the n-octanol-water partition coefficient are not available or if the log Pow is greater than 6.0, the substance is ranked on water solubility.

At each stage in the decision tree, it is necessary to ask a second question after a "yes" response is obtained and an initial estimate of a score for a specific substance is generated. That is, it is necessary to determine if the substance being considered has been shown to biomagnify through the food chain. If the substance has been shown to biomagnify, and if the initial score obtained from using BCF, Pow, or S data is less than 6, than 1 should be added to the initial score to elevate the rating value because of the biomagnification potential. In no instance should a substance be scored higher than 6.

For those substances for which there is no information on BCF, Pow, or S, a score of zero would be assigned under this scheme. The general rationale for assigning a "zero" in this instance is that in employing a screening mechanism, it is not desirable to impute knowledge concerning a substance when there is none. Finally, it is possible to "tag" substances for which there are no data available for further investigation. This investigation would allow, at least, a laboratory analysis of the water solubility of the substance, and could lead to a preliminary score for that substance.

The scheme for ranking substances for which only solubility data are available reflects the fact that this information is less certain than either the BCF or Pow data. Specifically, solubility data provide a good indication of those substances which are not likely to bioaccumulate, but information on the extent to which a substance may bioaccumulate is not easy to determine from solubility data alone. If a more refined screening is desired for those substances for which only S data is available, a detailed laboratory analysis of either the Pow or the BCF of the substance is required.

3.3 Illustration of Proposed Ranking Scheme

Appendix A contains a series of examples of how this scheme would be used to rank substances.

Table B-1 gives the measured BCFs for over 130 hazardous substances. It also indicates substances believed to biomagnify. Tables B-2 and B-3 present data on the log Pow. Table B-2 is taken

from a computerized data base which is maintained by and available from Technical Database Services, Inc. (1985). Table B-3 relies on either values reported in the open literature or on calculations performed by The MITRE Corporation. Data on water solubility are available in publications such as Verschueren (1983). Using these data, a series of substances were ranked to illustrate the use of the decision tree in Figure 4. This illustration is contained in Appendix A.

In this ranking scheme, hazardous substances with a high potential to bioaccumulate in the food chain would have one or more of the following characteristics:

- BCF of 10,000 or more
- Log Pow of greater than 5.5 to 6.0
- S less than 25 mg/liter

This classification of a substance in terms of its potential for bioaccumulation in the food chain is intended to be factored into a methodology for rating human food chain exposure in the HRS. This rating methodology is explained separately (Saari, 1986).

4.0 BIBLIOGRAPHY AND REFERENCES

Alexander, Martin, 1985. Biodegradation of Organic Chemicals. Environmental Science and Technology. 18(2):106-111.

Andelman, Julian B., 1973. Incidence, Variability and Controlling Factors for Trace Elements in Natural Fresh Waters (in) Trace Metals and Metal Organic Interactions in Natural Waters. Edited by P.C. Singer. Ann Arbor Science, Inc., Ann Arbor, MI.

Arbuckle, W.B., 1983. Estimating Activity Coefficients for Use in Calculating Environmental Parameters. Environmental Science and Technology 17(9):537-542.

Bahner, L.H., A. Rebekah, A. Rigby, and L.A. Faas, 1983. Bioavailability of Kepone from Sediments to Several Estuarine Species. Research and Development Abstracts. EPA/ERL Gulf Breeze Lab, FL.

Banerjee, Sujit, 1984. Solubility of Organic Mixtures in Water. Environmental Science and Technology 18(8):587-591.

Barnthouse, L.W., J.E. Breck and G.W. Suter, 1986. Development and Demonstration of a Hazard Assessment Rating Methodology for Phase II of the Installation Restoration Program. Oak Ridge National Laboratory, ORNL/TM-9857. Oak Ridge, TN.

Berthelin, J. and U. Dommergues, 1976. The Role of Heterotrophic Microorganisms in the Deposition of Iron and Carbon in Soil Profiles, in Environmental Biogeochemistry, Vol. 2, edited by J.O. Nriagu. Ann Arbor Science, Ann Arbor, MI.

Beveridge, A. and W.F. Pickering, 1983. The Influence of Surfactants on the Adsorption of Heavy Metal Ions by Clays. Water Research 17(2):215-225.

Black, John J., 1983. Testimony to House Subcommittee on Fisheries and Wildlife Conservation and the Environment. 98th Congress No. 98-40, Washington, DC.

Bourquin, A.W. and P.H. Prichard, 1983. Microbial Degradation of Pollutants in Estuarine/Marine Environments (in) Proceedings of Conference on Genetic Control of Environmental Pollutants. Wolfebord, H.H. (ed.). Plenum Press.

Bro-Rasmussen, F. and K. Christiansen, 1984. Hazard Assessment - A Summary of Analysis and Integrated Evaluation of Exposure and Potential Effects from Toxic Environmental Chemicals. Ecological Modeling 22(1-4):67-84.

Brown, Jeffrey, ed., 1985. Compound Evaluation and Analytical Capability Annual Residue Plan. U.S. Department of Agriculture, Food Safety and Inspection Service, Washington, DC.

Bruggeman, W.A., J. VanderSteen, and O.J. Hutzinger, 1982. Reversed-Phase Thin-Layer Chromatography of Polynuclear Aromatic Hydrocarbons and Chlorinated Bi-Phenyls: Relationship With Hydrophobicity as Measured by Aqueous Solubility and Octanol-water Partition Coefficient. Journal of Chromatography 238:335-346.

Callahan, M.A., et al., 1979. Water Related Environmental Fate of 129 Priority Pollutants. U.S. Environmental Protection Agency EPA-440/4-79-029a (prepared by Versar). Washington, DC.

Carey, A.E., C.B. Weersma, H. Tai, and W.G. Mitchell, 1973. Organochlorine Pesticide Residues in Soil and Crops of the Corn Belt Region, 1970. Pesticide Monitoring Journal 6(4):369-376.

Chaney, R.L., 1983. Food Chain Pathways for Toxic Metals and Toxic Organics in Wastes (in) Proceedings of 4th Life Science Symposium, Gatlinburg, TN, October 1981, Frances and Auerback (eds.).

Chiou, C.T., V.H. Freed, D.W. Schmedding, and R.L. Kohnert, 1977. Partition Coefficient and Bioaccumulation of Selected Organic Chemicals. Environmental Science and Technology 11(5):475-478.

Chiou, Cary T., 1985. Partition Coefficients of Organic Compounds in Lipid-Water Systems and Correlations with Fish Bioconcentration Factors. Environmental Science and Technology 19(1):57-62.

Cleveland, Mary E., 1983. Biotic and Abiotic Factors Affecting Sorption of Toxic Compounds to Natural Sediments. MS Thesis, University of W. Florida, Pensacola, FL.

Colwell, R.R., G.S. Sayler, J.P. Nelson, Jr., and A. Justice, 1977. Microbial Mobilization of Mercury in the Aquatic Environment (in) Environmental Biogeochemistry, Vol. 2. Edited by J.O. Nriagu. Ann Arbor Science, Ann Arbor, MI.

Connolly, J.P., M.E. Cleveland, and P.H. Pritchard, 1983. Validity of Partition Coefficient as the Adsorption Descriptor in Exposure Concentration Predictions: Studies with Kepone. Research and Development Abstracts. EPA/ERL Gulf Breeze Laboratory, FL.

Connor, Michael S., 1984. Comparison of the Carcinogenic Risks from Fish vs. Groundwater Contamination by Organic Compounds. Environmental Science and Technology 18(8):628-631.

Cooley, R.V. and P.L. McCarty, 1977. Kinetics of Microbiological Aerobic Decomposition of Methylmercury (in) Environmental Biogeochemistry, Vol. 2. Edited by Jerome O. Nriagu. Ann Arbor Science, Ann Arbor, MI.

Corey, J.C. and A.L. Boni, 1977. Summary of Plutonium Terrestrial Research Studies. Environmental Transport and Effects Research, Annual Report. DOE-DP-1489. Department of Energy, Washington, DC.

Daly, O.G., 1984. Water Pollution from Agriculture. Farm Food Research 15(1):4-6.

Dawson, S.V., H. Cabrera, and N.Y. Kado, 1983. Toxic Substances in the Atmospheric Environment. Journal Air Pollution Control Association 33(9):827-834.

DeSesso, J. et al. (1986). Hazard Ranking System Issue Analysis: Toxicity as a Ranking Factor (Draft), (MTR-86W128). The MITRE Corporation, McLean, VA.

Ditri, P.A. and F.M. Ditri, 1976. Mercury Contamination: A Human Tragedy. Wiley Interscience Publication. John Wiley and Sons, New York.

Dixon, Elizabeth and Gregory Holton, 1984. Foodchain: A Monte Carlo Model to Estimate Individual Exposure to Airborne Pollutants via the Foodchain Pathway (in) Computer Applications in Health Physics (Kathren et al., eds.) Proceedings 17th Mid-year Topical Symposium of the Health Physics Society: 4:129-135.

Domsch, K.H., 1984. Effects of Pesticides and Heavy Metals on Biological Processes in Soil. Plant Soil 76(1-3):367-78.

Dreesen, D.R. and J.M. Williams, 1982. Mobility and Bioavailability of Uranium Mill Tailings Contaminants. Environmental Science and Technology 16(10):702-709.

Drifmeyer, J.E. and W.E. Odum, 1975. Lead, Zinc, and Manganese in Dredge-Spoil Pond Ecosystems. Environmental Conservation 2(1):39-45.

Duke, W., 1982. Introduction: Proceedings of Conference on Meaningful Measures in Marine Pollution Effects. U.S. National Oceanic and Atmospheric Administration. Pensacola Beach, FL.

Fiksel, J. and M. Segal, 1982. An Approach to Prioritization of Environmental Pollutants. The Action Alert System Final Report (Rev). Arthur D. Little, EPA Cont. 68-01-3857, Cambridge, MA.

Filov, V.A., M.D. Golubev, E.I. Liublina, and N.A. Tolokontsev, 1979. Quantitative Toxicology. John Wiley and Sons, New York, NY.

Fish, R.H., F.E. Brinckman, and K.L. Jewett, 1982. Fingerprinting Inorganic Arsenic and Organoarsenic Compounds in In-Situ Oil Shale Retort and Process Waters Using a Liquid Chromatograph Coupled with an Atomic Absorption Spectrometer as a Detector. Environmental Science and Technology 16(3):17 5-179.

Fraser, J.L. and K.R. Lum, 1983. Availability of Elements of Environmental Importance in Incinerated Sludge Ash. Environmental Science and Technology 17(1):52-54.

Garten, C.T. and R.C. Dahlman, 1978. Plutonium in Biota from an East Tennessee Floodplain Forest. Health Physics 34:705-712.

Garten, C.T. and J.R. Trabalka, 1983. Evaluation of Models for Predicting Terrestrial Food Chain Behavior of Xenobiotics. Environmental Science and Technology 17(10):590-595.

Gerike, P. and W.K. Fischer, 1979. A Correlation Study of Biodegradability Determinations with Various Chemicals in Various Tests. Ecotoxicology and Environmental Safety 3:159-173.

Geyer, H., G. Politzki, and D. Freitag, 1984. Prediction of Ecotoxicological Behavior of Chemicals: Relationship Between n-Octanol/Water Partition Coefficient and Bioaccumulation of Organic Chemicals by Alga Chlorella. Chemosphere 13(2):269-284.

Geyer, H. et al., 1982. Prediction of Ecotoxicological Behavior of Chemicals: Relationship Between Physicochemical Properties and Bioaccumulation of Organic Chemicals in the Mussel Mytilus Edulis. Chemosphere 11:1121-1134.

Ghisalba, O., 1983. Chemical Wastes and Their Biodegradation. Experimentia 39(11):1247-57. Basel, Switzerland.

Gillett, J.W., 1983. A Comprehensive Prebiological Screen for Ecotoxicologic Effects. Environmental Toxicology and Chemistry 2:463-476.

Gunderson, Ellis, 1985. (Personal Communication). Food and Drug Administration. Washington, DC.

Guthrie, R.K. and E.M. Davis, 1979. Biomagnification of Heavy Metals by Organisms. Bulletin Environmental Contamination and Toxicology 21:53-61.

Guthrie, R.K., E.M. Davis, D.S. Cherry, and H.E. Murray, 1979. Biomagnification of Heavy Metals by Organisms in a Marine Microcosm. Bulletin Environmental Contamination and Toxicology 21:53-61.

Hansen, David J., 1982. Utility of Toxicity Tests to Measure Effects of Substances on Marine Organisms (in) Proceedings of Conference on Meaningful Measures of Marine Pollution Effects. National Oceanic and Atmospheric Administration, Pensacola Beach, FL.

Hanson, W.C., 1975. Ecological Considerations of the Behavior of Plutonium in the Environment. Health Physics 28:529-537.

Hardy, J.T., R.L. Schmidt, and C.W. Apts, 1981. Marine Sediments and Interstitial Water: Effects of Bioavailability of Cadmium to Gills of the Clam. Bulletin Environmental Contamination Toxicology 27:798-805.

Harshbarger, John, 1983. Testimony to House Subcommittee on Fisheries and Wildlife Conservation and the Environment. 98th Congress. HR No. 98-40. Washington, DC.

Hartley, D.M. and J.B. Johnston, 1983. Use of the Freshwater Clam (Corbicula manilensis) as a Monitor for Organochlorine Pesticides. Bulletin Environmental Contamination Toxicity 31:33-40.

Hatfull, R.S., 1983. Survey of Pesticide Residues in Foodstuffs, 1981. Journal Association of Public Analysts 21(1):19-24. Stafford, U.K.

Hawker, D.W. and D.W. Connell, 1985. Prediction of Bioconcentration Factors Under Non-Equilibrium Conditions. Chemosphere 14(11/12): 1835-1843.

Hildebrand, S.G. and R.M. Cushman, 1976. The Potential Toxicity and Bioaccumulation in Aquatic Systems of Trace Elements Present in Aqueous Coal Conversion Effluents (in) Trace Substances in Environmental Health Symposium. Edited by D.D. Hemphill. Univ. of Missouri, Columbia, MO.

Holdway, D.A., J.B. Sprague, and J.G. Dick, 1983. Bioconcentration of Vanadium in American Flagfish Over One Reproductive Cycle. Water Research 17(8):937-941.

Hutchison, T.C., A. Fedorenko, J. Fitchko, A. Kuja, J. Vanloon, and J. Lichwa, 1977. Movement and Compartmentation of Nickel and Copper in an Aquatic Ecosystem (in) Environmental Biogeochemistry, Vol. 2. Edited by J.O. Nriagu. Ann Arbor Science, Ann Arbor, MI.

Hushon, J.M., A.W. Klein, W.J.M. Strachan, and F. Schmidt-Bleek, 1983. Use of OECD Premarket Data in Environmental Exposure Analysis for New Chemicals. Chemosphere 12(6):887.

Hushon, J.M. and M.R. Kornreich, 1984. Scoring Systems for Hazard Assessment. Hazard Assessment of Chemicals: Current Developments 3:63-109. Academic Press.

ICF, Inc., 1985. Regulatory Impact Analysis of Reportable Quantity Adjustments Under Sections 102 and 103 of the Comprehensive Environmental Response, Compensation, and Liability Act (Vol. 1-5), prepared for U.S. Environmental Protection Agency, Office of Emergency and Remedial Response. Washington, DC.

ICF, Inc., 1985b (Draft). Superfund Public Health Evaluation Manual. Prepared for Office Emergency and Remedial Response U.S. Environmental Protection Agency, (Oct. 1, 1985). Cont. No. 68-01-7080. Washington, DC.

Interagency Testing Committee, 1977. Initial Report of the TSCA Interagency Testing Committee to the Administrator, Environmental Protection Agency, (Oct. 1, 1977). Federal Register 42(197):55026-55080.

Inter-Governmental Maritime Consultative Organization, 1973. Annex II of the International Conference on Marine Pollution. Regulations for the Control of Pollution by Noxious Liquid Substances in Bulk. Regulation 8, Appendix I, pp. 97-104. Washington, DC.

