5. POTENTIAL FOR HUMAN EXPOSURE

5.1 OVERVIEW

2-Hexanone is a volatile organic liquid that is very soluble in water. It is expected to be quite mobile in water and soils. Its rate of volatilization is likely to be moderately fast, but equilibration with sediments will be low. Biodegradation of 2-hexanone may occur slowly in water and soil, but bioconcentration is not expected.

Exposure of the general population to 2-hexanone is not likely to be high. However, persons living near hazardous waste sites or wood pulping, coal-gasification, or oil-shale processing plants may be exposed to 2 hexanone in contaminated environmental media. In the past, occupational exposures to 2-hexanone resulted from its manufacture and use. However, since 2-hexanone is not currently manufactured or used commercially in the United States, occupational exposures related to these activities are no longer of special concern.

The EPA has identified 1,177 NPL sites. 2-Hexanone has been found at 15 of the sites evaluated for the presence of this chemical. However, we do not know how many of the 1,177 NPL sites have been evaluated for the presence of 2-hexanone. As more sites are evaluated by the EPA, the number may change (View 1989). The frequency of these sites can be seen in Figure 5-1. Of these sites, 14 are located within the United States and 1 is located in the Commonwealth of Puerto Rico (not shown).

5.2 RELEASES TO THE ENVIRONMENT

Because 2-hexanone is not currently manufactured, imported, processed, or used for commercial purposes in the United States (EPA 1987b), releases to the environment are not likely to be high. Although it is reported to be released from wood pulping, coal-gasification, and oil-shale processing plants, levels resulting from these operations have been reported as being low. This compound is not listed in the Toxics Release Inventory (TRI).

