

5. POTENTIAL FOR HUMAN EXPOSURE

5.1 OVERVIEW

1,3-Butadiene is a high-volume, volatile hydrocarbon used in the production of commercial plastics and rubbers. The chemical reactivity of this monomer is utilized in its transformation into polymeric materials. 1,3-Butadiene is also present in gasoline.

1,3-Butadiene may be released to the environment as an intentional or fugitive emission during its production, use, storage, transport, or disposal. Large amounts of this hydrocarbon are released to the atmosphere from commercial processes. According to the SARA Section 313 Toxic Release Inventory (TRI), an estimated total of 9.2 million pounds of 1,3-butadiene were released to the atmosphere from manufacturing and processing facilities in the United States in 1987 (TRI 1989). This total compares to a total release of approximately 9.6 million pounds to air, soil, water, public treatment works, and off-site areas during the same year. TRI data can be found in Table 5-1. The quality of the TRI data must be viewed with caution because the 1987 data represent first-time reporting by these facilities. Only certain types of facilities were required to report. This is not an exhaustive list. 1,3-Butadiene is also released to the atmosphere in motor vehicle exhaust, cigarette smoke, the smoke of brush fires, the thermal breakdown or burning of plastics, and by volatilization from gasoline.

Large amounts of 1,3-butadiene are released to the atmosphere. Data on the detection of 1,3-butadiene in soil and water are scarce due to the lack of a reliable analytical method to detect this compound in these media. It has been qualitatively detected in drinking water. 1,3-Butadiene has been detected at three hazardous waste sites (View 1989). The states in which these hazardous waste sites are located can be found in Figure 5-1.

1,3-Butadiene is a highly volatile gas; therefore, it is expected to partition predominantly to the atmosphere. In the atmosphere, 1,3-butadiene is expected to undergo rapid destruction, primarily by photo-initiated reactions. The reaction with photochemically produced hydroxyl radicals has a calculated half-life of approximately 6 hours and is expected to be the dominant pathway for atmospheric removal. Destruction of atmospheric 1,3-butadiene by the gas-phase reaction with ozone and by the night-time reaction with nitrate radicals in urban areas is also expected to be significant.

Limited data have been located on the fate of 1,3-butadiene in soil or water. Based on its physical properties, rapid volatilization of 1,3-butadiene from either soil or water to the atmosphere is expected to dominate over all other potential environmental processes. Studies performed with pure cultures indicate that 1,3-butadiene may be susceptible to microbial attack. Based on estimated values, 1,3-butadiene is not expected to adsorb significantly to soil or sediment, nor is it expected to bioconcentrate in

TABLE 5-1. Releases to the Environment from Facilities That Manufacture or Process 1,3-Butadiene^a

State ^d	No. of facilities	Range of reported amounts released in thousands of pounds ^b						Off-site waste transfer
		Air	Underground injection	Water	Land	Total environment ^e	POTW ^c transfer	
AL	1	3.4-3.4	0-0	0.3-0.3	0-0	3.7-3.7	0-0	0.3-0.3
AR	1	0.3-0.3	0-0	0-0	0-0	0.3-0.3	0-0	0-0
CA	12	0-2.1	0-0	0-0.3	0-0	0-2.4	0-0	0-0.3
CO	2	0.3-0.8	0-0	0-0	0-0	0.3-0.8	0-0	0-0
CT	1	41.3-41.3	0-0	0.1-0.1	0-0	41.3-41.3	0-0	17-17
DE	2	24-78.3	0-0	0-0	0-0	24-78.3	0-0	0-0
GA	3	105-403.5	0-0	0-0	0-0	105-403.5	0-0	0-93
HI	1	0.5-0.5	No Data	0-0	0-0	0.5-0.5	0-0	0-0
IA	2	175-278	0-0	0-0.1	0-0	175-278	0-0	0-0
IL	7	0.1-113.8	0-0	0-0.3	0-0	0.1-113.8	0-0	0-0
IN	3	0.4-40.2	0-0	0-0	0-0	0.4-40.2	0-0	0-0
KS	3	0.2-0.4	0-0.1	0-0	0-0	0.2-0.4	0-0	0-0.1
KY	6	1.7-161	0-0	0-0.1	0-0.1	1.8-161	0-0.3	0-1.3
LA	16	0.1-150	0-0	0-0.2	0-0.1	0.1-150	0-0	0-181.7
MI	1	63.5-63.5	0-0	0-0	0-0	63.5-63.5	0-0	0-0
MN	1	0-0	0-0	0.1-0.1	0-0	0.1-0.1	0-0	0-0
MO	1	0.2-0.2	0-0	0-0	0-0	0.2-0.2	0.1-0.1	0.2-0.2
MS	2	0.5-2.2	0-0	0-0	0-0	0.5-2.2	0-0	0-0
MT	2	0.3-0.9	0-0	0-0	0-0	0.3-0.9	0-0	0-0
NC	2	0-9.6	0-0	0-0	0-0	0-9.6	0-0.1	0-0
NE	1	0-0	0-0	0-0	0-0	0-0	0-0	0-0
NJ	2	0.1-0.1	0-0	0-0	0-0	0.1-0.1	0-0	0-0
NY	3	0.1-65.8	0-0	0-0.1	0-0	0.1-65.8	0.1-0.1	0-0.3
OH	15	0-146.8	0-0	0-0.3	0-0.1	0.1-146.8	0-36	0-65.5
OK	3	0.1-1.9	0-0	0-0	0-0	0.1-1.9	0-0	0-0
PA	4	0-115.6	0-0	0-0.3	0-0	0.2-115.6	0-0	0-0
SC	1	14-14	0-0	0-0	0-0	14-14	0-0	0-0
TN	3	9.9-640.2	0-0	0-0	0-0	9.9-640.2	0-0.1	0-0
TX	49	0-960	0-0	0-430	0-2.9	0-1,392	0-0	0-1,802
VA	1	0.1-0.1	0-0	0-0	0-0	0.1-0.1	0-0	0-0
WA	2	4.2-5.7	0-0	0-0.1	0-0	4.2-5.7	0-0	0-0
WV	2	6.1-700	0-0	0-0.1	0-0	6.1-700	0-0	0-0

^aTRI 1989

^bData in TRI are maximum amounts released by each facility. Quantities reported here have been rounded to the nearest hundred pounds, except those quantities >1 million pounds, which have been rounded to the nearest thousand pounds.