Jenne, E.A. and S.N. Luoma, 1977. Biological Implications of Metals in the Environment (in) Wildung, R.E. and H. Drucker, pp. 110-143. NTIS, Springfield, VA.

Jewett, K.L., F.E. Brinckman, and J.M. Bellama, 1975. Chemical Factors Influencing Metal Alkylation in Water (in) Marine Chemistry in the Coastal Environment. Thomas M. Church, editor. American Chemical Society, Washington, DC.

Jones, W.E., 1975. Detection of Pollutants by Fish Tests. Water Treatment and Examination 24(2):132-139.

Jones, R. and M.S.E. Burgess, 1984. Zinc and Cadmium in Soils and Plants Near Electrical Transmission (Hydro) Towers. Environmental Science and Technology 18(10):731-734.

Kanazawa, J., 1981. Measurement of the Bioconcentration Factors of Pesticides by Freshwater Fish and Their Correlation with Physicochemical Properties or Acute Toxicities. Pesticide Sciences 12:417-424.

Kay, Stratford H., 1984. Potential for Biomagnification of Contaminants within Marine and Freshwater Food Webs. U.S. Army Engineer Waterways Experimental Station, Tech. Rept. D-84-7. Vicksburg, MS.

Keene, J.C., 1983. Managing Agricultural Pollution. Ecology Law Quarterly 11(2)135-88.

Kenaga, E.E., 1980. Correlations of Bioconcentration Factors. Environmental Science and Technology 14:533-556.

Kenaga, E.E. and C.A.I. Goring, 1980. Relationship Between Water Solubility, Soil Sorption, Octanol Water Partitioning and Bioconcentration of Chemicals in Biota. ASTM Spec. Tech. Publ. STP 707, 78. American Society for Testing and Materials, as cited by Mackay, (1982).

Kershaw, P.J., D.J. Swift, R.J. Pentreath, and M.B. Lovett, 1984. The Incorporation of Plutonium, Americium and Curium into Irish Sea Seabed by Biological Activity. Sci. of Total Environment 40:61-81.

Klein, W., H. Geyer, D. Freitag, and H. Rohleder, 1984. Sensitivity of Schemes for Ecotoxicological Hazard Ranking of Chemicals. Chemosphere 13(1):203-211.

Kneip, T.J. and G.J. Lauer, 1973. Trace Metal Concentration Factors in Aquatic Ecosystems (in) Chemical Analysis of the Environment and Other Modern Techniques, pp. 43-62. Edited by S. Akiya. Plenum Press.

Kobayashi, H. and B.E. Rittmann, 1982. Microbial Removal of Hazardous Organic Chemicals. Environmental Science and Technology 16(3):170A-183A.

Koch, R., 1984. A Theoretical-Methodological Approach Towards the Evaluation of Environmental Pollutants. Toxicological and Environmental Chemistry 7:331-346.

Kodric-Smit, M., Z. Smit, and K. Olie, 1980. Organochloride Contaminants in Human Milk from Yugoslavia, 1978. Pesticides Monitoring Journal 14:1-2.

Kraal, H. and W. Ernst, 1976. Influence of Copper High Tension Lines on Plants and Soils. Environmental Pollution 11:131-135.

Larsson, Per, 1984. Uptake of Sediment Released PCBs by the Eel Anguilla Anguilla in Static Model Systems. Ecological Bulletin 36:62-67.

Leckie, J. and R.O. James, 1974. Control Mechanisms for Trace Metals in Natural Waters (in) Aqueous Environmental Chemistry of Metals. Edited by A.J. Rubin. Ann Arbor Science, Ann Arbor, MI.

Lee, G.F. and R.A. Jones, 1977. Assessment of the Environmental Significance of Chemical Contaminants Present in Dredged Materials. Enviro. Qual. Consultants for New York District, U.S. Army Corps of Engineers, NY.

Lemons, John D., 1975. Distribution and Ratio Trends of Nutritious and Toxic Metals in a Desert Ecosystem. University of Wyoming. Ph.D. Dissertation.

Leo, A., C. Hansch, and D. Elkins, 1971. Partition Coefficients and Their Uses. Chemical Review 71(6):525-613.

Lombardo, P., 1979. Food and Drug Administration Chemical Contaminants Program: The Search for the Unrecognized Pollutant, in Nicholson, W.J. and A. Moore (eds.), 1979. Annals of the New York Academy of Sciences, Vol. 320. Health Effects of Halogenated Aromatic Hydrocarbons; International Symposium, New York, NY, June 24-27, 1978.

Lu, Po-Yung and Robert L. Metcalf, 1975. Environmental Fate and Biodegradability of Benzene Derivatives as Studied in Model Aquatic Ecosystem. Environmental Health Perspectives 10:269-284.

Lyman, W.J., W.F. Reihl, and D.H. Rosenblatt, 1982. Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Compounds. McGraw-Hill Book Co., New York, NY,

Macek, K.J., S.R. Petrocelli, and B.H. Sleight III, 1979. Considerations in Assessing the Potential for, and Significance of Biomagnification of Chemical Residues in Aquatic Food Chains (in) Aquatic Toxicology. American Society for Testing and Materials, Philadelphia, PA.

Mackay, D., 1981. Calculation of Environmental Partitioning and Persistence of Chemicals Using the Fugacity Approach. Environmental Science and Technology. Cited in Hushon et al., 1983.

Mackay, Donald, 1982. Correlation of Bioconcentration Factors. Environmental Science and Technology 16(5):274-278.

Mackay, D., A. Bobr, D.W. Chan, and W.Y. Shiu, 1982. Vapor Pressure Correlations for Low Volatility Environmental Chemicals 16(10):645-649.

Mathis, B.J. and T.F. Cummings, 1973. Selected Metals in Sediments, Water and Biota in the Illinois River. Journal of Water Pollution Control Federation 45:1573-1586. Cited in Wong and Tam (1984).

McKim, J.M., R.L. Anderson, D.A. Benoit, R.L. Spehar, and G.N. Stokes, 1976. Effects of Pollution on Freshwater Fish. Journal Water Pollution Control Federation 1976: 1544-1620.

Melius, Paul, 1981. Comparative Benzo(a)pyrene Metabolite Patterns in Fish and Rodents (in) Symposium on the Use of Small Fish Species in Carcinogenicity Testing, National Institutes of Health, Bethesda, MD.

Metcalf, R.L. et al., 1975. Laboratory Model Ecosystem Studies of the Degradation and Fate of Radiolabeled Tri-, Tetra-, and Pentachlorobiphenyl Compared with DDE. Archieves of Environmental Contammination and Toxicology 3:151-165.

Michigan Water Resources Commission, 1980. Critical Materials Register. Environmental Services Division, Department of Natural Resources, Pub. No. 4833-5324. Lansing, MI.

Michigan Water Resources Commission, 1984. Review Report Michigan Site Assessment System. September 1984. Environmental Services Division, Department of Natural Resources, Lansing, MI.

Miller, S.S., 1974. Water Pollution. American Chemical Society, Washington, DC.

Montgomery, R.L. and M.R. Palermo, 1983. Evaluation of Upper Mobile Dredged Material Disposal Plan. U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

Monti, C., E. O'Neill, and P. Ahearn, 1983. Modeling the Movement of Kepone Across Disturbed Sediment-Water Interface in Laboratory Systems (in prep.). Environmental Toxicology Chemicals. EPA/ERL, Gulf Breeze, FL.

Morel, F., R.E. McDuff, and J.J. Morgan, 1974. Interactions and Chemostasis in Aquatic Chemical Systems: Role of pH, pE, Solubility, and Complexation (in) Trace Metals and Metal-Organic Interactions in Natural Waters. Edited by Philip C. Singer. Ann Arbor Science, Ann Arbor, MI.

Moriarty, F., 1983. Ectoxicology: The Study of Pollutants in Ecosystems. London and New York, Academic Press.

Moriarty, F., 1984. Persistent Contaminants, Compartmental Models and Concentration Along Food Chains. Ecological Bulletin 36:35-45.

National Oceanic and Atmospheric Administration, National Ocean Service, 1985. Coastal Hazardous Waste Site Review. Prepared by the Ocean Assessments Division, Seattle, WA.

National Research Council, 1975. Assessing Potential Ocean Pollutants. Report to Ocean Affairs Board. National Academy of Sciences, Washington, DC.

National Research Council, 1985 and the Royal Society of Canada. The Great Lakes Water Quality Agreement. National Academy Press, Washington, DC.

Neeley, W.B., D.R. Bramson, and G.E. Blan, 1974. Partition Coefficient to Measure Bioconcentration Potential of Organic Chemicals in Fish. Environmental Science amd Technology 8:1113-1115.

Neubecker, T.A. and H.E. Allen, 1983. The Measurement of Complexation Capacity and Conditional Stability Constants for Ligands in Water. Water Research 17(1):1-14.

Niethammer, K.R., D.H. White, T.S. Baskett, and M. Sayre, 1984. Presence and Biomagnification of Organochlorine Chemical Residues in Oxbow Lakes of Northeastern Louisiana. Archives Environmental Contamination Toxicology 13:63-74.

Niewiadowska, A. and A. Sosyniak, 1983. Residues of Organochlorine Insecticides and Polychlorinated Biphenyls. Bulletin Veterinary Institute Pulawy 26(1-4):60-3. Poland.

Niimi, A.J. and B.G. Oliver, 1983. Biological Half Lives of Polychlorinated Biphenyl (PCB) Congeners in Whole Fish and Muscle of Rainbow Trout. Canadian Journal of Fisheries and Aquatic Sciences 40(9):1388-1394.

Oakes, T.W., B.A. Kelly, and J.C. Bird, 1982. Technical Background Information for the Environmental and Safety Report, Vol. 4: White Oak Lake and Dam. ORNL 5681. Oak Ridge National Laboratory, Oak Ridge, TN.

O'Connor, Joseph M., 1984. Polychlorinated Biphenyl Transport in Coastal Marine Foodwebs. EPA Gulf Breeze Lab EPA-600-S3-84-083. Gulf Breeze, FL.

O'Connor, J.M. and J.W. Rachlin, 1982. Perspectives on Metal in New York Bight Organisms: Factors Controlling Accumulation and Body Burden (in) Ecological Stress and the New York Bight: Science and Management, G.F. Mayer, editor. Estuarine Research Federation, Columbia, SC.

Odum, W.E., 1970. Utilization of the Direct Grazing and Plant Detritus Food Chains by the Striped Mullet (in) Marine Food Chains. pp. 222-240. Edited by J.H. Steele. Oliver and Boyd, Edinburgh, Scotland.

Ofstad, E.B. and K. Martinsen, 1983. Persistent Organochlorine Compounds in Seals. Ambio 12(5):262-4.

Ogata, M. and Y. Miyake, 1978. Disappance of Aromatic Hydrocarbons and Organic Sulphur Compounds from Fish Flesh Reared in Crude Oil Suspension. Water Research 12:1041-1044.

Oliver, B.G. and K.D. Nicol, 1982. Chlorobenzenes in Sediment, Water and Selected Fish from Lakes Superior, Huron, Erie and Ontario. Environmental Science and Technology, 16:532-536.

Oliver, B.G. and A.J. Niimi, 1983. Bioconcentration of Chlorobenzenes from Water by Rainbow Trout: Correlations with Partition Coefficients and Environmental Residues. Environmental Science and Technology 17(5):287-291.

Portier, R.J. and S.P. Meyers, 1980. Use of Microcosms for Analyses of Stress-Related Factors in Estuarine Ecosystems (in) International Wetlands Conference, New Delhi, India.

Potter, L., D. Kidd, and D. Standiford, 1975. Mercury Levels in Lake Powell: Bioamplification of Mercury in Man-Made Desert Reservoir. Environmental Science and Technology 9:41-46. Cited in Kay (1984).

Rapaport, R.A. and S.J. Eisenreich, 1984. Chromatographic Determination of Octanol-Water Partition Coefficients for 58 Polychloronated Biphenyl Congeners. Environmental Science and Technology 18:168.

Ray, S., B.M. Jessop, J. Coffin, and D.A. Swetnam, 1984. Mercury and Polychlorinated Biphenyls in Striped Bass from Two Nova Scotia Rivers. Water, Air, and Soil Pollution 21:15-23.

Reish, D.J., G.G. Geesey, F.G. Wilkes, P.S. Oshida, and A.J. Mearns, 1982. Marine and Estuarine Pollution. Journal Water Pollution Control Federation 54(6):786-811.

Reish, D.J., G.G. Geesey, F.G. Wilkes, P.S. Oshida, S. Rossi, and T.C. Ginn, 1983. Marine and Estuarine Pollution. Journal Water Pollution Control Federation 55(6):767-787.

Robberecht, H., H. Deelstra, and D. Vanden Berghe, 1983. Metal Pollution and Selenium Distributions in Soils and Grass. Science Total Environment 29(3):329-42.

Rubinstein, N.I., W.T. Gilliam, and N.R. Gregory, 1984. Dietary Accumulation of PCBs from a Contaminated Sediment, Source for Demersal Fish Species. U.S. Army Engineer Waterways Experiment Station WES/TR/D-84-6. Vicksburg, MS.

Saari, Sharon, 1986. Hazard Ranking System Issue Analysis: Potential Human Food Chain Exposure. (Draft). The MITRE Corporation, McLean, VA. Prepared for the Environmental Protection Agency, Washington, DC.

Shaw, G.R. and D.W. Connell, 1984. Physiochemical Properties Controlling Polychlorinated Biphenyl (PCB) Concentrations in Aquatic Organisms. Environmental Science and Technology 18(1):18-23.

Shelton, Daniel R. and James M. Tiedje, 1984. General Method for Determining Anaerobic Biodegradation Potential. Applied and Environmental Microbiology 47(4):850-857.

Sinderman, C.J., S.C. Esser, and E. Gould, 1982. Effects of Pollutants on Fishes (in) Ecological Stress and the New York Bight. Science and Management. G.F. Mayer, editor. Estuarine Research Federation. Columbia, SC.

Smith, J.H., D.C. Bomberger, and D.I. Haynes, 1981. Volatilization Rates of Intermediate and Low Volatility Chemicals from Water. Chemosphere 10:281-289. Cited in Gillett (1983).

Spacie, A. and I.C. Hamerlink, 1982. Alternative Models for Describing the Bioconcentration of Organics in Fish, Environmental Toxicology and Chemistry 1:309-320.

Suffet, I.H., 1975. Fate of Pollutants in the Air and Water Environments. Part 2: Chemical and Biological Fate of Pollutants in the Environment. John Wiley and Sons, NY.

Taymaz K., V. Yigit, and H. Ozbal, 1984. Heavy Metal Concentrations in Water Sediment and Fish from Turkey. Int. Jour. Environ. Anal. Chem. 16(4)253-66.

Technical Database Services, Inc., 1985. Log Pow Database. Pomona College, New York, NY.

Thayer, J.S., G.J. Olson, and F. Brinckman, 1984. Iodomethane as a Potential Metal Mobilizing Agent in Nature. Environmental Science and Technology 18(9):726-729.

Thomann, R.V. and J.P. Connolly, 1984. Model of PCB in the Lake Michigan Lake Trout Food Chain. Environmental Science and Technology 18(2):65-72.

Thompson, S.E., C.A. Burton, D.J. Quinn, and Y.C. Ng, 1972. Concentration Factors of Chemical Effluents in Edible Aquatic Organisms. Lawrence Livermore National Laboratory UCRL-50564, Rev. 1. University of California, Livermore, CA.

Tinsley, I.J., 1979. Chemical Concepts in Pollutant Behavior. John Wiley and Sons, Inc., NY.

Trabalka, J.R. and C.T. Garten, 1982. Development of Predictive Models for Xenobiotic Bioaccumulation in Terrestrial Ecosystems. ORNL-5869. Oak Ridge National Laboratory, TN.

Troup, B.N. and O.P. Bricker, 1975. Processes Affecting the Transport of Materials from Continents to Oceans in Marine Chemistry in the Coastal Environment. Edited by Thomas M. Church. American Chemical Society, Washington, DC.

