

APPENDIX B

PHYSICAL AND CHEMICAL PROPERTIES

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B.1 PHYSICAL AND CHEMICAL PROPERTIES OF POLYCHLORINATED BIPHENYLS

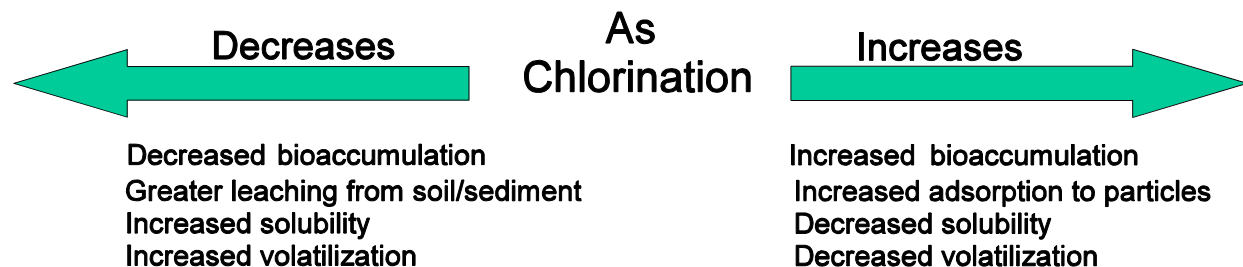
PCBs are a class of compounds in which 1 to 10 chlorine atoms are attached to the biphenyl structure. The 209 chlorobiphenyl congeners are classified according to degree of chlorination of the molecule, and the term isomer is used to identify different compounds with the same degree of chlorination. The mono-, di-, tri-, tetra-, penta-, hexa-, hepta-, octa-, nona-, and decachlorobiphenyl congeners can exist in 3, 12, 24, 42, 46, 42, 24, 12, 3, and 1 isomeric forms, respectively. According to the International Union of Pure and Applied Chemistry (IUPAC) system of nomenclature, the 209 PCB congeners are arranged in ascending numerical order, based on chlorine substitution, and assigned numbers from 1 to 209. Of the theoretical 209 congeners, only about 130 are likely to be found in commercial mixtures (Safe 1990).

From 1930 to 1977, PCBs were marketed in mixtures under the trade name Aroclor. The Aroclors are identified by a four-digit numbering code in which the first two digits indicate that the parent molecule is biphenyl and the last two digits indicate the chlorine content by weight percent. For example, Aroclor 1242 is a chlorinated biphenyl mixture of varying amounts of mono- through heptachlorinated homologs with an average chlorine content of 42 percent.

PCBs are highly stable under most environmental conditions. However, they differ in their properties and physicochemical behaviors depending on the number and pattern of chlorine substitutions in the individual congeners. These properties, such as vapor pressure, water solubility, and susceptibility to degradation, influence both the environmental fate and toxicity of PCBs.

PCBs in general are relatively insoluble in water, sorb strongly to soil and organic matter, and have a high potential for bioaccumulation. As the degree of chlorination increases, PCBs generally become less soluble, less volatile, and more strongly sorbed to soils and sediments. In addition, PCBs are very stable and persistent compounds in various environmental media, and the breakdown of PCBs in water and soil may take several years or even decades. Generally, persistence increases as the number of chlorine atoms increases. Although they are slow processes, volatilization and biodegradation account for the major routes of removal of PCBs from water and soil (Mackay and others 1992).

Recent research (*discussed in EPA 1996*) has found that certain PCB congeners are much more toxic than others with the same degree of chlorination. The most toxic congeners have three properties: (1) they have few ortho-substituted chlorines so the two aromatic rings can be in the same plane, (2) they have four or more chlorines, and (3) when in the coplanar state, the congener molecule appears to other molecules as if it were a 2,3,7,8-substituted tetrachlorodioxin or tetrachlorofuran. Therefore, these congeners behave in mammals and other species much as if they were the highly toxic dioxins and furans. Residual and bioaccumulated PCBs, with relatively more of the highly chlorinated congeners, including the coplanar congeners, will be more toxic than the original mixtures because they contain a higher proportion of the dioxin-like, coplanar PCB congeners.



PCBs in Air

The vapor pressures of PCBs indicate that they should exist primarily in the vapor phase in the atmosphere. Monitoring data indicate that 87 to 100 percent of the PCBs in the atmosphere are present in the vapor phase. The predominant congeners are the less toxic, less chlorinated ones. The atmosphere may effectively disperse PCBs within short distances from sources (Eisenreich and others 1981, Hermanson and Hites 1989). In the atmosphere, removal of vapor-phase PCBs is dominated by the reaction of PCBs with hydroxyl radicals by photolysis.

PCBs in air may also be present as both solid and liquid aerosols that eventually return to the land and water by either settling or washout by snow and rain. Adsorbed to particulates, PCBs can undergo long-range transport in the air. Because the vapor pressure of PCBs generally decreases with an increase in the degree of chlorination, the higher-chlorinated PCBs are more likely to be associated with the particulate-adsorption-phase in air than are the lower-chlorinated PCBs. Physical removal of PCBs from the atmosphere is accomplished by wet and dry deposition; dry deposition occurs only for PCBs associated in the particulate phase (HSDB 2000).

PCBs in Soil and Sediment

As reflected by their low water solubility and high soil (organic carbon) partition coefficients (K_{oc}), PCBs bind strongly to soil and sediments and may persist in this phase for many years. Adsorption of PCBs generally increases as the organic carbon and clay content of the soil and sediment increase. Conversely, evaporation from soil surfaces to air increases as organic matter and clay in soils decrease, due to the weaker sorption of PCBs. Volatilization rates will also be greater in moist soils due to the codistillation of PCBs with water. Leaching of PCBs from soil to groundwater is generally slow. PCBs may, however, leach significantly in the presence of organic solvents, as might occur at a hazardous waste site (Griffin and Chou 1981). The residual mixtures (after volatilization and leaching) will be enriched in the more chlorinated congeners. Storm water runoff will also transport PCBs from soil to surface water, in the water phase and as particulates.

There is no chemical process known to degrade PCBs in sediment and soil. However, biodegradation via dechlorination may occur under anaerobic conditions. Biodegradation rates are highly variable because they depend on a number of factors, including the amount of chlorination, concentration, type of microbial population, available nutrients, and temperature. In general, the rates of PCB dechlorination decrease as (1) the degree of chlorination increases and (2) the organic carbon content of the soil increases (Tiedje and others 1993).

PCBs in Water

In water, adsorption to sediments and suspended particulates is a major fate process that partitions PCBs from water to solid phases. Based on their water solubilities and partition coefficients, PCB solubility decreases with increased chlorination. A small amount of the PCBs may remain dissolved, but most tend to be adsorbed to particles and sediments. PCBs are freely soluble in nonpolar organic solvents and in biological lipids.

In water, transformation processes such as hydrolysis and oxidation do not significantly degrade PCBs. PCB degradation in water is primarily via photolysis, although biodegradation may be more important than photolysis in subsurface water. Biodegradation is also probably the ultimate degradation process for PCBs in sediments.

The values for the estimated Henry's law constants for PCBs indicate that volatilization is also a significant environmental transport process for PCBs dissolved in water. Adsorption to sediments significantly decreases the volatilization rate of highly chlorinated PCBs from the aquatic phase (EPA 1985b, Lee and others 1979).

Sediments containing PCBs at the bottom of a large body of water generally act as a reservoir from which PCBs may be released in small amounts to the water over a long period of time. Although adsorption and subsequent sedimentation may immobilize PCBs for relatively long periods of time in aquatic systems, redissolution into the water column has been shown to occur in the environment. Redissolution and release of PCBs from sediments is favored when PCB concentrations in the aquatic phase are depleted, for example as a result of volatilization. The rate of redissolution of PCBs from sediment to water will always be greater in summer than in winter because of more rapid volatilization from water (Larsson and Soedergren 1987).

PCBs in Plants, Animals, and Food

Accumulation of PCBs in terrestrial vegetation can occur in the following ways: uptake from soil through the root with translocation to the aerial parts of plants; deposition of atmospheric particulates on aerial plant surfaces; and uptake of airborne vapors by aerial plant parts.

PCBs in water bioaccumulate in fish and can reach levels hundreds of thousands of times higher than the levels in water. The bioaccumulation in aquatic animals may also depend on the water zone in which they predominantly reside. For example, because the concentration of PCBs in sediments is several orders of magnitude higher than in water, the bioaccumulation of PCBs in bottom-feeding (benthic) species is also expected to be high. Bioaccumulation is more pronounced in the fatty tissues of aquatic organisms than in the muscle or whole body.

As indicated by the PCB concentrations in higher trophic levels of aquatic organisms, PCBs biomagnify within the food web. There is also evidence that food web biomagnification occurs in several species of birds that feed on fish.

The more chlorinated congeners have higher bioconcentration and bioaccumulation factors, as well as lower biodegradation rates than the less chlorinated congeners. Therefore, the accumulated PCBs will be enriched in the heavier congeners.

By virtue of their large and mobile biomass, their position in food webs, and their biotransformation potential, insects have been suggested as significant contributors to the global transport and transformation of PCBs (Saghir and others 1994).

[Sources: Background information for the preceding section is from USDHHS. 1997. *Toxicological Profile for Polychlorinated Biphenyls* (Update). Agency for Toxic Substances and Disease Registry unless otherwise indicated.]

Table B-1. Origins and Physical and Chemical Properties of PCBs

PCBs					
Major Sources / Uses	<ul style="list-style-type: none"> • Current authorized uses limited to coolants and lubricants in electrical equipment (transformers, capacitors) • Historically used as an ingredient in hydraulic fluids, plasticizers, carbonless copy paper, fluorescent lamp ballasts, flame retardants, inks, adhesives, and other consumer products. Landfills not designed to handle hazardous wastes may contain these products and serve as PCB sources • One of the major sources today is environmental cycling of PCBs previously introduced into the environment; PCBs held in soil and sediments are released to water, PCBs in the water and soils volatilize to the atmosphere, PCBs in atmosphere are redeposited in soil and surface waters via wet and dry deposition. 				
Chemical and Physical Forms	Water	Soils and Sediments	Air	Biota	Other Commonly Released Forms
	<ul style="list-style-type: none"> • Primarily as PCBs adsorbed to sediments and suspended particulates 	<ul style="list-style-type: none"> • Primarily as PCBs adsorbed to soil particles and sediments; PCBs do not readily leach to water 	<ul style="list-style-type: none"> • Primarily as PCBs in the vapor phase • Also present as solid and liquid aerosols (airborne particulates) 	<ul style="list-style-type: none"> • Primarily found in fatty tissues in humans, wildlife, and aquatic organisms 	<ul style="list-style-type: none"> • There are 209 PCB congeners; the seven principal Aroclors (tradename) included: Aroclor 1221 Aroclor 1232 Aroclor 1016 Aroclor 1242 Aroclor 1248 Aroclor 1254 Aroclor 1260 (4)

Source for physical and chemical property data: EPA. 1993. Revised Draft Lake Michigan Lakewide Management Plan unless otherwise indicated.

Table B-2. Distribution and Fate of PCBs

PCBs					
Transport and Media Partitioning (physical distribution)					
Distribution and Fate in the Environment	<p>- Generally PCBs bind strongly to soil and sediments rather than remaining in dissolved phase; transport and deposition of PCBs in water is in the form of suspended particulates.</p> <p>- In air, most PCBs are in the vapor phase, although more highly chlorinated forms may be associated with particulates. Removal from atmosphere and deposition to water and land is by dry and wet deposition.</p>				
	Water (solid/liquid transfers)	Soils and Sediments (solid/liquid transfers)	Air		Living Organisms (bioaccumulation)
	Water Solubility ¹ : 0.57 mg/L (Aroclor 1016) or 0.010 mg/L (Aroclor 1254) (5)	Log K _{ow} ² : 5.4 (Aroclor 1016) or 6.2 (Aroclor 1254)	Volatility	Gas/Liquid transfers	
	<ul style="list-style-type: none"> Generally insoluble in water (more highly chlorinated⁶ forms are least soluble), and are therefore associated primarily with sediments. 	<ul style="list-style-type: none"> Binds to soils and sediments Soluble in organic solvents and may leach from landfills where solvents are present 	<p>Vapor Pressure ³: 7x10⁻⁴ mm Hg (Aroclor 1016) or 9x10⁻⁵ mm Hg (Aroclor 1254) except for photolysis in the atmosphere or shallow water</p> <ul style="list-style-type: none"> PCBs bound to soils, sediments, or particles in water are less volatile. 	<p>KH ⁴: 4.23x10⁻⁴ atm m³/mol at 25°C (Aroclor 1016) (5) and 3.79x10⁻³ atm m³/mol at 25°C (Aroclor 1254)</p> <ul style="list-style-type: none"> Volatilization is significant for dissolved PCBs in water. 	<p>BCF ⁵ (Aroclor 1242): >100,000 (fathead minnow)⁷</p> <ul style="list-style-type: none"> Retained in body tissue (bioaccumulative) More highly chlorinated forms are the most bioaccumulative

Table B-2. Distribution and Fate of PCBs (continued)

Distribution and Fate in the Environment (continued)	Transformations and Degradation/Persistence (chemical changes and distribution)			
	-Biodegradation is major removal route from soils, sediments, and aquatic environments but is a very slow process. No chemical degradation process is known.			
Water	Half-life: 2 to 6 yrs (b) • Photolysis in surface water layers • Biodegradation in deeper water or where associated with solids	Soils Half-Life: 2 to 6 yrs (b) • Biodegradation via microbial dechlorination	Sediments Half-life: 2 to 6 yrs (b) • Biodegradation	Air Residence time): 1 week to 6 years (b) • Degradation by photolysis
	Biota			

Sources:

- a Revised Draft Lake Michigan Lakewide Management Plan unless otherwise indicated.
- b Makay and others 1992.
- c USDHHS. 1997. Toxicological Profile for Polychlorinated Biphenyls. (ATSDR)
- d EC. 1997. Scientific Justification: Polychlorinated Biphenyls.
- e EPA 1998. Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities.

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.

- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures $>10^{-4}$ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures $<10^{-8}$ mm Hg should exist almost entirely in the particulate phase.
- ⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- ⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).
- ⁶ The number of chlorine atoms in PCB may range from 1 to 10, with the most commonly released Aroclor mixtures containing between 21 to 60 percent chlorine. The representative mixtures, Aroclor 1016 and Aroclor 1254; contain about 40 and 54 percent chlorine, respectively (EC 1997).
- ⁷ Fathead minnows are a ubiquitous fish species found in Lake Michigan and are commonly used as a marker species in bioaccumulation and toxicity studies.

B.2 PHYSICAL AND CHEMICAL PROPERTIES OF DIOXINS AND FURANS

Dioxins and furans are aromatic hydrocarbons that can have from one to eight chlorine substituents. There are 75 PCDD and 135 PCDF substituted forms (congeners) for a total of 210. The most toxic and consequently the most extensively studied of the dioxins is 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD). To simplify the assessment of toxicity data for PCDDs and PCDFs, a system has been developed to compare the relative toxicity of the congeners. As it is the most studied, the toxicity of 2,3,7,8-TCDD is used as a reference in relating the toxicity of the other 209 compounds (in terms of equivalent amounts of 2,3,7,8-TCDD). Using this system, the toxicity of airborne mixtures of PCDDs and PCDFs are expressed in terms of 2,3,7,8-TCDD toxic equivalents (TEQ) in mg/m^3 (EPA 1997).

Both the number of chlorine atoms and their positions determine the physical and chemical properties, and therefore, the fate and toxicity of a given substituted form (congener). The most toxic congener (2,3,7,8-TCDD) is extremely lipophilic, exhibiting a high degree of solubility in fats and is only sparingly soluble in water. The more chlorinated congeners are even more lipophilic and less soluble in water. Limited data also indicated that PCDDs and PCDFs are persistent in soils, sediments, and water. On the basis of the information available, it is concluded that the more highly chlorinated (that is, tetra-CDD/Fs and above) congeners are persistent in the environment (EC 1997).