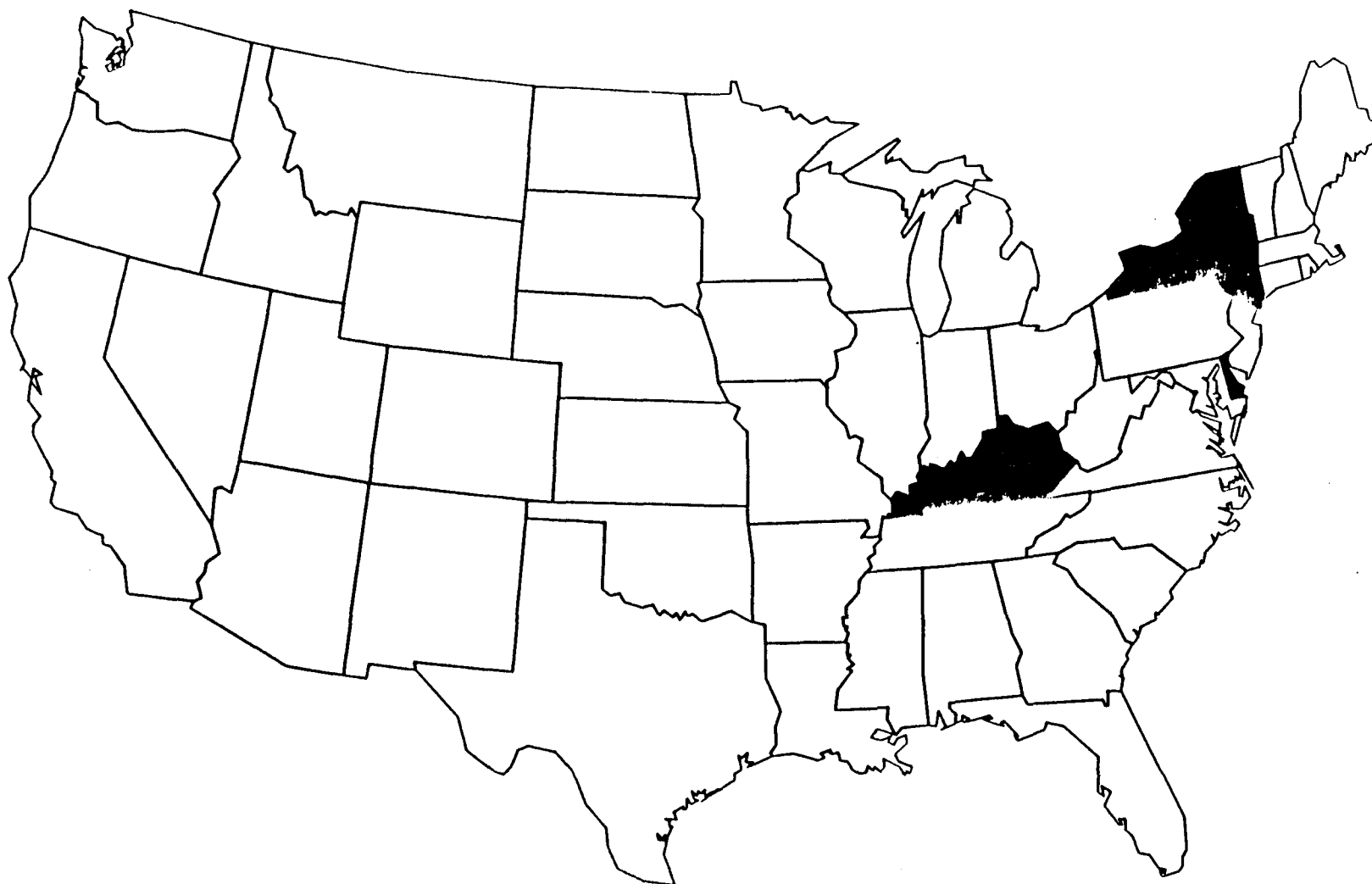
^cPublicly owned treatment works

^dPost office state abbreviation

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

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FIGURE 5-1. FREQUENCY OF NPL SITES WITH 1,3-BUTADIENE CONTAMINATION *



FREQUENCY  1 SITES

* Derived from View 1989

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fish or aquatic organisms; however, experimental data is necessary to verify these conclusions.

Although 1,3-butadiene undergoes rapid destruction in the atmosphere, it is almost always present at very low concentrations in urban and suburban areas. Automobile exhaust is a constant source of 1,3-butadiene release to the atmosphere. Because of the compound's presence in the atmosphere, the general population is exposed to ppb levels of 1,3-butadiene through inhalation. Exposure to 1,3-butadiene may also occur from the inhalation of gasoline fumes, cigarette smoke, or possibly the smoke from wood fires. Possible ingestion of contaminated drinking water may also lead to low levels of exposure, although we do not know the concentration of this compound in water samples, nor do we have a good understanding of its frequency of detection. The levels of 1,3-butadiene in soil are not known. Dermal exposure to low levels of 1,3-butadiene may occur for members of the general population if they spill gasoline on themselves. Elevated levels of exposure for the general population may occur for those near its site of manufacture or facilities where it is made into polymeric materials.

Occupational exposure to 1,3-butadiene is expected to be limited to those working at facilities that manufacture 1,3-butadiene or convert it into commercial polymers. Exposure by inhalation is expected to be the dominant pathway for exposure. Theoretically, dermal exposure to liquified 1,3-butadiene could occur during an explosion of a pressurized storage tank or some other catastrophic event; however, no such accidents have been reported in the available literature.