U.S. Department of Agriculture, 1985. Food Safety and Inspection Service. Compounds Evaluation and Analytical Capability: Annual Residue Plan. Washington, DC.

U.S. Environmental Protection Agency, 1977. Investigation of Selected Potential Environmental Contaminants. Halogenated Benzenes. PB-273-206. Office of Toxic Substances, Washington, DC.

U.S. Environmental Protection Agency, 1979. Office of the Environmental Criteria and Assessments, Cincinnati, OH. EPA Hazard Profiles prepared by Syracuse Research Corporation.

U.S. Environmental Protection Agency, 1980. Water Quality Criteria Documents. Federal Register, 45 FR 79318, 28 November 1980. PB 81-117-269 through 889.

U.S. Environmental Protection Agency, 1981. Water Quality Criteria Document: Polynuclear Aromatic Hydrocarbons. PB 81-117 806. Washington, DC.

U.S. Environmental Protection Agency, 1982a. National Oil and Hazardous Substances Contingency Plan. Federal Register, 47 FR 31179, 16 July 1982.

U.S. Environmental Protection Agency, 1982b. Handbook for Applying Section 403(C) Criteria of the Clean Water Act. Criteria and Standards Division, Washington, DC.

U.S. Environmental Protection Agency, 1984a. Draft Guidance and Methods for the Use of Acceptable Daily Intakes in Health Risk Assessment, Cincinnati, OH.

U.S. Environmental Protection Agency, 1984b. Review and Analysis of Hazard Ranking Schemes. Final Report by ENVIRON Corporation to EPA Office of Solid Waste, Washington, DC.

U.S. Environmental Protection Agency, 1984c. Review and Analysis of Hazard Ranking Schemes. Final Report by ENVIRON Corporation to EPA Office of Solid Waste, Washington, DC.

U.S. Environmental Protection Agency, 1985. Notification Requirements; Reportable Quantities Adjustments. Final Rule, Federal Register, 50 FR 13456-13522. April 4, 1985.

U.S. Food and Drug Administration, 1983. State Services Branch. Use of the FDA Surveillance Index in Planning Pesticide Residue Monitoring Programs, Rockville, MD.

U.S. Nuclear Regulatory Commission, 1977. Regulatory Guide 1.109. Calculation of Annual Doses to Man from Routing Releases of Reactor Effluents for the Purpose of Evaluating Compliance with 10 CFR 50. U.S. NRC, Office of Standards Development, Washington, DC.

Van AS, D., A.O. Fourie, and C.M. Vleggaar, 1973. Accumulation of Certain Trace Elements in Marine Organisms from the Sea Around the Cape of Good Hope (in) Radioactive Contamination of the Environment. International Atomic Energy Agency, Vienna, Austria.

van Gestal et al., 1985. Relation Between Water Solubility, Octanol/Water Partition Coefficients, and Bioconcentration of Organic Chemicals in Fish: A Review. Regulatory Toxicology and Pharmecology, 5:422-431.

Veith, G.D., D.L. DeFoe, and B.V. Bergstedt, 1979. Measuring and Estimating the Bioconcentration Factor of Chemicals in Fish. Journal Fisheries Research Board Canada 36:1040-1048.

Veith, G.D. and P. Kosian, 1983. Estimating Bioconcentration Potential from Octanol/Water Partition Coefficients. In Physical Behavior of PCBs in the Great Lakes (D. McKay et al., eds.), Chapter 15, pp. 269-282. Ann Arbor Science, Ann Arbor, MI.

Veith, G.D., K.J. Macek, S.R. Petrocelli, and J. Carroll, 1980. Aquatic Toxicology, pp. 116-129. ASTM STP 707. Edited by J.G. Eaton, P.R. Parrish, and A.C. Hendricks.

Versar, Inc., 1984. Final Draft Superfund Exposure Assessment Manual. Prepared for EPA Office of Solid Waste and Emergency Response by Versar Inc., Springfield, VA.

Versar, Inc., 1985. Assessment of Human Health Risk from Ingesting Fish and Crabs from Commencement Bay. EPA 910/9-85-129. Washington Department of Ecology, Olympia, WA.

Verschueren, Karl, 1983. Handbook of Environmental Data on Organic Chemicals, Second Edition. Van Nostrand Reinhold Company, New York, NY.

Wakeham, Stuart G., Alan C. Davis, and Jennifer L. Karas, 1983. Mesocosm Experiments to Determine the Fate and Persistence of Volatile Organic Compounds in Coastal Seawater. Environmental Science and Technology 17(10):611-617.

Walton, B.T. and N.T. Edwards, 1986. Accumulation of Organic Waste Constituents in Terrestrial Biota (in) Lochr and Malina (eds.). Land Treatment: A Hazardous Waste Management Alternative. Water Resources Symposium No. 13. University of Texas, Austin, TX.

Weatherley, A.H., P.S. Lake, and S.C. Rogers, 1980. Zinc Pollution and the Ecology of the Freshwater Environment (in) Zinc in the Environment. Edited by Jerome O. Nriagu. John Wiley and Sons, NY.

Weaver, Grant, 1984. PCB Contamination In and Around New Bedford, Massachusetts. Environmental Science and Technology 18(1):22A-27A.

Whelan, Gene and Yasuo Onishi, 1983. In-Stream Contaminant Interaction and Transport. 1983 International Symposium on Urban Hydrology, Hydraulics and Sediment Control, Lexington, KY.

Whelan, G. and B.L. Steelman, 1984. Development of Improved Risk Assessment Tools for Prioritizing Hazardous and Radioactive Mixed Waste Disposal Sites. PNL-SA-12708 (in) Proceedings of the 5th DOE Environmental Protection Information Meeting, Albuquerque, NM.

Whelan, G., B.L. Steelman, D.L. Strenge, and J.G. Droppo, 1986. Overview of the Remedial Action Priority System (RAPS). Pacific Northwest Laboratories. Presented at the First Workshop on Pollutant Transport and Accumulation, Los Angeles, CA.

Wiedemeyer, Gary, 1986. U.S. Fish and Wildlife Service, National Fishery Laboratory, Personal Communications. Seattle, WA.

Wood, J.M., 1980. The Role of pH and Oxidation Reduction Potentials in the Mobilization of Heavy Metals (in) Polluted Rain. Edited by T.Y. Toribara, M.W. Miller, and P.E. Morrow, Plenum Press, NY.

Wood, J.M., 1982. Chlorinated Hydrocarbons: Oxidation in the Biosphere. Environmental Science and Technology 16(5):291A-297A.

Wood, W.P., 1981. Comparisons of Environmental Compartmentalization Approaches. OECD Chemicals Group, Exposure Analysis (EXPO) Room. Doc. 80.21. Organization for Economic Cooperation and Development, Paris, France.

Wong, M.L. and F.Y. Tam, 1984. Sewage Sludge for Cultivating Freshwater Algae and the Fate of Heavy Metal at Higher Trophic Organisms. Archives Hydrobiology 100(4):423-30.

Young, D.R., Tsu-Kai J., and G.P. Hershelman, 1980. Cycling of Zinc in the Nearshore Marine Environment (in) Zinc in the Environment. Edited by J.O. Nriagu. John Wiley and Sons, NY.

APPENDIX A

CLASSIFICATION OF HAZARDOUS SUBSTANCES FOR POTENTIAL TO BIOACCUMULATE

This appendix illustrates the use of the decision tree presented in Figure 4 (Section 3). The substances included in this appendix were selected for their ability to illustrate the use of the decision tree rather than for any particular importance of the individual substances. Fifteen substances were chosen for this illustration. These substances include:

1. Acenaphthene
2. Benzo(a)pyrene
3. Cadmium
4. DDT
5. Dichloromethane
6. Dichlorobiphenyl
7. Copper
8. Vinyl chloride
9. Xylene
10. N-Pentane
11. Lorsban
12. Dichlorobiphenyl
13. Lead
14. Thiourea
15. Cyclohexanone

The process for following the decision tree presented in Section 3 is illustrated in Table A-1. In all instances, the BCF data should be used first, then the log Pow data, and if neither of these is available, the S data. For Benzo(a)pyrene, for example, the score based on the BCF would be 5. Since the substance has been reported to bioaccumulate, 1 is added to this factor for a final score of 6. For DDT, the score based on the BCF would be 6, the maximum allowable regardless of the fact the substance bioaccumulates.

TABLE A-1
BIOACCUMULATION RATING BASED ON PROPOSED RATING SCHEME

	Substance	BCF	Log Pow	S	Biomagnify	Rating Value
1.	Acenaphthene	387	--*	--	No	4
2.	Benzo(a)pyrene	2,177	--	0.003 mg/l	Yes	6
3.	Cadmium	1,000-3,999	--	--	Yes	6
4.	DDT	10,000	--	0.0031 mg/l	Yes	6
5.	Dichloromethane	5	--	20,000 mg/l	No	1
6.	Dichlorobisphenyl	214	--	--	No	4
7.	Copper	1,000	--	--	No	5
8.	Vinyl chloride	1.2	--	1,100 mg/l	No	2
9.	Xylene	21-23	3.15	198 mg/l	No	3
10.	N-Pentane	--	3.39	--	No	3
11.	Lorsban	--	4.96	--	No	5
12.	Dichlorobiphenyl	215	--	--	No	4
13.	Lead	924	--	--	No	4
14.	Thiourea	--	--	91.8 mg/l	No	4
15.	Cyclohexanone	--	3.44	55 mg/l	No	3

*Indicates data not readily available for inclusion in table.

APPENDIX B

SUMMARY OF DATA COLLECTED ON HAZARDOUS SUBSTANCES

Table B-1 presents the findings from a literature review to identify substances which may bioaccumulate in food chains. The automated EPA NPL technical data base was queried to identify substances found at NPL sites. Most of the substances subsequentially researched were found at five or more NPL sites. The collected literature was scanned to determine which of these substances have been reported to bioaccumulate in biota. Most of the tabulated BCF data are for fish, but several reflect measurements of plants or animals. Some BCFs contained in Table B-1 are generic values as presented in the referenced literature. BCFs are for edible tissue (e.g., meat or whole fish) not for liver concentrations.

Table B-2 presents a range of log Pow values from a computerized database (Technical Database Services, Inc., 1985).

For a limited number of substances found at waste sites, and which are not included in the computerized data base, MITRE calculated log Pow values or found log Pow values in the literature. These values are reported in Table B-3.

TABLE B-1

DATA COLLECTED ON HAZARDOUS SUBSTANCES AND POTENTIAL BIOACCUMULATION

Substance Name	CAS Number	Bioconcentration Factor	Biomagnifies	Source Number
Acenaphthene	00083-32-9	387 fish		3/22
		242		42
Acrolein	0107-02-8	344 fish		3/22
		215		42
Acrylonitrile	00107-13-1	48 fish		3/22
		30		42
Aldrin	00309-00-2	greater than 4000		4
		13,390 clam		31
		2-3.5 cattle		11/38
		3,000-11,000 fish		11
		4,600-6,300		22
Aluminum and compounds	07429-70-5	10,000-15,000	yes	10
		10 in fish		39
Aniline	0062-53-3	6 fish		26
		0.5		42
Anthracene	00120-12-7	917		25
		100-10,000		32
Antimony and compounds, NOS	07440-36-0	greater than 4,000		4
		less than 1		42/22
Antimony trioxide	1309-64-4	40 fish		32
		16,000 invertebrates		32
Arsenic and compounds	07440-38-2	700-999		4
		1-3 plants		9
		10,000 fish		17
		0-4 fish		22
		333 fish		39
		44 fish		42

TABLE B-1 (Continued)

Substance Name	CAS Number	Bioconcentration Factor	Biomagnifies	Source Number
Atrazine	01912-24-9	2-4	no	17
		less than 8		25
		3		33
Barium	07440-39-3	0.6-5.2		30
		4		35
Benzene	0071-43-2	3.5 eels		21
		less than 10 fish		33
		5.2		42
Benzidine	0092-87-5	38-44		22
		83		33
		87 fish		28
Benzoic acid	00065-85-0	21 fish	no	26
Benzo(a)pyrene	00050-32-8	37 mosquito		20
		2,177 snail		20
		930 fish	yes	20
		less than 1 plant		38
		30		42
Beryllium and	7440-41-7	2-100 fish	no	20/39
		19		22
		100		32
Biphenyl	00092-52-4	340		24
		437		25
Bis (2-chloroethyl) ether	0011-44-4	11 fish		3
		6.9 fish		28
Boron and compounds	07440-42-8	0.22 in fish		39
Bromine	07726-95-6	0.015-420 fish		23
Butylbenzyl phthalate	00085-68-7	772 fish		3
		279		22

TABLE B-1 (Continued)

Substance Name	CAS Number	Bioconcentration Factor	Biomagnifies	Source Number
Cadmium	074409-43-9	1,000-3,999	yes	4
		1,100-2,400 fish		13
		30,000 algae	no	17
		7.5 fish		17
		8.9 muscle		17
		649 freshwater fish		22
		226 saltwater fish		22
		1,220-2,040 oyster		22
		64-81 fish		42/28
Captan	00133-06-2	less than 300		4
Carbon tetrachloride	0056-23-5	30 fish		3
		17-39 fish		13
		30		22
		18		42
Cerium	07440-45-1	1-10 fish		23
Chlordane	00057-74-9	0.1-0.5 cattle		11
		8,000-11,400 fish		11
		4,702		22
		4,810 clam		31
		14,000		42
Chlorobenzene	00108-90-7	645 fish		12
		1,000-10,000		32
		12		24
		10		42
		650		26
Chlorobiphenyl	02051-62-9	490		24
Chloroform	00067-66-3	6 fish		3/22
2-Chlorophenol	00095-57-8	214 fish		3/22

TABLE B-1 (Continued)

Substance Name	CAS Number	Bioconcentration Factor	Biomagnifies	Source Number
Chromium and compounds	07440-47-3	8,500 algae		22
		300 algae	no	10
		less than 1-2.5 fish		22/17
		125-200 salt oyster		22
Cobalt and compounds	07440-48-4	6-10 plants		9
		6,760 fish	yes	34
		320 fish		39
Copper and compounds	07440-50-8	1 plant		9
		1,000-5,000 marine		10
		1-290 fish		22
		9,960 shellfish	no	22
		200-320 in fish		39
		36		42
Cyanides (NOS)	00057-12-5	none		22/43
		2.3		36/38
DDD	72-54-8	80×10^3		10
		1,000-100,000	yes	32
DDE,p,p'	00072-55-9	62×10^2-10^3	yes	18
		51,000 fish		28
		10,000-100,000		32
DDT,p,p'	00050-29-3	greater than 4,000		4
		0.9 cattle		11
		61,600-84,500 fish		11
		17,870		22
		16,950	yes	26/18
		54,000 fish		28
1,2-Dichlorobenzene	00095-50-1	56-89 fish		42/3
		60-215		22/24
1,3-Dichlorobenzene	00541-73-1	66 fish		3
1,4-Dichlorobenzene	00106-46-7	37-60 fish		42/3
		89-215		22/24

TABLE B-1 (Continued)

Substance Name	CAS Number	Bioconcentration Factor	Biomagnifies	Source Number
3,3-Dichlorobenzene		312 fish		28
Dichlorobiphenyl		215		24
1,2-Dichloroethane	00107-06-2	2 fish 1.2		3 42
1,1-Dichloroethylene	00075-35-4	5.6 fish		28
Dichloromethane	00075-09-2	5 fish		28
2,4-Dichlorophenol	00120-83-2	41 fish		28
2,4-Dichlorophenoxy-acetic acid (2-4-D)	00094-75-7	$17\text{-}45 \times 10^{-5}$ cattle 20 fish	no	11 11
1,3-Dichloropropene	00542-75-6	1.9 fish		28
Dieldrin	00060-57-1	greater than 4,000 1.6-3 cattle 4,400-5,800 fish 1,557 3,540 clam	yes no	4 11 11 22 31
Diethyl phthalate	00084-66-2	117 fish		3
Diethylhexyl phthalate	00117-81-7	38		22
Di-N-butyl phthalate	00084-74-2	14		22
Di-N-octyl phthalate	00117-84-0	9,400		22
Dimethyl phthalate	00131-11-3	57 fish		3
2,4-Dimethylphenol	00105-67-9	150 fish		3/22
Dinitrotoluene	2532-114-6	3.8 fish		28

