

5. POTENTIAL FOR HUMAN EXPOSURE

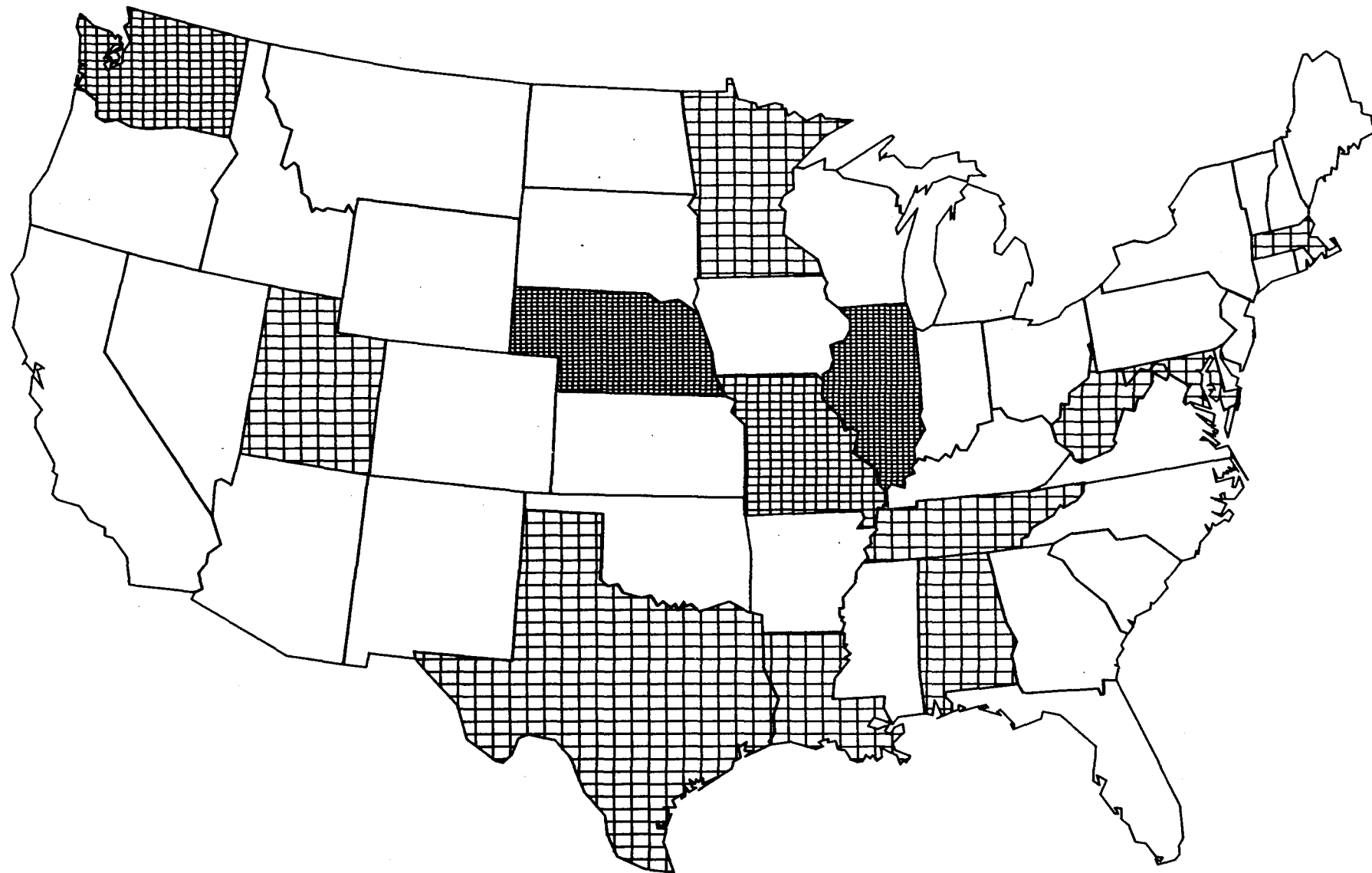
5.1 OVERVIEW

The nitroaromatic compounds 1,3-DNB and 1,3,5-TNB are used in the manufacture of explosives. They are formed as by-products during the manufacture of TNT. 1,3-DNB is also used in the manufacture of industrial solvents and dyes. Effluents from Army ammunition plants are primarily responsible for the releases of both compounds into the environment. When released to the air, both compounds have the potential to undergo photolysis. 1,3,5-TNB will also slowly react with photochemically generated hydroxyl radicals, but this is not a significant fate process. No data were located for 1,3-DNB regarding reaction with hydroxyl radicals. Both compounds are mobile in soil and can leach into the groundwater. Hydrolysis is not expected to be an important fate process since aromatic nitro compounds are generally resistant to chemical hydrolysis under environmental conditions. Both compounds are expected to undergo photolysis in water; however, no photolysis data were located for 1,3,5-TNB. The photolytic half-life of 1,3-DNB in water was 23 days. 1,3-DNB can undergo biodegradation under aerobic and anaerobic conditions in water and soil. 1,3,5-TNB is subject to biodegradation under aerobic conditions in water; however, no data were located regarding anaerobic biodegradation in water or anaerobic and aerobic biodegradation in soil. 1,3-DNB and 1,3,5-TNB have been detected in groundwater and soil in the vicinity of Army ammunition plants at levels ranging from ppb to ppm.

The general population is not likely to be exposed to either 1,3-DNB or 1,3,5-TNB. Exposure to both compounds is expected to be limited to areas around Army ammunition plants and other industries, such as dyestuff, and plastic and rubber manufacturing, where these compounds are used. The most likely route of exposure to these compounds is ingestion of contaminated drinking water.

Both 1,3-DNB and 1,3,5-TNB have been identified in 12 and 14 sites, respectively, of the 1,397 hazardous waste sites on the NPL (HazDat 1994). The frequency of these sites within the United States can be seen in Figure 5-1. It should be noted that the number of sites actually tested for 1,3-DNB and 1,3,5-TNB (from the total 1,397 sites) is unknown.

