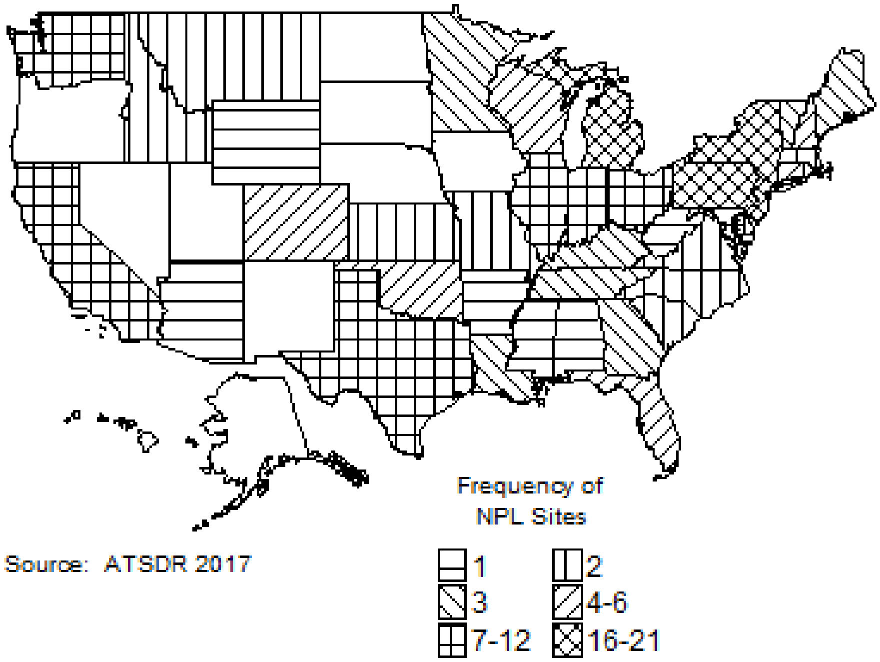
CHAPTER 5. POTENTIAL FOR HUMAN EXPOSURE

5.1 OVERVIEW

2-Hexanone has been identified in at least 224 of the 1,854 hazardous waste sites that have been proposed for inclusion on the EPA National Priorities List (NPL) (ATSDR 2017). However, the number of sites in which 2-hexanone has been evaluated is not known. The number of sites in each state is shown in Figure 5-1. Of these sites, 221 are located within the United States, 1 is located in the Guam, and 2 are located in Puerto Rico (not shown).

Figure 5-1. Number of NPL Sites with 2-Hexanone Contamination



- 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.
- Because 2-hexanone is not currently manufactured, imported, processed, or used for commercial purposes in the United States (EPA 1987), releases to the environment are not likely to be high.
- 2-Hexanone can be released to the air from activities involving the oil and gas industry if waste water is stored in open containment pits. It may be released to water by activities associated with the oil and natural gas industries and at hazardous waste sites.

- 2-Hexanone exists in the atmosphere as a vapor and is very soluble in water.
- The major fate mechanism of atmospheric 2-hexanone is photooxidation.
- 2-Hexanone may be biodegraded in soil.
- 2-Hexanone is expected to have high mobility in soil, and may therefore leach into groundwater.

5.2 PRODUCTION, IMPORT/EXPORT, USE, AND DISPOSAL

5.2.1 Production

No information is available in the TRI database on facilities that manufacture or process 2-hexanone because this chemical is not required to be reported under Section 313 of the Emergency Planning and Community Right-to-Know Act (Title III of the Superfund Amendments and Reauthorization Act of 1986) (EPA 2005).

In 1977, the combined U.S. production and import of 2-hexanone was between 453 and 4,500 metric tons (EPA 1981, 1987); no breakdown of these figures was provided. The only U.S. producer of 2-hexanone, the Tennessee Eastman Company division of Eastman Kodak, discontinued its production of 2-hexanone in 1979 and sold its remaining reserves by 1981 (EPA 1981, 1987; Lande et al. 1976). 2-Hexanone was commercially produced by the catalyzed reaction of acetic acid and ethylene under pressure (EPA 1987). 2-Hexanone may still be commercially produced in countries outside of the United States.

5.2.2 Import/Export

Currently, 2-hexanone is not produced or approved for commercial use in the United States, and consequently, there is no information on exports or imports (EPA 1987; HHS 2017).