Dioxins and Furans in Air

Although 2,3,7,8-TCDD has an extremely low vapor pressure it has been shown to be volatile and to occur in air in both the gas phase and particulate phase. In general, most PCDDs and PCDFs are not persistent atmospherically in the vapor phase but are persistent when associated with particulate matter. The physical and chemical properties of PCDDs and PCDFs indicate that most of the more highly chlorinated (tetra-CDD/Fs and above), less volatile PCDDs and PCDFs in the ambient atmosphere will be associated with the particulate phase (Mackay and others 1992). They are susceptible to photodegradation in the presence of ultraviolet light. TCDD may be transported long distances through the atmosphere, and particulates may be physically removed from the atmosphere by wet and dry deposition. There is also evidence that PCDDs and PCDFs are transported long distances in the atmosphere.

Partitioning affects the persistence of PCDDs and PCDFs in the atmosphere. Generally, PCDDs and PCDFs associated with particulate matter will be more persistent and have the potential to be transported long distances in the atmosphere. Atmospheric deposition is one of the major sources of PCDDs and PCDFs measured in the sediments of the Great Lakes (EPA 1994). Persistence of specific congeners, regardless of media partitioning, has also been observed to generally increase with the amount of chlorination of the molecule.

Dioxins and Furans in Soil

In soils, dioxins are generally bound tightly to the solid phase and are thus relatively immobile. Soil adsorption studies and monitoring of various soils contaminated by 2,3,7,8-TCDD have demonstrated that TCDD does not leach to groundwater. In this adsorbed phase, dioxins are also resistant to biodegradation and are relatively persistent in soils. Movement of dioxins from soils to surface waters by surface erosion of contaminated soil particles may be possible. Minor amounts of the more volatile (less chlorinated) dioxins are lost from the soil to the atmosphere through volatilization. TCDD exposed to sunlight on terrestrial surfaces may be susceptible to photodegradation. Volatilization from soil surfaces during warm, summer months may be a major mechanism by which TCDD is removed from soil.

Dioxins and Furans in Water

Photolysis and biological degradation are the key transformation processes affecting the persistence of PCDDs and PCDFs in water. The more highly chlorinated PCDDs and PCDFs are generally resistant to hydrolysis in the environment. The photolysis rates of PCDDs in natural water are enhanced by direct photosensitization or by indirect reactions of chemicals naturally occurring in water. Volatilization may also contribute to some dioxin loss from surface water.

Dioxins and furans, as reflected in high soil-water partition coefficients and low water solubilities, will tend to associate with the particulate phase in aquatic environments and will be removed from the water column by sedimentation. Once in sediments, as in soils, dioxins are resistant to biodegradation and are persistent. Aquatic sediments may be an important, and perhaps ultimate, environmental sink for all global releases of TCDD.

Dioxins and Furans in Plants, Animals, and Food

Although variability in bioaccumulation factors among congeners is significant, in general the more highly chlorinated (tetra-CCD/F and above) congeners of PCDDs and PCDFs accumulate in biota. The presence of dioxins and furans in human breast milk around the world and in animals at the top of the food chain also demonstrates that these substances biomagnify (EC 1997).

[Sources: Background information for the preceding section is from EPA, 1997. *Locating and estimating air emissions from sources of Dioxins and Furans*; and from HSDB 1998 unless otherwise indicated.]

Table B-3. Origins and Physical and Chemical Properties of Dioxins and Furans

Dioxins and Furans					
Major Sources / Uses	<ul style="list-style-type: none"> Dioxins and furans formed as a by-product during the incomplete combustion of materials containing carbon and chlorine compounds, including backyard burn barrels, manufacture of organic compounds (such as chlorinated solvents and pesticides), and chlorine bleaching process used in pulp and paper mills. Other sources include incinerators, vehicle exhaust, iron and steel manufacturing, cement kilns, crematoria, and chemical waste landfills. Natural sources include forest fires. 				
Physical and Chemical Forms	Water	Soils and Sediments	Air	Biota	Other Commonly Released Forms
	<ul style="list-style-type: none"> Adsorbed to suspended solids and sediments 	<ul style="list-style-type: none"> Associated with solid phase and organic matter 	<ul style="list-style-type: none"> Highly chlorinated congeners and associated with airborne particulates (tetra-CDDs and above) Less chlorinated forms also in vapor phase 	<ul style="list-style-type: none"> Accumulates in fatty tissue of humans and wildlife 	<ul style="list-style-type: none"> Released as congener mixtures 75 different polychlorinated (PCDD) dibenzo-p-dioxin congeners 135 different polychlorinated (PCDF) dibenzofuran congeners 2,3,7,8 -congeners more harmful (2,3,7,8-tetrachlorodibenzo - p-dioxin most toxic)

Source for physical and chemical property data: EPA. 1993 and Revised Draft Lake Michigan Lakewide Management Plan unless otherwise indicated

Table B-4. Distribution and Fate of Dioxins and Furans

Dioxins and Furans					
Transport and Media Partitioning (physical distribution)					
<p>Distribution and Fate in the Environment</p>	<ul style="list-style-type: none"> • Soils and sediments are primary sink • Also subject to long-range transport as particulates in the atmosphere, with removal by wet and dry deposition 				
	Water	Soils and Sediments (solid/liquid transfers)	Air		Living Organisms (bioaccumulation)
	Volatility	Gas/Liquid transfers			
<p>Water Solubility¹ (2,3,7,8 -TCDD): 0.419 $\mu\text{g/L}$ (2,3,7,8-TCDF): 0.483 $\mu\text{g/L}$</p> <ul style="list-style-type: none"> • Low water solubility • Lipophilic 	<p>$\text{Log } K_{ow}^2$: TCDD = 6.6 TCDF\approx 6.5</p> <ul style="list-style-type: none"> • Immobile in soils • Removal from water column by sedimentation 	<p>Vapor Pressure³ : TCDD = 3.38×10^{-8} mm Hg and TCDF\approx 1.50×10^{-8} mm Hg</p> <ul style="list-style-type: none"> • Vapor pressure decreases as chlorination increases • Less volatile forms partition to particulates in air 	<p>KH⁴ : TCDD = 1.6×10^{-5} atm $\ast \text{ m}^3/\text{mol}$ and TCDF\approx 8.6×10^{-6} atm $\ast \text{ m}^3/\text{mol}$</p> <ul style="list-style-type: none"> • Air deposition is important source to surface waters 	<p>BCF⁵ : 2, 3, 7, 8-TCDD = 2500 - 9300 (fathead minnow)⁶</p> <ul style="list-style-type: none"> • Bioaccumulates in fatty tissues, especially the more highly chlorinated congeners 	

Table B-4. Distribution and Fate of Dioxins and Furans (continued)

Distribution and Fate in the Environment (continued)	Transformations and Degradation/Persistence (chemical changes and distribution)				
	Water	Soils	Sediments	Air	Biota
<ul style="list-style-type: none"> • Persistence increases as chlorination increases • Generally not persistent in vapor phase, but generally persistent in soil, sediment, and water phases 	<ul style="list-style-type: none"> • Half-life: 2 days to 1.62 years (a) • Resistant to hydrolysis 	<ul style="list-style-type: none"> • Half-life: 1 to 3 years, up to 12 years (a) • Generally resistant to biodegradation • Persistent in soils 	<ul style="list-style-type: none"> • Half-life: 4.4 to 6.2 years, up to 30 to 170 years (a) • Persistent in sediment 	<ul style="list-style-type: none"> • Half-life: 1.6 to 10 days (vapor phase) • Breakdown via photodegradation for vapor phase • In particulate phase, photodegradation less important 	<ul style="list-style-type: none"> • Slowly metabolized

Source: Revised Draft Lake Michigan Lakewide Management Plan unless otherwise indicated

(a) Source for water solubility, log K_{ow} , vapor pressure, Henry's Law coefficient EPA 1998

(b) EC. 1997. Scientific Justification: Polychlorinated Biphenyls.

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures $>10^{-4}$ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures $<10^{-8}$ mm Hg should exist almost entirely in the particulate phase.
- ⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- ⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).
- ⁶ Fathead minnows are a ubiquitous fish species found in Lake Michigan and are commonly used as a marker species in bioaccumulation and toxicity studies.

B.3 PHYSICAL AND CHEMICAL PROPERTIES OF DIELDRIN/ALDRIN

Aldrin in its pure form is a white crystalline solid. Dieldrin in its pure form is a white crystalline solid and in its technical grade is a tan color. The chemical synthesis of dieldrin is by epoxidation of aldrin, and in the environment, aldrin is readily converted to dieldrin through biodegradation. In general, aldrin undergoes photolysis to dieldrin, which in turn may be degraded by ultraviolet radiation or microbial action into the more persistent photodieldrin (USDHHS 1993). Dieldrin is persistent because it is more resistant to biotransformation and abiotic degradation than aldrin, and as a result, it is found in low levels in all media.

Dieldrin/Aldrin in Air

Aldrin and dieldrin are released to the atmosphere through volatilization in the vapor phase from previously treated soil and evaporation from contaminated surface water. Gas-water transfers are strongly dependent on seasons, with net outputs in the summer and net inputs to surface waters typically observed in the winter (EPA 1997). Volatilization of aldrin from soil is more rapid when it is applied to the soil surface rather than incorporated into the soils. Once in the atmosphere, both chemicals may be transported great distances and may be removed by wet or dry deposition (USDHHS 1993). Atmospheric degradation of aldrin, by epoxidation by sunlight to photoaldrin, dieldrin, or photodieldrin, prevents accumulation of aldrin in the air. The estimated lifetime of dieldrin in the atmosphere, based on reactions with atmospheric hydroxyl radicals, is approximately 1 day. However, dieldrin may be more stable than implied by this lifetime if it is associated with particulate matter in the atmosphere. Under these conditions, wet and dry deposition may be more important loss processes (Bidleman and others 1990).

Dieldrin/Aldrin in Soil

Possible releases of aldrin and dieldrin to soil may come from the improper disposal of old stocks at landfill sites or as a result of the historical use of these compounds as insecticides. Because aldrin is converted to dieldrin so rapidly, aldrin concentrations in soils tend to be much lower than dieldrin concentrations, despite the fact that aldrin was applied more frequently (USDHHS 1993). Losses of dieldrin from soils may occur by volatilization to the atmosphere, by runoff to surface waters (as dieldrin-contaminated soil particles), or by degradation. The major degradation pathways include epoxidation of aldrin to dieldrin, biodegradation, and photodecomposition of dieldrin to photodieldrin. Dieldrin is much more resistant to biodegradation than aldrin and is relatively persistent in soil.

In general, aldrin/dieldrin are unlikely to leach appreciably from soil to water. Dieldrin is extremely nonpolar and, therefore, has a strong tendency to adsorb tightly to soil particles. Volatilization is the principal route of loss of dieldrin from soil; however, the process is relatively slow because of the low vapor pressure of dieldrin. Volatilization of aldrin is more rapid when it is applied to the soil surface rather than incorporated into the soil, and relatively rapid loss of both aldrin and dieldrin attributed to volatilization has been observed from soil during the first few months after the pesticide application.

Dieldrin/Aldrin in Water

Aldrin and dieldrin may be released to surface waters as a result of suspended solid transport in runoff from contaminated soils. Losses of dieldrin from water may occur by volatilization to the atmosphere, removal from the water column by sedimentation, or in small amounts by degradation. Due to their hydrophobic nature, aldrin and dieldrin can be expected to accumulate in sediments. Dieldrin is persistent in water.

Dieldrin/Aldrin in Plants, Animals, and Food

Aldrin is readily and rapidly converted to dieldrin, not only in the environment but also in plant and animal tissues (USDHHS 1993). Dieldrin readily bioaccumulates and biomagnifies. Dieldrin is extremely nonpolar and, therefore, has a strong tendency to adsorb tightly to lipids such as animal fat and plant waxes. Dieldrin bioconcentrates and biomagnifies through the terrestrial and aquatic food webs.

[Sources: Background information from USDHHS 1993. *Toxicological Profile for Aldrin/Dieldrin* (Update). Agency for Toxic Substances and Disease Registry unless otherwise indicated.]

Table B-5. Origins and Physical and Chemical Properties of Dieldrin/Aldrin

Dieldrin/Aldrin				
Major Sources / Uses	<ul style="list-style-type: none"> • Organochloride pesticide • Used on crops and as a termiticide • Used for locust and mosquito control and as a wood preservative • Most uses canceled in 1974, with last remaining use canceled in 1989 • Primary degradation product of aldrin (a related pesticide, canceled for all uses by 1991) 			
Physical and Chemical Forms	Water	Soils and Sediments	Air	Biota
	<ul style="list-style-type: none"> • Primarily bound to particulate phase, little in dissolved phase 	<ul style="list-style-type: none"> • Bound to soil solid phase and sediments 	<ul style="list-style-type: none"> • May be in vapor phase or associated with particulate matter 	<ul style="list-style-type: none"> • Accumulates in fatty tissue • Dieldrin also present as aldrin metabolite
				Other Commonly Released Forms
				<ul style="list-style-type: none"> • Aldrin readily converts to dieldrin in the environment

Source for physical and chemical property data: EPA BNS *Great Lakes Pesticide Report* unless otherwise indicated.

Table B-6. Distribution and Fate of Dieldrin/Aldrin

Dieldrin/Aldrin					
Transport and Media Partitioning (physical distribution)					
Distribution and Fate in the Environment	<ul style="list-style-type: none"> • Will reach surface water via particulate phase runoff • Airborne particulates subject to long-range transport • Removed from the atmosphere by wet and dry deposition 				
	Water	Soils and Sediments (solid/liquid transfers)	Air		Living Organisms (bioaccumulation)
	Water Solubility ¹ = 140 μg/L at 20°C	Log K _{oc} ² = 4.41	Volatility	Gas/Liquid transfers	BCF ³ : 100 to 10,000 for various aquatic species (a)
	<ul style="list-style-type: none"> • Hydrophobic • Adsorbs strongly to sediments 	<ul style="list-style-type: none"> • Adsorbs strongly to sediments • Immobile in most soils 	Vapor Pressure ³ = 1.31 x 10 ⁻⁹ mm Hg @ 25°C	KH ⁴ = 3.51 x 10 ⁻⁹ atm m ³ /mol a 25°C <ul style="list-style-type: none"> • Gas transfer from water strongly dependent on seasons (temperature dependent) 	<ul style="list-style-type: none"> • Bioconcentrates in fish

Table B-6. Distribution and Fate of Aldrin/Dieldrin (continued)

Dieldrin/Aldrin					
Transformations and Degradation/Persistence (chemical changes and distribution)					
Distribution and Fate in the Environment (continued)	Water	Soils	Sediments	Air	Biota
	<ul style="list-style-type: none"> • Hydrolysis not important • Persistent in water (associated with particulate phase) 	<ul style="list-style-type: none"> • Half-life: 1 month to 5 years • Epoxidation of aldrin to dieldrin • Biodegradation (Dieldrin is much more resistant to biodegradation than aldrin) 	<ul style="list-style-type: none"> • Epoxidation of aldrin to dieldrin • Dieldrin relatively persistent in sediments (dieldrin is much more resistant to biodegradation than aldrin) 	<ul style="list-style-type: none"> • Epoxidation of aldrin to dieldrin • Photodecomposition of dieldrin to photodieldrin 	<ul style="list-style-type: none"> • Aldrin converted to dieldrin in plant and animal tissues

(a) EPA. 1993. Revised Draft Lake Michigan Lakewide Management Plan.

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures $>10^{-4}$ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures $<10^{-8}$ mm Hg should exist almost entirely in the particulate phase.
- ⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- ⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).