5.2 RELEASES TO THE ENVIRONMENT

5.2.1 Air

The dominant sources for the release of 1,3-butadiene to the atmosphere are fugitive or accidental emissions during its manufacture, use, transport, and storage. Low levels of 1,3-butadiene are constantly emitted to the atmosphere from many sources including exhaust from motor vehicle engines using petroleum-based fuels.

A correlation of data from the EPA Air Toxic Emission Inventory with industrial source codes (SIC) indicates that volatile emissions of 1,3-butadiene are associated with 14 different industrial classifications, which are dominated by rubber and chemical products (Pacific Environmental Services 1987). Fugitive emissions of 1,3-butadiene from seals, valves, vents, flanges, and the like in petrochemical plants manufacturing this compound were estimated to be 1,112 metric tons/year (Hughes et al. 1979). The authors believed that this level of release was lower than that released by refineries. Emissions of 1,3-butadiene from equipment leaks and process vents in 1984 were estimated at 3.8 million pounds/year during its production, 5 million pounds/year during the synthesis of styrene-butadiene copolymers,

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900,000 pounds from polybutadiene production, and 86,000 pounds from neoprene/chloroprene production (Mulling 1990).

According to the TRI (1989), 155 facilities that manufacture or process 1,3-butadiene released an estimated 9,205,532 pounds of this compound to the atmosphere in 1987. The largest air emission from a single facility was 960,000 pounds. The quality of the TRI data must be viewed with caution because the 1987 data represent first-time reporting by these facilities. Only certain types of facilities were required to report. This is not an exhaustive list. TRI data can be found in Table 5-1.

1,3-Butadiene is a component of motor vehicle exhaust; this is a constant source of release to the atmosphere (Stump and Dropkin 1985). In high-traffic areas, the release of 1,3-butadiene to the atmosphere occurs continually. In a recent study, it was measured in the exhaust of typical automobiles and light trucks using both winter and summer gasoline formulations and accounted for up to 0.12% of total hydrocarbon emissions (Stump et al. 1989). An earlier study determined that the concentration of 1,3-butadiene in automobile exhaust was 20-60 ppb (Neligan 1962). 1,3-Butadiene has also been detected in the exhaust of diesel engines (Hayano et al. 1985) and high-altitude jet aircraft engines operating under simulated conditions (Katzman and Libby 1975). 1,3-Butadiene has also been identified in modern formulations of unleaded gasolines (Sigsby et al. 1987) and may be released to the atmosphere by direct volatilization from the fuel.

There are several minor sources for the release of 1,3-butadiene to the atmosphere; all involve the thermal breakdown of other materials. 1,3-Butadiene has been detected as a component of the sidestream smoke from cigarettes (Bartle et al. 1969; Blomberg and Widmark, 1975). The average amount of 1,3-butadiene in sidestream cigarette smoke is 205-361 µg/cigarette (Brunnemann et al., 1990), with an average airborne yield of 400 µg/cigarette (Lofroth et al. 1989). The burning of plastics or rubber has been shown to release small amounts of 1,3-butadiene (Miller 1978). In a test designed to simulate a real-life electrical overload condition, 1,3-butadiene was detected when polyurethane coated wire was heated to 250°C for 40 minutes, (Rigby 1981). 1,3-Butadiene has also been measured as a component of the smoke from a brush fire (Stephens and Burlison 1969), and as a stack emission from waste incinerators (Junk and Ford 1980). The concentrations of 1,3-butadiene were not presented in these studies.

5.2.2 Water

Very limited data on release of 1,3-butadiene to environmental waters were located in the available literature. According to the TRI (1989), 155 facilities that manufacture or process 1,3-butadiene discharged an estimated total of 432,857 pounds of 1,3-butadiene to surface water in 1987. A single facility was responsible for 430,000 pounds of this discharge.

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Transfer of 1,3-butadiene to publicly owned treatment works (POTWs) amounted to 56,490 pounds in 1987 (TRI 1989). The quality of the TRI data must be viewed with caution because the 1987 data represent first-time reporting by these facilities. Only certain types of facilities were required to report. This is not an exhaustive list.

5.2.3 Soil

Limited data on releases of 1,3-butadiene to soil were located in the available literature. According to the TRI (1989), 155 facilities that manufacture or process 1,3-butadiene released an estimated total of 3,672 pounds of 1,3-butadiene to land in 1987. However, the quality of the TRI data must be viewed with caution because the 1987 data represent firsttime reporting by these facilities. Only certain types of facilities were required to report. This is not an exhaustive list.

5.3 ENVIRONMENTAL FATE

5.3.1 Transport and Partitioning

Experimental data on the partitioning of 1,3-butadiene in the environment were not located in the available literature. The following discussion on the partitioning of 1,3-butadiene in the environment is based on the physical and chemical properties of this compound. The estimation techniques used in this discussion are well-established in the literature; however, without adequate experimental data, we do not know exactly how this compound will behave in the environment.

The high volatility of this compound suggests that it will partition predominantly to the atmospheric compartment, where it is not expected to be adsorbed to particulate matter to any significant extent (Eisenreich et al., 1981).

An estimated Henry's law constant of 7.05×10^{-2} atm/m³-mol at 25°C can be obtained using the method of Hine and Mookerjee (1975). Based on this value, the half-life for volatilization of 1,3-butadiene from a model river 1 m deep, flowing at 1 m/set, with a wind velocity of 3 m/set is 2.2 hours (Lyman et al. 1982). Based on an experimental log octanol/water partition coefficient of 1.99 (Hansch and Leo 1985), a calculated soil adsorption coefficient of 288 (Lyman et al. 1982) suggests that adsorption to sediment and suspended organic matter will not be a significant fate process. From the log octanol/water partition coefficient, a calculated bioconcentration factor of 19 (Lyman et al. 1982) indicates that 1,3-butadiene will not bioconcentrate in fish and aquatic organisms to any significant extent. However, no experimental data have been located to verify these theoretical values.