TABLE B-1 (Continued)

Substance Name	CAS Number	Bioconcentration Factor	Biomagnifies	Source Number
Dioxin	01746-01-6	10,000		32
		5,800		42
		greater than 4,000		4
		5,000 fish		28
		130-9,000 plants		32
Diphenylamine,N,N	00122-39-4	30 fish		28
1,2-Diphenylhydrazine	00122-66-7	25 fish		28
Endosulfan	00115-29-7	50-30,000	no	32
Endrin	00072-20-8	greater than 4,000		4
		1.2-1.3 cattle		11
		1,400-4,050 fish	yes	11
		0.4 lobster		15
		1,324		22
Ethylbenzene	00100-41-4	37.5 fish		28
Fluoranthene	00206-44-0	1,150 fish		28
		100-10,000		32
Fluorene	00086-73-7	1,300 fish		28
Heptachlor	00076-44-8	10,630 clam		31
		15,700 fish		28
		greater than 4,000		4
		0.4-0.6 cattle		11
		2,000-17,400 fish		11
		9,500 freshwater fish		22
		7,500 saltwater fish		22
Heptachlor epoxide	01024-57-3	10^2-10^4		32
		2,330 clam		31
		14,400 fish		28/22/27

TABLE B-1 (Continued)

Substance Name	CAS Number	Bioconcentration Factor	Biomagnifies	Source Number
Hexachlorobenzene	00118-74-1	1,166 fish	yes	12/43
		8,600		24
		22,000		22
		1,166		24
		5,500-21,900		27
Hexachlorobutadiene	00087-68-3	19		22
		3-4.3		42/28
		1000		32
Hexachlorocyclo-hexane (NOS)	00608-73-1	10-500		20
		480 fish		20
		130 oyster		20
		352 fish		22
Hexachlorocyclo-pentadiene	00077-47-4	300-699		4
		448 fish		20
		11		22
		300-2,000		32
Hexachloroethane	00067-72-1	139 fish		3
		87		42
Iron and compounds	07439-89-6	1,000-5,000 fish		10/38
		10,000-100,000 invertebrates		10
		100 fish		39
Isophorone	00078-59-1	7 fish		22/3
		7-16 fish		36
Kepone	00143-50-0	5,000-7,000 oyster		40
		440-1,060 crab		40
		4,500-11,700 shrimp	yes	35/40
		3.9-10.5	yes	17
		8,400 (estimate from water solubility)		24
		2,600-7,600		29

TABLE B-1 (Continued)

Substance Name	CAS Number	Bioconcentration Factor	Biomagnifies	Source Number
Lead	07439-92-1	0.1 plants		14
		17 snail		22
		0.2-2 plants		9
		0.1-0.3 fish		14
		42-45 fish		22
		924 bivalves		22
		300 fish		39
		49		42
Lindane	00058-89-9	0.4-0.7 cattle		11
		2,610		31
		325-560 fish		11
		130-170 shellfish		20
		352 fish		22
		754		33
Magnesium and compounds	07439-95-4	50-93		39
Manganese and compounds	07439-96-5	0.2-0.3 fish		14
		660 fish	no	39
Mercury	10045-94-0	greater than 4,000-5,500	yes	4/28
		13,000	yes	42
		1,000-10,000		10/22
Mercuric chloride	07487-94-7	1,800-4,994 fish		22
		10,000 oyster		22
Methoxychlor	00072-43-5	less than 300		4
		0 cattle		11
		185-1,550 fish		11
		8,300		25
Methyl mercuric chloride		11,000-85,700 fish	yes	22
Methyl parathion		45 fish		28

TABLE B-1 (Continued)

Substance Name	CAS Number	Bioconcentration Factor	Biomagnifies	Source Number
Mirex	02385-85-8	84 fish	yes	15
Molybdenum	07439-98-7	44-50 plants		9
		10 fish		39
		20-100 marine		10
Naphthalene	00091-20-3	100		20
		131		25
		427		25
		5,000 copepods	yes	22/17
		10		42
Nickel and compounds	07440-02-0	greater than 4,000		4
		425-467 plants		9
		100-200		10
		300 fish	no	17
		30 fish		22
		84 oyster		22
		47		42
Nitrobenzene	00098-95-3	29 fish		26
		3		42
4-Nitrophenol	00100-02-7	57		33
		3		42
N-Nitrosodi-phenylamine	00086-30-6	217 fish		3
Parathion	00056-38-2	24		42
Pentachlorobenzene	00608-93-5	3,400 fish		1
		5,000		24
		3,400		22
		2,125 fish		28
Pentachloroethane	00076-01-7	67 fish		3

TABLE B-1 (Continued)

Substance Name	CAS Number	Bioconcentration Factor	Biomagnifies	Source Number
Pentachlorophenol	00087-86-5	greater than 4,000		4
		296 fish		12/26
		770		25
		200 (approximately)		22
		1,050 fish		33
		31		33
Phenanthrene	00085-01-8	325		25
		2,630		28
		100-10,000		32
Phenol	00108-95-2	1.4		42
Plutonium		350		34
Plutonium-238		1-15 fish		1
		230-520 shellfish		1
Plutonium-239	15117-48-3	6×10^{-5} land		5
		1,000 marine	yes	13
		2-15 fish muscle		13
		1,100 fish gut		13
Polychlorinated biphenyls	01336-36-3	4×10^{5}		2
		greater than 4,000		4
		2,500 shrimp		2
		10^{5}-10^{6}		16
		10,400	yes	22
		31,200	yes	42
Pyrene	00129-00-0	2,700		25
		2,800 (log Pow estimate)		22
		10,000		32
Radium and compounds	07440-14-4	0.9×10^{3}		6
		5-16 plants		9

TABLE B-1 (Continued)

Substance Name	CAS Number	Bioconcentration Factor	Biomagnifies	Source Number
Selenium	07782-49-2	1-40		8
		16 fish		28
		78-104 plants		9
		8-20 fish	yes	22/41
		167 fish	no	39/17
Silver	07440-22-4	10-3,000 fish		20
		3,080 fish		28
		28 fish		22
Sodium	07440-23-5	0.067-100 fish		23
Strontium	07440-24-6	171	yes	6
		1-10 soft tissue		10
		1,000 bone		10
		200		34
Sulfur	07704-34-9	2-5 marine		10
1,2,4,5-Tetrachloro-benzene	00095-94-3	1,800 fish		3
		1,125 fish		28
		4,500		24
1,1,2,2-Tetrachloro-ethane	00079-34-5	5-8 fish		3/42
		42 fish		28
1,1,2,2-Tetrachloro-ethene	00127-18-4	100	no	32/20
		greater than 100 in liver		32/20
2,3,4,6-Tetrachloro-phenol	00058-90-2	240 fish		28
Thallium	07440-28-0	100,000		32
		116		42

TABLE B-1 (Continued)

Substance Name	CAS Number	Bioconcentration Factor	Biomagnifies	Source Number
Tin and compounds	07440-31-5	0.5 fish		17
		3.5 invertebrates		17
		3,000 fish		39
		1,000		39
Titanium and compounds	07440-32-6	40-1,000 marine		10
Toluene	00108-88-3	13.2 eel		21
		11		42
Toxaphene	08001-35-2	greater than 4,000		4
		10,000 fish	yes	18
		4,372-6,150		22
		26,400		24
		13,100		42
Trichlorobenzene	00050-31-7	1,700 in fish		39
1,2,3-Trichloro-benzene	00087-61-6	182 fish		22
		890-2,300		24/33
1,2,4-Trichloro-benzene	00120-82-1	100-1,000		32
		2,800 fish		28
		491		24/33
		183 fish		17
		890-2,300		27
1,1,1-Trichloro-ethane	00071-55-6	9 fish		3
		11		42
		5-5.6 fish		28
1,1,2-Trichloro-ethane	00079-00-5	4.5		3/42

TABLE B-1 (Continued)

Substance Name	CAS Number	Bioconcentration Factor	Biomagnifies	Source Number
Trichloroethylene	00079-01-6	88 fish		33
		11-17		42/22
		2.7		23
Trichlorophenol	25167-82-2	110-150 fish		28
Trichlorophenoxy acetic acid (2,4,5-T)	00093-76-5	$4\text{-}19 \times 10^{-4}$ cattle	no	11
		25-43 fish		11
Tris	00126-72-7	2.7		23
Uranium and compounds	07440-61-1	3-6 plants		9
		10 fish		9/39
		less than 0.03 animals		9
Vanadium and compounds	07440-62-2	7-11 plants		9
		20-100 marine		10
		2-28 fish		13
Vinyl chloride	00075-01-4	1.2		42
Xylene	01330-20-7	21.4-23.6 eel		21
Zinc and compounds	07440-66-6	less than 300	no	4
		47		42
		1,000-5,000		10
		0.33-0.48	yes	14/37
		60-100		22
Zirconium	07440-67-7	3.3-200		23

TABLE B-1 (Concluded)

Sources:

(1) National Research Council, 1975
(2) Thomann & Connolly, 1984
(3) Veith et al., 1980
(4) Michigan Water Resources Commission, 1984
(5) Garten & Dahlman, 1978
(6) Lemons, 1975
(7) Dawson et al., 1983
(8) Robberecht et al., 1983
(9) Dreesen & Williams, 1982
(10) Wilber, 1969 (in Brown, 1985)
(11) Kenaga, 1980
(12) U.S. EPA, 1977
(13) Holdway et al., 1983
(14) Drifmeyer & Odum, 1975
(15) Reish et al., 1982
(16) Weaver, 1984
(17) Kay, 1984
(18) Niethammer et al., 1984
(19) Oliver and Nicol, 1982
(20) Callahan et al., 1979
(21) Ogata & Miyake, 1978
(22) U.S. EPA, 1980 (updated with 1985 final)
(23) U.S. NRC, 1977
(24) Kenaga & Goring (in Lyman, 1982)
(25) Southworth et al., (in Lyman, 1982)
(26) Lu & Metcalf, 1975
(27) Vieth et al., 1979
(28) ICF, Inc., 1985
(29) Reish et al., 1983
(30) Guthrie & Davis, 1979
(31) Hartley and Johnson, 1983
(32) Ghisalba, 1983
(33) Klein et al., 1984
(34) Oakes et al., 1982
(35) Bahner et al., 1983
(36) U.S. EPA, 1979
(37) Guthrie et al., 1979
(38) U.S. EPA, 1985
(39) Hildebrand and Cushman, 1976
(40) Macek et al., 1979
(41) Wiedemeyer, 1986
(42) ICF, Inc., 1985b
(43) Oliver and Niimi, 1983

TABLE B-2

LOGARITHM N-OCTANOL-WATER COEFFICIENTS

Substance Name	CAS Number	Log Pow
1,1,1-TRICHLOROETHANE /BPA/	71-55-6	2.49
1,1,2,2-TETRACHLOROETHANE	79-34-5	2.39
1,1,2-TRICHLOROTRIFLUOROETHANE	76-13-1	3.16
1,1-DICHLOROETHANE /BPA/	75-34-3	1.79
1,1-DICHLOROETHYLENE/VINYLIDINE CHLORIDE/	75-35-4	2.13
1,2,3-TRICHLOROBENZENE	87-61-6	3.99
1,2,3-TRIMETHYLBENZENE	526-73-8	3.66
1,2,4,5-TETRACHLOROBENZENE	95-94-3	4.82
1,2,4-TRICHLOROBENZENE	120-82-1	4.12
1,2,4-TRIMETHYLBENZENE	95-63-6	3.78
1,2,5,6-DIBENZANTHRACENE	53-70-3	6.50
1,2-DIBROMOETHANE	106-93-4	1.96
1,2-DICHLOROETHANE /BPA/	107-06-2	1.48
1,2-DICHLOROETHYLENE -CIS	156-59-2	1.86
1,2-DICHLOROETHYLENE -TR	156-60-5	2.09
1,3,5-TRIMETHYLBENZENE/MESITYLENE/	108-67-8	3.42
1,3,5-TRINITROBENZENE	99-35-4	1.18
1,3-BUTADIENE /BPA/	106-99-0	1.99
1,3-DICHLOROBENZENE	541-73-1	3.38
1,4-NAPHTHOQUINONE	130-15-4	1.78

(Source: Technical Database Services, Inc., 1985)

TABLE B-2 (Continued)

Substance Name	CAS Number	Log Pow
1-BUTENE /BPA/	106-98-9	2.40
1-CHLOROBUTANE /BPA/	109-69-3	2.64
1-ETHYL-1-NITROSOUREA/ENU/	759-73-9	-0.15
1-ETHYL-2-METHYLBENZENE	611-14-3	3.53
1-METHYL-1-NITROSOUREA	684-93-5	-0.16
1-PROPENE,1-PHENYL	637-50-3	3.35
2,2'-DICHLOROETHYLETHER	111-44-4	1.29
2,2,2-TRICHLORO-1,1-ETHANEDIOL/CHLORALHYDRATE	302-17-0	1.61
2,3,4,5-TETRACHLOROPHENOL	4901-51-3	5.05
2,3,4,6-TETRACHLOROPHENOL	58-90-2	4.10
2,3,4-TRICHLOROPHENOL	15950-66-0	3.51
2,3,4-TRICHLOROPHENOL	15950-66-0	3.51
2,3,5,6-TETRACHLOROPHENOL	935-95-5	4.88
2,3,5-TRICHLOROPHENOL	933-78-8	4.56
2,3,6-TRICHLOROPHENOL	933-75-5	3.46
2,3-DICHLOROPHENOL	576-24-9	2.52
2,4,5-TRICHLOROPHENOL	95-95-4	3.72
2,4,6-TRICHLOROPHENOL	88-06-2	3.62
2,4,6-TRINITROTOLUENE	118-96-7	1.60
2,4-DICHLOROPHENOL	120-83-2	3.30

TABLE B-2 (Continued)

Substance Name	CAS Number	Log Pow
2,4-DIMETHYLPHENOL	105-67-9	2.30
2,4-DINITROPHENOL	51-28-5	1.50
2,4-DINITROTOLUENE	121-14-2	1.98
2,5-DICHLOROPHENOL	583-78-8	3.20
2,6-DICHLOROPHENOL	87-65-0	2.34
2-BUTANONE	78-93-3	0.29
2-HEXANONE	591-78-6	1.38
2-NITROGUANIDINE	556-88-7	-0.89
2-PENTANONE	107-87-9	0.91
2-PICOLINE/2-METHYL PYRIDINE/	109-06-8	1.11
3,3'-DICHLOROBENZIDINE	91-94-1	3.51
3,4,5-TRICHLOROPHENOL	609-19-8	4.01
3,4-DICHLOROPHENOL	95-77-2	2.86
3-METHIO-4-AMINO-6-T-BU-1,2,4-TRIAZINE-5-ONE	21087-64-9	1.70
3-METHIO-4-AMINO-6-T-BU-1,2,4-TRIAZINE-5-ONE	21087-64-9	1.70
4,4'-I-PROPYLIDENE-DIPHENOL/DIPHENYLOLPROPANE	80-05-7	3.32
4,4'-PCB	2050-68-2	5.58
4,4'-STILBENEDIOL,A,A'-DIETHYL/DES/	56-53-1	5.07
4-AMINOPYRIDINE	504-24-5	0.26
4-NITROQUINOLINE-1-OXIDE	56-57-5	1.02

TABLE B-2 (Continued)