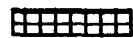
FIGURE 5-1. FREQUENCY OF NPL SITES WITH 1,3-DNB and 1,3,5-TNB CONTAMINATION *



FREQUENCY



1 SITE
2 SITES
3 SITES



2 SITES

*Derived from HazDat 1994

5.2 RELEASES TO THE ENVIRONMENT

5.2.1 Air

Because 1,3-DNB and 1,3,5-TNB are used in the manufacture of explosives, industrial solvents, plastics, rubber, and dyes, they may be released to air as a result of such uses (Hallas and Alexander 1983). It has been reported by DuPont that approximately 60 pounds of 1,3-DNB are released into the atmosphere annually during processing of the compound (EPA 1991b). According to TR192 (1994) data given in Table 5-1, an estimated total of 1,251 pounds of 1,3-DNB, amounting to 100% of the total environmental release, was discharged to the air from the two manufacturing and processing facilities in the United States in 1992. The TRI data should be used with caution since only certain types of facilities are required to report. This is not an exhaustive list.

Since 1,3-DNB has a very low vapor pressure, insignificant amounts would volatilize from water (HSDB 1994; Lyman et al. 1982). Therefore, the amount of 1,3-DNB that might enter the air through evaporation from aquatic effluent streams would be minuscule.

5.2.2 Water

Both 1,3-DNB and 1,3,5-TNB are formed as by-products during the manufacture of TNT and can be released to water in discharges from TNT production facilities and munitions plants (ATSDR 1989a, 1989b; Mitchell and Dennis 1982; Spanggord et al. 1982a). 1,3,5-TNB is also formed as a by-product in TNT photolysis (Army 1987b). 1,3-DNB has been detected in the commercial product TNT and can therefore be present in effluents from munitions blending and loading operations (Mitchell and Dennis 1982). 1,3-DNB can also be produced in water by the photoconversion of the munitions by-product 2,4-dinitrotoluene (Higson 1992). 1,3-DNB is one of many nitroaromatic compounds used in the manufacture of dyes and industrial solvents and may be released to water as a result of such uses (Hallas and Alexander 1983). 1,3-DNB can be released to water through wastes and waste discharges from the dye manufacturing process (Dey and Godbole 1986).