If released to soil, 1,3-butadiene is expected to volatilize rapidly from either moist or dry soil to the atmosphere. This follows from the estimated

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lack of any appreciable adsorption to soil, and consideration of 1,3-butadiene's calculated Henry's law constant for moist soil or its vapor pressure, 2,100 mmHg at 25°C (Daubert and Danner 1985), for dry soil. Both values suggest a rapid rate of volatilization from their respective media.

The calculated soil adsorption coefficient of 288 (Hansch and Leo 1985; Lyman et al. 1982) suggests that 1,3-butadiene may display moderate mobility in soil (Swann et al. 1983). However, the expected rapid rate of volatilization and the possibility of rapid degradation in soil suggest that there is little potential for 1,3-butadiene to leach into groundwater. But until adequate groundwater monitoring for 1,3-butadiene has been performed, the partitioning of 1,3-butadiene in soil cannot be adequately addressed.

5.3.2 Transformation and Degradation

5.3.2.1 Air

Butadiene is a reactive, electron-rich chemical that is expected to undergo rapid reactions with the electrophilic oxidants typically present in the atmosphere: ozone, photochemically produced hydroxyl radicals, nitrate radicals, and molecular oxygen. Among these, the most rapid reaction in the atmosphere is with photochemically produced hydroxyl radicals.

The atmospheric destruction of 1,3-butadiene by photo-initiated processes has been established empirically by early studies. These studies typically involved irradiating urban air samples in atmospheric chambers of varying complexity and monitoring the disappearance of each constituent. Using this technique, 1,3-butadiene, at an average concentration of 12.4 ppb, disappeared in 6 hours when irradiated with natural sunlight during October (Kopczynski et al. 1972). In another study, a half-life of 2 hours was determined for the atmospheric removal of 1,3-butadiene using natural sunlight in October or November (Altshuller et al. 1970). In smog chamber studies, the sunlight oxidation of 1,3-butadiene led to the formation of fairly potent eye irritants, suggesting destruction of this compound with concomitant formation of oxygenated species (Dimitriades et al. 1975; Heuss and Glasson 1968). It is believed that the destruction of 1,3-butadiene occurs by photo-initiated bimolecular processes rather than direct photochemical degradation (Kopczynski et al. 1972). It is important to note that the rate of destruction of 1,3-butadiene when it was irradiated with natural light depended on the time of day in which the irradiation occurred. Furthermore, these studies were performed in October and November, when the amount and the intensity of available sunlight is diminished over that of summer months; thus, these values probably represent the high end of the compound's atmospheric lifetime. The individual processes responsible for the destruction of 1,3-butadiene in the atmosphere are discussed below.

Numerous studies have determined the rate constant for the gas-phase reaction of 1,3-butadiene with photochemically produced hydroxyl radicals

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(Atkinson 1985; Atkinson and Aschmann 1984; Atkinson et al. 1977, 1979; Maldotti et al. 1980). The experimental rate constant 6.85×10^{-11} cm³/molecule-sec at 26°C (Atkinson et al. 1977) is representative. Given an average hydroxyl radical concentration of 5×10^5 molecule/cm³ (Atkinson 1985), the half-life for this second-order process is 5.6 hours. In an attempt to classify the potential for atmospheric destruction of organic compounds by hydroxyl radicals, a rating system based on nonreactive methane (class I) to highly reactive compounds (class V) was established (Darnall et al. 1976). In this classification system, 1,3-butadiene was assigned between classes IV and V, signifying its high reactivity towards photochemically produced hydroxyl radicals.

Gas-phase 1,3-butadiene also reacts with ozone in the atmosphere. Rate constants ranging from 6.7×10^{-18} to 8.4×10^{-18} cm³/molecule-sec at 25°C have appeared in the literature (Atkinson and Carter 1984; Jaspar et al. 1974). Using an average atmospheric ozone concentration of 7×10^{11} molecules/cm³ (Atkinson and Carter 1984), half-lives ranging from 1.4 to 1.7 days can be calculated for this second-order process. Therefore, the reaction of 1,3-butadiene with ozone is expected to contribute to the overall destruction of atmospheric 1,3-butadiene. The initial products from the reaction of 1,3-butadiene with ozone are acrolein, formaldehyde, acetylene, ethylene, and formic anhydride (Niki et al. 1983). All of these products are susceptible to secondary reactions with ozone and other atmospheric oxidants.

1,3-Butadiene can also be destroyed in the atmosphere by the reaction with ground-state, triplet oxygen. Rate constants for this addition reaction range from 1.9×10^{-11} to 2.07×10^{-11} cm³/molecule-sec (Atkinson and Pitts 1977; Gaffney and Levine 1979; Nip et al. 1979), in a reaction that appears to be essentially independent of temperature (Nip et al. 1979). Given the average atmospheric concentration of oxygen of 2.54×10^4 molecules/cm³ (Graedel et al. 1986), the half-life for the destruction of 1,3-butadiene by this process can be calculated as 15-16 days. Although this reaction will not be significant under conditions where the facile pathways described above are operating, it may occur under conditions where they are not.

The night-time degradation of 1,3-butadiene is also expected to occur via the gas-phase reaction with nitrate radicals; this tends to be significant in urban areas, where the concentration of this oxidant is typically higher than in rural areas (Altshuller and Cohen 1964; Gay and Bulfalini 1971; Maldotti et al. 1980). A rate constant of 5.4×10^{-14} cm³/molecule-sec at 22°C has been determined for this reaction. This corresponds to a half-life of 14.9 hours using an average atmospheric nitrate radical concentration of 2.4×10^8 molecule/cm³ (Atkinson et al. 1984), typical of mildly polluted urban centers. Acrolein has been identified as a primary product of this reaction.

In summary, there are four gas-phase pathways that can destroy 1,3-butadiene in the atmosphere. Depending on local conditions, any one or all of these reactions may occur. Destruction of atmospheric 1,3-butadiene by

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the gas-phase reaction with photochemically produced hydroxyl radicals is expected to be the dominant photo-initiated pathway. Destruction by nitrate radicals is expected to be a significant night-time process in urban areas.