5.2.3 Use

2-Hexanone is not currently manufactured, processed, or used for commercial purposes in the United States (EPA 1987; HHS 2017). 2-Hexanone had been used as a solvent for many materials, primarily in the lacquer industry as a solvent for lacquers and varnish removers. It had also been used as a solvent for ink thinners, resins, oils, fats, and waxes, and as a medium evaporating solvent for alkyd, vinyl, and nitrocellulose acrylate coatings. 2-Hexanone had also been used as an intermediate in the synthesis of organic chemicals (ACGIH 1986; EPA 2009a). 2-Hexanone has been studied as a possible oxygenate in blended diesel fuels; however, it absorbs water and is susceptible to gum formation (McCormick et al. 2015).

5.2.4 Disposal

No data were located regarding the disposal of 2-hexanone or on regulations and guidelines regarding its disposal. The favored method for disposal of ketones is incineration (Lande et al. 1976).

5.3 RELEASES TO THE ENVIRONMENT

The Toxics Release Inventory (TRI) data should be used with caution because only certain types of facilities are required to report (EPA 2005). This is not an exhaustive list. Manufacturing and processing facilities are required to report information to the TRI only if they employ ≥10 full-time employees; if their facility is included in Standard Industrial Classification (SIC) Codes 10 (except 1011, 1081, and 1094), 12 (except 1241), 20–39, 4911 (limited to facilities that combust coal and/or oil for the purpose of generating electricity for distribution in commerce), 4931 (limited to facilities that combust coal and/or oil for the purpose of generating electricity for distribution in commerce), 4939 (limited to facilities that combust coal and/or oil for the purpose of generating electricity for distribution in commerce), 4953 (limited to facilities regulated under RCRA Subtitle C, 42 U.S.C. section 6921 et seq.), 5169, 5171, and 7389 (limited S.C. section 6921 et seq.), 5169, 5171, and 7389 (limited to facilities primarily engaged in solvents recovery services on a contract or fee basis); and if their facility produces, imports, or processes ≥25,000 pounds of any TRI chemical or otherwise uses >10,000 pounds of a TRI chemical in a calendar year (EPA 2005).

Because 2-hexanone is not currently manufactured, imported, processed, or used for commercial purposes in the United States (EPA 1987), releases to the environment are not likely to be high. Although it is reported to be released from currently operating wood pulping, coal-gasification, and *in situ* oil-shale processing[1] plants via liquid waste water containing 2-hexanone or as a volatilized gas from waste water into the surrounding air, levels resulting from these operations have been reported as being low (ATSDR 2008; Pellizzari et al. 1979). In the past decade, there has been an increase in oil and natural gas production due to the development of horizontal drilling and hydraulic fracturing (EIA 2016). There is some evidence that 2-hexanone may be released from these operations; however, the data are limited.

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[1] *In situ* shale oil processing involves drilling into oil shale strata and heating rocks to release crude shale oil, shale gas, and water (referred to as termed retorting).

5.3.1 Air

There is no information on releases of 2-hexanone to the atmosphere from manufacturing and processing facilities because these releases are not required to be reported (EPA 2005).

Limited studies were located regarding the amount of 2-hexanone released to the atmosphere. 2-Hexanone was detected at a maximum average concentration of 1,700 μg/m^3 in the air emissions of eight municipal solid waste composting disposal facilities in the United States (Eitzer 1995). Kumar et al. (2011) also reported 2-hexanone to be a volatile organic compound emission from green waste composting. Municipal solid waste composting facilities collect waste, including yard waste, food scraps, farm waste, cardboard, newspaper, and sewage treatment plant solids, from non-industrial sources such as residential homes, restaurants, retail centers, and office buildings. Therefore, the 2-hexanone detected in air emissions is likely produced from the microbial digestion of large bioorganic compounds.

2-Hexanone can be released to the air from activities involving the oil and gas industry if waste water is stored in open containment pits. For example, a report from an environmental nonprofit group reported that 2-hexanone was detected in air samples above oil and gas waste water open containment ponds located in Kern County, California at a concentration of 12 μg/m^3 (Grinberg 2014). Hawthorne and Sievers (1984) measured 2-hexanone at levels of 0.22–3.6 ng/mL in air samples above shale oil waste water retort water and gas condensate. Since 2-hexanone is no longer produced in the United States (EPA 1987) or used commercially (EPA 1987; Lande et al. 1976; O’Donoghue 1985), atmospheric emissions from industrial sources are likely to be small.

5.3.2 Water

There is no information on releases of 2-hexanone to water from manufacturing and processing facilities because these releases are not required to be reported (EPA 2005).

