

5. POTENTIAL FOR HUMAN EXPOSURE

5.1 OVERVIEW

There are no known natural sources of hexachlorobutadiene which contribute to environmental levels. The main source of hexachlorobutadiene in the United States is its production as a by-product of chlorinated hydrocarbon synthesis. An estimated 100,000 pounds of this by-product are released to the environment each year. The majority of hexachlorobutadiene-containing waste is disposed of by incineration, with lesser amounts disposed by deep well injection and landfill.

Literature data regarding the fate and transport of hexachlorobutadiene are limited. Much of the available information consists of modeling based on the physical and chemical properties of hexachlorobutadiene, and the monitoring data. These data indicate that hexachlorobutadiene will bind to soil particles and sediments, and is found in air and water bound to particulates. Some volatilization of hexachlorobutadiene from surface waters and soils may also occur. The bioconcentration of hexachlorobutadiene has been reported in fish and shellfish with considerable variability between species (EPA 1976; Oliver and Niimi 1983; Pearson and McConnell 1975).

Data regarding the transformation and degradation of hexachlorobutadiene are limited. Much of the available information consists of modeling based on the monitoring data and by analogy to structurally similar compounds. Hexachlorobutadiene may react with reactive oxygen species in air for which the half-life has been estimated to range from months to years. Under aerobic conditions, but not anaerobic conditions, hexachlorobutadiene undergoes complete biodegradation in water. The observations in water are believed to hold true for soils as well.

Low levels of hexachlorobutadiene can be detected in air, water, and sediment. Atmospheric levels of hexachlorobutadiene in rural and urban air samples typically range from 2 to 11 ppt, with a mean value of 2-3 ppt. Higher levels can be detected at areas near industrial and chemical waste disposal sites and production sites. Hexachlorobutadiene is infrequently detected in ambient waters, but has been detected in drinking water at levels of 2-3 ppt. Sediments contain higher levels of hexachlorobutadiene than the waters from which they were obtained. Foodstuffs generally do not

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contain detectable levels of hexachlorobutadiene, with the exception of fish, in which concentrations of 0.1-4.7 mg/kg have been reported.

Hexachlorobutadiene has been detected in human adipose tissue and blood samples. These data indicate that exposure to hexachlorobutadiene does occur in humans, however route-specific estimates of hexachlorobutadiene exposure were not located. Based on monitoring data, individuals who work in hexachlorobutadiene-producing facilities, live at or near hazardous waste facilities, or consume large amounts of hexachlorobutadiene-contaminated fish may have above-average exposures to hexachlorobutadiene.

Hexachlorobutadiene has been identified in at least 45 of the 1,350 hazardous waste sites that have been proposed for inclusion on the EPA National Priorities List (NPL) (HazDat 1993). However, the number of sites evaluated for hexachlorobutadiene is not known. The frequency of these sites within the United States can be seen in Figure 5-1.

5.2 RELEASES TO THE ENVIRONMENT

5.2.1 Air

There are no known natural sources of hexachlorobutadiene which contribute to environmental levels. The predominant source of hexachlorobutadiene is inadvertent production from the synthesis of certain chlorinated hydrocarbons (EPA 1982b). In 1975, the production of hexachlorobutadiene in the United States was estimated to be 8 million pounds, with 0.1 million pounds released to the environment (NSF 1975). Sixty-eight percent of the 27 million pounds of hexachlorobutadiene waste generated in the United States in 1982 was disposed of by incineration. This process typically obtains a 99.99% destruction efficiency, indicating that approximately 1,900 pounds were released to the atmosphere. According to TRI90 (1992), an estimated total of 4,906 pounds (2.2 metric tons) of hexachlorobutadiene, amounting to 82% of the total environmental release, was discharged to the air from manufacturing and processing facilities in the United States in 1990 (see Table 5-1). The TRI data should be used with caution since only certain types of facilities are required to report. This is not an exhaustive list.

TABLE 5-1. Releases to the Environment from Facilities
that Manufacture or Process Hexachlorobutadiene^a