Substance Name	CAS Number	Log Pow
6-AMINOCHRYSENE	218-01-9	4.98
7,12-DIMETHYLBENZ(A)ANTHRACENE	57-97-6	5.80
A,A,A-TRICHLOROTOLUENE	98-07-7	2.92
A-CHLOROTOLUENE	100-44-7	2.30
A-NAPHTHYLAMINE	134-32-7	2.25
A-NAPHTHYLTHIOUREA/ANTU/	86-88-4	1.66
ACENAPHTHENE	83-32-9	3.92
ACETANILIDE,4-ETHOXY/PHENACETIN/	62-44-2	1.58
ACETIC ACID	64-19-7	-0.17
ACETIC ACID, ETHYL ESTER	141-78-6	0.73
ACETIC ACID, METHYL ESTER	79-20-9	0.18
ACETIC ACID,BUTYL ESTER	123-86-4	1.82
ACETIC ACID,PROPYL ESTER	109-60-4	1.24
ACETONE	67-64-1	-0.24
ACETONITRILE	75-05-8	-0.34
ACETOPHENONE	98-86-2	1.73
ACETYLENE /BPA/	74-86-2	0.37
ACRIDINE	260-94-6	3.40
ACRYLAMIDE	79-06-1	-0.67
ACRYLIC ACID, BUTYL ESTER	141-32-2	2.36

TABLE B-2 (Continued)

Substance Name	CAS Number	Log Pow
ACRYLIC ACID, METHYL ESTER	96-33-3	0.80
ACRYLIC ACID,ETHYL ESTER	140-88-5	1.32
ACRYLONITRILE	107-13-1	-0.92
ADIPIC ACID	124-04-9	0.08
ALACHLOR/LASSO/	15972-60-8	3.52
ALACHLOR/LASSO/	15972-60-8	3.52
ALDICARB/TEMIK/	116-06-3	0.70
ALLYL ALCOHOL	107-18-6	0.17
ANILINE	62-53-3	0.90
ANILINE,N-METHYL	100-61-8	1.82
ANTHRACENE	120-12-7	4.45
ARGON /BPA/	7440-37-1	0.74
AZOBENZENE,4-DIMETHYLAMINO	60-11-7	4.58
B-NAPHTHYLAMINE	91-59-8	2.28
BENZALDEHYDE	100-52-7	1.48
BENZENE	71-43-2	2.13
BENZIDINE	92-87-5	1.34
BENZO(A)PYRENE	50-32-8	5.97
BENZOIC ACID	65-85-0	1.87
BENZONITRILE	100-47-0	1.56

TABLE B-2 (Continued)

Substance Name	CAS Number	Log Pow
BENZOPHENONE	119-61-9	3.18
BENZOTHIAZOLE	95-16-9	2.01
BIPHENYL	92-52-4	3.95
BROMOBENZENE	108-86-1	2.99
BROMOCHLOROMETHANE	74-97-5	1.41
BUTANE /BPA/	106-97-8	2.89
BUTANOL	71-36-3	0.88
BUTOXYETHANOL	111-76-2	0.83
BUTYL BENZOATE	136-60-7	4.21
BUTYLAMINE	109-73-9	0.88
BUTYLBENZENE	104-51-8	4.26
BUTYLBENZYLPHTHALATE	85-68-7	3.97
BUTYRALDEHYDE	123-72-8	0.88
CAPTAN	133-06-2	2.35
CARBOFURAN	1563-66-2	2.32
CARBON TETRACHLORIDE /BPA/	56-23-5	2.83
CHLORAMBUCIL/NCS 3088/	305-03-3	1.70
CHLOROBENZENE	108-90-7	2.84
CHLORODIFLUOROMETHANE/FREON-22/ BPA/	75-45-6	1.08
CHLOROFORM	67-66-3	1.97

TABLE B-2 (Continued)

Substance Name	CAS Number	Log Pow
CHLOROTRIFLUOROMETHANE/FREON 13/BPA/	75-72-9	1.65
CYCLOHEXANE /BPA/	110-82-7	3.44
CYCLOHEXANOL	108-93-0	1.23
CYCLOHEXANONE	108-94-1	0.81
CYCLOHEXYLAMINE	108-91-8	1.49
CYCLOPROPYLBENZENE	873-49-4	3.27
CYTOXAN/CYCLOPHOSPHAMIDE/	50-18-0	0.63
DDE	72-55-9	4.87
DDT	50-29-3	3.98
DECANE	124-18-5	5.01
DEMETONTHIOL	298-04-4	1.93
DI-(P-AMINOPHENYL)METHANE	101-77-9	1.59
DI-2-ETHYLHEXYLPHTHALATE	117-81-7	3.98
DI-I-PROPANOLAMINE	110-97-4	-0.82
DIBENZOFURAN	132-64-9	4.12
DIBUTYL ETHER	142-96-1	3.21
DICHLORODIFLUOROMETHANE/FREON-12/BPA/	75-71-8	2.16
DICHLOROFLUOROMETHANE/FREON-21/ BPA/	75-43-4	1.55
DICOFOL	115-32-2	3.54
DIETHANOLAMINE	111-42-2	-1.43

TABLE B-2 (Continued)

Substance Name	CAS Number	Log Pow
DIETHYLAMINE	109-89-7	0.57
DIETHYLPHTHALATE	84-66-2	2.47
DIMETHOATE	60-51-5	0.50
DIMETHOXYMETHANE	109-87-5	0.00
DIMETHYLAMINE	124-40-3	-0.38
DIMETHYLFORMAMIDE	68-12-2	-1.01
DIMETHYLPHTHALATE	131-11-3	1.56
DINOSEB	88-85-7	2.30
DIOXANE	123-91-1	-0.42
DIPHENYLAMINE	122-39-4	3.34
DIPHENYLNITROSAMINE	86-30-6	3.13
DIPROPYLAMINE	142-84-7	1.73
DIPROPYLNITROSAMINE	621-64-7	1.36
DODECANOIC ACID/LAURIC ACID/	143-07-7	4.20
ETHANE /BPA/	74-84-0	1.81
ETHANE-1,2-DIOL/ETHYLENE GLYCOL/	107-21-1	-1.93
ETHANOLAMINE	141-43-5	-1.31
ETHION	563-12-2	5.07
ETHYL CHLORIDE/BPA/	75-00-3	1.43
ETHYL ETHER	60-29-7	0.77

TABLE B-2 (Continued)

Substance Name	CAS Number	Log Pow
ETHYLAMINE	75-04-7	-0.13
ETHYLBENZENE	100-41-4	3.15
ETHYLENE	74-85-1	1.13
ETHYLENE OXIDE /BPA/	75-21-8	-0.30
FLUORANTHENE	206-44-0	5.20
FLUORENE	86-73-7	4.18
FLUOROACETAMIDE	640-19-7	-1.05
FLUOROFORM/BPA/	75-46-7	0.64
FORMALDEHYDE	50-00-0	0.35
FORMALDEHYDE	50-00-0	0.35
FORMIC ACID	64-18-6	-0.54
FURAN /BPA/	110-00-9	1.34
FURFURAL	98-01-1	0.41
GLYCEROL /BPA/	56-81-5	-1.76
GLYCERYL TRINITRATE	55-63-0	1.62
HEPTANE	142-82-5	4.66
HEXACHLORO-1,3-BUTADIENE	87-68-3	4.74
HEXACHLOROBENZENE	118-74-1	4.13
HEXACHLOROCYCLOHEXANE, ALPHA ISOMER//124/356/	319-84-6	3.80
HEXACHLOROCYCLOHEXANE,BETA ISOMER//135/246/	319-85-7	3.78

TABLE B-2 (Continued)

Substance Name	CAS Number	Log Pow
HEXACHLOROCYCLOHEXANE/BHC/ GAMMA ISOMER	58-89-9	3.61
HEXACHLOROCYCLOPENTADIENE	77-47-4	5.04
HEXACHLOROETHANE	67-72-1	3.82
HEXACHLOROPHENE /PKA2=11.33/	70-30-4	2.62
HEXANE	110-54-3	3.90
HYDRAZINE	302-01-2	-2.07
HYDRAZOBENZENE	122-66-7	2.94
HYDROCYANIC ACID /BPA/	74-90-8	-0.25
I-BUTANOL	78-83-1	0.76
I-PROPANOL	67-63-0	0.05
I-PROPYLAMINE	75-31-0	-0.03
IMIDAZOLIDONE,2-THIO/ETHYLENETHIOUREA/	96-45-7	-0.66
INDENE	95-13-6	2.92
ISOPROPYLBENZENE	98-82-8	3.66
M-CHLOROPHENOL	108-43-0	2.50
M-DIHYDROXYBENZENE/RESORCINOL/	108-46-3	0.80
M-DINITROBENZENE	99-65-0	1.49
M-XYLENE	108-38-3	3.20
MALATHION	121-75-5	2.89
MALEIC ACID HYDRAZIDE /3,6-DIHYDROXYPYRIDAZIN	123-33-1	-0.84

TABLE B-2 (Continued)

Substance Name	CAS Number	Log Pow
METHACRYLIC ACID, ETHYL ESTER	97-63-2	1.94
METHACRYLIC ACID, METHYL ESTER	80-62-6	1.38
METHACRYLONITRILE	126-98-7	0.68
METHANE /BPA/	74-82-8	1.09
METHANOL	67-56-1	-0.64
METHOMYL	16752-77-5	1.08
METHOMYL	16752-77-5	1.08
METHOXYCHLOR	72-43-5	3.31
METHYL BROMIDE /BPA/	74-83-9	1.19
METHYL CHLORIDE/BPA/	74-87-3	0.91
METHYL IODIDE	74-88-4	1.69
METHYLAMINE	74-89-5	-0.57
METHYLHYDRAZINE	60-34-4	-1.05
METOLACHLOR	51218-45-2	3.13
METOLACHLOR	51218-45-2	3.13
MORPHOLINE	110-91-8	-1.08
MUSCIMOL	2763-96-4	-2.39
N,N-DIMETHYLANILINE	121-69-7	2.31
N-METHYLCARBAMATE,1-NAPHTHYL	63-25-2	2.36
N-NITROSODIBUTYLAMINE	924-16-3	1.92

TABLE B-2 (Continued)

Substance Name	CAS Number	Log Pow
N-NITROSODIETHYLAMINE	55-18-5	0.48
N-NITROSODIMETHYLAMINE	62-75-9	-0.57
N-NITROSOPIPERIDINE	100-75-4	0.63
N-NITROSOPYRROLIDINE	930-55-2	-0.19
NAPHTHALENE	91-20-3	3.59
NITROBENZENE	98-95-3	1.85
NITROETHANE	79-24-3	0.18
NITROMETHANE	75-52-5	-0.33
NONANE	111-84-2	4.51
O-AMINOPHENOL	95-55-6	0.62
O-CHLOROPHENOL	95-57-8	2.17
O-CHLOROTOLUENE	95-49-8	3.42
O-DIBUTYLPHTHALATE	84-74-2	4.72
O-DICHLOROBENZENE	95-50-1	3.38
O-DINITROBENZENE	528-29-0	1.58
O-DIOCTYLPHTHALATE	117-84-0	5.22
O-ETHYL CARBAMATE/URETHANE/	51-79-6	-0.15
O-HYDROXYBENZOIC ACID/SALICYLIC ACID/	69-72-7	2.26
O-METHYLBENZENESULFONAMIDE	88-19-7	0.84
O-NITROPHENOL	88-75-5	1.26

TABLE B-2 (Continued)

Substance Name	CAS Number	Log Pow
O-PHTHALIC ACID	88-99-3	0.73
O-TOLIDINE	119-93-7	2.34
O-XYLENE	95-47-6	2.77
OCTANE	111-65-9	5.18
OCTANOL	111-87-5	3.15
P-AMINOPHENOL	123-30-8	0.04
P-CHLOROANILINE	106-47-8	1.83
P-CHLOROBIPHENYL	2051-62-9	4.90
P-CHLOROPHENOL	106-48-9	2.35
P-DICHLOROBENZENE	106-46-7	3.39
P-DIHYDROXYBENZENE/HYDROQUINONE/	123-31-9	0.59
P-DINITROBENZENE	100-25-4	1.46
P-NITROANILINE	100-01-6	1.39
P-NITROPHENOL	100-02-7	0.76
P-NITROTOLUENE	99-99-0	2.37
P-XYLENE	106-42-3	3.15
PARALDEHYDE	123-63-7	0.67
PARAOXON	311-45-5	1.69
PARATHION	56-38-2	2.15
PENTACHLOROBENZENE	608-93-5	5.52

TABLE B-2 (Continued)

Substance Name	CAS Number	Log Pow
PENTACHLOROETHANE	76-01-7	3.05
PENTACHLORONITROBENZENE/QUINTOZENE/	82-68-8	4.22
PENTACHLOROPHENOL	87-86-5	5.01
PENTANE /BPA/	109-66-0	3.23
PENTANOL	71-41-0	1.40
PHENANTHRENE	85-01-8	4.46
PHENOL	108-95-2	1.48
PHENOL,4-CHLORO,3-METHYL	59-50-7	3.10
PHENOXYACETIC ACID,2,4,5-TRICHLORO	93-76-5	3.13
PHENOXYACETIC ACID,2,4-DICHLORO	94-75-7	2.81
PHENTERMINE	122-09-8	1.90
PHENYLARSONIC ACID /PKA2=8.48/	98-05-5	0.06
PHENYLMERCURIC ACETATE	62-38-4	0.71
PHENYLTHIOUREA	103-85-5	0.73
PHORATE/THIMET/	298-02-2	3.56
PHOSPHINE SULFIDE,TRIS-(1-AZIRIDINYL)/NSC 639	52-24-4	0.53
PHOSPHORIC ACID	7664-38-2	-1.86
PHTHALIC ANHYDRIDE	85-44-9	1.60
PIPERAZINE	110-85-0	-1.17
PROARGYL ALCOHOL/2-PROPYN-1-OL/	107-19-7	-0.38

TABLE B-2 (Continued)

Substance Name	CAS Number	Log Pow
PROPANOL	71-23-8	0.30
PROPENAL/ACROLEIN/	107-02-8	-0.01
PROPIONALDEHYDE	123-38-6	0.59
PROPIONIC ACID	79-09-4	0.33
PROPIONITRILE	107-12-0	0.16
PROPYLAMINE	107-10-8	0.48
PROPYLENE /BPA/	115-07-1	1.77
PROPYLENE OXIDE	75-56-9	0.03
PYRENE	129-00-0	4.88
PYRIDINE	110-86-1	0.62
QUINOLINE	91-22-5	2.02
QUINONE	106-51-4	0.20
STYRENE	100-42-5	2.95
TEREPHTHALIC ACID	100-21-0	2.00
TETRACHLOROETHYLENE	127-18-4	3.40
TETRAFLUOROMETHANE /BPA/	75-73-0	1.18
TETRAHYDROFURAN /BPA/	109-99-9	0.46
THIOPHENOL	108-98-5	2.52
THIOUREA	62-56-6	-0.98
TOLUENE	108-88-3	2.69

TABLE B-2 (Concluded)

Substance Name	CAS Number	Log Pow
TRICHLOROETHYLENE	79-01-6	2.29
TRICHLOROFLUOROMETHANE/FREON-11/BPA/	75-69-4	2.53
TRIETHYLAMINE	121-44-8	1.44
TRIETHYLPHOSPHATE	78-40-0	0.80
TRIFLURALIN	1582-09-8	3.06
TRIMETHYL ORTHOFORMATE	149-73-5	0.25
TRIS-(2,3-DIBROMOPROPYL)-PHOSPHATE	126-72-7	3.71
UREA	57-13-6	-1.09
VINYL ACETATE	108-05-4	0.73
WARFARIN	81-81-2	0.05

TABLE B-3

LOGARITHM OF N-OCTANOL-WATER COEFFICIENTS (LOG POW) FOR SELECTED ORGANIC CHEMICALS FOUND AT NATIONAL PRIORITIES LIST SITES

Substance Name	Log Pow	Source
Acenaphthalene	3.74	U.S. EPA, 1981
Benz(A)anthracene	5.61	U.S. EPA, 1981
Benzo(B)fluoranthene	6.06	U.S. EPA, 1981
Benzo(K)fluoranthene	6.06	U.S. EPA, 1981
1,12-Benzoperylene	6.51	U.S. EPA, 1981
Creosote (coal tar)	3.98	Callahan et al., 1979
Chrysene	4.98	Leo et al., 1971
Dibenz(A,H)acridine	5.73	U.S. EPA, 1981
m-Dichlorobenzene	3.44	Veith et al., 1980
Beta hexachlorocyclohexane (Beta BHC)	3.80	Callahan et al., 1979
Delta hexachlorocyclohexane (Delta BHC)	4.14	Callahan et al., 1979
3-Methylcholanthrene	6.97	U.S. EPA, 1981
1-Methylphenanthrene	5.00	U.S. EPA, 1981
Methylnaphthalene	4.22	MITRE*
Napthol	2.84	Leo et al., 1971
2-Pentanone (Methyl propyl ketone)	0.84	MITRE*
2,3-Phenylene pyrene	6.51	U.S. EPA, 1981
1,2,3,4-Tetrachlorobenzene	4.60	Chiou, 1985
Tribromomethane (Bromoform)	2.39	MITRE*
Trimethyl benzene	4.04	MITRE*
2,3,4-Trinitrotoluene (TNT)	2.01	MITRE*
2,4,5-Trinitrotoluene (TNT)	2.01	MITRE*

*Calculated by Leo's Fragment Constant Method as specified in Lyman et al., 1982.