2-Hexanone may be released to water by activities associated with the oil and natural gas industries and at hazardous waste sites. 2-Hexanone was detected in process water from a coal gasification site (7 μg/L) located in Wyoming and condensate water (202 μg/L) from the low-BTU gasification of coal from a facility in West Virginia (Pellizzari et al. 1979). It was also detected in retort water (55 μg/L) from an *in situ* oil shale processing location in Wyoming (Pellizzari et al. 1979). It was analyzed for, but not detected in, flowback water (the water that is returned to the surface following the hydraulic fracturing) from 19 natural gas hydraulic fracturing locations in West Virginia and Pennsylvania as well as flowback water from 5 locations in Texas (Hayes 2009; RPSEA 2012). 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 5.5.2), indicating that this is a source of 2-hexanone release to the environment.

5.3.3 Soil

There is no information on releases of 2-hexanone to soil from manufacturing and processing facilities because these releases are not required to be reported (EPA 2005).

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 5.5.3).

5.4 ENVIRONMENTAL FATE

5.4.1 Transport and Partitioning

Air. 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 estimates the tendency of a chemical to partition between its vapor phase and water. An estimated value for Henry's law constant of 2-hexanone is 9.32×10^{-5} atm-m^3/mol at 25°C (HSDB 2009). 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.

Water. 2-Hexanone is very soluble in water, approximately 17.2 g/L (Yalkowsky and Yan 2003). The Henry's law constant indicates that a fraction of 2-hexanone will volatilize from water. Estimated half-lives in model river and lake water are about 7 hours and 7 days, respectively (Thomas 1990). Based on its estimated organic carbon partition coefficient (K_{oc}) value of 77, 2-hexanone is expected to have high mobility in soil (Thomas 1990), and may therefore leach into groundwater. This may be a particular concern if contaminated waste water or flowback water is stored in unlined containment ponds or disposed of via underground injection.

2-Hexanone is not likely bioconcentrated by organisms in water. An octanol/water partition coefficient (log 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. Generally, a log K_{ow} range of 2–7 describes most chemicals of interest with the potential to partition to fatty tissues. The log K_{ow} of 2-hexanone is 1.38 (Hansch et al. 1995). Therefore, this low value suggests that 2-hexanone is not likely to partition to fatty tissues. Further, 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. Generally, a BCF value <30 is considered to have low bioconcentration potential. A BCF of 4 was calculated for 2-hexanone (EPA 2012a), suggesting that bioconcentration in aquatic organisms is not expected to be 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.

5.4.2 Transformation and Degradation

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 photochemically induced transformation of 2-hexanone by hydroxyl radicals in the atmosphere has been measured at 9.01×10^{-12} cm^3/ molecule-set (Atkinson 1989). Using an average concentration of atmospheric hydroxyl radicals of 5×10^5 molecules/cm^3 (Atkinson 1989), the calculated atmospheric half-life of 2-hexanone is about 2.4 days. 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.

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

Sediment and 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.

Other Media. No studies were located for the environmental fate of 2-hexanone in other media.

5.5 LEVELS IN THE ENVIRONMENT

Reliable evaluation of the potential for human exposure to 2-hexanone depends, in part, on the reliability of supporting analytical data from environmental samples and biological specimens. Concentrations of 2-hexanone in unpolluted atmospheres and in pristine surface waters are often so low as to be near the limits of current analytical methods. In reviewing data on 2-hexanone levels monitored or estimated in the environment, it should also be noted that the amount of chemical identified analytically is not necessarily equivalent to the amount that is bioavailable.

Table 5-1 shows the lowest limit of detections that are achieved by analytical analysis in environmental media. An overview summary of the range of concentrations detected in environmental media is presented in Table 5-2.

Table 5-1. Lowest Limit of Detection Based on Standards[a]

Media	Detection limit	Reference
Air	0.454 μg (0.227 mg/m^3)	NIOSH 1984; OSHA 1995
Drinking water	No data	
Surface water and groundwater	<10 μg/kg	Badings et al. 1985
Whole blood	No data	Anderson and Harland 1980; White et al. 1979

[a] Detection limits based on using appropriate preparation and analytics. These limits may not be possible in all situations.