B.4 PHYSICAL AND CHEMICAL PROPERTIES OF CHLORDANE

Chlordane is an organochlorine pesticide chemically related to aldrin, dieldrin, heptachlor, and endosulfan. However, it is more volatile than the others and was once used as a fumigant.

Chlordane in Air

When released to the atmosphere, chlordane exists predominately in the vapor phase and is susceptible to rapid photodegradation in this state. Chlordane degrades in the atmosphere by both photolysis and oxidation. The amount of chlordane bound to particulates in the atmosphere relative to the amount in the vapor phase is temperature dependent (more is present in the particulate phase in colder, arctic regions). Although chlordane exists primarily in the vapor phase, the small amount bound to particles appears to be significant in terms of long-range atmospheric transport of chlordane.

Even though there has been no recent use of chlordane for termite control, studies have detected chlordane in the indoor air of homes treated for termites up to 15 years after application.

Chlordane in Soil

When released to soil, chlordane persists for long periods, although only limited degradation information is available. Chlordane has been found in soils for up to 20 years after application. Chlordane, like many of the persistent chlorinated hydrocarbons, persists much longer in heavy soils with high organic content when compared to loamy sandy soil (USDHHS 1994). It has been suggested that chlordane is very slowly biotransformed in the environment, which is consistent with the long persistence periods observed under field conditions.

Chlordane in Water

When released to water, chlordane does not significantly undergo hydrolysis, oxidation, or direct photolysis. As a result, chlordane is highly persistent in aquatic ecosystems. Based on the low solubility and high K_{ow} of chlordane, any chlordane present in the water column is likely bound to particles and can be assumed to partition to sediments.

Chlordane in Plants, Animals, and Food

Although chlordane is very bioaccumulative, long-term monitoring studies have indicated a decline in the concentrations of chlordane in fish from the mid-1970s through the early 1990s. Studies of herring gull eggs have reported a slightly different trend. Chlordane levels in herring gull eggs increased or remained constant from the mid-1970s to 1980 before dropping dramatically.

[Sources: Some background information for the preceding section is from USDHHS. 1994. *Toxicological Profile for Chlordane* (Update). Agency for Toxic Substances and Disease Registry unless otherwise indicated.]

Table B-7. Origins and Physical and Chemical Properties of Chlordane

Chlordane					
Major Sources / Uses	<ul style="list-style-type: none"> • Pesticide used on field crops and later under restricted use as a termiticide • All commercial uses canceled since 1988 • Current sources from historical use and hazardous waste sites 				
Primary Forms	Water	Soils and Sediments	Air	Biota	Other Commonly Released Forms
	<ul style="list-style-type: none"> • Isomer mixtures • Primarily bound to soils or water-borne particulates 	<ul style="list-style-type: none"> • Isomer mixtures bound to solid phase 	<ul style="list-style-type: none"> • Exists predominantly in vapor phase • Particulate phase binding is temperature dependent (more adsorption in colder regions) 	<ul style="list-style-type: none"> • Chlordane is metabolized to oxychlordane in fish 	<ul style="list-style-type: none"> • Technical grade chlordane is mixture of > 140 related compounds • Major constituents: cis-(α-chlordane) and trans-(γ-chlordane) chlordane

Source for physical and chemical property data: EPA 1998. *Great Lakes Binational Toxics Strategy Pesticide Report*. December unless otherwise indicated.

Table B-8. Distribution and Fate of Chlordane

Transport and Media Partitioning (physical distribution)				
<ul style="list-style-type: none"> Physical and chemical properties differ among isomers and uncertainty exists regarding transport of specific compounds Adsorption to sediments is the major fate process 				
Water	Soils and Sediments (solid/liquid transfers)	Air		Living Organisms (bioaccumulation)
		Volatility	Gas/Liquid transfers	
Water Solubility ¹ = 550 µg/L @25°C <ul style="list-style-type: none"> Low solubility 	Log K _{oc} ² = 4.71 <ul style="list-style-type: none"> Partitions to soil and sediments Generally immobile 	Vapor Pressure ³ = 2.7 x 10 ⁻⁵ mmHg <ul style="list-style-type: none"> Vapor pressures change as the more volatile compounds in the mixture volatilize Volatility is temperature dependent 	KH ⁴ = 2.6 x 10 ⁻⁵ atm m ³ / mol at 25 °C	BCF ⁵ : 38,000 (fathead minnow ⁶ at 32 days) (a) <ul style="list-style-type: none"> Strongly bioaccumulated in fish and other aquatic organisms

Distribution and Fate in the Environment

Table B-8. Distribution and Fate of Chlordane (continued)

Transformations and Degradation/Persistence (chemical changes and distribution)					
Physical and chemical properties differ amongst isomers and therefore there is uncertainty regarding degradation of specific compounds					
Generally resistant to both chemical and biological degradation					
Distribution and Fate in the Environment (continued)	Water	Soils	Sediments	Air	Biota
	<ul style="list-style-type: none"> • Hydrolysis, direct oxidation, direct photolysis not significant • Very persistent in adsorbed state 	<ul style="list-style-type: none"> • Mean half-life: 3.3 years (a) • Very persistent • Very slowly biotransforms 	<ul style="list-style-type: none"> • Very persistent 	<ul style="list-style-type: none"> • Half-life: 1.3 to 6.2 hours (vapor phase), 1.3 days (other phases) • Degrades by photolysis and oxidation 	<ul style="list-style-type: none"> • Metabolized to oxychlordane

(a) EPA. 1993. *Revised Draft Lake Michigan Lakewide Management Plan*

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures $>10^{-4}$ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures $<10^{-8}$ mm Hg should exist almost entirely in the particulate phase.
- ⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- ⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).
- ⁶ Fathead minnows are a ubiquitous fish species found in Lake Michigan and are commonly used as a marker species in bioaccumulation and toxicity studies.

B.5 PHYSICAL AND CHEMICAL PROPERTIES OF DDT AND ITS METABOLITES

DDT is normally found associated with DDD and DDE. The latter two are impurities in the newly synthesized DDT and products of degradation, including on-column transformations during analysis and metabolism. All three compounds have substantially similar chemical, physical, and biological properties. DDT remains in use in public health work in many countries but not the United States or Canada.

DDT in Air

DDT may be present in the atmosphere as a result of volatilization from soil and water. DDT remains in the air only a short time. Once in the atmosphere, DDT will eventually photooxidize to carbon dioxide, hydrochloric acid, and hydroxyl radicals. Cortes and others (1998) report atmospheric half-lives at Sleeping Bear Dunes (IADN monitoring station for Lake Michigan) as 2.3 years for DDT and 2.6 years for DDE and DDD. Small particles that carry DDT or its degradation products may also be distributed through the atmosphere. Both wet and dry deposition are significant mechanisms of removal of DDT and its metabolites from the atmosphere.

DDT in Soil

DDT is persistent in soil and does not leach or move easily to groundwater. Routes of loss and degradation include runoff, volatilization, photolysis and biodegradation (aerobic and anaerobic). These processes generally occur very slowly. DDE and DDD are the initial breakdown products of DDT in the soil environment. Both sister compounds are also highly persistent and have chemical and physical properties similar to DDT. Due to its extremely low solubility in water, DDT will be retained to a greater degree by soils and soil fractions with higher proportions of organic matter. DDT residues in surface soils are much more likely to be broken down or otherwise dissipated than in subsurface deposits.

Volatilization losses of DDT from soil depends on the amount of DDT applied, the proportion of soil organic matter, proximity to the soil-air interface, and the amount of sunlight. Volatilization of DDT, DDE, and DDD is known to account for considerable losses of these compounds from soil surfaces. Their tendency to volatilize from the soil surface can be predicted by their relatively high vapor pressures.

DDT in Water

DDT reaches surface waters primarily by runoff, atmospheric transport, drift, or by direct application (for example, to control mosquito-borne malaria). DDT, DDE, and DDD are only slightly soluble in water. The main degradation and loss pathways in the aquatic environment are volatilization, photodegradation, adsorption to water-borne particulates (including sedimentation), and uptake by aquatic organisms that accumulate DDT and DDT metabolites in their tissues. Volatilization of DDT, DDE, and DDD is known to account for considerable losses of these compounds from the water surface.

DDT in Plants, Animals, and Food

DDT, DDE, and DDD are highly lipophilic, which combined with an extremely long half-life, has resulted in bioaccumulation (that is, levels in organisms exceed those levels occurring in the surrounding environment). In aquatic systems, DDT and its metabolites are bioconcentrated in aquatic organisms and biomagnify in the food web. The evaluation of DDT trends in wildlife is complicated by the fact that

some studies report total DDT (DDT and the sum of metabolites), whereas other studies may report DDT, DDE, and DDD separately (DHHS 1994).

A study of the biomagnification of polychlorinated biphenyls (PCB), toxaphene, and the DDT family of metabolites in southeastern Lake Michigan found that DDE was the most strongly biomagnified compound, increasing 28.7 times in average concentration from plankton to fish. The same study determined that DDE is the predominant form of DDT in the Lake Michigan ecosystem, accounting for more than 75 percent of total DDT. (Evans and others 1991)

Table B-9. Origins and Physical and Chemical Properties of DDT

DDT					
Physical and Chemical Forms	Water	Soils and Sediments	Air	Biota	Other Commonly Released Forms
	<ul style="list-style-type: none"> DDT and metabolites primarily bound to water-borne particles and sediments 	<ul style="list-style-type: none"> DDT and metabolites bound to solid phase 	<ul style="list-style-type: none"> Gaseous, vapor phase 	<ul style="list-style-type: none"> Primarily found in fatty tissues and eggs of fish-eating birds 	<ul style="list-style-type: none"> Technical DDT: p,p-DDT (85 percent) o,p-DDT (15 percent) DDE as trace contaminant

Source for physical and chemical property data: EPA 1998. *Great Lakes Binational Toxics Strategy Pesticide Report*. December, unless otherwise indicated.

Table B-10. Distribution and Fate of DDT

DDT			
Transport and Media Partitioning (physical distribution)			
<ul style="list-style-type: none"> Major processes for transfer are air-water exchange and sorption in biota and sediments 			
Distribution and Fate in the Environment	Water	Soils and Sediments (solid/liquid transfers)	Air
	Volatility	Gas/Liquid transfers	Living Organisms (bioaccumulation)
	Water Solubility ¹ = 3.4 $\mu\text{g/L}$ @ 25 °C <ul style="list-style-type: none"> Highly insoluble in water Soluble in most organic solvents 	Log K_{oc}^2 = 5.83 <ul style="list-style-type: none"> Adsorbs to soil and water-borne particulates 	Vapor Pressure ³ = 3.9 x 10 ⁻⁷ torr at 20 °C <ul style="list-style-type: none"> Semivolatile Will partition to atmosphere
			KH ⁴ = 5.37 x 10 ⁻⁵ atm m ³ /mol @ 25 °C <ul style="list-style-type: none"> Air-water exchange significant process in deposition to surface water
			BCF ⁵ : 317,000 (largemouth bass) (a) <ul style="list-style-type: none"> Very lipophilic Readily bioaccumulates

Table B-10. Distribution and Fate of DDT (continued)

Distribution and Fate in the Environment (Continued)		Transformations and Degradation/Persistence (chemical changes and distribution)				
		<ul style="list-style-type: none"> In general, very persistent and resistant to degradation Major degradation products are DDE and DDD, both of which are highly persistent and have physical and chemical properties similar to those of DDT. 				
		Water	Soils	Sediments	Air	Biota
		<ul style="list-style-type: none"> Half-life: 7-350 days (b) Mainly photolysis 	<ul style="list-style-type: none"> Half-life: 2-15 yrs (b) Very persistent Slow degradation by photolysis and biodegradation (aerobic and anaerobic) 	<ul style="list-style-type: none"> Half-life: 16.6 days - 31.3 years (b) Slow biodegradation 	<ul style="list-style-type: none"> Half-life: 17.7 hours to 7.4 days (b) Will photo oxidize to CO₂ and hydroxyl radicals 	<ul style="list-style-type: none"> Very persistent

(a) EPA. 1993. Revised Draft Lake Michigan Lakewide Management Plan

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures >10⁻⁴ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures <10⁻⁸ mm Hg should exist almost entirely in the particulate phase.
- ⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- ⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).

B.6 PHYSICAL AND CHEMICAL PROPERTIES OF MERCURY

Mercury is an element, a metal that occurs naturally in the environment in several forms. Most of the mercury found in the environment is inorganic mercury, in the form of metallic mercury and inorganic mercury compounds.

In its metallic or elemental form (Hg^0), mercury is a shiny, silver-white, odorless liquid. Some evaporation of metallic mercury occurs at room temperature to form mercury vapor, a colorless, odorless gas. In the ionic form, mercury exists in one of two oxidation states (or valences): Hg^{+1} , or the mercurous ion, and Hg^{+2} , or the mercuric ion. Of the two states, the higher oxidation state (Hg^{+2}) is the more stable. Ionic mercury combines with other elements, such as chlorine, sulfur, or oxygen, to form inorganic mercury compounds or “salts.”

Mercury can also form a chemical bond with carbon to create the organomercurial compounds methylmercury, dimethylmercury, phenylmercury, and thimerosal (Merthiolate). It is customary to refer to mercury with bonds to carbon as “organic” mercury. Like the inorganic mercury compounds, both methylmercury and phenylmercury exist as “salts” (for example methylmercuric chloride or phenylmercuric acetate). The most common forms of mercury naturally found in the environment are metallic mercury, mercuric sulfide, mercuric chloride, and methylmercury.

Environmental cycling of mercury includes conversion between inorganic and organic forms, as well as phase transfers between the gaseous (atmospheric); solid (soils, sediments, and airborne particulates); and aqueous (dissolved and sediment bound) states.

The natural global biogeochemical cycling of mercury is characterized by degassing of the mineral mercury from soils and surface waters, long-range transport in the atmosphere, wet and dry deposition of mercury back to land and surface waters, and sorption of the compound to soil or sediment particulates.

The form of mercury found in the environment can be changed slowly by microorganisms and natural processes. Particulate-bound mercury can be transformed and mobilized by biotic and abiotic oxidation and reduction and can be converted to insoluble mercury compounds and precipitated. Inorganic mercury can also be methylated by microorganisms indigenous to soils and fresh water. This bioconversion between inorganic and organic forms is mediated by various microbial populations under both aerobic and anaerobic conditions. Overall, these transformations may convert mercury into more volatile or soluble forms that reenter the atmosphere or are taken up by biota and bioaccumulated in terrestrial and aquatic food webs.

The specific state (that is, solid, liquid, or gas) and form (for example, inorganic or organic) in which the compound is found in an environmental medium depends on several factors, including pH, temperature, aerobic or anaerobic condition, and microbial activity.

Mercury in Air

Over 95 percent of the mercury found in the atmosphere is elemental mercury (Hg^0), which is gaseous. This is the form involved in long-range atmospheric transport of the compound. Approximately 5 percent of atmospheric mercury is associated with particulates, which have a shorter atmospheric residence time, are removed by dry or wet deposition, and may show a regional or local distribution pattern (Nater and Grigal 1992). Metallic mercury released to the atmosphere in vapor form can be

transported long distances before wet and dry deposition processes return the compound to land and water surfaces.

Wet deposition is the primary method of removal of mercury from the atmosphere and may account for virtually all of the mercury content in remote lakes that do not receive inputs from other sources (such as industrial effluents) (Hurley and others 1991, Swain and others 1992). Most inert mercury (Hg^{+2}) in precipitation is bound to aerosol particulates, which are relatively immobile when deposited on soil or water. In addition to wet and dry deposition processes, mercury may also be removed from the atmosphere by sorption of the vapor form to soil or water surfaces (EPA 1984b)

The primary form of atmospheric mercury, metallic mercury vapor (Hg^0), is oxidized by ozone to other forms (such as Hg^{+2}) in the removal of the compound from the atmosphere by precipitation. Other mercury compounds vary in stability and susceptibility to chemical transformation. The main atmospheric transformation process for organomercurials appears to be photolysis (EPA 1984b).