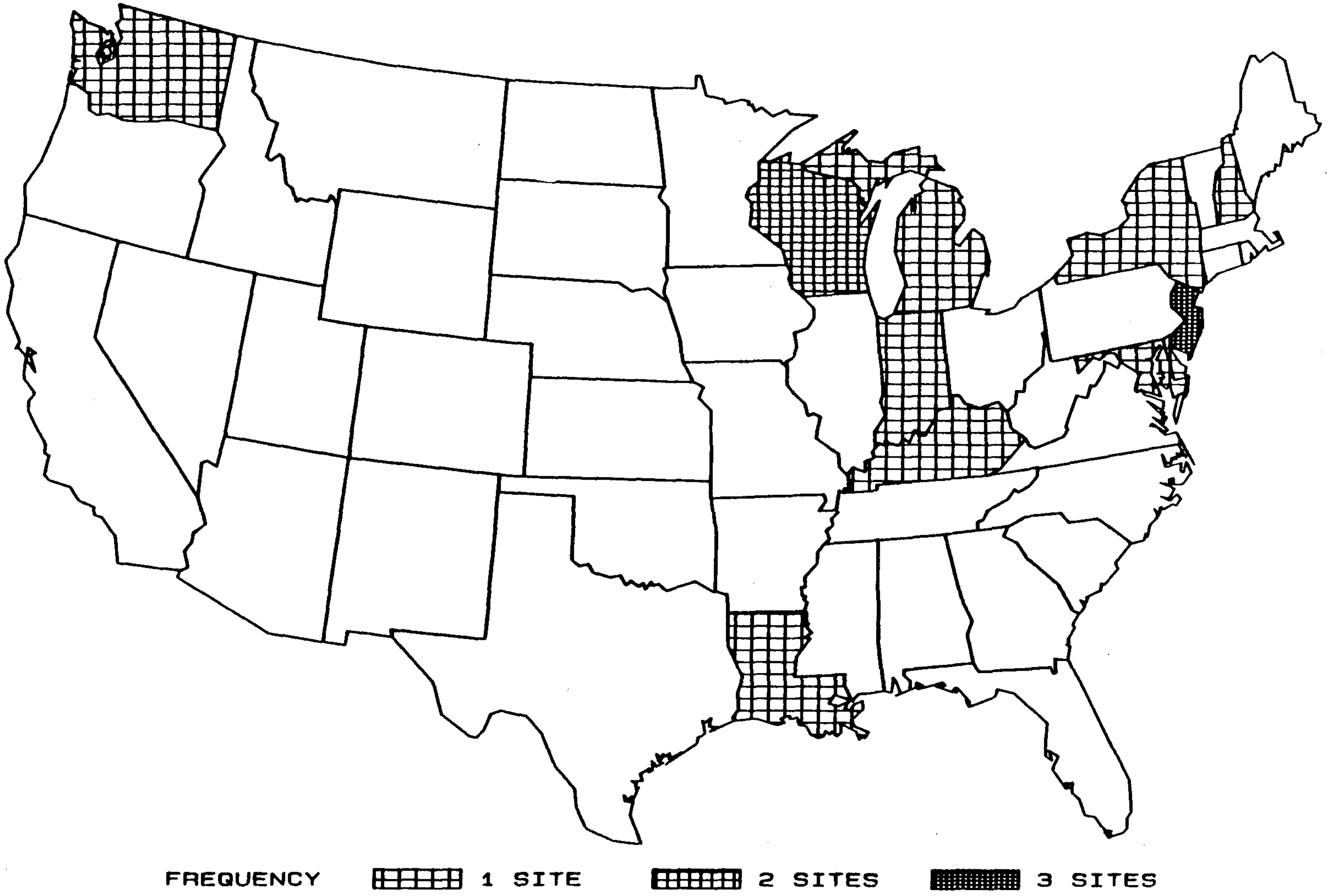
5.2.1 Air

No studies were located regarding the amount of 2-hexanone released to the atmosphere. However, since 2-hexanone is no longer produced in the United States (EPA 1987b) or used commercially (EPA 1987b; Lande et al. 1976; O'Donoghue 1985), atmospheric emissions from industrial sources are likely to be small.

5.2.2 Water

2-Hexanone is released to water by industrial facilities and at hazardous waste sites. 2-Hexanone was detected in 2 of 3 effluents from coal gasification plants and in 1 of 2 effluents from oil shale processing plants

FIGURE 5-1. FREQUENCY OF NPL SITES WITH 2-HEXANONE CONTAMINATION *



* Derived from View 1989

at mean concentrations ranging from 7 to 202 ppb (µg/L) (Pellizzarri et al. 1979). The compound has also been tentatively identified in 1 of 63 industrial effluents (Perry et al., 1979), the effluent from a chemical plant (Shackelford and Keith 1976), and in one municipal landfill leachate at 0.148 ppm (mg/L) in a study of leachates from 58 municipal and industrial landfills (Brown and Donnelly 1988).

2-Hexanone has also been detected in both groundwater and surface water at hazardous waste sites (CLPSD 1989) (see Section 5.4.2), indicating that this is a source of 2-hexanone release to the environment.

5.2.3 Soil

Soils or sediments may become contaminated with 2-hexanone by landfilling with 2-hexanone-containing solid wastes or by the discharge of contaminated water. 2-Hexanone has been detected in soil samples from hazardous waste sites (CLPSD 1989) (see Section 5.4.3).

5.3 ENVIRONMENTAL FATE

5.3.1 Transport and Partitioning

2-Hexanone exists in the atmosphere as a vapor. Liquid 2-hexanone is volatile; its vapor pressure has been measured as 1.53×10^{-2} atm (11.6 mmHg) at 25°C (Ambrose et al. 1975). Because 2-hexanone is very soluble in water, a large fraction of 2-hexanone released to the atmosphere, may dissolve in water vapor (such as clouds and rain drops). A Henry's law constant (H) estimates the tendency of a chemical to partition between its vapor phase and water. A value for H may be calculated by dividing the vapor pressure of 2-hexanone by its solubility in water at the same temperature (Mabey et al. 1982). In this case, an estimated value for H is $4.4\text{-}7.7\times10\text{-}^{-5}$ atm-m^3/mole at about 25°C. The magnitude of this value suggests that a large fraction of vapor-phase 2-hexanone will dissolve in water, and that precipitation may be an important physical removal mechanism. An analogous air-water partition coefficient measured for 2-hexanone at 37°C was approximately 2.3×10^{-4} atm-m^3/mole (Sato and Nakajima 1979), which indicates that precipitation will also be an important removal mechanism at this higher temperature.