Table 5-2. Summary of Environmental Levels of 2-Hexanone

Media	Low	High	For more information
Outdoor air (ppbv)	0.11 μg/m^3	15 μg/m^3	Section 5.5.1
Ground water (ppb)	87 μg/L	150 μg/L	Section 5.5.2
Food (ppb)	1 μg/kg	18 μg/kg	Section 5.5.4
Soil	40 μg/kg	440 μg/kg	Section 5.5.3

Detections of 2-hexanone in air, water, and soil at NPL sites are summarized in Table 5-3.

Table 5-3. 2-Hexanone Levels in Water, Soil, and Air of National Priorities List (NPL) Sites

Medium	Median[a]	Geometric mean[a]	Geometric standard deviation[a]	Number of quantitative measurements	NPL sites
Water (ppb)	74	71.4	21.6	29	25
Soil (ppb)	58.5	244	40.5	20	16
Air (ppbv)	5.37	5.67	27.8	10	8

[a] Concentrations found in ATSDR site documents from 1981 to 2017 for 1,854 NPL sites (ATSDR 2017). Maximum concentrations were abstracted for types of environmental media for which exposure is likely. Pathways do not necessarily involve exposure or levels of concern.

5.5.1 Air

Limited studies were located that measured or estimated the concentration of 2-hexanone in ambient air. 2-Hexanone was detected, but not quantified, in air samples collected from Whitaker’s Forest in the Sierra Nevada Mountains, California in 1990 (Helmig and Arey 1992).

2-Hexanone and several other volatile organic compounds (VOCs) were monitored for in Garfield County, Colorado where several natural gas hydraulic fracturing wells had been operating at the time of the study (ATSDR 2008). Natural gas needs to be separated from fluids and other gases that may release VOCs into the surrounding air. In addition, fracking water may contain small amounts of chemicals containing VOCs used during the hydraulic fracturing process, and these may volatilize to ambient air if the water is stored in uncovered wells at the location. 2-Hexanone was detected in 14.8% of grab samples collected at all of the monitoring sites in Garfield County at levels ranging from 0.7 to 15.0 μg/m^3, with an average concentration of 1.7 μg/m^3 (ATSDR 2008). It was concluded that noncancer adverse health effects were not likely to occur from exposure to the levels of 2-hexanone measured at these sites, based on comparison with the ATSDR chronic health guidelines. In addition to grab samples, 14 fixed sites were monitored for a 24-hour period once per month or once per quarter; this included 8 locations near oil and gas drilling facilities, 4 urban locations, and 2 rural background locations. 2-Hexanone was detected in at least 4% of the samples from three of the oil and natural gas drilling locations and two of the urban locations. It was detected in <4% of the samples in both the rural background sites.

2-Hexanone was detected in ambient air during a monitoring study in the Commonwealth of Pennsylvania to determine the effect that natural gas exploration had on air quality (PA DEP 2011). Levels of 2-hexanone in air related to Marcellus Shale natural gas activities were determined to be at levels similar to, or slightly greater than, levels observed in areas not impacted by hydraulic fracturing operations. Annual average concentrations of 2-hexanone at these locations ranged from 0.11 to 2.1 μg/m^3. 2-Hexanone was detected in air samples above oil and gas waste water open containment ponds located in Kern County, California at a concentration of 12 μg/m^3 (Grinberg 2014).

In the past, workplace air concentrations in facilities where 2-hexanone was manufactured or used as a solvent ranged from 1 to 156 ppm (4.1–640 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 the federal government has set certain regulations and guidelines to help protect people from the possible health effects of 2-hexanone in the workplace, it is unlikely that current workplace air concentrations are as high as they were in the past. The Occupational Safety and Health Administration (OSHA) has set a Permissible Exposure Limit (PEL) of 100 ppm (100 parts of 2-hexanone in 1 million parts of air) as a time-weighted average (TWA) to this chemical in workplace air during an 8-hour work period, over a 40-hour workweek (OSHA 2018a). The National Institute for Occupational Health and Safety (NIOSH) has set a Recommended Exposure Limit (REL) of 1 ppm

(TWA) 2-hexanone in workplace air as an average exposure during a 10-hour work period (NIOSH 2018) for up to a 40-hour workweek. The American Conference of Governmental Industrial Hygienists (ACGIH) recommends a 5 ppm (TWA) Threshold Limit Value (TLV) for 2-hexanone in workplace air as an average during an 8-hour workday (ACGIH 2001, 2003, 2015). ACGIH also has a 15-minute short-term exposure limit (STEL) of 10 ppm.