Facility	Location ^b	Reported amounts released in pounds						
		Air	Underground injection	Water	Land	Total environment ^c	POTW ^d transfer	Off-site waste transfer
DOW CHEMICAL CO.	PITTSBURG, CA	0	0	0	0	0	0	0
VULCAN CHEMICALS	WICHITA, KS	49	330	0	0	379	0	8
VULCAN MATERIALS CO. CHEMICALSDIV. GEISMAR FACILITY	GEISMAR, LA	842	0	10	0	852	0	295
DOW CHEMICAL CO. LOUISIANA DIV.	PLAQUEMINE, LA	51	0	0	0	51	0	0
PPG INDUSTRIES INC.	WESTLAKE, LA	3,345	0	705	0	4,050	0	73,022
MALLINCKRODT SPECIALTY CHEMICALS CO.	SAINT LOUIS, MO	550	0	0	0	550	940	7,000
OCCIDENTAL CHEMICAL CORP. NIAGARA PLANT	NIAGARA FALLS, NY	25	0	0	0	25	18	20
DOW CHEMICAL CO. TEXAS OPERATIONS	FREEPORT, TX	44	0	0	0	44	0	4,000

^aDerived from TRI90 (1992)

^bPost Office state abbreviations

^cThe sum of all releases of the chemical to air, land, water, and underground injection wells by a given facility.

^dPOTW = publicly owned treatment works

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5.2.2 Water

Hexachlorobutadiene may be released to underground and surface waters through discharge from industrial facilities, by leaching from industrial discharges, by leaching from landfills or soils, or by urban runoff. Hexachlorobutadiene was detectable in 1.6% of 1,190 industrial effluent samples reported in the EPA Storage and Retrieval (STORET) database (Staples et al. 1985). The median concentration for all samples, including nondetects was < 6 ppb. This chemical was also detected in leachate from an industrial landfill at a concentration of 0.109 ppm (Brown and Donnelly 1988) and from a hazardous waste site (Hauser and Bromberg 1982). In 1982, of the 27 million pounds of hexachlorobutadiene waste produced in the United States as a by-product of chlorinated hydrocarbon production, 9 million pounds was disposed of by deep well injection (EPA 1982b). According to TR190 (1992), an estimated total of 715 pounds (0.3 metric tons) of hexachlorobutadiene, amounting to 12% of the total environmental release, was discharged to the water from manufacturing and processing facilities in the United States in 1990 and 330 pounds (about 6%) was disposed of by underground injection (see Table 5-1).

5.2.3 Soil

Hexachlorobutadiene may be released to soil by disposal of wastes in landfill operations. In 1982, only 0.2% of the 27 million pounds of hexachlorobutadiene waste produced as a by-product of chlorinated hydrocarbon-synthesis was disposed of in landfill operations (EPA 1982b). These data indicate that the release to soil was approximately 54,000 pounds. According to TR190 (1992), no hexachlorobutadiene was discharged to the soil from manufacturing and processing facilities in the United States in 1990 (see Table 5-1). The TRI data should be used with caution since only certain types of facilities are required to report. This is not an exhaustive list.

5.3 ENVIRONMENTAL FATE

5.3.1 Transport and Partitioning

Hexachlorobutadiene can exist in the atmosphere as a vapor or adsorbed to airborne particulate matter. The atmospheric burden of hexachlorobutadiene has been estimated to be 3.2 and 1.3 million kg/year for the northern and southern hemispheres, respectively (Class and Balls&miter 1987).

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Significant dispersion of hexachlorobutadiene has been confirmed by the detection of hexachlorobutadiene at areas which are far removed from release sources (Class and Balls&miter 1987). A high partition coefficient ($\log K_{oc}$) value of 3.67 (Montgomery and Welkom 1990) for hexachlorobutadiene indicates that adsorption to soils with high organic carbon content can occur. Wind erosion of contaminated surface soils can then lead to airborne hexachlorobutadiene-containing particulate matter. Levels of hexachlorobutadiene have been detected in fly ash from the incineration of hexachlorobutadiene-containing hazardous waste (Junk and Ford 1980). The transport of particulate matter is a function of particle size and wind speed, however no data were located regarding the transport of hexachlorobutadiene-containing particles in air.

Transport and partitioning of hexachlorobutadiene in water involves volatilization to the atmosphere and sorption to soil and sediments particulates. The high partition coefficient ($\log K_{ow}$) of 4.78 (Montgomery and Welkom 1990) for hexachlorobutadiene leads to preferential partitioning to sediments and biota over water. Environmental surveys generally report higher levels of hexachlorobutadiene in sediments than in the waters that contain them (Elder et al. 1981; EPA 1976; Oliver and Charlton 1984). Hexachlorobutadiene has a vapor pressure of 0.15 mmHg (25°C) (Montgomery and Welkom 1990), indicating that volatilization from water occurs. Volatilization is reduced by adsorption to organic material in the water.