2-Hexanone is very soluble in water, approximately 20-35 g/L (Morrison and Boyd 1974; Verschueren 1983). The magnitude of the estimated Henry's law constant ($4.4\text{-}7.7\times10^{-5}$ atm-m^3/mole) indicates that 2-hexanone will volatilize from water, with a half-life in river water of about 10-15 days (Mabey et al. 1982). Volatilization will be slower from lakes or ponds (Mabey et al. 1982). There is no information on whether 2-hexanone in water is expected to partition to soils and sediments.

2-Hexanone will probably not be bioconcentrated by organisms in water. An octanol/water partition coefficient (K_{ow}) estimates the partitioning of a chemical between octanol and water. Octanol is believed to best imitate the fatty structures in plants and animal tissues. The K_{ow} of 2-hexanone is approximately 20-40, based on its solubility in water (Hassett et al. 1983). These low values suggest that 2-hexanone will not partition to fatty tissues.

A bioconcentration factor (BCF) relates the concentration of a chemical in plants or animals to the concentration of that chemical in the medium in which they live. A BCF of about 7 was calculated for 2-hexanone (Lande et al. 1976) using the empirical regression of Neely et al. (1974). This low BCF indicates that bioconcentration is probably not an important fate mechanism for 2-hexanone released into the environment. Biomagnification of 2-hexanone is also not expected to occur to any great extent (Lande et al. 1976). However, no experimental data on the biomagnification potential of 2-hexanone were located to corroborate these assumptions.

5.3.2 Transformation and Degradation

5.3.2.1 Air

The major fate mechanism of atmospheric 2-hexanone is photooxidation. This ketone is also degraded by direct photolysis (Calvert and Pitts 1966), but the reaction is estimated to be slow relative to reaction with hydroxyl radicals (Laity et al. 1973). The rate constant for the photochemicallyinduced transformation of 2-hexanone by hydroxyl radicals in the troposphere has been measured at 8.97×10^{-12} cm^3/ molecule-set (Atkinson et al. 1985). Using an average concentration of tropospheric hydroxyl radicals of 6×10^5 molecules/cm^3 (Atkinson et al. 1985), the calculated atmospheric halflife of 2-hexanone is about 36 hours. However, the half-life may be shorter in polluted atmospheres with higher OH radical concentrations (MacLeod et al. 1984). Consequently, it appears that vapor-phase 2-hexanone is labile in the atmosphere.

5.3.2.2 Water

2-Hexanone is a ketone, and ketones are generally not degraded by hydrolysis (Lande et al. 1976; Morrison and Boyd 1974). Based on its reactions in air, it seems likely that 2-hexanone will undergo photolysis in water, however no information was located. Based on studies with microorganisms (see Section 5.3.2.3), it is probable that 2-hexanone will be biodegraded in water.

5.3.2.3 Soil

2-Hexanone may be biodegraded in soil. 2-Hexanone has been shown to be degraded by hydrocarbon-utilizing mycobacteria (Lukins and Foster 1963; Perry -1968). Similarly, certain yeasts have been isolated that can use 2-hexanone as a carbon source (Lowery et al. 1968). In a study using acclimated microbial cultures, 2-hexanone was significantly biodegraded (Babeu and Vaishnav 1987). An experimental 5-day biological oxygen demand (BOD) determination was about 61% of the theoretical BOD value. Although these studies have demonstrated that 2-hexanone may be biodegraded under ideal conditions, no information was located on its biological half-life in soils.

5.4 LEVELS MONITORED OR ESTIMATED IN THE ENVIRONMENT

5.4.1 Air

No studies were located which measured or estimated the concentration of 2-hexanone in ambient air.