Mercury in Soil and Sediment

Mercury compounds in soils may undergo the same chemical and biological transformations described below for surface waters. Mercuric (Hg^{+2}) mercury usually forms various complexes with chloride and hydroxide ions in soils, and the specific complexes formed depend on the pH, salt content, and composition of the soil solution. Formation and degradation of organic mercurials in soils appear to be mediated by the same types of microbial processes occurring in surface waters and may also occur through abiotic processes (Anderson 1979).

In general, mercury in soil is stable for long periods of time, usually stays on the surface of the sediments or soil, and does not move through the soil to groundwater. Inorganic mercury sorbed to particulate material is not readily desorbed. Thus, freshwater and marine sediments are important repositories for inorganic forms of the compound, and leaching is a relatively insignificant transport process in soils. This strong adsorption of mercury to particulate matter also means that the transport of mercury-contaminated particulates carried in surface runoff is an important mechanism for moving mercury from soil to water.

Mercury in Water

Mercury cycling occurs in freshwater lakes with the concentrations and speciation of the mercury depending on limnological features and water stratification. The top water layer may be saturated with volatile elemental mercury, although sediments are the primary source of the mercury in surface waters.

Mercury in water can exist in the +1 and +2 valence states as a number of complex ions with varying water solubilities. Mercuric mercury, present as complexes, is probably the predominant form of mercury present in surface waters. The transport and partitioning of mercury in surface waters and soils is influenced by the particular form of the compound. Highly insoluble salts, such as mercury sulfide, are the most stable and least mobile form of mercury.

Volatile forms of mercury (such as metallic mercury and dimethylmercury) evaporate to the atmosphere, whereas solid forms partition to particulates in the soil or water column and are transported downward to the sediments in the water column.

The most important transformation process in the environmental fate of mercury in surface waters is biotransformation. Any form of mercury entering surface waters can be microbially converted to methylmercuric ion given favorable conditions. Methylmercury is the usual organic form of mercury

created by these natural processes. It is soluble, mobile, and quickly enters the aquatic food chain. Methylmercury is accumulated to a greater extent in biological tissue than are inorganic forms of mercury, and it can accumulate in certain fish to levels that are many times greater than in the surrounding water.

Transformation of methylmercury compounds back to volatile elemental mercury may also occur as a result of microbial demethylation. Anaerobic conditions, as may be found in sediments, favor the demethylation of methylmercury. Abiotic reduction of mercuric mercury to metallic mercury in aqueous systems can also occur. This reduction process is enhanced by light and occurs under both aerobic and anaerobic conditions.

Mercury in Plants, Animals, and Food

Methylmercury in surface waters is rapidly accumulated by aquatic organisms. The biomagnification potential for methylmercury in fish is influenced by the pH and dissolved oxygen content of the water. The biological half-life of methylmercury in mussels is estimated to be 1,000 days (Cossa 1989). Bioaccumulation of methylmercury in aquatic food webs is of interest because it is generally the most important source of nonoccupational human exposure to the compound (EPA 1984b).

[Sources: Background information in the preceding section is from USDHHS. 1993. *Toxicological Profile for Mercury* (Update). Agency for Toxic Substances and Disease Registry unless otherwise indicated.]

Table B-11. Origins and Physical and Chemical Properties of Mercury

Mercury					
Major Sources / Uses	<ul style="list-style-type: none"> • Naturally occurring substance. • Used in batteries, thermometers, electric switches, fluorescent lamps, and as a catalyst in oxidation of organic compounds. • Other anthropogenic releases include combustion of fossil and other fuels, mining, smelting, manufacturing, and past agricultural use. • Environmental cycling of historically released mercury compounds is an important source of mercury loadings to Lake Michigan. 				
Physical and Chemical Forms	Water	Soils and Sediments	Air	Biota	Other Commonly Released Forms
	<ul style="list-style-type: none"> • Inorganic salts (chelates and complexes) and methyl mercury • Associated with solid phase (particulates and sediments) 	<ul style="list-style-type: none"> • Elemental (Hg⁰) (gaseous) • Inorganic mercury salts (Hg⁺, Hg⁺²) (solids: such as mercuric sulfide, mercuric chloride) bound to solid phase 	<ul style="list-style-type: none"> • Most is elemental mercury (Hg⁰) gas • Small amount associated with solid phase (air-borne particulates) 	<ul style="list-style-type: none"> • Hg metabolized to methyl-mercury (organic Hg) by microorganisms • Accumulates as methyl-mercury 	<ul style="list-style-type: none"> • Phenylmercuric (organic) acetate formerly used as fungicide • Methyl-mercury compounds formerly man-made for use as fungicides

Source for physical and chemical property data: USDHHS 1993. Toxicological Profile for Mercury. ATSDR unless otherwise indicated.

Table B-12. Distribution and Fate of Mercury

Transport and Media Partitioning (physical distribution)				
<ul style="list-style-type: none"> Major transport mechanisms include outgassing of the element from soils and surface waters, long-range transport in the atmosphere, wet and dry deposition, sorption to soils and sediment particles, and bioaccumulation. 				
Water	Soils and Sediments (solid/liquid transfers)	Air		Living Organisms (bioaccumulation)
		Volatility	Gas/Liquid transfers	
<p>Water Solubility¹ = 0.056 mg/L (inorganic element)</p> <ul style="list-style-type: none"> Water solubility varies among inorganic complexes. Methyl-mercury is soluble. 	<p>Log K_{oc}² = additional information needed</p> <ul style="list-style-type: none"> In general, the dominant transport process is sorption of nonvolatile forms to soils and sediments with little resuspension to the water column. Methyl-mercury is mobile in soils. 	<p>Vapor Pressure³: inorganic = .002 mmHg at 25 °C organic = .0085 mmHg at 25 °C</p> <ul style="list-style-type: none"> More volatile forms evaporate to atmosphere 	<p>$KH^4 = 7.1 \times 10^{-3}$ atm- m³/mol (inorganic element)</p> <ul style="list-style-type: none"> More volatile forms (Hg⁰ and dimethyl-Hg) evaporate to atmosphere 	<p>BCF⁵: inorganic = 1,800- 4,994 organic = 10,000- 81,670 (b)</p> <ul style="list-style-type: none"> Very bioaccumulative
Distribution and Fate in the Environment				

Table B-12. Distribution and Fate of Mercury (continued)

Transformations and Degradation/Persistence (chemical changes and distribution)				
Distribution and Fate in the Environment (continued)	- Mercury (as an element) cannot be further broken down. - Other forms are converted by biotic and abiotic oxidation and reduction, bioconversion between organic and inorganic forms, and photolysis of organic compounds.			
	Water	Soils	Sediments	Air
	<ul style="list-style-type: none"> Bioconversion is most important (methylation). 	<ul style="list-style-type: none"> Bioconversion and abiotic reduction (especially in the presence of organic matter) 	<ul style="list-style-type: none"> Same as soils and surface waters 	<ul style="list-style-type: none"> Hg⁰ oxidized by ozone to Hg⁺¹ and Hg⁺² Particulate-bound is more stable
				Biota
				<ul style="list-style-type: none"> Methyl-mercury is persistent. May be transformed back to elemental-mercury in tissues

Sources:

- (a) USDHHS. 1993. Toxicological Profile for Mercury. ATSDR unless otherwise indicated.
- (b) EPA. 1993. Revised Draft Lake Michigan Lakewide Management Plan.

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures >10⁻⁴ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures <10⁻⁸ mm Hg should exist almost entirely in the particulate phase.
- ⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- ⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).

B.7 PHYSICAL AND CHEMICAL PROPERTIES OF LEAD

Natural lead is found in many minerals, with the highest concentrations in sulfides. Since it is the ultimate, stable product of natural radioactive decay, lead is also found in minerals derived from such compounds. Virtually all natural lead is in the plumbous (Pb^{+2}) oxidation state.

Most manmade lead is in the metallic (Pb^0) state or the plumbous state. There are also a few plumbic (Pb^{+4}) compounds. Environmental transformations between oxidation states are rare, and occur slowly. However, the forms have generally similar characteristics, including minimal to negligible water solubility and volatility. A few compounds (acetate, nitrate, chloride, others) are fairly soluble in water, but these will be rapidly precipitated as the sulfate, carbonate, or similar insoluble salt. Synthetic organolead compounds, such as tetraethyl lead, are volatile, but are relatively unstable and are converted to inorganic salts within years. Since these organolead compounds have been phased out over the last few decades, they are now of minimal importance.

Lead in Air

Lead in air is in the particulate phase, entering as airborne dust, and then washed out if it does not settle out first. Relatively soluble compounds may be transformed to the oxide, or carbonate salts, but no other changes are expected.

Lead in Soil and Sediment

Lead in soil is relatively stable and immobile. Therefore, deposits from airborne lead will form a highly contaminated surface layer over a minimally contaminated mass. Deposits of the metal will corrode, forming the more insoluble salts, such as the sulfate, phosphate, sulfide, and oxide depending on the exact soil chemistry.

Lead in Water

Almost all of the lead in water will be in the sediment phase, since most compounds have low solubility and the lead in the soluble compounds will be precipitated by the anions in the water. Minimum soluble concentrations occur at pH 5 to pH 6. Lead metal will dissolve, especially at low pH, move some distance, and then be precipitated.

In addition, there are reports that some lake sediment microorganisms can transform inorganic lead compounds to methyl lead compounds. However, this occurs with only some sediments and the rate is measurable only if the lead is initially present as a soluble compound.

Lead in Plants, Animals, and Food

Lead is passively absorbed by plants and animals. Once absorbed, it will then be deposited wherever the organisms deposit calcium. Therefore, plants will not have very much lead. However, mammals, birds, fish, and other animals will accumulate lead in their skeletons and oysters, mussels, snails, and similar animals will accumulate lead in their shells. Older individuals will have more than younger ones. In aquatic communities, the benthic organisms and the algae will generally have the highest concentrations.

Table B-13. Origins and Physical and Chemical Properties of Lead

Lead				
Major Sources / Uses	<ul style="list-style-type: none"> • Widely distributed metal, in sulfide and other minerals • The largest single use for lead is in storage batteries • Lead metal and alloys are used in cable sheaths, solder, type metal, bearings, bullets, radiation shielding, and so on. • Lead oxide and other compounds are used in optical glass, ceramics, pigments, and other uses. Tetraethyl lead as a gasoline additive and lead pigments in household paints are now obsolete. 			
Physical and Chemical Forms	Water	Soils and Sediments	Air	Biota
	<ul style="list-style-type: none"> • Inorganic salts associated with the solid phase (particulates and sediments) 	<ul style="list-style-type: none"> • Inorganic salts bound to, or part of, the mineral matrix 	<ul style="list-style-type: none"> • Inorganic salts in the solid phase (particulates) 	<ul style="list-style-type: none"> • Bioaccumulated in calcium-containing organs, such as bones and shells
				Other Commonly Released Forms
				<ul style="list-style-type: none"> • Older tetraethyl lead releases are now probably mineralized to inorganic lead.

Source for physical and chemical property data: USDHHS 1993. *Toxicological Profile for Lead*. ATSDR unless otherwise indicated.

Table B-14. Distribution and Fate of Lead

Transport and Media Partitioning (physical distribution)					
Distribution and Fate in the Environment	Water	Soils and Sediments (solid/liquid transfers)	Air		Living Organisms (bioaccumulation)
			Volatility	Gas/Liquid transfers	
	Water Solubility ¹ = 10 mg/L (litharge form of PbO)	Log K _{oc} ² = additional information needed	Vapor Pressure ³ : 10 mmHg at 1,025°C (litharge)	KH ⁴ = additional information is needed	log BCF ⁵ : = 42 (fish) = 536 (oysters) = 2,570 (mussels) but some species much higher, such as 726 (rainbow trout) and 6,600 (eastern oyster)
	<ul style="list-style-type: none"> Other salts are generally similar 				

Table B-14. Distribution and Fate of Lead (continued)

Transformations and Degradation/Persistence (chemical changes and distribution)					
Distribution and Fate in the Environment (continued)	Water	Soils	Sediments	Air	Biota
	<ul style="list-style-type: none"> Generally relatively immobile in the solid phase 	<ul style="list-style-type: none"> Generally relatively immobile in the solid phase 	<ul style="list-style-type: none"> Generally relatively immobile in the solid phase 	<ul style="list-style-type: none"> Generally relatively immobile in the solid phase 	<ul style="list-style-type: none"> Generally relatively immobile in the solid phase

Sources:

- (a) USDHHS. 1993. Toxicological Profile for Mercury. ATSDR unless otherwise indicated.
- (b) EPA. 1993. Revised Draft Lake Michigan Lakewide Management Plan.

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures $>10^{-4}$ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures $<10^{-8}$ mm Hg should exist almost entirely in the particulate phase.
- ⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- ⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).

B.8 PHYSICAL AND CHEMICAL PROPERTIES OF CADMIUM

Cadmium is a naturally occurring element in the earth's crust. Pure cadmium is a soft, silver-white metal; however, cadmium is not usually found in the environment as a metal. It is usually found as a mineral combined with other elements such as oxygen (cadmium oxide), chlorine (cadmium chloride), or sulfur (cadmium sulfate, cadmium sulfide). These compounds are solids that may dissolved in water but do not evaporate or disappear from the environment. All soils and rocks, including coal and mineral fertilizer, have some cadmium in them. Cadmium is often found as part of small particles present in air. You cannot tell by smell or taste that cadmium is present in air or water because it does not have any definite taste or odor.

Cadmium and cadmium compounds have negligible vapor pressures, but may exist in air as suspended particulate matter derived from sea spray, industrial emissions, combustion of fossil fuels, or the erosion of soils. Cadmium emitted to the atmosphere from combustion processes is usually associated with very small particulates that are in the respirable range (less than 10 μm) and are subject to long-range transport. These cadmium pollutants may be transported from 100 to a few thousand km and have a typical atmospheric residence time of about 1 to 10 days before deposition occurs. Larger cadmium-containing particles from smelters and other pollutant sources are also removed from the atmosphere by gravitational settling, with substantial deposition in areas downwind of the pollutant source. Cadmium deposition in urban areas is about one order of magnitude higher than in rural areas of the United States.

Cadmium is more mobile in aquatic environments than most other heavy metals, such as lead. In natural waters, most cadmium will exist as the hydrated ion ($\text{Cd}^{+2} 6\text{H}_2\text{O}$). Cadmium complexed with humic substances is also an important form of cadmium in polluted waters. Cadmium concentration in water is inversely related to the pH and the concentration of organic material in the water. Because cadmium exists only in the +2 oxidation state, aqueous cadmium is not strongly influenced by the oxidizing or reducing potential of the water. However, under reducing conditions, cadmium may form cadmium sulfide which is poorly soluble and tends to precipitate.

Precipitation and sorption to mineral surfaces and organic materials are the most important removal processes for cadmium compounds. Sediment bacteria may also assist in the partitioning of cadmium from water to sediments. Both cadmium-sensitive and cadmium-resistant bacteria reduced the cadmium concentration in the water column from 1 ppm to between 0.2 and 0.6 ppm, with a corresponding increase in cadmium concentration in the sediments that is at least one order of magnitude higher than in the overlying water. However, cadmium may also re-dissolve from sediments under varying ambient conditions of pH, salinity, and redox potential. Cadmium is not known to form volatile compounds, so partitioning from water to the atmosphere does not occur.

Cadmium in soils may leach into water, especially under acidic conditions. Cadmium-containing soil particles may also be entrained into the air or eroded into water, resulting in dispersion of cadmium into these media.

Cadmium in Air

Little information is available on the atmospheric reactions of cadmium. The common cadmium compounds found in air (oxide, sulfate, chloride) are stable and not subject to photochemical reactions. Cadmium sulfide may photolyze to cadmium sulfate in aqueous aerosols. Transformation of cadmium among types of compounds in the atmosphere is mainly by dissolution in water or dilute acids.