The transport and partitioning of hexachlorobutadiene in soils involve volatilization and adsorption. An estimated high partition coefficient ($\log K_{oc}$) of 3.67 (Montgomery and Welkom 1990) for hexachlorobutadiene in soil indicates that soil adsorption can occur, particularly in soils with a high organic carbon content. Sorption was the predominant fate process for hexachlorobutadiene during anaerobic digestion of sludges (Govind et al. 1991). Data indicate that hexachlorobutadiene is mobile in sandy soils which have relatively low organic-carbon contents (Piet and Zoeteman 1980). Volatilization from surface soils is relatively low; binding to the organic carbon content of the soil further reduces hexachlorobutadiene release.

In rainbow trout the bioconcentration factor (BCF) was dependent on water concentration (Oliver and Niimi 1983). At low concentrations of 0.10 ng/L a BCF of 5,800 was obtained, compared to a value of 17,000 obtained with higher water concentrations of 3.4 ng/L. Hexachlorobutadiene preferentially accumulates in the liver of fish (Pearson and McConnell 1975). In mussels, the BCF was determined to be between 900 and 2,000 (Pearson and McConnell 1975). However, lower values were obtained

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for algae, crayfish, and bass (160, 60, and 29, respectively) (EPA 1976). The EPA is reviewing new BCF data and has recommended a value of 392 (EPA 1989a).

5.3.2 Transformation and Degradation

5.3.2.1 Air

No data were located regarding the transformation and degradation of hexachlorobutadiene in air. Based on the monitoring data, the tropospheric half-life of hexachlorobutadiene was estimated by one author to be 1.6 years in the northern hemisphere (Class and Ballschmiter 1987). However, analogy to structurally similar compounds such as tetrachloroethylene indicates that the half-life of hexachlorobutadiene may be as short as 60 days, predominantly due to reactions with photochemically produced hydroxyl radicals and ozone (Atkinson 1987; Atkinson and Carter 1984). Oxidation constants of $< 10^3$ and $6 \text{ (m}^3 \text{ hr)}^{-1}$ were estimated for reactions with singlet oxygen and peroxy radicals, respectively (Mabey et al. 1982).

5.3.2.2 Water

Data concerning the transformation and degradation of hexachlorobutadiene in waters are limited. Under aerobic conditions, hexachlorobutadiene underwent complete biodegradation after 7 days in water inoculated with domestic sewage (Tabak et al. 1981). Biodegradation of hexachlorobutadiene also occurred during anaerobic digestion of wastewater sludges, although sorption was the predominant fate process (Govind et al. 1991). However, biodegradation did not occur in anaerobic waters (Johnson and Young 1983). Based on monitoring data, the half-life of hexachlorobutadiene in rivers and lakes was estimated to be 3-30 days and 30-300 days, respectively (Zoeteman et al. 1980). Data regarding the hydrolysis or photolysis of hexachlorobutadiene in water were not located.

5.3.2.3 Sediment and Soil

Data regarding the transformation and degradation of hexachlorobutadiene in soil were not located. However, based on the observation that hexachlorobutadiene was completely biodegraded in water under aerobic conditions (Tabak et al. 1981), biodegradation probably occurs in nonarid soils as well.

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5.4 LEVELS MONITORED OR ESTIMATED IN THE ENVIRONMENT

5.4.1 Air

In the United States, the reported average concentration of hexachlorobutadiene, based on 72 samples from urban and source dominated areas, was 36 ppt ($0.38 \mu\text{g}/\text{m}^3$) (Shah and Heyerdahl 1988; Shah and Singh 1988). Hexachlorobutadiene levels ranging from 2 to 11 ppt were reported in a number of cities (Pellizzari 1978; Singh et al. 1980; Singh et al. 1982). Higher levels of hexachlorobutadiene were reported in Niagara Falls, with concentrations of up to 37 ppt detected in ambient air levels and up to 38 ppt detected in the basement air of homes near industrial and chemical waste disposal sites (Pellizzari 1982).

Occupational exposures can be significantly higher for individuals who work at plants that produce chlorinated hydrocarbons. Maximum air levels off plant property, at a plant boundary, and within a plant were reported to be 22 ppt, 938 ppt, and 43,000 ppt, respectively (Li et al. 1976).

5.4.2 Water

Hexachlorobutadiene has been detected in some surface waters but the incidence of detection is low. It was detected in 0.2% of 593 ambient water samples in the STORET database with a median level for all samples of less than 10 ppb (Staples et al. 1985). Hexachlorobutadiene was detected in 1 of 204 surface water sites sampled across the United States with a concentration of 22 ppb (Ewing et al. 1977). Low levels of hexachlorobutadiene were detected in the Niagara River at 0.82 ppt (Oliver and Charlton 1984). Hexachlorobutadiene was not detected in rainwater (Pankow et al. 1984) or urban storm water runoff (Cole et al. 1984) in a number of U.S. cities. It has not been detected in open ocean waters; however, the coastal waters of the Gulf of Mexico were reported to contain 3-15 ppt (Sauer 1981).