5.5.2 Water

2-Hexanone was 1 of 70 VOCs monitored for in influent water and flow-back water at 19 hydraulic fracturing locations located in Pennsylvania and West Virginia (Hayes 2009). 2-Hexanone was not detected in the samples collected. It was also not detected in flowback water from five hydraulic fracturing operations in North Texas (RPSEA 2012).

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). 2-Hexanone was detected, but not quantified, in groundwater near a forest waste site in Otisville, Michigan in 1987 (EPA 1988). Groundwater samples collected from the Biscayne Aquifer Superfund sites in Florida contained 2-hexanone at maximum concentrations of 150 μg/L (from the entire study area) and 110 μg/L (from well fields) (Canter and Sabatini 1994). 2-Hexanone was detected in 0.3, 11.1, 3.6, and 1.4% of hazardous waste site groundwater samples collected from 1981 to 1986 in EPA Regions 1, 2, 9, and 10, respectively (Plumb 1992).

2-Hexanone was detected at an unauthorized hazardous waste disposal site in Lang Township, New Jersey in two well water samples collected in 1985 at an average concentration of 7,135 μg/L (maximum concentration of 14,000 μg/L) and in onsite lagoon surface water samples at an average concentration of 20 μg/L (maximum concentration of 30 μg/L) (EPA 1986). This compound was also identified in a study of drinking water concentrates and advanced waste treatment concentrates (Lucas 1984). Richardson et al. (1999) reported that 2-hexanone was identified in drinking water that had been treated by ozone disinfection.

5.5.3 Sediment and 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). 2-Hexanone was detected at an unauthorized hazardous waste disposal site in Lang Township, New Jersey in surface and subsurface soil samples collected in 1985 at concentrations of 440 and 46 μg/kg, respectively (EPA 1986). In residential topsoil samples taken from a 0.5-acre area at the Dona Park Residential site located immediately south of a former smelting and refining plant in Corpus Christi, Texas, 2-hexanone was detected at 274 mg/kg (TCEQ 2011). No other data were located regarding estimation of 2-hexanone in soils or sediments.

5.5.4 Other Media

2-Alkanones and 2-alkanols are formed naturally in some foods as a byproduct of the degradation of free fatty acids (Dumont and Adda 1978; Girolami and Knight 1955). 2-Hexanone has been identified among the natural volatile components of several foods, including blue and Beaufort cheeses, nectarines, roasted filberts (hazelnuts), beef, and chicken muscle (Day and Anderson 1965; Dumont and Adda 1978; Grey and Shrimpton 1967; Kinlin et al. 1972; Ramarathnam et al. 1991; Takeoka et al. 1988); levels were not stated in these reports. It has been detected in canned cream, canned kernel, frozen kernel, and fresh kernel cooked corn products at concentrations of 1, 2, <5, and <1 ppb, respectively (Buttery et al. 1994). 2-Hexanone was also 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.

5.6 GENERAL POPULATION 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 after its discontinuation in 1979 (EPA 1987), widespread or high-level exposure of the general population to 2-hexanone is not likely. 2-Hexanone has been detected in air samples at locations in which hydraulic fracturing has occurred, suggesting that nearby populations could be susceptible to inhalation exposure. No data were located indicating that 2-hexanone has been detected in groundwater at these locations.

According to surveys conducted by NIOSH, the number of employees potentially exposed to 2-hexanone dropped from 41,600 in the early 1970s to 1,100 in the early 1980s (RTECS 2009). Neither the National

Occupational Hazard Survey (NOHS) nor the National Occupational Exposure Survey (NOES) databases contain information on the frequency, concentration, or duration of exposures of workers to any chemicals listed. 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 commercial use of this chemical (EPA 1987). It is unlikely that many persons are currently occupationally exposed to 2-hexanone, other than as a degradation product resulting from wood pulping, *in situ* oil shale processing, or coal gasification operations. NIOSH does not list 2-hexanone among the chemicals considered in an occupational exposure evaluation of coal gasification plants (NIOSH 1978).

5.7 POPULATIONS WITH POTENTIALLY HIGH EXPOSURES

Populations with potentially high exposure to 2-hexanone include people living near or working in areas affected by oil and natural gas activities, or living near the hazardous waste sites where 2-hexanone is likely present. The most likely exposure routes are ingestion or dermal contact with water contaminated from these sources or inhalation of 2-hexanone that has volatilized from contaminated water or soil. Individuals may still be exposed by ingestion, inhalation, skin absorption from use of consumer products manufactured prior to 1982 such as lacquers, primers, sealers, and thinners that contain 2-hexanone, or through currently imported products containing 2-hexanone, including foods.