Cadmium in Soil and Sediment

Transformation processes for cadmium in soil are mediated by sorption from and desorption to water, and include precipitation, dissolution, complexation, and ion exchange. Important factors affecting transformation in soil include the cation exchange capacity, the pH, and the content of clay minerals, carbonate minerals, oxides, organic matter, and oxygen.

Cadmium in Water

In fresh water, cadmium is primarily present as the cadmium(+2) ion, although at high concentrations of organic material, more than half may occur in organic complexes. In reducing environments, cadmium precipitates as cadmium sulfide. Photolysis is not an important mechanism in the aquatic fate of cadmium compounds, nor is biological methylation likely to occur.

Cadmium in Plants, Animals, and Food

Aquatic and terrestrial organisms bioaccumulate cadmium. Cadmium concentrates in freshwater and marine animals to concentrations hundreds to thousands of times higher than in the water. Reported bioconcentration factors (BCFs) range from 113 to 18,000 for invertebrates and from 3 to 2,213 for fish. Bioconcentration in fish depends on the pH and humus content of the water.

The data indicate that cadmium bioaccumulates in all levels of the food chain. Cadmium accumulation has been reported in grasses and food crops, and in earthworms, poultry, cattle, horses, and wildlife. However, since cadmium accumulates primarily in the liver and kidneys of vertebrates, biomagnification through the food chain may not be significant. Although some data indicate increased cadmium concentrations in animals at the top of the food chain, comparisons among animals at different trophic levels are difficult, and the data available on biomagnification are not conclusive. Uptake of cadmium from soil by feed crops may result in high levels of cadmium in beef and poultry (especially in the liver and kidneys). This accumulation of cadmium in the food chain has important implications for human exposure to cadmium, whether or not significant biomagnification occurs.

Table B-15. Origins and Physical and Chemical Properties of Cadmium

Cadmium						
Major Sources / Uses	<ul style="list-style-type: none"> • Naturally occurring substance • Used for nickel-cadmium batteries and metal plating • Releases result from combustion of fossil fuel, incineration of municipal or industrial wastes, or land application of sewage sludge or fertilizer. 					
Physical and Chemical Forms	Water	Soils and Sediments		Air	Biota	Other Commonly Released Forms
	<ul style="list-style-type: none"> • Generally found as hydrated ion (Cd(+2) 6H₂O), complexed with humic substances is also an important form. 	<ul style="list-style-type: none"> • Usually found adsorbed onto soil 		<ul style="list-style-type: none"> • Found only as solid particles 	<ul style="list-style-type: none"> • Bioaccumulates in all levels of the food chain 	

Table B-16. Distribution and Fate of Cadmium

Transport and Media Partitioning (physical distribution)					
Distribution and Fate in the Environment	Water	Soils and Sediments (solid/liquid transfers)	Air		Living Organisms (bioaccumulation)
			Volatility	Gas/Liquid transfers	
	Insoluble	Log Koc ² = Not available	Vapor pressure ³ = 1 mmHg at 394 ° C	KH ⁴ = Not available	BCF ⁵ = Not available
	Primarily present as the cadmium (+2) ion, although at high concentrations of organic material, more than half may occur in organic complexes.	May leach into water, especially under acidic conditions.	Cadmium and cadmium compounds have negligible vapor pressures.	Particulates may dissolve in atmospheric water droplets and be removed from air by wet deposition.	Bioaccumulates in all levels of the food chain.
Transformations and Degradation/Persistence (chemical changes and distribution)					
Distribution and Fate in the Environment (continued)	Water	Soils	Sediments	Air	Biota
	In reducing environments, cadmium precipitates as cadmium sulfide.	Transformation processes are mediated by sorption from and desorption to water.	Bacteria may assist in partitioning from water to sediments.	Found only in the particulate (solid) form	Accumulated, but does not biomagnify

Source: USDHHS. 1993. *Toxicological Profile for Cadmium*, April.

Footnote Information:

¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.

Table B-16. Distribution and Fate of Cadmium (continued)

- 2 Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- 3 Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures $>10^{-4}$ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures $<10^{-8}$ mm Hg should exist almost entirely in the particulate phase.
- 4 KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- 5 BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).

B.9 PHYSICAL AND CHEMICAL PROPERTIES OF CHROMIUM

Chromium has a rather complicated chemistry with three common and several uncommon oxidation states. Natural chromium is found in the chromic (Cr^{+3}) form, generally in association with iron. Highest concentrations are in basic and ultrabasic igneous rocks, with much lower concentrations in granitic (siliceous) igneous rocks. Chromium ore is converted to either the metal (Cr^0) or the chromate (Cr^{+6}) form. Most chromium is used as the metal in stainless steel and many other alloys. Some of the chromite (Cr^{+3}) ore is refined and used in refractories. A small part of the total chromium is converted to chromate (Cr^{+6}) and other chromium compounds. These are used primarily as pigments (Cr^{+3} and Cr^{+6}); leather tanning (Cr^{+3}); metal finishing (Cr^{+6}); and wood preserving (Cr^{+6}); as well as a wide array of minor uses.

Environmentally, the three oxidation states have quite different chemical properties. Chromium metal is practically inert, as one would expect from its use in stainless steel. Salts in the chromic state (Cr^{+3}) are relatively insoluble, so they are almost inert; however, chromate salts (Cr^{+6}) are relatively water soluble. Dissolved chromate is an oxidizing material, which will react in time to produce a chromic chemical and the oxidized substrate. Thus Cr^{+3} is the ultimate form of environmental chromium. However, this process takes a considerable period of time, so the environmental processes of chromate are significant.

Chromium in Air

Airborne chromium is found in the solid phase. Natural sources include dust and volcanic emissions. The major manmade source is combustion of fuels; other sources include emissions from cement kilns and from cooling towers that use chromium water treatments. Chromium in air remains in the solid phase. The only likely reactions involve chromate (Cr^{+6}), which can oxidize organic matter and other material that it contacts.

Chromium in Soil

Chromium metal and chromic (Cr^{+3}) salts are stable in soil. Chromate (Cr^{+6}) salts are slowly reduced to the chromic state, with the reaction proceeding faster in acidic soils. In shallow soils, the chromate typically reacts with organic carbon. In deeper soils, where conditions are anaerobic, the chromate will react with sulfide (S^{-2}) or ferrous (Fe^{+2}) iron. The chromate salts can move by dissolution in water and movement with the water. However, chromic salts are found in practically insoluble salts and organic complexes and are, therefore, immobile.

Chromium in Water

The properties of chromium in water are substantially similar to those in soil. The chromic and metallic chromium is part of the solid phase, sediment and particulate, while much of the chromate is dissolved. There may be some chromic-organic complexes which are soluble and stable. The chromate then reacts with a suitable substrate and is reduced to an insoluble chromic salt.

Chromium in Plants, Animals, and Food

In plants, chromium is taken up with water and remains in the plant after evapotranspiration of the water. Since chromate is much more soluble, it is the predominant species entering the plant, but it is readily reduced to the chromic form.

Chromium is a necessary component of some metabolic enzymes in mammals as well as other animals. Therefore, uptake and excretion of surplus chromium are under active control. However, the net result of animal chromium metabolism is substantially similar to the passive processes in plants.

Table B-17. Origins and Physical and Chemical Properties of Chromium

Chromium				
Major Sources / Uses	<ul style="list-style-type: none"> • Chromium salts are widely distributed, especially with iron salts. • The main use of chromium is the metal as a component in stainless steel and other alloys. • Chromium salts are used in refractories, pigments, leather tanning, wood preserving, and other fields. 			
Physical and Chemical Forms	Water	Soils and Sediments	Air	Biota
	<ul style="list-style-type: none"> • Inorganic salts are generally insoluble, associated with the solid phase (particulates and sediments) 	<ul style="list-style-type: none"> • Part of the mineral matrix 	<ul style="list-style-type: none"> • Part of the solid phase (airborne particulates) 	<ul style="list-style-type: none"> • Limited uptake
				Other Commonly Released Forms

Source for physical and chemical property data: USDHHS 1993. *Toxicological Profile for Chromium*. ATSDR unless otherwise indicated.

Table B-18. Distribution and Fate of Chromium

Transport and Media Partitioning (physical distribution)					
<ul style="list-style-type: none"> The major mechanisms are dissolution and precipitation 					
Distribution and Fate in the Environment	Water	Soils and Sediments (solid/liquid transfers)	Air		Living Organisms (bioaccumulation)
			Volatility	Gas/Liquid transfers	
	Water Solubility ¹ = Chromic (+3) oxide = practically insoluble Chromium (+6) trioxide = 671 g/L <ul style="list-style-type: none"> Other salts have similar solubilities 	Log K_{oc} ² = additional information needed	Vapor Pressure ³ : Negligible	KH ⁴ = additional information needed	log BCF ⁵ : = 1 (trout), 86 to 192 (mollusks)
			<ul style="list-style-type: none"> Chromium is expected to remain in the solid phase 		

Table B-18. Distribution and Fate of Chromium (continued)

Transformations and Degradation/Persistence (chemical changes and distribution)					
Distribution and Fate in the Environment (continued)	Water	Soils	Sediments	Air	Biota
	<ul style="list-style-type: none"> The primary processes are dissolution of Cr⁺⁶, reduction to Cr⁺³, and precipitation 	<ul style="list-style-type: none"> Cr⁺⁶ will dissolve and act as in water. Cr⁺³ has minimal mobility 	<ul style="list-style-type: none"> Same as soils 	<ul style="list-style-type: none"> Remains part of solid phase 	Once absorbed, converted to Cr ⁺³ and excreted.

Sources:

- (a) USDHHS. 1993. Toxicological Profile for Mercury. ATSDR unless otherwise indicated.
- (b) EPA. 1993. Revised Draft Lake Michigan Lakewide Management Plan.

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures >10⁻⁴ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures <10⁻⁸ mm Hg should exist almost entirely in the particulate phase.
- ⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- ⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).

B.10 PHYSICAL AND CHEMICAL PROPERTIES OF COPPER

Copper is one of the first metals used by man. Most of the copper used by man is found as the pure metal (electrical wiring, pipe, and son on) or as alloys (brass, bronze, bell metal, German silver, and many others). However, most natural copper and some manufactured copper is found in salts, including chlorides, sulfides, carbonates (the green coating seen on copper roofing), and complex salts. Cuprous salts (Cu^{+1}) are known, but the cupric salts (Cu^{+2}) are more common. When cuprous salts are dissolved in water, they generally disproportionate into the metal and the cupric form.

Copper in Air

Neither copper metal nor any of its salts has a readily measured vapor pressure. Therefore, copper will be found in air as part of the particulates (solid phases). The primary source of natural airborne copper is windblown dust. Other sources include volcanoes, decaying vegetation, and forest fires. Manmade sources include metal production (iron and steel and various other metals, in addition to copper), waste incineration, coal combustion, and others. The combustion sources (including most metal production processes) generally release cupric oxide, while the other sources do not change the chemical species. In all cases, the particulates, including their copper, are eventually deposited on soil, water, or vegetation.

Copper in Soil

Most environmental copper is present in the soil; where traces of copper (typically tens of parts per million) are found in many rocks and in the soils derived from those rocks. Manmade copper is initially found on surface deposits from airborne deposition.

Copper in soil is relatively immobile. There is little, if any, mobilization at $\text{pH} > 3$ except for the few soluble salts such as copper sulfate. Dissolved copper from such soluble salts generally precipitates as copper carbonate (if exposed to air), binds to the organic matter in the soil, or is bound by other ions. Therefore, in ordinary conditions, copper in soil will move only as a component of a particle.

Copper in Water

Metallic copper will dissolve in water especially in relatively soft, acidic water. Such “aggressive water” will rapidly erode copper pipes and fittings, producing a solution of cupric oxide. Dissolved copper in surface water precipitates rapidly, becoming part of the solid phase, both sediment and suspended matter. Once in that state, the copper behaves as in soil, with minimal dissolved cupric ions. The exact nature of the chemical state varies with the nature of the solid phase. Some will be bound to humic acid and similar material while other copper will be part of a mineral matrix.

Copper in Plants, Animals, and Food

Some copper is taken up by all plants and animals. In plants, uptake seems to be passive. That is, copper in the water the plant takes in will be distributed about the plant and then precipitated when the water is lost by evapotranspiration. Most plants are not affected by copper. Therefore, if high concentrations of copper exist in the water from deposition, deliberate (such as use as a pesticide) or otherwise, plants may contain so much copper that animals eating them are poisoned.

Copper is an essential micronutrient for mammals and other animals. Terrestrial animals (including humans) have mechanisms that take up enough copper from food and reject or excrete the surplus.

Therefore, toxicity is rare except for extremely high concentrations. However, aquatic animals are much more susceptible to copper toxicity, leading to the use of copper salts as molluscicides. In addition, many microorganisms, both terrestrial and aquatic, are also susceptible to copper toxicity, leading to its use as fungicide and algicide in fields, orchards, lakes, and streams.

Table B-19. Origins and Physical and Chemical Properties of Copper

Copper					
Major Sources / Uses	<ul style="list-style-type: none"> • Naturally occurring substance, as metal and (especially) salts • Metal very widely used in electrical wiring and plumbing • Salts have been used for pigments in paints and ceramics, and as pesticides of various types, especially antifouling paints, algicides, and fungicides. Copper salts are also used in nutritional supplements with many alloys used for coins and various machinery parts. 				
Physical and Chemical Forms	Water	Soils and Sediments	Air	Biota	Other Commonly Released Forms
	<ul style="list-style-type: none"> • Inorganic salts • Associated with solid phase (particulates and sediments) 	<ul style="list-style-type: none"> • Inorganic salts bound to solid phase • Element may be present in particulate form 	<ul style="list-style-type: none"> • Bound to solid phase (air-borne particulates) 	<ul style="list-style-type: none"> • Essential micronutrient in animals 	<ul style="list-style-type: none"> • Salts have been used on algicides in streams and reservoirs.

Source for physical and chemical property data: USDHHS 1990. Toxicological Profile for Copper. ATSDR unless otherwise indicated.

Table B-20. Distribution and Fate of Copper

Transport and Media Partitioning (physical distribution)				
<ul style="list-style-type: none"> Data are for copper sulfate, a common, soluble commercial salt 				
Water	Soils and Sediments (solid/liquid transfers)	Air		Living Organisms (bioaccumulation)
		Volatility	Gas/Liquid transfers	
Water Solubility ¹ = 143 g/L	Log K_{oc} ² = additional information needed	Vapor Pressure ³ : Very low organic = .0085 mmHg at 25°C	KH ⁴ = Additional information needed	BCF ⁵ : Not available
<ul style="list-style-type: none"> Water solubility varies considerably among salts; most are much less soluble 	<ul style="list-style-type: none"> Dominant transfer process is sorption to soils and sediment with little resuspension in water column due to density. 			

Distribution and Fate in the Environment

Table B-20. Distribution and Fate of Copper (continued)

Distribution and Fate in the Environment (continued)	Transformations and Degradation/Persistence (chemical changes and distribution)				
	Water	Soils	Sediments	Air	Biota

Sources:

- (a) USDHHS, 1993. Toxicological Profile for Mercury. ATSDR unless otherwise indicated.
- (b) EPA, 1993. Revised Draft Lake Michigan Lakewide Management Plan.

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures $>10^{-4}$ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures $<10^{-8}$ mm Hg should exist almost entirely in the particulate phase.
- ⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- ⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).

B.11 PHYSICAL AND CHEMICAL PROPERTIES OF ZINC

Natural zinc is found as bivalent compounds, especially as sulfides, carbonates, and oxides. The major use of zinc is as the metal. The primary useful property of the metal is its corrosion resistance, so chemical transformations are relatively unimportant.

Zinc in Air

Zinc is in air in the particulate phase. It is removed by wet and dry deposition.