Table 5-1. Releases to the Environment from Facilities that Manufacture or Process 1,3-DNB

Reported amounts released in pounds per year								
State ^a	City	Facility	Air	Water	Underground Land Injection	Total Environment ^b	POTW Transfer	Offsite Waste Transfer
MS	PASCAGOULA	FIRST CHEMICAL CORP.	10			10		105
NJ	DEEWATER	DU PONT CHAMBERS WORKS	1,241			1,241		5
Totals			1,251			1,251		110

Source: TRI92 1994

^aPost office state abbreviations used^bThe sum of all releases of the chemical to air, land, water, and underground injection wells by a given facility

POTW = Publically Owned Treatment Works

5.2.3 Soil

Both 1,3-DNB and 1,3,5-TNB may be released to soil in waste discharges from the manufacture of TNT, or from the disposal of TNT wastes, or wastes from munitions plants (Army 1981, 1984b; ATSDR 1987, 1989c; Spalding and Fulton 1988). 1,3-DNB can be released to soil through wastes and waste discharges from the dye manufacturing process (Dey and Godbole 1986).

1,3-DNB and 1,3,5-TNB were not listed in the CLPSD of chemicals detected in soil samples taken at NPL sites only (CLPSD 1989).

5.3 ENVIRONMENTAL FATE

5.3.1 Transport and Partitioning

The estimated vapor pressure of 1,3-DNB is <1.0 mm Hg at 20°C (HSDB 1994), indicating that 1,3-DNB will exist entirely in the vapor phase in the atmosphere (Eisenreich et al. 1981). Based on a vapor pressure of 3.2×10^{-6} mm Hg at 25°C (see Table 3-2) 1,3,5-TNB is expected to exist partly in the vapor phase and partly in the particulate phase (Eisenreich et al. 1981). The transport of vapor phase 1,3-DNB from the atmosphere to the terrestrial surface is likely to occur mainly by wet deposition, while 1,3,5-TNB is likely to be transported by both wet and dry deposition (Bidelman 1988).

The partitioning of 1,3-DNB in water between water and the suspended solid and sediment has been estimated. Simulation studies based on the octanol-water partition coefficient predict that $>99\%$ of 1,3-DNB will remain in the water column and $<1\%$ will be adsorbed to suspended solid and sediment (EPA 1991b). 1,3,5-TNB with an octanol-water partition coefficient value lower than 1,3-DNB (see Table 3-2), is expected to exist almost exclusively in the water column.

Henry's law constant for 1,3-DNB was estimated to be 2.33×10^{-6} atm-m³/mol (HSDB 1994). Based on this value, volatilization from deep quiescent water bodies is expected to be a slow fate process for 1,3-DNB (Lyman et al. 1982). Henry's law constant for 1,3,5-TNB was estimated to be 3.08×10^{-9} atm-m³/mol at 25°C using a group structural estimation method (Hine and Mookerjee 1975; HSDB 1994). Based on this value, 1,3,5-TNB is essentially nonvolatile (Lyman et al. 1982). This means

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that it is very unlikely that large amounts of either 1,3-DNB or 1,3,5-TNB would be released into the air from contaminated waters.

The soil organic carbon adsorption coefficient (K_{oc}) values for 1,3-DNB and 1,3,5-TNB were calculated to be 213.8 and 75.86, respectively (Army 1987b). Based on these K_{oc} values, 1,3-DNB and 1,3,5-TNB are expected to exhibit moderate and high mobility, respectively, in soil; thus, both compounds can leach into groundwater (Swann et al. 1983). However, nitroaromatic compounds show stronger binding toward clay minerals in soil as a result of complex formation between electron donor groups present at mineral surfaces and electron accepting properties of nitroaromatics (Haderlein and Schwarzenbach 1993). This effect is expected to significantly decrease the mobility of such compounds in soil (Haderlein and Schwarzenbach 1993).