5.3.2.2 Water

Data on the degradation of 1,3-butadiene in aquatic systems are limited. Experimental data are restricted to microbial degradation studies performed under aerobic conditions. The bulk of these data were obtained from isolated Bacterial strains, not with mixed microbial populations typically found in natural systems. 1,3-Butadiene biodegraded when inoculated with methane-utilizing, or methanotrophic, organisms under aerobic conditions. Cell suspensions of these bacteria oxidized 1,3-butadiene to 3,4-epoxybutene (Hou et al. 1979, 1980; Patel et al. 1982a). None of the authors reported further degradation of the epoxide to the corresponding diol.

Bacteria isolated from lake water and raised on propane also oxidized 1,3-butadiene to 3,4-epoxybutene (Hou et al. 1983). 1,3-Butadiene was listed as a synthetic organic chemical that should degrade in a biological sewage treatment system, provided that suitable acclimation could be achieved, although no experimental details were provided (Thorn and Agg 1975).

A Nocardia species isolated from water and soil completely degraded 1,3-butadiene to acetic acid under aerobic conditions (Watkinson and Somerville 1976). The proposed route for this degradation involves initial stereospecific epoxidation to but-3-ene-1,2-epoxide followed by ring opening to but-3-ene-1,2-diol, oxidation to the corresponding α -keto acid (2-ketobutyrate-3-ene), loss of CO₂ to acrylic acid, hydroxylation to 2-hydroxypropionic acid, oxidation to pyruvic acid, and loss of CO₂ to acetic acid. This pathway is described in Figure 5-2 (Verschueren 1983; Watkinson and Somerville 1978). Although this pathway is reasonable, experimental evidence establishing the formation of all the key intermediates was not provided. Most importantly, cleavage of the initially formed epoxide was not rigorously established. No data were located on the biodegradation of 1,3-butadiene under anaerobic conditions.

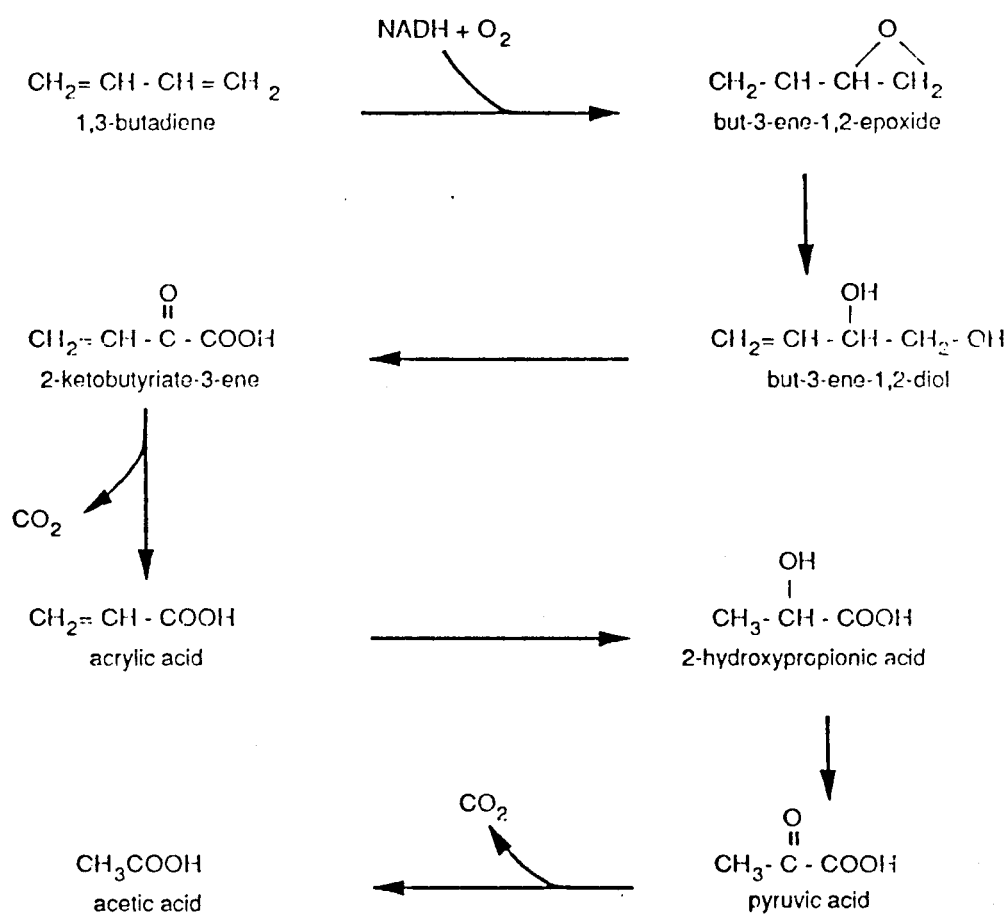
5.3.2.3 Soil

As is the case for the degradation of 1,3-butadiene in water, very limited data on the destruction of this compound in soil could be located in the available literature. The experimental data obtained from pure culture studies on the microbial degradation of 1,3-butadiene suggest that this compound can biodegrade in soil.

Methane-utilizing bacteria isolated from the soil of an oil refinery epoxidized 1,3-butadiene under aerobic conditions (Hou et al. 1979; Patel et al. 1979, 1982a, 1982b). Cell suspensions of Mycobacterium obtained from soil and raised on ethylene oxidized 1,3-butadiene under aerobic conditions;

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FIGURE 5-2. Catabolic Pathway for the Biodegradation of 1,3-B. by *Norcardia* Cultures in Aqueous Media*



*Source: Verschueren 1983; Watkinson and Somerville 1976

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however, cultures raised on ethane or succinate did not (DeBont et al. 1979). Microorganisms isolated from soil (Nocardia, Mycobacterium, Xanthobacter, and Pseudomonas) and raised on gaseous alkenes oxidized 1,3-butadiene to the corresponding epoxide under aerobic conditions (VanGinkel et al. 1987). These bacteria may convert the initially formed epoxide to the diol, although no evidence was presented to support this point.