Zinc in Soil and Sediment

In soil, zinc is part of the mineral matrix. Due to its solubility in water, it will slowly leach with the water phase. The rate of this movement depends on the local environmental conditions, especially the anions present and the pH.

Zinc in Water

The nitrate, chloride, and similar salts of zinc are very soluble, but soon precipitate as the oxide, sulfide, carbonate, or other slightly soluble species. The amount of zinc in the dissolved phase will depend on pH (least dissolved at near-neutral pH7), the presence of organic molecules that can bind the zinc ion, and the concentrations of precipitating anions. Regardless, the bulk of the zinc will be in the solid phase.

Zinc in Plants, Animals, and Food

Zinc is an essential mineral for essentially all life, so it can be found in most tissues. Aquatic organisms will have zinc concentrations considerably above the concentration of the dissolved zinc. However, the organisms control mechanisms generally prevent biomagnification up the food chain. Terrestrial organisms do not bioconcentrate zinc.

Table B-21. Origins and Physical and Chemical Properties of Zinc

Zinc				
Major Sources / Uses	<ul style="list-style-type: none"> • Zinc is widely distributed in the earth's crust, primarily as the sulfide, carbonate and oxide salts. • The main use of zinc is as a protective coating for other metals, as in "galvanized iron." Zinc alloys include brass, bronze, and current penny coins. • Zinc compounds have many uses, from smoke bombs through batteries and wood preservatives to food supplements and drugs. 			
Physical and Chemical Forms	Water	Soils and Sediments	Air	Biota
	<ul style="list-style-type: none"> • Inorganic salts primarily in the solid phase (particulates and sediments) 	<ul style="list-style-type: none"> • Inorganic salts, relatively immobile 	<ul style="list-style-type: none"> • Part of the solid phase 	<ul style="list-style-type: none"> • Essential element to all biota. Some accumulation can occur.
				Other Commonly Released Forms

Source for physical and chemical property data: USDHHS 1994. *Toxicological Profile for Zinc* (update). ATSDR unless otherwise indicated.

Table B-22. Distribution and Fate of Zinc

Transport and Media Partitioning (physical distribution)					
<ul style="list-style-type: none"> Major transport mechanisms include outgassing of the element from soils and surface waters, long-range transport in the atmosphere, wet and dry deposition, sorption to soils and sediment particles, and bioaccumulation. 					
Distribution and Fate in the Environment	Water	Soils and Sediments (solid/liquid transfers)	Air		Living Organisms (bioaccumulation)
			Volatility	Gas/Liquid transfers	
	Water Solubility ¹ = 6.5 mg/L (zinc oxide)	Log K _{oc} ² = additional information needed	Vapor Pressure ³ : 1 mmHg at 487 °C (metal). Salts are even less volatile	KH ⁴ = Addition ^{al} information needed	BCF ⁵ : Typical numbers are 1,000 for plants and fish and 10,000 for invertebrates.
	<ul style="list-style-type: none"> Most other salts have similar solubility, but zinc sulfide is essentially insoluble. 				<ul style="list-style-type: none"> Very bioaccumulative

Table B-22. Distribution and Fate of Zinc (continued)

Transformations and Degradation/Persistence (chemical changes and distribution)					
Distribution and Fate in the Environment (continued)	Water	Soils	Sediments	Air	Biota
	<ul style="list-style-type: none"> The concentration of zinc in water depends on the other ions present. Sulfide decreases water concentrations while high pH and high organic concentrations will increase dissolved zinc. 	<ul style="list-style-type: none"> Generally bound to the mineral mass 	<ul style="list-style-type: none"> Generally bound to the mineral mass 	<ul style="list-style-type: none"> Generally bound to the mineral mass 	<ul style="list-style-type: none"> Zinc is an essential part of several essential enzymes. Most organisms have mechanisms to control zinc concentrations, but these can be overwhelmed by high environmental concentrations.

Sources:

- (a) USDHHS. 1993. Toxicological Profile for Mercury. ATSDR unless otherwise indicated.
- (b) EPA. 1993. Revised Draft Lake Michigan Lakewide Management Plan.

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures $>10^{-4}$ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures $<10^{-8}$ mm Hg should exist almost entirely in the particulate phase.
- ⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- ⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).

B.12 PHYSICAL AND CHEMICAL PROPERTIES OF ARSENIC

Arsenic is a silver-gray, brittle, crystalline, metallic-looking substance that exists in three allotropic forms: yellow, black, and gray. It is odorless and nearly tasteless. Arsenic is naturally occurring in the environment at low levels. It is found mostly in compounds with oxygen, chlorine, and sulfur, which form inorganic arsenic compounds. Arsenic in plants and animals combines with carbon and hydrogen to form organic arsenic compounds. Organic arsenic is usually less harmful than inorganic arsenic. Arsenic has several oxidation states. The most common are As^{+3} (arsenous), which includes arsenite (AsO_2^-) salts, and As^{+5} (arsenic), which includes arsenate (AsO_4^{3-}) salts.

Arsenic exists in both the gas and particulate matter phases. The majority of atmospheric arsenic is highly respirable inorganic arsenic particulate matter smaller than 2.5 micrometers. Heating of most arsenic-containing compounds in the presence of air results in the oxidation of the arsenic bound in the mineral, producing primarily arsenic trioxide. Conditions in the ambient atmosphere favor oxidation, so inorganic arsenic compounds are generally expected to predominate in unimpacted ambient air.

The inorganic arsenic compounds are solids at normal temperatures and are not likely to volatilize. In water, they range from quite soluble (sodium arsenite and arsenic acid) to practically insoluble (arsenic trisulfide). Arsenic is soluble in nitric acid, cold hydrochloric acid, and sulfuric acid. It is insoluble in water and nonoxidizing acids. Arsenic compounds are generally nonvolatile except for gaseous arsine and arsenic trioxide. Arsenic trioxide is a solid at room temperature but sublimates at 193 °C.

Some organic arsenic compounds are gases or low-boiling point liquids at normal temperatures. Poisonous gas is produced by arsenic in a fire. Arsenic near acid or acid mist can release arsine, a very deadly gas.

Synonyms for arsenic are arsenic-75, metallic arsenic, arsenic black, arsenicals, and colloidal arsenic.

Transport and partitioning of arsenic depends upon its chemical form. The major transport fate for arsenic is sorption or complexation to soils and sediments. Suspended particulates reach surface waters by wet and dry deposition.

Arsenic as a free element is rarely encountered in natural waters. Soluble inorganic arsenate predominates under normal conditions because it is thermodynamically more stable in water than arsenite.

Arsenic in Air

Because arsenic is naturally occurring in the environment, low levels of arsenic are present in the air. Levels in air are usually about 0.02 to 0.10 micrograms per cubic meter. The atmospheric lifetime of inorganic, particulate-phase arsenic is typically 5 to 15 days due to wet and dry deposition.

Combustion and high-temperature processes are the major sources of inorganic arsenic emissions to the atmosphere. Manufacturing of copper and other metals often releases inorganic arsenic into the air, as does the burning of most fossil fuels, which frequently contain low levels of arsenic. There are also low levels of arsenic in cigarette smoke.

Natural processes that release inorganic arsenic to the air include volcanoes and the weathering of arsenic-containing minerals and ores.

Arsenic in Soil and Sediment

Low levels of arsenic are naturally present in all media, although soil usually contains the highest quantities, with average levels of about 5,000 parts per billion. Elevated levels of arsenic in soil and sediment are due either to natural mineral deposits or to contamination from anthropogenic activities.

Arsenic in Water

Arsenic is naturally occurring in water in amounts of about 2 parts per billion. Arsenic and its salts have low solubility in water. Concentrations of less than 1 milligram will mix with a liter of water. Arsenic is persistent in water, with a half-life of more than 20 days.

Natural mineral deposits in some geographic areas contain large quantities of arsenic, which may result in elevated levels of inorganic arsenic in water. Some chemical waste disposal sites also contain large quantities of arsenic. If the material is not properly stored or contained at the site, arsenic may leach into the water. Widespread application of pesticides may lead to water or soil contamination.

Arsenic in Plants, Animals, and Food

Except where soil arsenic contact is high (around smelters and where arsenic-based pesticides have been applied heavily), arsenic does not accumulate in plants to toxic levels. Where soil arsenic content is high, growth and crop yields can be decreased. Arsenic has a high chronic toxicity to aquatic life and moderate chronic toxicity to birds and land animals.

The concentration of arsenic found in fish tissue is expected to be somewhat higher than the average concentration of arsenic in the water from which the fish was taken. Fish and shellfish build up organic arsenic in their tissues, but most of the arsenic in fish is not toxic. Mammals, including man, excrete arsenic by depositing it in the dermis (for example, the skin, hair, and nails).

[Sources: Information for parts of the preceding section are from the Environmental Defense Fund website <http://www.scorecard.org/>; National Safety Council; Environmental Health Center website <http://www.nsc.org/>; the EPA website <http://mail.odsnet.com/TRIFacts/>; and USDHHS 1998. Toxicological Profile for Arsenic; ATSDR website <http://atsdr.cdc.gov/>; the National Safety Council, Environmental Health Center website <http://www.nsc.org/>; and the Environmental Defense Fund website <http://www.scorecard.org/>.]

Table B-23. Origins and Physical and Chemical Properties of Arsenic

Arsenic					
Major Sources / Uses	Water	Soils and Sediments	Air	Biota	Other Commonly Released Forms
Physical and Chemical Forms	<ul style="list-style-type: none"> Generally found as dissolved arsenates; some precipitates may be found 	<ul style="list-style-type: none"> Usually found on arsenates adsorbed onto soil 	<ul style="list-style-type: none"> Found only as solid particles 	<ul style="list-style-type: none"> Found in trace concentrations in most biota. Mammals excrete arsenic in hair. 	
	<ul style="list-style-type: none"> Naturally occurring substance Used on lead and other alloys, glass, semiconductors, pesticides, and herbicides Other releases include combustion of coal and tobacco, mining and smelting, manufacturing, and past agricultural use 				

Source: NLM. 2000. Hazardous Substances Databank (HSDB). Downloaded February 4, 2000.

Table B-24. Distribution and Fate of Arsenic

Transport and Media Partitioning (physical distribution)					
Data are for arsenic pentoxide, parent compound of arsenic acid and arsenate salts					
	Water	Soils and Sediments (solid/liquid transfers)	Air		
			Volatility	Gas/Liquid transfers	
Distribution and Fate in the Environment	Water solubility ¹ = 1,500,000 mg/L	Log Koc ² = Not available	Vapor pressure ³ = Not available	KH ⁴ = Not available	BCF ⁵ = 0 to 7
	Solubility varies considerably among compounds. Arsenite compounds are generally less soluble, and less common in the environment than the corresponding arsenates.	Arsenite compounds are generally transformed to arsenates. Arsenates are well adsorbed on hydrous oxides of aluminum and iron.	Except for the reactive gas arsine, arsenic compounds are essentially nonvolatile solids.	Deposition of particulates is the only significant process.	Most plants and animals readily absorb soluble compounds. Biomagnification does not occur.
Transformations and Degradation/Persistence (chemical changes and distribution)					
Only major transformation is arsenite to arsenate in all environments except extremely reducing ones.					
Distribution and Fate in the Environment (continued)	Water	Soils	Sediments	Air	Biota
	Oxidation to arsenate and dissolution occur.	Oxidation to arsenate, adsorption to soils, and dissolution in waste occur.	Oxidation to arsenate, adsorption to sediments, and dissolution in waste occur.	Found only in the particulate (solid) form	Accumulated and excreted, but does not biomagnify

Source: NLM. 2000. Hazardous Substances Databank (HSDB). Downloaded February 4, 2000.

Table B-24. Distribution and Fate of Arsenic (continued)

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures $>10^{-4}$ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures $<10^{-8}$ mm Hg should exist almost entirely in the particulate phase.
- ⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- ⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).

B.13 PHYSICAL AND CHEMICAL PROPERTIES OF CYANIDE

Hydrogen cyanide, HCN, is a colorless or pale blue liquid or gas with a strong, irritating, bitter almond odor. Its boiling point is 25.6 °C. It is miscible and soluble in water. When it is exposed to heat, flame, or oxidizers, a very dangerous fire hazard can occur. Potassium cyanide, KCN, is a white granular powder. Sodium cyanide, NaCN, is a nonflammable, white crystalline powder. Both potassium cyanide and sodium cyanide have a slight, bitter, almond odor (www.glc.org/air/scope/ 1995). Some plants produce toxic cyanide-containing organic compounds, such as amygdalin in almonds and some fruit pits, as well as cyanide itself in cassava (manioc).

Cyanide in Air

The single largest source of cyanide in air is vehicle exhaust. Other sources of release to the air may include emissions from chemical processing industries, steel and iron industries, metallurgical industries, metal plating and finishing industries, and petroleum refineries. Cyanides may also be released from public waste incinerators, from landfills, and during the use of cyanide-containing pesticides. Cyanides are also released in high concentrations when nitrogen-containing plastics, silk, wool, paper, and other materials are burned (ATSDR 1989).

The usual atmospheric form is gaseous hydrogen cyanide. This is relatively stable and can be transported long distances before it is removed by wet deposition.

Cyanide in Soil

Cyanides are generally not persistent when released to water or soil and are not likely to accumulate in aquatic life. They rapidly evaporate and are broken down by microbes. They do not bind to soils and may leach to groundwater. In water and soil, cyanide compounds generally form hydrogen cyanide that goes into the air and remains there for several years (EPA 1998).

The largest sources of cyanide released to soil are primarily from the disposal of cyanide wastes in landfills and the use of cyanide-containing road salts (EPA 1986).

Cyanide in Water

The major sources of cyanide releases to water are publicly owned wastewater treatment works, iron and steel production plants, and metal finishing and organic chemical industries. Much smaller amounts of cyanide may enter water through stormwater runoff in locations where cyanide-containing road salts are used. Groundwater can be contaminated by the movement of cyanide through soil from landfills (ATSDR 1989).

Because hydrogen cyanide is a weak acid, the fate of cyanide depends on pH. However, when the pH is less than 9.2, the cyanide is primarily in the mobile, volatile acid form. Only a higher pH will produce major concentrations of the less volatile salt form.

Cyanide in Plants, Animals, and Food

Cyanides compounds are not accumulated in fish. Cyanide occurs naturally as cyanoglycosides or as the free ion in a variety of fruits, vegetables (such as cassava), and grains. In the United States, only low levels of cyanide are taken in from eating because foods with high cyanide levels are not a major part of the American diet.

Table B-25. Origins and Physical and Chemical Properties of Cyanide

Cyanide					
Major Sources / Uses	<ul style="list-style-type: none"> • Found in some plants (cherries, peaches, apricots, apples, and pears) as cyanoglycosides in the seeds • Product of incomplete combustion of nitrogen-containing material, such as wool, tobacco, and some plastics • Used as chemical intermediates, electroplating, and pesticides. Cyanamides were formerly used as fertilizers. 				
Chemical and Physical Forms	Water	Soils and Sediments	Air	Biota	Other Commonly Released Forms
	Usually found as inorganic salts or as organic cyanides (nitriles). At pH ≤ 9.2, much will volatilize as HCN.	Usually found as inorganic salts. At pH ≤ 9.2, much will volatilize as hydrogen cyanide.	Found as hydrogen cyanide gas	Usually metabolized to thiocyanate and excreted	

Source: NLM. 2000.