In the past, workplace air concentrations in facilities where 2-hexanone was manufactured or used as a solvent ranged from 1 to 156 ppm (4.1 to 640 mg/m^3) (ACGIH 1986), and air concentrations up to 1,636 mg/m^3 were measured in the operations areas of some facilities (Bierbaum and Marceleno 1973; Marceleno et al. 1974). However, because 2-hexanone is no longer produced or used commercially in the United States, and because OSHA has reduced the Permissible Exposure Limit (PEL) to 5 ppm (20 mg/m^3) (OSHA 1989), it is unlikely that current workplace air concentrations are as high as they were in the past.

5.4.2 Water

Data estimating 2-hexanone concentrations in water are sparse. 2-Hexanone was identified in one of three groundwater samples at a concentration of 87 μg/L (ppb) near a hazardous waste site in Florida (Myers 1983). This compound was also identified in a study of drinking water concentrates and advanced waste treatment concentrates (Lucas 1984).

2-Hexanone has been detected in both surface water and groundwater at hazardous waste sites. Data from the Contract Laboratory Program (CLP) Statistical Database indicate that 2-hexanone was found at 2% of the sites at a geometric mean concentration of 7.5 μg/L (ppb) in positive surface water samples and 12 μg/L (ppb) in positive groundwater samples (CLPSD 1989). This database provides data from both NPL and non-NPL waste sites.

5.4.3 Soil

2-Hexanone was detected in soil samples at 3% of hazardous waste sites (both NPL and non-NPL) at a geometric mean concentration of 40 μg/kg (ppb) in positive samples (CLPSD 1989). No other data were located regarding estimation of 2-hexanone in soils or sediments.

5.4.4 Other Environmental Media

2-Hexanone has been identified among the natural volatile components of several foods including blue and Beaufort cheeses, nectarines, roasted filberts, and chicken muscle (Day and Anderson 1965; Dumont and Adda 1978; Grey and Shrimpton 1967; Kinlin et al. 1972; Takeoka et al. 1988); levels were not stated in these reports. It has also been detected in milk and cream at concentrations ranging from 0.007 to 0.018 ppm (7-18 ppb) and in bread (Lande et al. 1976). Because few quantitative data are available, it is not known if food is an important source of human exposure to 2-hexanone.

No studies were located regarding the occurrence of 2-hexanone in any other media.

5.5 GENERAL POPULATION AND OCCUPATIONAL EXPOSURE

Human exposure to 2-hexanone may occur by inhalation, ingestion, or dermal exposure. Exposure to small amounts of 2-hexanone may occur by ingestion of foods in which it has been detected. However, since this compound is no longer manufactured or used commercially in the United States, widespread or high-level exposure of the general population to 2-hexanone is not likely.

According to surveys conducted by NIOSH, the number of employees potentially exposed to 2-hexanone dropped from 41,600 in the early 1970s (NOHS 1989) to 1,100 in the early 1980s (NIOSH 1989). Neither the NOHS nor the NOES databases contain information on the frequency, concentration, or duration of exposures of workers to any of the chemicals listed therein. These surveys provide only estimates of the number of workers potentially exposed to chemicals in the workplace. This dramatic reduction in the extent of occupational exposure parallels the halt of production and the reduction in use of this chemical (EPA 1987b). It is unlikely that many persons are currently occupationally exposed to 2-hexanone, other than as a degradation product resulting from wood pulping, oil shale processing, or coal gasification operations. The NIOSH does not list 2-hexanone among the chemicals considered in an occupational exposure evaluation of coal gasification plants (NIOSH 1978b).

5.6 POPULATIONS WITH POTENTIALLY HIGH EXPOSURES

Populations with potentially high exposure to 2-hexanone include people living near or working in coal gasification, oil shale processing or wood pulping operations, or living near the hazardous waste sites at which 2-hexanone is likely to occur. The most likely exposure routes are ingestion of or dermal contact with water contaminated from these sources or inhalation of 2-hexanone which has volatilized from contaminated water or soil.

Individuals may still be exposed by inhalation or skin absorption from consumer products manufactured prior to 1982 such as lacquers, primers, sealers, and thinners that contain 2-hexanone.

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 2-hexanone 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 2-hexanone.

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 or eliminate the uncertainties of human health assessment. In the future, the identified data needs will be evaluated and prioritized, and a substance-specific research agenda will be proposed.