Low levels of hexachlorobutadiene (less than 1 ppb) may be found in drinking water (EPA 1989a). Finished drinking water samples from two U.S. cities were found to contain 1.6 ppt and 2.7 ppt, respectively (Lucas 1984). Hexachlorobutadiene was also detected in groundwater at 6 of 479 waste disposal sites in the United States (Plumb 1991).

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5.4.3 Sediment and Soil

Hexachlorobutadiene adsorbs to sediments in contaminated water. Sediments from the Niagara River were found to contain 2.9-11 $\mu\text{g}/\text{kg}$ (Oliver and Charlton 1984). Sediments from the Great Lakes were reported to contain levels of hexachlorobutadiene typically ranging from 0.08 to 120 $\mu\text{g}/\text{kg}$ (Fox et al. 1983; Oliver and Bourbonniere 1985; Oliver and Charlton 1984). Data regarding the levels of hexachlorobutadiene in soils were not located. Hexachlorobutadiene was not detectable in any of 196 sediment samples reported on the STORET database (Staples et al. 1985). The median detection limit was < 500 ppb.

5.4.4 Other Environmental Media

Hexachlorobutadiene was detected in several foodstuffs in the United Kingdom (McConnell et al. 1975) and Germany (Kotzias et al. 1975), but it was not detected in the United States in milk, eggs, or vegetables even when the samples were obtained from within a 25-mile radius of facilities producing chlorinated hydrocarbons (Yip 1976; Yurawecz et al. 1976). Fish samples from the Mississippi River were found to contain hexachlorobutadiene levels ranging from 0.1 to 4.7 mg/kg (Laska et al. 1976; Yip 1976; Yurawecz et al. 1976). Fish from the Great Lakes generally did not contain detectable levels of hexachlorobutadiene (Camanzo et al. 1987; DeVault 1985) with the exception of trouts from Lake Ontario, which were reported to contain 0.06-0.3 mg/kg (Oliver and Niimi 1983). Hexachlorobutadiene was not detectable in any of 51 biota samples reported on the STORET database (Staples et al. 1985).

Hexachlorobutadiene was not detected in sewage influents (Levins et al. 1979) or in sewage samples (EPA 1990g).

5.5 GENERAL POPULATION AND OCCUPATIONAL EXPOSURE

The general population can be exposed to low levels of hexachlorobutadiene in air, food, and water. Estimates of source or route-specific exposures to humans were not located. Hexachlorobutadiene has been detected in human adipose tissue with a concentration ranging from 0.8 to 8 $\mu\text{g}/\text{kg}$ wet weight (McConnell et al. 1975; Mes et al. 1982). Higher concentrations were reported in human liver samples with values ranging from 5.7 to 13.7 $\mu\text{g}/\text{kg}$ wet weight (McConnell et al. 1975). These data

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indicate that exposure to hexachlorobutadiene occurs in humans, but do not identify sources or routes of exposure. Although exposure from foods *is* probably a minor route of exposure, people who consume large amounts of fish obtained from contaminated waters may be exposed to significant quantities of hexachlorobutadiene. Similarly, persons who live in source-dominated areas or work in plants that produce chlorinated hydrocarbons may be exposed to significant levels of hexachlorobutadiene in the air. No information was found on the number of workers potentially exposed to hexachlorobutadiene.

5.6 POPULATIONS WITH POTENTIALLY HIGH EXPOSURES

People who live in source-dominated areas (at or near hazardous waste sites or chlorinated hydrocarbon production plants) and workers in these areas are potentially exposed to high levels of hexachlorobutadiene. Individuals who consume large amounts of fish from contaminated waters may also be exposed to above-average levels of hexachlorobutadiene.

5.7 ADEQUACY OF THE DATABASE

Section 104(i)(5) of CERCLA, as amended, directs the Administrator of ATSDR (in consultation with the Administrator of EPA and agencies and programs of the Public Health Service) to assess whether adequate information on the health effects of hexachlorobutadiene is available. Where adequate information is not available, ATSDR, in conjunction with the NTP, is required to assure the initiation of a program of research designed to determine the health effects (and techniques for developing methods to determine such health effects) of hexachlorobutadiene.

The following categories of possible data needs have been identified by a joint team of scientists from ATSDR, NTP, and EPA. They are defined as substance-specific informational needs that if met would reduce the uncertainties of human health assessment. This definition should not be interpreted to mean that all data needs discussed in this section must be filled. In the future, the identified data needs will be evaluated and prioritized, and a substance-specific research agenda will be proposed.