A Nocardia species isolated from soil and water degraded 1,3-butadiene under aerobic conditions to acetic acid (Watkinson and Somerville 1976). The proposed sequence for this transformation is described in Section 5.3.2.2 and presented in Figure 5-2. No data on the degradation of 1,3-butadiene under anaerobic soil conditions were located in the available literature.

5.4 LEVELS MONITORED OR ESTIMATED IN THE ENVIRONMENT

5.4.1 Air

In an analysis of the ambient air monitoring data for the United States contained in published and unpublished experimental reports from 1970 to 1987, Shah and Heyerdahl (1988) compiled median daily concentrations for volatile organic compounds. For 1,3-butadiene, the median concentrations are 0.29 ppb in urban areas, 0.32 ppb in suburban areas, and 0.10 ppb in rural areas. The value for rural areas must be interpreted carefully, as it is based on only two data points. The suburban and urban values are based on 196 and 385 data points, respectively. Representative data on the concentration of 1,3-butadiene in urban and remote areas can be found in Table 5-2. Reports on the detection of 1,3-butadiene in urban areas have also been published from areas monitored in the Netherlands (Guicherit and Schulting 1985), Australia (Mulcahy et al. 1976), and South Africa (Louw et al. 1977).

On a monitoring trip in 1986, the Texas Air Control Board (1990) measured ambient air concentrations within a mile of a petrochemical complex in Allendale, Texas, suspected of exceeding air quality limits. The average concentration of 1,3-butadiene was 100 ppb, with the highest daily and hourly average measured at 143 and 905 ppb, respectively. A 1989 monitoring trip to Port Neches, Texas, found that air samples within 1 mile of another petrochemical complex had a highest 1 hour average 1,3-butadiene concentration of 642 ppb and a highest 12-hour average concentration of 240 ppb. This manufacturing plant was also suspected of exceeding air quality limits. The highest single value for 1,3-butadiene measured in this study was 1,740 ppb. Residential areas were located near the monitoring stations used in these two studies.

1,3-Butadiene has been detected in indoor air samples. The concentrations of 1,3-butadiene in a tavern were 11 and 19 $\mu\text{g}/\text{m}^3$ (4.98 and 8.60 ppb) in two separate studies, while the outside air concentration was less than or equal to 1 $\mu\text{g}/\text{m}^3$ (0.45 ppb) at the same time (Lofroth et al. 1989). The difference in the indoor versus outdoor concentration may be

TABLE 5-2. Detection of 1,3-Butadiene in Air

Media type/location	Sampling dates	No. of samples	Concentration (ppb)		Reference
			Range	Mean	
<u>Urban</u>					
Houston, TX	1973	9	ND-150 ^a	33.4 ^a	Lonneman et al. 1979
	1974	7	8.0-57	27.2	
	1974	4	ND-8.4	3.0	
Los Angeles, CA	1968	NS	NS	12.4 ^a	Kopczynski et al. 1972
Riverside, CA	1965-66	8	ND-2.0	NS	Stephens and Burleson 1967
Los Angeles, CA	1960	16	ND-9	3.1	Neligan 1962
Boone, NC	1981-82	3	ND-0.34 ^a	0.11	Seila et al. 1984
Boone, NC (downtown)		3	0.34-5.0	4.2	
Boone, NC (outskirts)		3	0.11-0.22	0.15	
<u>Remote</u>					
Roan Mt., NC	1981-82	3	ND-0.22 ^a	0.74	Seila et al. 1984
Grandfather Mt., NC		3	ND-0.15	0.37	
Linville Gorge, NC		3	ND-0.45	0.19	

^aData reported in ppbC (parts per billion carbon). Converted to ppb using the conversion factor 1 ppb = 1.12 ppbC (54.1 ppb/48.4 ppbC)

ND = below detection limit

NS = not stated

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ascribed to the presence of 1,3-butadiene in cigarette smoke. The concentration of 1,3-butadiene in a smoke-filled bar was 2.7-4.5 $\mu\text{g}/\text{m}^3$ (1.2-2.0 ppb) (Brunnemann et al. 1990). 1,3-Butadiene was also detected in a public building in Riverside, California, in 1965 at a concentration of 9.0 ppb, although its source was not specified (Stephens and Burleson 1967).

5.4.2 Water

Limited data on the occurrence of 1,3-butadiene in water were located in the available literature. 1,3-Butadiene was found in 1 of 204 water samples taken in 1975-76 from surface waters near known industrialized areas across the United States. The single positive sample was obtained in the Carquinez Strait, Posta Corta, California, at an approximate concentration of 2 ppb (Ewing et al. 1977).

No specific data on its presence in drinking water, such as monitoring dates or concentration, were located; however, 1,3-butadiene has been qualitatively detected in U.S. drinking water (EPA 1978; Kraybill 1980).

5.4.3 Soil

No data on the occurrence of 1,3-butadiene in soil were located in the available literature.

5.4.4 Other Environmental Media

1,3-Butadiene is used to manufacture synthetic rubber and plastics that are frequently used for food packaging. Because residual 1,3-butadiene may be present in the polymers used to make the containers, both the packaging and the food contained therein have been analyzed. In one study, 1,3-butadiene at a concentration of 8-9 ng/g (ppb) was detected in 3 of 3 brands of olive oil packaged in 1,3-butadiene rubber-modified acrylonitrile-acrylic bottles (McNeal and Breder 1987). Analysis of the bottles themselves found 1,3-butadiene residues as high as 6600 ng/g (ppb). Soft-plastic packaging tubs used as containers for potato salad, cottage cheese, and yogurt had residual 1,3-butadiene levels in the range 21-1700 ng/g (ppb). However, no 1,3-butadiene was detected in any of the food packed in these containers (detection limit 1 ppb). Chewing gum made with a 1,3-butadiene rubber base did not show residual traces of this diene (McNeal and Breder 1987). Soft plastic margarine tubs from five major name brands in the United Kingdom contained 1,3-butadiene residues ranging from 5 to 310 $\mu\text{g}/\text{kg}$ (ppb), but none of the monomer was detected in the margarine samples themselves (detection limit 0.2 $\mu\text{g}/\text{kg}$) (Startin and Gilbert 1984). The authors concluded that migration of the 1,3-butadiene monomer from plastic packaging to food is unlikely to present a problem. Residual levels of 1,3-butadiene in food containers are closely regulated by the Food and Drug Administration.