Table B-26. Distribution and Transport of Cyanide

Cyanide					
Transport and Media Partitioning (physical distribution)					
Distribution and Fate in the Environment	Water (solid/liquid transfers)	Soils and Sediments (solid/liquid transfers)	Air		Living Organisms (bioaccumulation)
			Volatility	Gas/Liquid transfers	
		Water Solubility ¹ ; Miscible (1,000,000 mL/L)	Log K _{ow} ² ; -0.25	Vapor Pressure ³ ; 630 mm Hg at 20°C	KH ⁴ ; 1.33 x 10 ⁻⁴ atm-m ³ /mol at 25°C
Transformations and Degradation/Persistence (chemical changes and distribution)					
	Water	Soils	Sediments	Air	Biota
	- Half-life: NA	Half-Life: NA	Half-life: NA	Half-life: 1 year	Usually rapidly degraded

Data are for hydrogen cyanide (NLM 2000).

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures >10⁻⁴ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures <10⁻⁸ mm Hg should exist almost entirely in the particulate phase.
- ⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- ⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).

B.14 PHYSICAL AND CHEMICAL PROPERTIES OF HEXACHLOROBENZENE

Hexachlorobenzene (HCB) is a halogenated aromatic hydrocarbon also known as pentachlorophenyl chloride, perchlorobenzene, and perchloryl phenyl. Former trade names of HCB include Anticarie, Bunt-Cure, No Bunt, and Sanocide. HCB exists as either a white, crystalline solid or a clear liquid and is practically insoluble in water. When heated to decomposition, HCB emits toxic fumes of chlorides. HCB is a persistent environmental chemical due to its chemical stability and resistance to biodegradation. A moderate rate of volatilization, as expected from the Henry's law constant value, makes this a significant mechanism of transfer from water, plant, and soil surfaces.

HCB in Air

In the atmosphere, HCB can exist in the vapor phase and in association with particulates. Degradation is very slow (estimated half-life with hydroxyl radicals is 2.6 years). Physical removal of HCB from the atmosphere occurs by both wet and dry deposition, although the compound is hydrophobic and therefore somewhat resistant to wet deposition, unless sorbed to particles. Atmospheric pathways are a major transport mechanism for HCB and can operate over large distances (possibly hemispheres).

HCB in Soil

HCB persists in soils for extended periods of time as indicated by the reported half-life of more than 6 years. This persistence is due to the strong adsorption to soil. HCB generally does not leach to water. Transport to groundwater is slow but varies with the organic makeup of the soil, as HCB tends to bind more strongly to soils with high organic content. Where bioremediation methods are proposed at waste disposal sites to reduce carbon-containing contaminants, the lipid content of remedial bacteria may cause HCB absorbed to soils to repartition to the bacteria and move into groundwater.

HCB in Water

HCB has a moderate vapor pressure and a very low solubility in water. If released to water, HCB will significantly partition from the water column to sediment and suspended matter, and it may build up in bottom sediments. Volatilization from the water column is rapid; however, the strong adsorption to sediment can result in long periods of persistence.

HCB in Plants, Animals, and Food

Bioconcentration and biomagnification of HCB in aquatic species are expected to be important on the basis of a high octanol/water partition coefficient (K_{ow}) value. Biological concentration factor (BCF) values of 16,200 for fathead minnows; 21,900 for green sunfish; and 5,500 for rainbow trout exposed to HCB. Biomagnification of HCB was also reported within aquatic food webs, with catfish (the highest trophic level species) accumulating over 10 times more HCB than the next highest trophic level investigation (snails); snail species accumulated 1.5 to 2 times more HCB than the lowest trophic level species in the food web.

Root crops and other plants (sugar beets, carrots, turnips, wheat, and pasture grass) have been shown to accumulate HCB from the soil. Concentrations of HCB in plants and agricultural crops can be directly transferred to humans by direct consumption and can be indirectly transferred to humans via consumption of dairy products or meat from animals consuming contaminated pasture grass.

Table B-27. Origins and Physical and Chemical Properties of HCB

HC					
HC					
Major Sources / Uses	<ul style="list-style-type: none"> • Currently released to the environment as a by-product from the manufacture and use of chlorinated solvents, pesticides and tires; it is also formed and released from diverse combustion and incineration processes. • Prior to 1985 HCB was used as a fungicide for seeds, although those uses have been voluntarily canceled and it is no longer produced as a pesticide in the United States. However, HCB is known to be a minor contaminant in several currently used pesticides, such as dacthal, picloram, pentachlorophenol, and chlorothalonil. • Long-range transport and subsequent deposition from within the United States and from other continents contribute to the environmental burden in geographically diverse aquatic systems. 				
Chemical and Physical Forms	Water	Soils and Sediments	Air	Biota	Other Commonly Released Forms
	<ul style="list-style-type: none"> • Readily volatilizes from the surface of water and adsorbs to sediments and suspended particulates 	<ul style="list-style-type: none"> • Adsorbs to soil particles and sediments and generally does not leach to water; subject to volatilization at the soil surface 	<ul style="list-style-type: none"> • May undergo slow photolytic degradation or be transported and removed from air via wet and dry deposition 	<ul style="list-style-type: none"> • Primarily found in fatty tissues in humans, wildlife, and aquatic organisms 	

Source for physical and chemical property data: EPA 1993. Revised Draft Lake Michigan Lakewide Management Plan, unless otherwise indicated.

Table B-28. Distribution and Fate of HCB

HC B				
Transport and Media Partitioning (physical distribution)				
<ul style="list-style-type: none"> Volatilization from water to air and sedimentation of adsorbed particulates are the major removal processes from water. HCB will also volatilize from the surface of soil, but it will accumulate and become trapped by overlying sediments. Subject to long-range transport in the atmosphere, with removal by wet and dry deposition 				
Water (solid/liquid transfers)	Soils and Sediments (solid/liquid transfers)	Air		
	Volatility	Gas/Liquid transfers	Living Organisms (bioaccumulation)	
Water Solubility ¹ : 0.0086 mg/L <ul style="list-style-type: none"> Low water solubility enhances volatilization from water 	Log K_{oc} ² : 4.90 Log K_{ow} ³ : 5.50 <ul style="list-style-type: none"> Binds to soils and sediments; volatilizes from surface Soluble in organic solvents, may desorb from resuspended bottom sediments 	Vapor Pressure ³ : 1.23 x 10 ⁻⁵ mm Hg <ul style="list-style-type: none"> Adsorbed particulates will be removed via wet and dry deposition 	KH ⁴ : 5.35 x 10 ⁻⁴ atm m ³ /mol at 25°C (a) <ul style="list-style-type: none"> Partitions between vapor and solid phases 	BCF ⁵ : 106,840 (worm); 24,800 (freshwater algae); 1,254 to 20,000 (trout) <ul style="list-style-type: none"> Retained in body tissue (bioaccumulative) Studies indicate that HCB biomagnifies through the food web (b)
Distribution and Fate in the Environment				
Transformations and Degradation/Persistence (chemical changes and distribution)				
- Chemical and biological degradation are not considered to be important removal processes from water or sediments				
Water	Soils	Sediments	Air	Biota
Half-life: 2.7-6 years (c)	Half-Life: > 6 years (d) <ul style="list-style-type: none"> Aerobic degradation 	Half-life: > 6 years (d) <ul style="list-style-type: none"> Aerobic degradation 	Half-life: 2-6 years (d) <ul style="list-style-type: none"> Degradation by photolysis and photo-oxidation 	<ul style="list-style-type: none"> Additional information needed

(a) EPA, 1993. Revised Draft Lake Michigan Lakewide Management Plan, unless otherwise indicated.
 (b) USDHHS. 1998. Toxicological Profile for Hexachlorobenzene (ATSDR).
 (c) Oliver, B.G., and A.J. Niimi. 1988. Environ. Sci. Technol. Volume 22. Pages 388 to 397.

Table B-28. Distribution and Fate of HCB (continued)

- (d) Mackay and others. 1992. Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume I. Lewis Publishers. Chelsea, Michigan. Howard and others. 1991. Handbook of Environmental Degradation Rates. Ed. H. Taup. Lewis Publishers. Chelsea, Michigan. Mackay and others. 1992.

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures $>10^{-4}$ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures $<10^{-8}$ mm Hg should exist almost entirely in the particulate phase.
- ⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- ⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).

B.15 PHYSICAL AND CHEMICAL PROPERTIES OF TOXAPHENE

Toxaphene, usually found as a solid or gas, is a mixture of more than 175 chlorinated components. These components, produced by the chlorination of camphene (a compound found in turpentine and many essential oils), result in a mixture averaging 67 to 69 percent chlorine by weight.

Because toxaphene is a mixture of polychlorinated camphene derivatives of varying physical and chemical properties and environmental behaviors, the environmental fate of toxaphene is complicated. However, in general, toxaphene is persistent in air, water, soil, and sediment, and is a bioaccumulative substance. It tends to partition to the solid phase in terrestrial and aquatic systems, although loss to the atmosphere via evaporation is also a significant process. Once volatilization has occurred, numerous studies indicate that the atmosphere is the most important environmental medium for toxaphene transport. Information on the environmental fate of toxaphene in various media is summarized below.

Toxaphene in Air

Due to its volatility and persistence, toxaphene is widely distributed in the atmosphere. In addition, it can be transported long distances, as evidenced by the presence of toxaphene in Canadian air masses that had originated in the southern United States (EPA 1997). Atmospheric toxaphene has been observed to exist predominantly in the apparent gas phase (greater than 90 percent) (Hoff and others 1992a), although some may be associated with airborne particulates (USDHHS 1998). In addition, toxaphene concentrations in the air, like many pesticides, tend to vary seasonally, with summer concentrations approximately 4 times higher than winter concentrations (Hoff and others 1992a). Although wet and dry deposition of toxaphene may occur, research indicates that loading of toxaphene by gas exchange may be more than one order of magnitude higher than the input by wet or dry deposition (USDHHS 1998).

Toxaphene in Soil

Toxaphene is relatively immobile in soil, due to its low water solubility and strong absorption. In ordinary conditions, it is relatively stable, with a long half-life. However, biodegradation is faster in anaerobic saline marsh soils and during the summer in inland areas.

Toxaphene in Water

Aquatic toxaphene is strongly sorbed to sediments. No significant hydrolysis and photolysis occur. However, it can be biodegraded in anaerobic sediments and it will volatilize from shallow streams.

Toxaphene in Plants, Animals, and Food

Toxaphene readily bioaccumulates in aquatic organisms, with bioconcentration factors of 3,000 to 33,000 for various fish species. The accumulated toxaphene is mostly in the fatty tissues. No major accumulation is known in plants, but one study reports a bioaccumulation factor of 5 in chickens given dosed feed.

Table B-29. Origins and Physical and Chemical Properties of Toxaphene

Toxaphene					
Major Sources / Uses	<ul style="list-style-type: none"> • Insecticide used to control insect pests on cotton and livestock and biocide used to kill unwanted fish in lakes. • Most United States uses canceled in 1982, with remaining uses canceled in 1990. • Long-range atmospheric transport from environmental reservoirs is an important source of toxaphene in Lake Michigan. 				
Chemical and Physical Forms	Water	Soils and Sediments	Air	Biota	Other Commonly Released Forms
	<ul style="list-style-type: none"> • Primarily bound to water-borne particulates and sediments 	<ul style="list-style-type: none"> • Bound to solid phase 	<ul style="list-style-type: none"> • Exists predominantly in vapor phase (some as air-borne particulates) 	<ul style="list-style-type: none"> • Found in fatty tissue 	<ul style="list-style-type: none"> • Manufactured insecticide containing over 175 congeners (majority contain 6 to 10 chlorines) • Also known as chlorinated camphene, polychlorocamphene, and camphechlor

Source for physical and chemical property data: EPA. 1998. *Great Lakes Binational Toxics Strategy Pesticide Report*, unless otherwise indicated.

Table B-30. Distribution and Fate of Toxaphene

Toxaphene					
Transport and Media Partitioning (physical distribution)					
Distribution and Fate in the Environment	<ul style="list-style-type: none"> • Long-range atmospheric transport and loading via gas absorption is the major pathway of toxaphene in Lake Michigan. • Non-atmospheric sources (for example, tributaries) may also be important in northern Lake Michigan. 				
	Water (solid/liquid transfers)	Soils and Sediments (solid/liquid transfers)	Air		Living Organisms (bioaccumulation)
	Water Solubility ¹ : 3 mg/L at 25C	Log K _{oc} ² : 2.5 - 5.0 Log K _{ow} = 3.3	Volatility	Gas/Liquid transfers	BCF ⁵ : 37,000 to 69,000 (fathead minnow) ⁶ (b)
	• Slightly soluble in water	• Sorbed to solid phase	Vapor Pressure ³ : 5 x 10 ⁻⁶ mm Hg at 20C • Volatile; evaporation from soils to atmosphere is an important transport process	KH ⁴ : 0.005-0.21 atm m ³ /mol at 25 C • Air-water exchange is important transport process	• Lipophilic • Bioconcentrates in fatty tissue

Table B-30. Distribution and Fate of Toxaphene (continued)

Transformations and Degradation/Persistence (chemical changes and distribution)					
Distribution and Fate in the Environment (continued)	Persistent in air, water, soil, and sediment Bioaccumulative				
	Water	Soils	Sediments	Air	Biota
	Half-life: > 200 days <ul style="list-style-type: none"> Resistant to hydrolysis and photolysis Biodegradation occurs relatively rapidly in anaerobic sediments, but not in aerobic sediments or surface waters 	Half-Life: 1 to 14 years <ul style="list-style-type: none"> Persistent under aerobic conditions Biodegradation occurs relatively rapidly under anaerobic conditions (for example, in flooded soils) 	Half-life: information needed <ul style="list-style-type: none"> Biodegradation occurs relatively rapidly in anaerobic sediments 	<ul style="list-style-type: none"> Very resistant to degradation by direct photolysis Degraded (vapor phase) by photochemically produced hydroxyl radicals (half-life: 4 to 5 days) 	<ul style="list-style-type: none"> Bioaccumulative

(a) EPA. 1998. *Great Lakes Binational Toxics Strategy Pesticide Report* unless otherwise indicated.

(b) EPA. 1993. Revised Draft Lake Michigan Lakewide Management Plan.

(c) USDHHS. 1998. Toxicological Profile for Toxaphene.

Footnote Information:

- Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures $>10^{-4}$ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures $<10^{-8}$ mm Hg should exist almost entirely in the particulate phase.
- KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.

Table B-30. Distribution and Fate of Toxaphene (continued)

- ⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).
- ⁶ Fathead minnows are a ubiquitous fish species found in Lake Michigan and are commonly used as a marker species in bioaccumulation and toxicity studies.

B.16 PHYSICAL AND CHEMICAL PROPERTIES OF PAHs

Polynuclear aromatic hydrocarbons (PAH) are the primary products of the incomplete combustion of organic materials. PAHs are principle constituents of soot, automobile and diesel exhaust, creosote (coal tar), tobacco smoke, asphalt, and similar mixtures. Benzo(a)pyrene (B[a]P) is the best-studied of the PAHs and, as far as is known, the most toxic. Its chemical and physical properties are similar to those of other commonly found PAHs. Therefore, B[a]P will be used as a prototype PAH in this discussion.

PAHs in Air

Atmospheric PAH concentrations consist, in great part, of lower molecular weight forms that can account for greater than 90 percent of the total atmospheric load. The balance of the load then is accounted for by the higher molecular weight forms bound to sediment particles. Essentially all PAHs are found in the particulate phase. B[a]P, and many other forms of PAHs are subject to long-range transport, depending on particle size and climactic conditions, which in turn determine the rates of wet and dry deposition. See <http://www.epa.gov/grtlakes/bns/baphcb/stepbap.html> for more information.

Photooxidation of gas phase PAHs caused daytime atmospheric concentrations of PAHs to be 75 percent less than nighttime concentrations, introducing a diurnal fluctuation. Furthermore, atmospheric PAH concentrations exhibit a seasonal fluctuation. According to concentrations observed as part of the Atmospheric Exchange Over Lakes and Oceans (AEOLOS) Project, PAH levels were highest during July and lowest during January. PAH levels are frequently higher during the winter months due to greater fossil fuel combustion for heating.