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5.7.1 Identification of Data Needs

Physical and Chemical Properties. The physical and chemical properties of hexachlorobutadiene are sufficient to make estimations on its fate in the environment. No data regarding the odor threshold of hexachlorobutadiene in water were located.

Production, Import/Export, Use, Release, and Disposal. Hexachlorobutadiene is not produced for commercial purposes in the United States, however small amounts are imported from Germany. Hexachlorobutadiene is mainly produced as a by-product of chlorinated hydrocarbon synthesis and is a primary component of "hex-wastes" (EPA 1982b). Its uses as a pesticide and fumigant have been discontinued. Hexachlorobutadiene is disposed chiefly by incineration, and to a lesser extent by deep well injection and landfill operations (EPA 1982b). More recent production and release data would be helpful in estimating human exposure to hexachlorobutadiene.

According to the Emergency Planning and Community Right-to-Know Act of 1986, 42 U.S.C. Section 11023, industries are required to submit chemical release and off-site transfer information to the EPA. The Toxics Release Inventory (TRI), which contains this information for 1990, became available in May of 1992. This database will be updated yearly and should provide a list of industrial production facilities and emissions.

Environmental Fate. Much of the environmental fate information on hexachlorobutadiene consists of modeling based on its physical and chemical properties and its similarity to related compounds. Further studies which determine the extent to which hexachlorobutadiene volatilizes from surface waters and soils, and the effects of organic-carbon content on this process would be helpful. Studies which experimentally determine the specific reactions and rates which drive the degradation of hexachlorobutadiene in air, water, and soil would be valuable. Data are lacking on hexachlorobutadiene adsorption to soil or its biodegradation in this medium. More information on the fate of the compound in soil would be useful since this medium may be a pathway of exposure for populations living near emission sources.

Bioavailability from Environmental Media. Toxicity studies in animals indicate that absorption of hexachlorobutadiene through the gastrointestinal tract, respiratory tract, and skin can occur. Studies

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which identify the relationship between absorption and the matrix of soils, sediments, and foods would be useful in establishing whether or not absorption is significantly affected by such factors.

Food Chain Bioaccumulation. Bioconcentration factors have been determined for algae, shellfish, and fish and exhibit a wide range (29-17,000) (EPA 1976; Oliver and Niimi 1983; Pearson and McConnell 1975). This wide range may be explained in part by species differences in metabolism or differences in concentrations tested. Studies also indicate that hexachlorobutadiene preferentially accumulates in the livers of fish. Further studies which might explain the wide range of BCF values would be helpful. No information was located regarding the bioaccumulation of hexachlorobutadiene in plants or aquatic organisms. More information is needed to determine the importance of terrestrial/aquatic food chain bioaccumulation as a potential human exposure pathway.

Exposure Levels in Environmental Media. Data are available on the occurrence of hexachlorobutadiene in air, water, and foodstuff. The majority of the monitoring data on hexachlorobutadiene are outdated and therefore more recent information on the levels typically found in the environment would allow for more accurate estimation of human exposures, and could also serve to indicate time-dependent trends when compared with older data. No data were located regarding the occurrence of hexachlorobutadiene in groundwater or soil.

Reliable monitoring data for the levels of hexachlorobutadiene in contaminated media at hazardous waste sites are needed so that the information obtained on levels of hexachlorobutadiene in the environment can be used in combination with the known body burden of hexachlorobutadiene to assess the potential risk of adverse health effects in populations living in the vicinity of hazardous waste sites.

Exposure Levels in Humans. Hexachlorobutadiene has been detected in human adipose tissues and blood (Bristol et al. 1982; Mes et al. 1985). Studies which establish a correlation between exposure levels in environmental media and the resulting levels in human tissues and excreta would be valuable in predicting exposures and corresponding health risks in humans who live at or near hazardous waste sites and who are likely to be exposed to hexachlorobutadiene.

This information is necessary for assessing the need to conduct health studies on these populations.

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Exposure Registries. No exposure registries for hexachlorobutadiene were located. This substance is not currently one of the compounds for which a subregistry has been established in the National Exposure Registry. The substance will be considered in the future when chemical selection is made for subregistries to be established. The information that is amassed in the National Exposure Registry facilitates the epidemiological research needed to assess adverse health outcomes that may be related to exposure to this substance.

5.7.2 On-going Studies

No on-going studies were located regarding the environmental fate or potential for human exposure to hexachlorobutadiene.