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5.5 GENERAL POPULATION AND OCCUPATIONAL EXPOSURE

1,3-Butadiene is almost always present in the air at low levels due to its emission from motor vehicles. Therefore, the general population is probably routinely exposed to ppb levels of this compound, although adverse health effects have not been noted at this level of exposure. Exposure to 1,3-butadiene by the general population is expected to be dominated by inhalation. Low level exposure by ingestion of contaminated drinking water may also occur as 1,3-butadiene has been qualitatively detected in U.S. drinking water supplies (EPA 1978; Kraybill 1980).

Inhalation of 1,3-butadiene by the general population may also occur due to other sources. 1,3-Butadiene has been identified in cigarette smoke; therefore, smokers and those nearby are exposed to this compound (Lofroth et al. 1989; Bartle et al. 1969; Blomberg and Widmark 1975; Brunnemann et al. 1990). Limited data suggest that 1,3-butadiene is present in the smoke from brush fires (Stephens and Burleson 1969), suggesting that inhalation of the smoke from wood fires will lead to low level exposure to 1,3-butadiene. Its presence in waste incinerator emissions (Junk and Ford 1980) suggests that exposure to the general population may occur for those living nearby. Due to its presence in gasoline formulations (Sigsby et al. 1987; Stump et al. 1989), members of the population who pump their own gasoline may inhale small amounts of 1,3-butadiene. The concentration of 1,3-butadiene in gasoline vapor is 4.4 ppb (IARC 1986). Small amounts of 1,3-butadiene are produced by the thermal degradation of polyurethane-coated wire, an event that may occur during an electrical overload (Rigby 1981). The thermal degradation of other 1,3-butadiene-based plastics or rubbers may produce 1,3-butadiene (Miller 1978), also leading to low-level exposure of the general population by inhalation.

If the mean daily urban air concentration of 1,3-butadiene is 0.29 ppb, as determined in an analysis and compilation of experimental reports of ambient monitoring data obtained from 1970 to 1987 (Shah and Heyerdahl 1988), a nonoccupational daily intake of 12.8 μg per person can be obtained based on an average human intake of 20 m^3 air/day.

No data are available that quantify general population exposure to 1,3-butadiene by other routes of intake, such as ingestion of contaminated drinking water. Given that residues of 1,3-butadiene have been found in plastic and rubber food containers and in a few samples of the food contained in these containers (McNeal and Breder 1987), very low-level exposure to the general population may occur by ingestion of contaminated foods packaged in these containers. 1,3-Butadiene has been identified as a constituent of modern gasoline formulations, and the general population may receive dermal exposure to 1,3-butadiene upon contact with gasoline (Sigsby et al. 1987), although the rate of absorption of 1,3-butadiene through the skin has not been investigated.

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According to the National Occupational Exposure Survey (NOES) conducted by NIOSH between 1980 and 1983, 9,456 workers, of which 286 are women, were estimated to be exposed to 1,3-butadiene (NIOSH 1989). The NOES database does not contain information on the frequency, concentration, or duration of exposure of workers to any chemicals listed therein. These surveys provide only an estimate of the number of workers potentially exposed to chemicals in the workplace. Occupational exposure to 1,3-butadiene is expected to be limited to inhalation of this compound, although dermal contact with liquified 1,3-butadiene may occur during a large spill, tank explosion, pipeline rupture, or similar catastrophic event, although no reports of this type have been reported in the available literature. Specific industrial classifications or job descriptions involving exposure to 1,3-butadiene are provided below.

A field study conducted in the process control room of a styrenebutadiene rubber plant using 12 different sampling locations concluded that the 1,3-butadiene concentration ranged from 0.044 to 6.5 ppm over a 3-day testing period (Jones and Harris 1983). Health hazard evaluation surveys conducted by NIOSH at six facilities utilizing 1,3-butadiene found that the air concentration ranged from 0.06 ppm to 39 ppm. These facilities manufactured helmets, visors, synthetic rubber, rubber tires and tubes, automotive weather stripping, braided hoses, or plastic components for aircraft. According to this NIOSH report, workers involved in the industrial classifications listed in Table 5-3 have been potentially exposed to 1,3-butadiene (NIOSH 1984). A walk-through survey of 11 monomers, 17 polymers, and 2 end-user plants found that personal exposures ranged from less than 0.006 ppm to 374 ppm (Fasen et al. 1990).

Environmental sampling at two Texas styrene butadiene rubber plants had time-weighted average concentrations of 1,3-butadiene ranging from 0.11 to 4.17 ppm (mean, 1.24 ppm) and 0.34 to 174 ppm (mean, 13.5 ppm) for samples taken in 1977 (Meinhardt et al. 1982). The range of 1,3-butadiene concentrations for individuals at the plant is given in Table 5-4.

5.6 POPULATIONS WITH POTENTIALLY HIGH EXPOSURES

High levels of exposure to 1,3-butadiene are likely to be limited to those resulting from an occupationally related use of this compound. Inhalation is the most likely route of high exposure to 1,3-butadiene. 1,3-Butadiene is stored and transported in pressurized tanks, and it is possible that high levels of exposure by inhalation or dermal contact with the liquified gas may occur during the loading and unloading of these tanks, or by the accidental rupture of these tanks. However, no such accidents have been reported in the available literature.