5.7.1 Data Needs

Physical and Chemical Properties. The physical and chemical property data available for 2-hexanone are sufficient to allow a limited estimation of the potential environmental fate of this chemical. The estimated Henry's law constant (Mabey et al, 1982) and K_{oc} (Hassett et al. 1983) need to be verified experimentally to help confirm the estimates of partitioning in environmental media. Since there does not seem to be a consensus on the solubility of 2-hexanone in water (reported values range from about 20-35 g/L) (Morrison and Boyd 1974; Verschueren 1983), additional measurements would be useful to more accurately predict the environmental fate of this compound.

Production, Import/Export, Use, and Disposal. 2-Hexanone is no longer produced, imported, or used commercially in the United States (EPA 1987b). Any future manufacture or use is required to be reported to EPA (EPA 1987b). Data from these reports would be helpful in estimating the potential for human exposure to this compound. No data on disposal of 2-hexanone were located. Information on disposal practices for wastes containing 2-hexanone is necessary for estimations of human exposure from this source. No regulations govern the disposal of 2-hexanone.

Environmental Fate. The probable transport and partitioning of 2-hexanone in environmental media have been predicted based on estimated partition coefficients. Experimental confirmation of these values would help to increase the accuracy of transport and partitioning assessments. The loss mechanisms of 2-hexanone transformations in the atmosphere are fairly-well understood (Atkinson et al. 1985; Calvert and Pitts 1966; Laity et al. 1973; MacLeod et al. 1984), but the reaction pathways and environmental fates of the transformation products are not known. Very little is known about the fate of 2-hexanone in water or soil (Babeu and Vaishnav 1987; Lande et al. 1976; Lowery et al. 1968; Lukins and Foster 1963; Perry 1968). Data on photodegradation and biodegradation of 2-hexanone in surface water and biodegradation of 2-hexanone in groundwater and soil may be helpful in assessing the persistence of 2-hexanone in these media.

Bioavailability from Environmental Media. Information on absorption by humans and other animal species indicates that it is well absorbed via the oral and dermal routes (DiVincenzo et al. 1977, 1978). 2-Hexanone has also been demonstrated to be well absorbed by humans and animals following inhalation exposure (DiVincenzo et al. 1978). Information on its bioavailability from contaminated soils would be useful in assessing the risk from exposure to this medium by populations in the vicinity of hazardous waste sites.

Food Chain Bioaccumulation. There are no data on the bioaccumulation of 2-hexanone in food chains. This lack of data may not be a major limitation in the database because it is unlikely that 2-hexanone is bioconcentrated by plants, aquatic organisms, or animals at lower trophic levels based on its high water solubility (Lande et al. 1976). However, data confirming that bioconcentration does not occur would help to more accurately assess the probability of bioaccumulation of 2-hexanone.

Exposure Levels in Environmental Media. Very few data are available regarding the presence of 2-hexanone in any environmental media (CLPSD 1989; Lucas 1984; Myers 1983). Although high levels of this compound are not expected to occur in ambient air, water, or soil, concentrations of 2-hexanone in these media near effluent sources or hazardous waste sites would be helpful in assessing the potential extent and magnitude of human exposures. Exposure Levels in Humans. No information has been located on exposure levels of humans to 2-hexanone in the workplace or in the vicinity of hazardous waste sites. It would be useful to collect information on levels of exposure to 2-hexanone in the environment and associated blood, urine or tissue levels of 2-hexanone and/or its metabolites in the exposed populations. Additional information relating those levels to the subsequent development of health effects would also be extremely useful.

Exposure Registries. No exposure registries for 2-hexanone were located. This compound is not currently one of the compounds for which a subregistry has been established in the National Exposure Registry. The compound 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 the exposure to this compound.

5.7.2 On-going Studies

Remedial investigations and feasibility studies conducted at the 15 NPL sites known to be contaminated with 2-hexanone will add to the available database in the categories of exposure levels in humans, exposure levels in the environmental media, and exposure registries.

No other on-going studies were located on the fate, transport, or potential for human exposure for 2-hexanone.