PAHs in Soil and Sediment

PAHs are found in nearly all soils. They are tightly bound to the soil and sediment particles and have little mobility. It is believed that PAHs in soils are a result of local or long-range air transport and subsequent deposition. Background PAH levels are generally the highest in urban soils and adjoining nearshore sediment due to the presence of large concentrations of anthropogenic activity in the urban corridors. Other, more direct sources of PAHs in soils include sludge disposal from public wastewater treatment plants, automotive exhaust, irrigation with coke oven effluent, leachate from bituminous coal storage sites, and use of contaminated soil compost and fertilizers. Soils directly adjacent to highways are susceptible to contamination from vehicle exhaust and wearing of tires and asphalt. Finally, the soils in or near landfill sites and industrial sites, such as creosote producing, wood-preserving, coking, and former gas manufacturing plants, all have the potential for high PAH levels.

PAHs in surface water sediments are widespread and are the main source of contamination in most surface waters, because PAHs adhere to soil particles and do not easily dissolve in water. In the National Sediment Quality Survey, PAHs were among four contaminants detected the most often at levels with probable adverse human health effects.

PAHs in Water

As stated above, the main source of PAH contamination in surface water is in the sediment. PAHs released to surface waters generally tend to remain in the sediments near their sites of deposition. Therefore, lakes, rivers, estuaries, and coastal environments near industrial or urban centers will contain the greatest amount of PAH contamination.

PAHs in Plants, Animals, and Food

PAHs can accumulate in plants and aquatic and terrestrial organisms. Plants take up PAHs from the soil with their roots or from the air through their foliage. Uptake rates are species-specific, but the biomagnification rates are generally low. Aquatic organisms ingest PAHs through water, sediments, and food, but they are generally able to metabolize PAHs and excrete the by-products. Some aquatic organisms such as molluscs do not metabolize PAHs as readily as other fish and crustaceans. Biomagnification was not observed among increasing trophic level aquatic organisms. Terrestrial animals may ingest PAHs through the food web or by direct soil ingestion, but biomagnification was not observed.

Table B-31. Origins and Physical and Chemical Properties of PAHs

PAHs					
Major Sources / Uses	<ul style="list-style-type: none"> • Product of incomplete combustion of carbon-containing material (such as coal, biomass, forest fires, and natural gas) • Only uses are as a component of coke and similar fuels and of asphalt 				
Chemical and Physical Forms	Water	Soils and Sediments	Air	Biota	Other Commonly Released Forms
	Adsorbed to suspended sediment	Adsorbed, especially in organic carbon	On particulates, especially those from combustion	Metabolized in mammals to more toxic forms	

Source: NLM. 2000.

Table B-32. Distribution and Fate of PAHs

Transport and Media Partitioning (physical distribution)				
<ul style="list-style-type: none"> • Soils and sediments are the primary sink. • Also subject to long-range transport as particulates in the atmosphere, with removal by wet and dry deposition. • All figures below given for B(a)P, a commonly regulated form of PAH. 				
Water (solid/liquid transfers)	Soils and Sediments (solid/liquid transfers)	Air		Living Organisms (bioaccumulation)
	Volatility	Gas/Liquid transfers		
Water Solubility ¹ : 0.0019 mg/L <ul style="list-style-type: none"> • Low water solubility 	Log K_{ow} ² : 6.13 <ul style="list-style-type: none"> • Immobile in soils • Removal from water column by sedimentation 	Vapor Pressure ³ : 4.89x10 ⁻⁹ mm Hg at 20 °C	KH ⁴ : 8.36 x 10 ⁻⁷ atm- m ³ /mol <ul style="list-style-type: none"> • Air deposition is important source to surface waters. 	BCF ⁵ : 10 to 10,000 <ul style="list-style-type: none"> • Biomagnification is not significant in plants and aquatic or terrestrial organisms.
Transformations and Degradation/Persistence (chemical changes and distribution)				
Water	Soils	Sediments	Air	Biota
Half-life: NA	Half-Life: 1 to 8 years	Half-life: 12 to 300 weeks	Residence time: NA	NA

Note: All information from ATSDR 1995 unless otherwise noted.

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures >10⁻⁴ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures <10⁻⁸ mm Hg should exist almost entirely in the particulate phase.

Table B-32. Distribution and Fate of PAHs (continued)

⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.

B.17 PHYSICAL AND CHEMICAL PROPERTIES OF ATRAZINE

The chemical structure of atrazine with its triazine nucleus, two amine groups, and single chloro group, is very different from the organochlorine pesticides (such as aldrin, DDT, and toxaphene) and similar compounds (PCBs, dioxins, and furans). Atrazine's structure leads to different physical properties, such as relatively high water solubility and distinct patterns of partitioning among phases.

In recent years, atrazine has been the most heavily used pesticide in the United States. The primary usage is as a pre- and early post-emergence herbicide for corn, pastures, trees, and non-crop areas.

Atrazine in Air

Atrazine exists in both the vapor and particulate phases. The vapor part will be degraded rapidly by photochemically-produced hydroxyl radicals. In contrast, particulate atrazine is quite stable and will remain until removed by wet or dry deposition. Long-range atmospheric transport is known to occur, and atrazine has been detected hundreds of kilometers from the nearest site of use.

Atrazine in Soil

Atrazine has a wide range of mobility in soil, depending on the soil characteristics. Volatility is negligible, but the atrazine is susceptible to dissolution and leaching. The extent of the dissolution depends on the soil particle size and organic content.

Atrazine will biodegrade, especially in moist soils. However, chemical degradation, primarily hydrolysis, is a more important process. The rate of hydrolysis is minimal in neutral conditions but increases rapidly under both acidic and basic conditions. Laboratory studies using only variations on pH have produced hydrolysis half-lives ranging from hours to centuries. Low moisture, high clay content, and high organic matter content also increase hydrolysis rates. Photolysis can occur in surface soils, but is rarely significant.

Atrazine in Water

The high solubility and low vapor pressure of atrazine result in no volatilization from water. Some atrazine, but not all, is adsorbed on sediments. There is minimal potential for biodegradation, so chemical degradation is more important. The primary process is the same acid- and base-catalyzed hydrolysis discussed for soil.

Atrazine in Plants, Animals, and Food

Little bioaccumulation and no biomagnification occur with atrazine. In fact, many measured bioconcentration factors are less than 1. Some uptake into plants does occur, so atrazine has been detected, at quite low concentrations, in market-basket food analyses. Corn and some other plants can completely metabolize atrazine.

Table B-33. Origins and Physical and Chemical Properties of Atrazine

Atrazine					
Major Sources / Uses	<ul style="list-style-type: none"> Released into the environment via effluents at manufacturing sites and at points of application where it is employed as a herbicide 				
Chemical and Physical Forms	Water	Soils and Sediments	Air	Biota	Other Commonly Released Forms
	<ul style="list-style-type: none"> Not expected to adsorb strongly to sediments Volatilization is not environmentally important 	<ul style="list-style-type: none"> Moderately to highly mobile in soils with low clay or organic matter content 	<ul style="list-style-type: none"> Initially found in both vapor and gas phases, but vapor phase is rapidly degraded 	<ul style="list-style-type: none"> Absorbed mainly through plant roots, but also foliage, and it accumulates in new leaves 	<ul style="list-style-type: none"> Irritating hydrogen chloride and toxic oxides of nitrogen may be formed upon combustion

Source for physical and chemical property data: EPA. 1993. Revised Draft Lake Michigan Lakewide Management Plan, unless otherwise indicated.

Table B-34. Distribution and Fate of Atrazine

Atrazine					
Transport and Media Partitioning (physical distribution)					
Despite its mild solubility in water, atrazine has a high potential for groundwater contamination					
Distribution and Fate in the Environment	Water (solid/liquid transfers)	Soils and Sediments (solid/liquid transfers)	Air		Living Organisms (bioaccumulation)
	Water Solubility ¹ : 30 mg/L	Log K_{ow} ² : 2.61 Log K_{oc} : 1.7 to 3.1 (measured)	Volatility	Gas/Liquid transfers	
• Moderately soluble in water	• High potential for groundwater contamination	Vapor Pressure ³ : 2.78×10^{-7} mm Hg at 25 °C	KH ⁴ : 2.63×10^9 atm m ³ mol ⁻¹	log BCF ⁵ : -0.1 to 0.3 (fathead minnow); 0.5 (whitefish)	• Not expected to bioconcentrate

Table B-34. Distribution and Fate of Atrazine (continued)

Transformations and Degradation/Persistence (chemical changes and distribution)				
Chemical hydrolysis, followed by biodegradation, may be the most important removal route in soils and aquatic environments.				
Water	Soils	Sediments	Air	Biota
<p>Half-life: varies depending upon conditions (such as, pH, organic carbon content)</p> <p>Hydrolyzes rapidly under acidic or basic conditions but slowly at neutral pH</p>	<p>Half-Life: 60 to >100 days (longer in cold or dry conditions)</p> <p>Highly persistent in soil</p> <p>May hydrolyze in either acidic or basic soils yet is fairly resistant to hydrolysis at neutral pH; addition of organic material increases the rate of hydrolysis</p>	<p>Half-life: <i>additional information needed</i></p>	<p>Atmospheric half-life: 2.6 hour at an atmospheric concentration of 5×10^5 hydroxyl radicals/cm³</p> <p>Reactions with photochemically produced hydroxyl radicals in the atmosphere may be important.</p>	<p>In plant species, atrazine increases arsenic uptake. May also inhibit photosynthesis or be metabolized.</p>
<p>Distribution and Fate in the Environment (continued)</p>				

- (a) EPA. 1993. Revised Draft Lake Michigan Lakewide Management Plan unless otherwise indicated
- (b) USDHHS. 1997. Toxicological Profile for Atrazine

Footnote Information:

- ¹ Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- ² Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- ³ Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures $>10^{-4}$ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures $<10^{-8}$ mm Hg should exist almost entirely in the particulate phase.
- ⁴ KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.

Table B-34. Distribution and Fate of Atrazine (continued)

⁵ BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).

B.18 PHYSICAL AND CHEMICAL PROPERTIES OF SELENIUM

In nature, selenium is found in the -2 (selenide), 0 (selenium), +4 (selenite), and +6 (selenate) oxidation states. Selenium has sorptive affinity for hydrous metal oxides, clays, and organic materials. Speciation is determined by pH and potential of the solution. Elemental selenium is favored by low pH and reducing conditions. Selenium chemistry is similar to sulfur chemistry. Natural selenite is usually a component of sulfide minerals.

Selenium in Air

Selenium is present in coal and fuel oil and is emitted in flue gas and fly ash during combustion. When released to the atmosphere, selenium is expected to exist predominantly in the particulate phase. Particulate-phase selenium is physically removed from the atmosphere by wet and dry deposition.

Selenium in Soil and Sediment

In soils, the behavior of selenium is affected by oxidation-reduction conditions, pH, hydrous oxide content, clay content, organic materials, and the presence of competing anions. In sediments, reduced and tightly bound selenium will remain relatively immobile unless the sediments are chemically or biologically oxidized (TOXNET 1999).

Selenium in Water

Selenium occurs in water as a result of the natural weathering of soils and rocks and from the mining and smelting of certain ores. When released into water, selenium is expected to form oxyanions and exhibit anionic chemistry. Selenium and its compounds have water solubilities ranging from low to moderate. Concentrations up to 1,000 milligrams will mix with a liter of water. Selenium is highly persistent in water, with a half-life greater than 200 days (EPA 1986).

Selenium in Plants, Animals, and Food

Trace amounts of selenium are essential for plants and animals. Plants easily take up selenate compounds from water and change them to organic selenium compounds such as selenomethionine. The toxicity of selenium depends on whether it is in the biologically active oxidized form, such as occurs in alkaline soils. These conditions can increase plant uptake of the metal. Plants grown in soils that contain high levels of selenium and selenium compounds can accumulate selenium and may be toxic to grazing livestock (1997). However, such plants are usually found only in semi-arid to arid alkaline soils, so they are not relevant to the Great Lakes area.

Selenium can collect in animals that live in water containing high levels of it. The concentration of selenium found in fish tissues is expected to be somewhat higher than the average concentration of selenium in the water from which the fish were taken (ATSDR 1997).

Table B-35. Origins and Physical and Chemical Properties of Selenium

Selenium					
Major Sources / Uses	<ul style="list-style-type: none"> Widely found in sulfide ores and fossil fuels and is released during smelting, burning, and similar operations. Uses include in photoelectric cells, in semiconductors, in ceramics, in pigments, as an insecticide, as a topical drug, and as a feed additive. 				
Physical and Chemical Forms	Water	Soils and Sediments	Air	Biota	Other Commonly Released Forms
	Generally found as selenite ion. Other oxidation states may occur.	Found as insoluble heavy metal selenides or as soluble alkali selenites and selenates.	Most found in particulate form. Selenium dioxide (from fuel combustion) is reduced to elemental selenium.	Some bioorganisms will convert to dimethyl selenide, a gas. Higher organisms treat it like sulfur.	The varied chemistry of selenium compounds controls its partitioning among media.

Source: NLM. 2000.

Table B-36. Distribution and Fate of Selenium

Transport and Media Partitioning (physical distribution)				
Data are given for selenium dioxide, parent of selenious acid and the selenites. Other known environmental forms include all the common oxidation states, including gases and solids				
Distribution and Fate in the Environment	Water	Soils and Sediments (solid/liquid transfers)	Air	
			Volatility	Gas/Liquid transfers
	Water soluble ¹ = 4,000,000 g/L	Log Koc ² = NA	Vapor presence ³ = NA Sublimes at 340 to 350 °C	KH ⁴ = NA
	Most common compounds are relatively soluble in water.	Except for insoluble heavy metal selenides, it is highly mobile due to its water solubility, and for dimethyl selenide, its volatility.	Most compounds are nonvolatile, but some oxides and organic species are gases.	Depends on chemical form
				BCF ⁵ = NA
				Some plants bioaccumulate, creating highly toxic forage.

Table B-36. Distribution and Fate of Selenium (continued)

Distribution and Fate in the Environment (continued)	Transformations and Degradation/Persistence (chemical changes and distribution)				
	Water	Soils	Sediments	Air	Biota
	Half-life = NA	Half-life = NA	Half-life = NA	Half-life = NA	Half-life = NA

Source for physical and chemical property data: NLM. 2000.

Footnote Information:

- 1 Water Solubility: the maximum concentration of a chemical that dissolves in pure water.
- 2 Log K_{oc} (Organic Carbon Partitioning Coefficient) or Log K_{ow} (Octanol-water partition coefficient): both measure a material's tendency to adsorb to soil/organic matter/sediment. High K_{oc} values indicate a tendency for the material to be adsorbed by the solid phase rather than remain dissolved in solution. Strongly adsorbed molecules will not leach or move unless the soil particle to which they are adsorbed moves (as in erosion). K_{oc} values <500 indicate little or no adsorption and a potential for leaching.
- 3 Vapor Pressure: a measure of volatility. Organic compounds with vapor pressures $>10^{-4}$ mm Hg should exist almost entirely in the vapor phase in the atmosphere, while organic compounds with vapor pressures $<10^{-8}$ mm Hg should exist almost entirely in the particulate phase.
- 4 KH (Henry's Gas Law Coefficient): reflects the physical solubility of a given gas. Defined as the ratio of the aqueous phase concentration of a chemical in moles per liter (mol/L) to the partial pressure of the substance in the gas phase in atmospheres (atm). Soluble gases have large Henry's law coefficients. When considering the behavior of atmospheric gases in equilibrium with large natural bodies such as lakes, Henry's law is generally accepted as a good approximation.
- 5 BCF (Bioconcentration Factor): A measure of the tendency for a chemical to accumulate in tissues of an organism (such as fish) to levels that are greater than that in the medium (such as water). Defined as the ratio of the concentration of the substance in the living organism in milligrams per kilogram (mg/kg) to the concentration of the substance in the surrounding environment in milligrams per liter (mg/L).