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TABLE 5-3. Industrial Workers Potentially Exposed to 1,3-Butadiene^a

Industry	Number of workers exposed
Paper and allied products	1,221
Chemicals and allied products	44,980
Petroleum and coal products	84
Rubber and plastic products	9,086
Primary metal industries	55
Fabricated metal products	96
Machinery, except electrical	1210
Electrical equipment and supplies	121
Transportation equipment	175
Instruments and related products	145
Miscellaneous manufacturing industries	2244
Miscellaneous business services	5339
Medical and other health services	493

^aDerived from NIOSH 1984

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TABLE 5-4. Air Concentrations of 1,3-Butadiene in a Styrene Butadiene Rubber Plant^a

Affected individuals	Concentration (ppm)
Technical services personnel	0.21-114.6
Production foreman	1.16 (1 sample)
Head production operator	0.25-69.61
Production operator	0.23-33.21
Operator helper	0.26-1.81
Pipefitter	0.18-1.78
Electrician	0.18-0.34
Maintenance mechanic	0.19-44.38
Carpenter	0.20-30.60
Common laborer	0.17-8.22
Instrument man	0.17-174.14

^aDerived from Meinhardt et al. 1982

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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 1,3-butadiene is available. Where adequate information is not available, ATSDR, in conjunction with the National Toxicology Program (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 1,3-butadiene.

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 properties of 1,3-butadiene are well documented (Sax and Lewis 1987; Windholz et al. 1983), and its environmental fate can be estimated from these properties (Lyman et al. 1982). Experimental verification of these calculated values used to determine the partitioning of 1,3-butadiene in the environment are necessary to establish accurate levels of human exposure.

Production, Import/Export, Use, and Disposal. The trends in the production and use of 1,3-butadiene are well documented (Kirshenbaum 1978; Chemical Marketing Reporter 1980; USITC 1988), and there do not appear to be any critical information gaps. 1,3-Butadiene monomer does not occur in most products used in the home, although residues of this compound in commercial packages, especially food containers (McNeal and Breder 1987), are not well described. Although it is clear that the majority of 1,3-butadiene is released to the atmosphere (TRI 1989), data on the release of 1,3-butadiene are not well correlated with specific sources. The disposal of 1,3-butadiene appears to be a straightforward process (HSDB 1989); however, the amount of 1,3-butadiene released or destroyed annually is not well documented. As the TRI program is improved, this type of information will become more readily available.

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 Toxic Release Inventory (TRI), which contains this information for 1987, became available in May of 1989. This database will be updated yearly and should provide a list of industrial production facilities and emissions.

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Environmental Fate. The fate of 1,3-butadiene in the atmosphere is well understood (Atkinson 1985; Atkinson and Carter 1984; Atkinson et al. 1984; Kopczynski et al. 1972). The fate of 1,3-butadiene in soil and water is not well understood, and partitioning from these media has to be determined from the physical and chemical properties of this compound (Lyman et al. 1982). A reliable method capable of detecting 1,3-butadiene in soil and water was not located in the available literature, and it is not clear whether 1,3-butadiene is absent from these media or simply not yet detected. The persistence of 1,3-butadiene in soil and water is not known, and the degree of partitioning from one environmental compartment to another can only be estimated. Exposure via ingestion or dermal contact to populations surrounding hazardous waste sites cannot, therefore, be accurately determined. Experimental data that addresses the partitioning of 1,3-butadiene in the environment, its potential to enter drinking water supplies, and its lifetime in soil and water are necessary to completely characterize the environmental fate of this compound.

Bioavailability from Environmental Media. Numerous toxicokinetic and toxicity studies in humans and animals have demonstrated the bioavailability of 1,3-butadiene from air. No data on the bioavailability of 1,3-butadiene from other sources (water or soil, for example) were located in the available literature. In conjunction with the data needs for determining 1,3-butadiene in environmental media, bioavailability studies from environmental media would be useful.

Food Chain Bioaccumulation. In theory, 1,3-butadiene is not believed to bioconcentrate significantly in fish and aquatic organisms; thus, it is not expected to biomagnify in the food chain (Hansch and Leo 1985; Lyman et al. 1982). No data addressing this point, however, were located in the available literature. Validation of these theories by valid experimental studies will aid in establishing a quantitative determination of 1,3-butadiene exposure to the general public.

Exposure Levels in Environmental Media. Data on the levels of 1,3-butadiene in environmental media are limited. Extensive data on the occurrence of 1,3-butadiene in ambient air samples are available (Shah and Heyerdahl 1988), but recent data appear to be lacking. Further, current correlations between the levels of 1,3-butadiene in the atmosphere and its sources of release are not available. Levels of 1,3-butadiene at hazardous waste sites are not available. Data on the occurrence of 1,3-butadiene in water samples are limited (Ewing et al. 1979). The presence of 1,3-butadiene in drinking water has been noted in the literature, but no concentrations or frequency of detection are available (EPA 1978; Kraybill 1980). The concentration of 1,3-butadiene in soil, water, and air at hazardous waste sites is not known (CLPSD 1989); therefore, the potential for exposure to populations residing nearby cannot be established. The development of reliable analytical techniques for the analysis of 1,3-butadiene in soil and

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water will establish unambiguously the levels at which this compound is found in environmental media.

Exposure Levels in Humans. Limited data on levels of occupational exposure to 1,3-butadiene were available in the literature; however, occupational exposure to this compound appears to be limited to a readily definable group of industrial classifications (NIOSH 1984, 1989). Exposure levels for the general population are not well defined. No data on its presence in human tissue were located. Studies that correlate personal exposure with daily activities are necessary to establish adequately exposure levels for 1,3-butadiene. Biological monitoring studies cannot be performed until acceptable experimental techniques are developed. Exposure levels for those living near hazardous waste sites are not available and should be established.

Exposure Registries. No exposure registries for 1,3-butadiene were located. This compound is not currently one for which a subregistry has been established in the National Exposure Registry, but it 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 the compound.

5.7.2 On-going Studies

On-going atmospheric monitoring studies for 1,3-butadiene performed by S. Sigsby have been identified (EPA 1989b), although no other specific information was provided.

Remedial investigations and feasibility studies conducted at the NPL sites known to be contaminated with 1,3-butadiene could add to the available database on exposure levels in environmental media, exposure levels in humans, and exposure registries, and may increase knowledge regarding the fate of 1,3-butadiene in the environment. No other long-term research studies pertaining to the environmental fate of 1,3-butadiene or to occupational or general population exposures to 1,3-butadiene were identified.