APPENDIX C

ECOLOGICAL FACTORS WHICH AFFECT BIOACCUMULATION

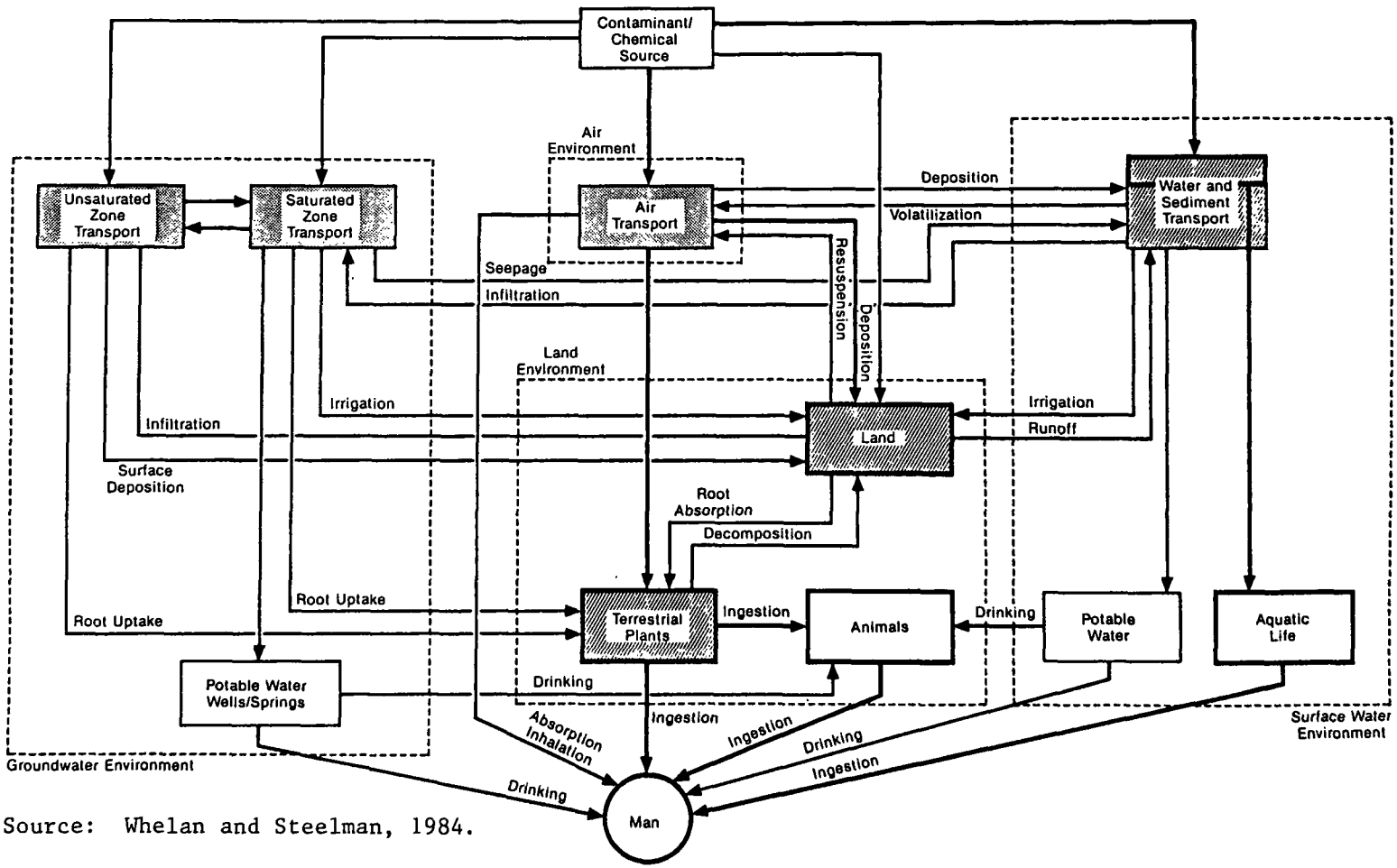
The biological processes and ecological interactions within aquatic and terrestrial systems are complex and not completely understood. Figure C-1 (Whelan and Steelman, 1984) is a simple schematic which shows the various environmental factors that can affect the transport of a chemical through the environment to eventually reach man. As Figure C-1 illustrates, the ecosystem involves complex interactions among the biotic and abiotic (non-living) components of the environment. The food chain is only one of those interconnected links. The physical/chemical fate of pollutants in the ecosystem influences, and is influenced by, the biological processes.

Because of the complexity of ecosystems and the diversity of organisms, there is no easy method to evaluate the availability of substances to either aquatic or terrestrial plants and animals or to man (Jenne and Luoma, 1977; Fraser and Lum, 1983). Nonetheless, a large body of scientific information, reflected in the tables in Appendix B, points out the potential for substances to bioaccumulate from the environment to human food organisms. Some substances clearly are found in biotic tissues at concentrations thousands of times greater than in the environment.

The preferred method of assessing the potential for a substance to enter the food chain is the direct measurement of the

Figure C-1

Schematic Diagram Illustrating the Interactions Between Media and the Movement of Contaminants to Human Targets



Source: Whelan and Steelman, 1984.

bioconcentration factor and/or the biomagnification of the substance in food organisms. However, as Table B-1 illustrates, there can be a wide diversity of bioconcentration factors measured for a specific substance reported in the literature. The reasons for such wide diversity are discussed below.

C.1 Ecological Factors

The ecological factors which affect the behavior of pollutants through the food chain include diversity, competition, niche, uptake modes, mobility, availability, and trophic level. It is the latter which is most important, especially for those substances which biomagnify in the food chain. If, at each increasing trophic level from producer (plants) to consumer (grazer) to predator (carnivore), the substance is concentrated at levels higher than in the food source or the surrounding environment, and if man is at the top of the food chain, then the threat to man is of concern.

Not all hazardous substances show consistent results for measurements of bioconcentration and subsequent magnification. Furthermore, some substances act differently in terrestrial ecosystems than they do in aquatic environments. For example, plutonium has a reported bioconcentration factor of over 1,000 in the marine ecosystem, but it is virtually unavailable to biota in terrestrial ecosystems (because it remains in the soil) (Corey and Boni, 1977; Garten and Dahlman, 1978; Hanson, 1975; National Research Council, 1975).

Ecosystems can change the form of the hazardous substance from that which was released into the environment to another form in tissue. For example, antimony may be released into the water in its elemental form or in any of a variety of compounds, but it is found in fish as antimony trioxide. Another example is mercury, which when converted to methylmercury in the environment, becomes more toxic (see Appendix D). The organism itself may take compound X and convert it to compound Y. For example, fish convert benzo(a)pyrene, a pollutant reported at many NPL sites, into metabolites strongly suspected of being carcinogenic and which have been found in edible portions of fish (Harshbarger, 1983; Melius, 1981).

C.2 Species and Individual Variability

There are distinctive characteristics of species which complicate the uptake process even further. Separate species have different niches in the environment; they eat different foods and live in widely varied habitats. Sole or flounder, for example, are bottom feeders and are more likely to be exposed to toxic substances found in sediments. Salmon, on the other hand, are anadromous (spawn in rivers) and may pass through a contaminated bay only once or twice in a lifetime. Menhaden are found in estuaries mainly in the juvenile stage, and so would only be exposed to coastal pollution as a juvenile, not as an adult. Various species are found on different trophic levels, and some, mullet for example, can feed at several trophic levels (Odum, 1970). A fish in a natural

environment may alter its feeding habits, eating vegetation one season, insects during another, and juvenile fish when available.

Within one species, there may also be wide individual variations which influence the levels of substances found in tissues. Physiological factors such as size, age, sex, condition, and metabolism all affect the results reported in the literature. Many hazardous substances concentrate in fatty tissue. Therefore, a female or an animal in good condition may store these substances. A starving individual, however, may be forced to use its fatty tissue and release the stored substances. In the case of PCB bioaccumulation in lake trout, older and larger individuals would be expected to have the greatest body burden because they are the top predator (Thomann and Connolly, 1984). Some individuals may metabolize a chemical, change it to another form, or excrete it rapidly (McKim et al., 1976).

Another factor which influences the results of biotic measurements is the tissue analyzed. Some authors report results from analyses of whole fish, some from fatty tissue, and some from edible meat, while others report the results from liver tissue. One study (Versar, 1985) reported that the worst-case scenario from a risk analysis for the Commencement Bay (Washington) food chain was for ingestion of fish liver. Although the population that eats fish liver is believed to be small, no data were available for the amount of liver consumed (Versar, 1985). Liver concentrations of hazardous

substances are usually high, because that is where those substances are metabolized. It is also easily measured. However, as mentioned above, fish liver is rarely ingested; therefore, the majority of results reported in Appendix B are for concentrations found in edible tissue or muscle.

C.3 Experimental Methods Used in Ecology

Bioconcentration factors reported in the literature also vary widely based on whether the data were collected in the laboratory or collected in the field. In the field, the uptake into the food web is influenced by numerous natural phenonmena including water quality, weather, trophic level, population competition, and availability of other food. In a laboratory experiment, the researcher is able to control many of the variables, including the water quality (pH, temperature, salinity) as well as the number of species present. He may, for example, set up a simple food chain from water to Daphnia to bluegills.

One important environmental variable which affects results is the duration of exposure. The exposure can be controlled in the laboratory where fish for instance, may be held in the experimental tank for as little as a few hours or days. In the field the duration is generally unknown, but similar fish could be exposed to the pollutant over a lifetime. Duke (1982) cautions scientists about the risks of extrapolating the results from laboratory experiments to the environment. Fish, when removed from a

contaminated environment, may be able to depurate or to purify their tissues when placed in clean water. This protective feature complicates field data, where the fish may live only a portion of their entire life cycle in a polluted environment.

Bourquin and Pritchard (1983) reported that certain organics (e.g., phthalates) are known to degrade biologically in the laboratory; however, in the field they tend to accumulate in the environment, even within ecological niches which appear to be optimal for degradation. In addition, the degradative processes in estuarine and marine environments may differ significantly from those in other aquatic environments.

Another variable, which makes comparisons of direct measurements difficult, is that the sampling and analysis methods used are quite often unique to a given study. One researcher might collect samples from local fishermen, while another uses random sampling from an entire bay. One researcher might collect samples over a four-day period, while another might collect his samples over a four-season period. One study may have results from 10 samples, while another reports results from 100 samples. All of these variations in sampling protocol may yield different results.

After sampling, additional variables are introduced by the preparation of the sample and by the analytical method used, further diversifying results. For some of the newer organic chemicals introduced into the environment (xenobiotics), there may not be an

analytical method of detection yet developed, there may be only one technique known, or the analysis may be very expensive. The results reported in the literature may, therefore, be very limited. On the other hand, data on many pesticides and metals are relatively easy to obtain, so there are a number of published studies available for these substances. For example, there are dozens to hundreds of published research reports on the bioaccumulation of DDT and cadmium, but very few on dioxins (TCDD), and none were found on asbestos. Substances, such as pesticides, which biologists have known about for decades, have a large body of research data published to support the conclusion that they do or do not biomagnify in the food chain. For other hazardous substances, data are limited and their biomagnification potentials are unknown at this time.

C.4 Metals in Sediments and Their Availability to Biota

Metals are persistent, remaining in the ecosystem for a very long time. Scientific debates continue as to whether or not those metals are available to biota for uptake into the food chain.

Sinderman et al. (1982) report that all three media (i.e., the settled particles, interstitial waters, and water immediately overlying the bottom) can provide major sources of metals to benthos in their natural habitat. Metals which are dissolved or adsorbed to particles are both potentially available, since filter feeders take in both sediments and water while feeding. The result is that the filter feeding organisms taken from contaminated zones have, on

average, ten times more metals in them than those biota found in other regions (Sinderman et al., 1982). The same result was reported by Taymaz et al. (1984) whose data suggest that a relationship exists between heavy metal content in shoreline sediments and in benthic fish.

The heavy metals may be either in dissolved form or adsorbed to particles. If dissolved, then the likely route of exposure in fish is across gill membranes or by direct ingestion. When water is ingested, both suspended solids and dissolved metals can be ingested. When food is ingested, particularly for bottom feeding fish, the adsorbed metals are ingested along with the benthos. Some benthic organisms, for example filter feeders and detritis feeders, ingest the sediments themselves. When an animal takes in the slurry mixture at the interface between sediments and water, the slurry contains the solid sediments, the organic detritis, as well as the interstitial waters between the particles. Metals may be found in all of those components, and since the sediment layer acts as a "sink" for heavy metals, this sediment interface becomes an important consideration (Taymaz et al., 1984).

The persistence of metals in sediments is related to the presence of organic matter and clay fractions since these affect sorption (Drifmeyer and Odum, 1975; Sinderman et al., 1982). This would be particularly important in the food chain of detritis feeders (e.g., shrimp and crabs). Even sandy sediments have a

proportion of silt and clay and retain metals, though in lesser amounts. Clay and silty bottom sediments may constitute a considerable reservoir of heavy metals in the ecosystem. In their food chain studies, Drifmeyer and Odum (1975) found there was a decrease in metal content within sediments as the particle size increased, which is consistent with the metals being adsorbed on the surface of the particles.

As noted above and discussed further below, a number of researchers have shown that adsorbed metals are available and are incorporated into biotic tissue. This is particularly true for bottom feeders, filter feeders, and immobile shellfish. However, the U.S. Army Corps of Engineers studies on dredged material (Lee and Jones, 1977; Montgomery and Palermo, 1983) report metals are not released to water, but instead remain tightly bound to the sediments.

Hardy et al. (1981) reported sediments serve as a "sink" for removal of dissolved cadmium from water. Bioaccumulation was related to the soluble Cd^{+2} ion concentration. The interstitial waters in sediments are high in dissolved organics which may complex with the cadmium and thus reduce availability.

Drifmeyer and Odum (1975) studied dredged spoil pond ecosystems and the uptake of lead, zinc and manganese via the detritis food chain. Detritus was a significant factor in the bioaccumulation of lead in that one-third to one-half of the lead was passed on via the detritis food chain. The grass shrimp, for example, eat

particulates with a high lead content, and thus, serve as a source of heavy metals to the mummichog fish. The mummichogs, in turn, had high levels of lead in those areas where sediments were contaminated.

Guthrie and Davis (1979) reported results from water, sediments, and benthos in the Gulf of Mexico, Texas. Data from the Gulf revealed that concentrations of 9 out of the 10 heavy metals studied were higher in the sediments than in the water column. Furthermore, zinc was present in higher concentrations in bottom organisms (e.g., worms and oysters) than in sediments. Oysters had significantly higher concentrations of zinc, copper, and arsenic than were present in the water samples. Clams had significantly higher concentrations of arsenic when compared to water samples taken from the same locations. Crabs had high levels of both arsenic and copper, which were believed to have come from both water and sediment sources.

O'Connor and Rachlin (1982) report different results for the Atlantic coast. The sediment concentrations did not correlate with metals measured in exposed organisms. However, these authors did indicate the geographic trends in metals in benthos of the Atlantic coast tend to correspond with the general trends for metals in those coastal sediments. O'Connor and Rachlin (1982) further suggest that increasing levels of metals in the environment would result in increased levels of metals in organisms.

These illustrations serve to explain why such diverse results are found in Appendix B, where the bioconcentration factors are

listed for both organic and inorganic hazardous substances. While not an invariant paramater for a given substance, the bioconcentration factor is well documented by published research papers, and it is an accepted indicator of which hazardous substances are relatively more important in the food chain.

APPENDIX D

CHEMICAL/PHYSICAL FACTORS WHICH AFFECT BIOACCUMULATION

As discussed in Appendix C, direct measurement of the bioaccumulation of hazardous substances in food chain organisms is complex, expensive and not always consistent. Furthermore, data are not available for all substances. In Section D.1, physical/chemical characteristics which may be used as indicators of the potential for an organic substance to bioaccumulate in the food chain are examined. Such characteristics could be used for assessing the potential for a substance to enter the food chain in the absence of the more direct measurements described in Section 2 of the main body of this report. These alternative characteristics could also be used to confirm direct measurement data in cases where there may be some question concerning the validity of those measurements.

Bioaccumulation information for inorganic chemicals is often reported in terms of a particular element present (usually a metal cation such as mercury, copper, etc.) and not in terms of a particular chemical species. The uptake and accumulation of the metal elements usually depends on the particular chemical species present (i.e., whether it is a hydrated or unhydrated ion, a covalent compound such as methylmercury, or a soluble ionic compound such as mercury chloride). However, as discussed in Section D.2, once a substance is released into the environment, it is likely to be physically and/or chemically and/or biologically altered by

complex natural processes. Therefore, the particular chemical species initially present at a site is not necessarily of importance in an initial ranking of its potential to accumulate in the food chain.

D.1 Organic Chemicals

A literature review indicated that for organic chemicals, the characteristics which may affect their potential to bioaccumulate include biodegradability, volatility, solubility, soil adsorption coefficient, and n-octanol-water partition coefficient. The first two influence the persistence of the substance in the environment; the more persistent substances have a greater opportunity to bioaccumulate. These two characteristics are discussed in the following two sections. The latter three characteristics are discussed in Section 2.

D.1.1 Biodegradability

Biodegradability refers to the propensity of a chemical to be degraded by microorganisms in the environment. It is an important characteristic to be considered in evaluating the fate of a chemical because if a chemical is biodegradable in a few hours or days, then the likelihood of its causing harm to public health through the food chain is reduced in comparison with chemicals that persist for months or years (Wood, 1982). If a substance is not biodegraded, then it is more likely to be persistent and more available for biotic uptake.

For a variety of reasons, however, biodegradation does not appear to be useful as a measure of the accumulation of a substance in food chain organisms. Laboratory biodegradation study results may not reflect conditions in the field where oxygen, oxidation reduction potential, temperature, pH, competing organisms, and chemical concentrations all affect the biodegradation process (Kobayashi and Rittmann, 1982). Residual concentrations of a substance left after the bulk of the substance has been degraded may still be subject to bioconcentration and could accumulate in the food chain to harmful levels. Finally, no published correlations relating bioaccumulation to biodegradability were identified.

D.1.2 Volatility

The volatility of a chemical substance is its propensity to vaporize and enter the atmosphere and is recognized as another indicator of the environmental fate of that substance (Mackay et al., 1982; Gillett, 1983; Suffet, 1975; Filov et al., 1979). Volatility could also be considered as a measure of persistence in the local environment. Substances which volatilize and dissipate quickly are not as readily available to biota for uptake.

The fundamental physical property of a chemical substance, which is an indicator of its tendency to volatilize, is its vapor pressure. However, vapor pressure data are not always readily available for substances or for mixtures of substances. Further, Mackay et al. (1982) report that many of the published vapor

pressure data may be erroneous. The limited availability of volatility or vapor pressure data and the lack of any reported consistent relationship between volatility and accumulation in food chain organisms limits the usefulness of volatility as a measure of the potential of a substance to accumulate in the food chain.

Thus, volatility and biodegradation were judged not to be useful as indicators of the bioaccumulation potential of hazardous substances in food chain organisms. They are considered to be more a measure of environmental persistence than of bioaccumulation, but they could be useful for fine tuning the food chain hazard classification of a chemical as suggested by Gillett (1983). For example, if two or more substances have similar bioconcentration factors, consideration of their environmental persistence based on biodegradeability or volatility could be used to establish a hazard ranking relative to each other. More persistent substances are usually those which are more likely to be taken up into the food chain. Thus, substances which volatilize or which degrade in the environment are not as potentially available to man via the food chain as are more persistent substances. Note however, that the current HRS includes a persistence factor and the use of persistence to rank substances in the proposed bioaccumulation ranking factor might be undesirable if the current HRS persistence factor were to remain unchanged.

D.2 Inorganic Chemicals

Among the elements identified at NPL sites are: aluminum, antimony, arsenic, boron, cadmium, chromium, cobalt, copper, iron, lead, manganese, mercury, molybdenum, nickel, plutonium, radium, selenium, silver, strontium, tin, titanium, uranium, vanadium, and zinc. The uptake and accumulation in the food chain of such elements may depend on the particular chemical species present, i.e., whether it is the pure element or a compound such as methylmercury, mercury chloride, copper sulphate, etc. However, once a substance is placed in a waste site or subsequently released into the environment, it is likely to be physically and/or chemically and/or biologically altered by natural processes into other forms that may be more or less available for uptake and accumulation in the food chain. Thus, even if a substance is initially present in a waste site in a form that is not readily biologically available, there is potential for it to be transformed to one that is readily available, and vice versa.

For example, natural waters are complex systems containing a variety of organic and inorganic matter from the natural decay and degradation of plants and animals, from soil erosion, and from human activities. The chemical and physical interaction of released chemical elements and their compounds with the organic and inorganic matter affects the behavior of the substances and their impact on the environment. Humic and fulvic acids, which constitute the major

portion of natural organic matter present in natural waters, reduce the biological availability of many metals by forming complexes with them (Neubecker and Allen, 1983; Morel et al., 1974).

Oily organic pollutants can concentrate at the surface of a body of water. The elements iron, lead, copper, and nickel have been found to concentrate in this organic surface layer (Andelman, 1973). Once concentrated, the metal and organic pollutants can enter the food chain when surface feeders ingest the hazardous substances along with food.

Natural waters also contain a number of inorganic compounds which can react with another inorganic substance that is released into the water. Chlorides, sulfates, fluorides, sulfides, phosphates, carbonates, and bicarbonates are among the more common species of inorganic compounds found in natural waters. A wide variety of soluble and insoluble compounds of released metals, for instance, can be formed depending on the inorganic compounds present in the water and on such factors as the acidity or alkalinity of the water and the oxidation-reduction environment. In a reducing environment, for example, toxic hexavalent chromium is reduced to less harmful trivalent chromium. In an acidic environment with sulfide present, mercuric ions combine with sulfides to form insoluble mercuric sulfide. If the water is alkaline, soluble mercury-sulfide complexes can form (Leckie and James, 1974). Insoluble substances tend generally to be less biologically

available than soluble substances. However, if they remain suspended in the water (e.g., in a fast moving stream) they can be ingested by fish or adsorbed onto the fish gills. In quiescient water, insoluble substances will settle in the sediment, where they may be taken up by benthic organisms and bottom feeding fish.

Physical adsorption of metal ions on suspended clay particles is another important process that can affect the bioavailability of the metal as discussed in Appendix C. Metal uptake varies with clay characteristics, the concentration and chemical form of the metal species, and the solution pH (Beveridge and Pickering, 1983).

Microorganisms present in the environment can also alter the form and availability of inorganic chemicals introduced into the environment. Bacteria are involved in the immobilization of iron by transforming the ferrous form of iron to the ferric form which precipitates as ferric hydroxide (Berthelin and Dommergues, 1976). Microbial immobilization of aluminum and silicon also occurs (Berthelin and Dommergues, 1976). Bacteria are also implicated in the conversion of mercury to methylmercury. Microorganisms are also present in the environment that can convert methylmercury into inorganic mercury forms (Cooley and McCarty, 1977).

The physical form in which a potentially hazardous substance is released to the environment is another factor that must be considered in evaluating its fate and effect in that environment. Its initial form may inhibit or delay the conversion process;

conversely, it may enhance the likelihood of transport and rapid conversion in the environment. For example, solid massive forms of metals such as iron, aluminum, copper, or zinc will slowly corrode from exposure to air and other chemicals in the natural environment. Leachate containing the metals can subsequently enter the soil and nearby waterways. Aqueous solutions of inorganic chemicals, if accidentally released, can move relatively quickly into the soil and/or nearby waterway. Once in the environment, the fate of the substance will be affected by the local environmental conditions as well as its initial chemical form.

In natural waters, the behavior and bioavailability of released inorganic compounds will be controlled by the chemical, physical, and biological characteristics of the particular body of water. These characteristics can be different for the same body of water at different times of the year. They will be different for lakes, estuaries, and oceans. They will also differ among aquatic ecosystems and soil types in different geographical locations (Andelman, 1973; Troup and Bricker, 1975).

D.3 Summary

Characteristics of a chemical substance which might be used in the absence of bioconcentration factor data to assess the potential of the substance to accumulate in the food chain were examined. Characteristics examined included biodegradability, volatility, n-octanol-water coefficient, solubility, and soil adsorption

coefficient. For organic substances, the logarithm of the n-octanol-water partition coefficient (log Pow) provides a satisfactory alternative measurement, because a significant correlation has been found between it and the bioconcentration factor. The correlation shows that, in general, as the bioconcentration factor increases the log Pow increases.

Biodegradation and volatility are measures of the persistence of a substance in the environment and may affect the potential of a substance to bioaccumulate, in that more persistent chemicals have a greater opportunity to bioaccumulate. However, the persistence of a substance in the environment is already considered in the HRS, and therefore, use of these characteristics in a bioaccumulation ranking factor was considered redundant.

As discussed in Section 2, the properties of water solubility and soil adsorption partition coefficients have been shown to have significant correlations with the bioconcentration factor, comparable to those of the log Pow.

Bioaccumulation information for inorganic compounds is usually reported in terms of a particular element present, usually the metal cation (e.g., mercury, copper, etc.), and not in terms of the particular chemical species. Uptake and accumulation of the metals generally depends on the particular species present, i.e., whether the pure element or a particular compound of the element is present. However, once a substance is released into the environment

it is likely to be physically, chemically, or biologically altered by natural processes into other forms. Even if a substance is initially present at a wastes site in a biologically unavailable form, it is possible for it to be transformed to another form which is biologically available. For this reason, it is considered unnecessary to consider the specific chemical species present at a hazardous wastes site in an initial ranking of the potential for an inorganic substance to accumulate in the food chain. This methodology is for use as a screening tool when very little data is available at a site.

APPENDIX E

GLOSSARY OF TERMS USED

accumulation	- Uptake of a substance from the environment
anadromous	- Fish which spawn in rivers, but live in the ocean
annual production	- Amount or rate of energy storage by plants over a year
availability	- Being present in a physical or chemical form that allows the substance to be taken up by biota
BCF	- Bioconcentration factor
benthic	- Bottom dwelling
benthos	- Bottom dwelling organisms
bioaccumulation	- Uptake of a substance from the environment (including the food chain) via a biological process to be incorporated into tissue at concentrations higher than those found in the surrounding environment
bioconcentration	- The process by which substances present in solution enter aquatic organisms directly through the gills or epithelial tissue. This process causes an increase in concentration of the substance in biota above that in its ambient environment (e.g., fish have higher concentrations than water; worms have higher concentrations than soil)
bioconcentration factor (BCF)	- Ratio of the concentration of a substance in biota to its concentration in the ambient environment
biodegradability	- Extent to which a substance can be decomposed by organisms
biodegradation	- Decomposition of an organic substance by living organisms

biological half-life	- Time it takes an animal (organism) to degrade, metabolize, convert or excrete 50% of a substance
biomagnification	- Process whereby the tissue concentration of a bioaccumulated substance increases at each step in the food chain, as the substance moves through two or more trophic levels
body burden	- The total amount of pollutant measured in all tissues
chemical index	- Score developed by NOAA which compares the toxicity of a compound to its persistence
competition	- The struggle by individuals or populations for resources in short supply
complexation	- Loosely defined as the reaction of two soluble species to form a third. In this report, it refers to the combination of metal cations with molecules or anions containing free pairs of electrons
consumers	- Grazers or herbivores in the food chain
default value	- A value to assign when no other data are available
diversity	- Number of species (richness) compared to the numbers of individuals of each species present (evenness) in a community
food web	- Interconnected food chains in a complex ecosystem
log Pow	- Logarithm of the n-octanol-water partition coefficient
magnification	- Increase in concentration of a substance in higher tropic levels of the food chain, also known as biomagnification
methylated metal	- An organometallic compound in which the organic molecular group is a methyl radical, i.e., CH_3
mobility	- Ability of a substance to be transported through the environment

net production	- Total biomass produced and stored by all plants and animals over an area during a specified time, usually over a year
niche	- The role of a species role in the environment, i.e., where it lives and what it eats
n-octanol-water partition coefficient	- This partitition is a measure of the preferential partitioning of a substance between n-octanol and water (measured in a laboratory test or calculated by one of several methods)
nonessential element	- An element that is not necessary for nutrition in biota
Automated EPA NPL technical data base	The automated EPA National Priorities List technical data base contains information on information on sites evaluated with the HRS
organometallic	- Referring to a class of compounds made up of the combination of an organic molecular group and a metallic atom where the metallic atom is bonded to the carbon atom of the organic molecular group, e.g., tetraethyl lead
pathway	- In the HRS, a possible migration route (i.e., ground water, surface water, or air)
persistent	- Long lasting in the environment, not easily degraded
photoxidation	- An oxidation reaction activated by light energy
Pow	- n-octanol-water partition coefficient
primary producers	- Organisms (e.g., plants) which can synthesize organic compounds from inorganic compounds. The source of energy is either light or chemical energy derived from the oxidation of inorganic compounds
primary production	- The organic material produced by the primary producers

protocol	- Series of specified steps followed in scientific procedure from the gathering of samples to analytical technique used and recording of results
secondary production	- The production of herbivorous animals
soil adsorption coefficient	- A ratio of the concentration of a substance on the soil adsorbent to the concentration of the substance in the environment surrounding the soil
solubility	- A property of a substance by virtue of which it forms mixtures with other substances which are chemically and physically homogeneous throughout
species	- May refer to a subcategory of classification of organisms, lower than genus; or may refer to a specific chemical compound
standing crop	- Total amount of biomass of all aquatic species within an area
steric effects	- The size and the shape of a molecule, affecting its uptake, e.g., ability to pass through a membrane
targets	- Population potentially affected by releases of hazardous substances
translocation	- Movement of materials in solution in plants from one location to another
trophic level	- Position in the food chain; e.g., plants (producers), herbivores (consumers), predators (carnivores)
uptake	- Absorbing or incorporating substance into living tissue
unavailable	- Being present in a physical or chemical form that does not allow the substance to be taken up by biota
waste characteristics score	- In the HRS, a point score currently based upon rating factors such as waste quantity, toxicity and persistence

xenobiotics	- Exogenously derived substances with no nutritive value to organisms, especially the synthetic organic chemicals (Walton and Edwards, 1986)
yield	- Part of the biotic production which is removed or expected to be harvested by man

APPENDIX F

OTHER METHODS REVIEWED

In examining the human food chain issue, a review of the technical literature was made to determine if there was an existing method of assessing the potential threat to humans due to exposure to hazardous substances in the human food chain. This appendix discusses why and how some existing methodologies incorporate bioaccumulation as a factor in assessing or ranking hazardous substances. It also presents a brief discussion of sources which discuss the use of bioaccumulation in hazard ranking systems.

F.1 Hazard Assessment Rating Methodology II (HARM II)

HARM II (Barnthouse et al., 1986) is an extension of the HARM system, intended to "permit the use of site-specific monitoring data to refine priorities for further study" at U.S. Air Force waste sites. Bioaccumulation is considered in order to estimate the total human intake of hazardous substances from the site per day. Bioaccumulation is defined using three terms:

Concentration Factor - The ratio of concentration of a substance in fish to the concentration in water.

Bioaccumulation Factor - The multiplier when an organism's pathways of exposure include both direct uptake from water and uptake from contaminated food.

Bioconcentration Factor - The multiplier used when the organism's pathway of exposure is only direct uptake from water.

All three are based on the concentration in fish at steady state. A hierarchy is established in HARM II for determining the

bioaccumulation factor to be used in scoring a site. Concentration factors based on field data are most preferable. Bioaccumulation factor or bioconcentration factor data measured in the laboratory may be used if concentration factors based on field data are not available. Finally, if no other data are available, a regression equation and log n-octanol-water partition coefficient data are used.

The bioaccumulation factor (BAF) determined above is then used to determine a final contaminant hazard score. This is done differently depending on whether or not an observed release of contaminants has occurred at the site. If an observed release has occurred, the BAF is used to calculate the estimated human daily food intake of contaminated food each hazardous substance presents at the site. Human health hazard quotients for all substances are eventually summed, indexed, normalized, and multiplied by a waste quantity factor to determine a final contaminant hazard score.

If an observed release has not occurred, each substance at the site is evaluated independently. The logarithm of the health effects benchmark and the BAF are indexed. The index values are then summed for each substance. The sum for the highest scoring substance is normalized and multiplied by a persistence factor value and a waste quantity multiplier to determine the final contaminant hazard score.

Principal differences between the HARM II and proposed scheme presented in Figure 4 are:

- HARM II does not use biomagnification data.
- HARM II states that a log Pow of less than 5 will not be important in food chains. Figure 4 assumes a log Pow of 3.2 or greater is important.
- HARM II uses log Pow to calculate the log BCF using a regression equation. Figure 4 uses the log Pow directly.

F.2 Remedial Action Priority System (RAPS)

RAPS is a computer-based methodology to integrate and analyze complex processes on DOE mixed waste sites. It was developed by Whelan et al. (1986) at Pacific Northwest Laboratory to prioritize hazardous and radioactive waste sites for further site investigation. When first presented in 1984, the RAPS did not consider the food chain. However, in the 1986 version of the model, RAPS uses the concentration of the contaminant in the media of exposure, daily ingestion rates, and a conversion factor to determine an individual risk factor. Instead of a bioconcentration factor, RAPS uses a "transfer factor" (e.g., water-feed-meat) for agricultural systems, as presented in U. S. Nuclear Regulatory Commission (1977).

The data used as a basis for the transfer factor data are from 1968 and 1972 reports on radioactive material transfer, and only data on elements are included. NRC (1977) reports bioaccumulation factors (using 1972 data) as calculated from concentrations of elements in fish compared to concentrations of those elements in invertebrates. These factors are to be used in absence of site-specific data. This is not the way BCFs are generally calculated today, as it disregards direct uptake from water.

The NRC does use a more standard bioaccumulation factor to calculate doses to man via liquid effluent pathways. This bioaccumulation factor is for nuclides in the pathway, expressed "as the ratio of the concentration in biota (in pCi/kg) to the radionuclide concentration in water (in pCi/liter) in liters/kg" (NRC, 1977).

RAPS calculates the dose to man from aquatic food chains also. Average daily intake is estimated using bioconcentration factors and the average daily ingestion rates for aquatic foods. One must have the concentration data for the contaminant in the food (e.g., mg/kg or pCi/kg) to complete the calculated risk factor.

In Whelan et al. (1986), it appears the NRC transfer factors are used to determine concentrations in meat and milk. Bioconcentration factors are used to the aquatic food chain to estimate average daily intake of substances. Whelan et al. (1986) does not state how to determine bioaccumulation, but other "standard parameter values" in RAPS are from NRC (1977), so we assume RAPS uses the NRC data on bioaccumulation factors. RAPS does not address the individual differences between substances which have biomagnification potential or those with high bioconcentration factors.

F.3 Food Chain Model

Dixon and Holton (1984) of Oak Ridge National Laboratory developed a model called FOODCHAIN, a Monte Carlo computer model for estimating exposure to airborne pollutants via the food chain pathway. The model calculates regression equations for ingestion of

milk and beef based on the log Pow correlations with bioconcentration factors from Kenaga and Goring (1980).

Garten and Trabalka (1983) and Trabalka and Garten (1982) raised several questions concerning practices used by Kenaga (1980) in his correlations for substances in terrestrial systems. In fact, such dependence upon the Pow for a terrestrial methodology may be the weakest point in the FOODCHAIN model. Furthermore, this model requires data on the concentration of substances in foods. The Monte Carlo modeling then generates 1,000 exposure results through random sampling of food concentrations. The results are applicable to individual exposures to pollutants. This model requires site specific data in order to be able to rank sites. It does not address the real differences between substances known to biomagnify and does not use bioconcentration factors as measured in the field or laboratory.

F.4 Action Alert System

The "Action Alert System" (Fiksel and Segal, 1982) was developed to rank environmental pollutants for further study. For the calculation of ingestion risk, Fiksel and Segal depend upon the correlation of solubility with bioconcentration factors based on Kenaga (1980). While food chain effects is beyond the scope of this system, the authors state it is possible to derive a bioconcentration factor for fish. They multiply the BCF with ambient water concentrations to estimate the contamination levels in fish. This

is then used with average consumption rates to estimate the amount of the pollutant ingested in food. There are two weaknesses in this approach: (1) one needs to know ambient water concentrations, and (2) dependence solely upon water solubility to estimate the BCF. No use is made of log Pow data, measured BCF data, or the biomagnification process.

An optional module to the Action Alert System was designed to assess food residues based upon the bioaccumulation factor and ambient water concentration for estimating fish contamination. These data then were used to predict amount of residue ingested in food to estimate per capita risk. Action Alert uses an experimentally-derived bioaccumulation factor (BF), which measures the ratio in equilibrium of pollutant concentration in fish to the concentration in the surrounding aquatic medium. The BF multiplied by the water concentration would give the fish contamination (ppm). This is then multiplied by per capita fish consumption to give the amount of contaminant ingested in fish per day. This is added to terrestrial residues consumed in foods to estimate risk.

To estimate risk from pesticides on food, Action Alert depends upon water solubility, based upon Kenega (1980) who correlated solubility with bioconcentration. To calculate water solubility the model estimates from regression equations using n-octanol-water partition coefficients following correlations by Chiou et al. (1977).

F.5 Predictive Model for Xenobiotic Bioaccumulation in Terrestrial Ecosystems

Trabalka and Garten (1982) provided a critical review of predictive models for xenobiotic bioaccumulation in terrestrial ecosystems. This analysis of models for estimating the fate of xenobiotics was directed toward those substances transferred from environmental sources to terrestrial vetebrates (i.e., birds and mammals) via the ingestion pathway (e.g., soil to plant to consumers). This was done to determine the "necessary and sufficient information required to predict, within reasonable limits, toxicity and environmental fate prior to manufacture" of such toxic materials. The review included a number of models which correlate the bioconcentration factor to the log n-octanol-water coefficient and water solubility.

Trabalka and Garten (1982) developed a Terrestrial Hybrid Model, based on NRC regulatory models, which used several types of bioconcentration factors (BF). These BFs were used to predict the concentration of xenobiotics in carnivorous animals. Examples of how bioconcentration factors (BF) are defined in the terrestrial model are listed below:

Simple Compartment Model

BF_{PA} = BF of xenobiotic in product (tissue, organ, secretion) of herbivorous animal from consumption of plant product

BF_{WP} = BF of xenobiotic in product of plant from uptake from soil interstitial water

Complex Compartment Model

BF_{AA} = BF of xenobiotic in carnivorous animal product from consumption of herbivorous animal product

BF_{FP} = BF of xenobiotic in product of plant from exposure to foliar contamination

BF_{SA} = BF of xenobiotic in herbivorous animal product from incidental ingestion of soil

These are applied in estimating uptake through the terrestrial food chain (e.g., pasture to cattle).

Trabalka and Garten (1982) then go on to analyze aquatic food chain models and correlations. In their data base, used to determine bioaccumulation in fish, the following BFs are defined, with methods given for BF determination in the laboratory:

1. BF(FW) = BF in freshwater fish from water-only exposure systems, typically flowing-water systems which maintain a reasonably constant exposure regime and continually removing metabolities; ratio of concentration of parent xenobiotic in fish (wet weight)/concentration of parent xenobiotic in water.

2. BF(ME) = BF in fish from static-model ecosystems which receive a single dose of the contaminant, which were maintained for approximately 30 days following initial exposure, and which contained a sand or soil substrate; ratio of concentration of parent xenobiotic in fish (wet weight)/concentration of parent xenobiotic in water.

3. BF(MA) = BF in fish from static-model aquatic systems which differed from the above in not having a sand or soil substrate and which were exposed for a total time of three days or less; BF calculated in the same manner.

4. BF(MP) = BF in fish from static-model ecosystems; ratio of concentration of total xenobiotic (including metabolites) in fish (wet weight)/concentration of parent xenobiotic in water.

5. BF(MM) = BF in fish from static-model ecosystems; ratio of concentration of total xenobiotic (including metabolites) in fish (wet weight)/concentration of total xenobiotic in water.

These bioconcentration factors are then included in a number of correlations with water solubility and log n-octanol-water coefficients. These authors concluded the n-octanol-water partition coefficient is a "highly satisfactory index of bioaccumulation potential in fish and terrestrial vertebrates (uptake from diet) for xenobiotics which do not accumulate by covalent reaction."

F.6 Michigan Site Assessment Systems (SAS)

The State of Michigan uses the SAS to rank the relative hazard posed by release sites for purposes of assigning priority for site evaluation and response actions (Michigan, 1983).

In scoring environmental fate, the SAS uses the following for bioaccumulation evaluation:

Score	Criteria
10	Fish Bioconcentration Factor* greater than 4,000 or Log Pow greater than 6
5	Fish Biocentration Factor = 700-4,000 or Log Pow = 4.5-6
0	Fish Bioconcentration Factor less than 700 or Log Pow 4.5

This score is then used with other factors to calculate a potential toxicity score for each chemical. This factor is then normalized and added to other site assessment screening factors for a total score.

*No guidance is given concerning derivation of the fish bioconcentration factor.

F.7 U.S. Department of Agriculture (USDA)

The U.S. Department of Agriculture (USDA, 1985) uses a compound evaluation ranking method for pesticides, animal drugs, and "unavoidable environmental contaminants." This method applies an A-B-C-D score to substances found in meat and poultry. The main reasons for a high score of A are high toxicity and carcinogenicity. Other criteria include: amount of actual or probable use; conditions of use related to residues at slaughter; potential for misuse to result in harmful residues; and the toxicity of the residue. While bioaccumulation is not mentioned in those criteria, background information on these substances ranked may includes statements, such as for PCBs, concerning bioaccumulation in the food chain. A proposed new ranking scheme, the Prototype Compound Evaluation System (CES) will subdivide these A-B-C-D categories further based upon hazard and exposure data. No mention is made of bioaccumulation potential.

F.8 National Academy of Sciences (NAS)

In 1975, a comprehensive review "Assessing Potential Ocean Pollutants," was published by the NAS (National Research Council, 1975). This report summarizes a number of earlier studies and reports biological concentration factors for many chemicals and radioisotopes. This report also summarizes fate and effect data for many compounds in soils and air, biodegradation processes, toxicity, and effects of the chemicals in the marine environment.

F.9 U.S. Food and Drug Administration (USFDA)

While the USDA monitors meat and poultry, the U.S. Food and Drug Administration Surveillance Index (USFDA, 1983) was developed for monitoring substances in other foods. About 160 pesticides have been classified in categories I to V, mainly on the basis of potential health risk and potential for occurrence as residues in foods. Use of the FDA method would be applicable to only a portion of the food chain problem. The FDA monitors foods other than meat and poultry, and their ranking index only applies to pesticides in foods.

The criteria used by FDA to score pesticides include:

- Annual production
- Use on corps
- Potential for environmental contamination and entering food chains
- Types of food containing residue
- Relative toxicity
- Chemistry, including metabolites
- Propensity to biomagnify in edible tissue
- Biological half-life
- Persistence
- Non-dietary exposure
- Per capita consumption
- Knowledge of existing incidence
- Special regulatory interests

Using these criteria, USFDA assigns a pesticide to one of five classes to determine priority for monitoring in human foods. Class I represents a high health hazard based on toxicological data or bioaccumulation potential.

Lombardo (1979) described another FDA program, the Chemical Contaminants Program, which selects industrial chemical types for study. Criteria used in this program included in bioaccumulation potential and oil-water partition coefficients. FDA's "primary indicator organism is freshwater fish, as most problem contaminants evenually find their way into this segment of the human food chain" (Lombardo, 1979). Using these data, FDA then establishes Action Levels or Tolerances for deleterious substances in seafood.

F.10 Inter-Governmental Maritime Consultative Organization (IMCO)

In 1973 IMCO published Annex II of the International Conference on Maritime Pollution. Appendix I of the Annex provides guidelines for the categorization of noxious liquid substances into four groups (A, B, C, and D) based upon probable tainting of seafoods and reduction of amenities. Cateogry A substances are bioaccumulative and are liable to produce a major health hazard.

These categories of noxious liquid substances are then used to regulate discharges from ships to the sea. No definitions of bioaccumulation are given, nor are methods given for determining this factor. Substances which bioaccumulate are either categorized

as A or B. This list of substances was used initially to indicate which ones may be found in fish.

F.11 Other Ranking Methods

Almost 60 methods for ranking the degree of hazard of substances are reviewed in Review and Analysis of Hazard Ranking Systems (U.S. Environmental Protection Agency, 1984c). In those methods which used bioaccumulation as one of the criteria for ranking hazardous substances, it was most often used as a modifier to address the fate of a substance in the environment. The more complex and sophisticated models require concentration data in water, and this is multiplied by the bioconcentration factor of the substance. Where the bioconcentration factor is unknown, the n-octanol-water partition coefficient is often used as a backup. One method recommended a laboratory test to determine the potential accumulation of substances into biota.

Hushon et al. (1983) and Hushon and Kornreich (1984) provide an extensive list of internationally published methodologies for ranking substances based upon the degree of hazard. A majority of these methods rely heavily on the n-octanol-water partition coefficient (Bro-Rasmussen and Christiansen, 1984; Mackay, 1981 and 1982; Wood, 1981; Hushon et al., 1983; Lu and Metcalf, 1975; Veith et al., 1979). The following methods use bioaccumulation as a scoring factor in ranking the degree of hazard of substances:

1. Ranking for European Economic Community Water Pollutants: to select chemicals for further study.

2. American Society for Testing and Materials Committee (d-19): to determine impacts of chemicals an aquatic life.

3. EPA Action Alert: previously discussed.

4. MITRE (for Federal Republic of Germany): to select chemicals for environmental trends monitoring.

5. Office of Technology Assessment: to identify possible food contaminants.

6. Michigan Critical Materials Register: to score chemicals of concern.

7. EPA Office of Toxic Substances: to select chemicals presenting environmental risk under TSCA.

Many other methods, however, were developed to rank substances based upon toxicity criteria but not bioaccumulation.

The reportable quantities support documents (EPA, 1985; ICF, 1985) provide substantial data on the CERCLA hazardous substances, including their toxicity and other factors which influence the fate of the substances in the environment. The documents consider the bioaccumulation potential, but do not quantify or apply the data. The tables only list substances which bioaccumulate in biota.

Some ranking methods, such as the "reportable quantities" documents (ICF, 1985) or those reviewed by Hushon and Kornreich (1984), use bioaccumulation as a "yes it does" or "no it does not" factor, and instead place more emphasis on toxicity to distinguish among substances.

In 1975, a comprehensive review "Assessing Potential Ocean Pollutants," was published by the NAS (National Research Council, 1975). This report summarizes a number of earlier studies and reports biological concentration factors as reported in the literature for many chemicals and radioisotopes. The report also summarizes fate and effect data for many compounds in soils and air biodegradation processes, toxicity, and effects of the chemicals in the marine environment.