The logarithm of the n-octanol/water partition coefficient ($\log K_{ow}$) is a useful preliminary indicator of the bioconcentration potential of a compound. The calculated $\log K_{ow}$ values for 1,3-DNB and 1,3,5-TNB are 1.52 and 1.18 (Deneer et al. 1987), respectively, suggesting a low potential for bioaccumulation. An experimental bioconcentration factor (BCF) of 1,3-DNB for the guppy, *Poecilia reticulata*, was reported to be 74.13 (Deneer et al. 1987). This BCF indicates that bioaccumulation in aquatic organisms is not an important fate process. BCF data were not located for 1,3,5-TNB.

The uptake, distribution, and metabolism of 1,3-DNB were studied in hydroponically grown mature soybean plants (McFarlane et al. 1987a). Initial uptake rate constants of 1,3-DNB by soybean plants determined by measuring either chemical loss from solution, ^{14}C concentration in plants, or root uptake were similar, ranging from 17 to 22.2 mL/minute. 1,3-DNB remained mostly in the roots, and ^{14}C was slowly translocated to the shoots. Examination of ^{14}C in the leaves indicated that the translocated chemicals were probably degradation products rather than 1,3-DNB and were metabolized in the roots. The degradation products, however, were not identified (McFarlane et al. 1987a).

No studies were located regarding plant uptake of 1,3,5-TNB.

5.3.2 Transformation and Degradation

5.3.2.1 Air

Based on an estimated reaction rate constant of 1.3×10^{-15} cm³/mol-second at 25 °C and an average hydroxyl radical concentration of 5.0×10^5 molecule/cm³, the half-life for the reaction of 1,3,5-TNB vapor with photochemically generated hydroxyl radicals in the atmosphere has been estimated to be 34 years (Atkinson 1985, 1987; HSDB 1994). No data were located regarding the photooxidation of 1,3-DNB. Although no data were located regarding direct photolysis of 1,3-DNB or 1,3,5-TNB, both compounds have the potential to photolyze when exposed to sunlight because both can absorb light at wavelengths greater than 290 nm (EPA 1976; Mill and Mabey 1985).

5.3.2.2 Water

No data were located regarding the hydrolysis of 1,3-DNB and 1,3,5-TNB. However, neither compound is expected to undergo hydrolysis since aromatic nitro compounds are generally resistant to chemical hydrolysis under environmental conditions (Lyman et al. 1982). The transformation of 1,3-DNB in water due to reactions with oxidants present in natural bodies of water is not expected to be important in environmental fate processes (EPA 1991b).

If released to water, 1,3-DNB and 1,3,5-TNB may be subject to direct photolysis when exposed to sunlight because both compounds can absorb light at wavelengths greater than 290 nm (EPA 1976; Mill and Mabey 1985). However, no data were located regarding the photolysis of 1,3,5-TNB in water. The photolytic half-life of 1,3-DNB in pure water was calculated to be 23 days (Simmons and Zepp 1986). A three- to four-fold increase in the rate of photoreaction of 1,3-DNB was observed in ambient waters containing natural humic substances or in distilled water containing dissolved humic materials compared to reaction without humic substances (Simmons and Zepp 1986). This enhancement of the reaction rate has been attributed to catalysis of the photoreaction by photosensitization effects of humic substances.

The biodegradation of 1,3-DNB in water requires the presence of microorganisms that are acclimated to 1,3-DNB (EPA 1991b). Therefore, biodegradation of 1,3-DNB is not likely to occur in pristine waters. A mixed bacterial culture, with *Pseudomonas* predominating, adapted to metabolize phenol as

the sole source of carbon had the ability to degrade 100 mg/L 1,3-DNB and 1,3,5-TNB under aerobic conditions (Chambers et al. 1963). Both compounds were slowly oxidized, and 1,3-DNB was degraded at a slower rate than 1,3,5-TNB. Cultures to which 1,3-DNB and 1,3,5-TNB were added had oxygen uptake values ranging from 1.8 to 2.0 times the endogenous rates after 210 and 180 minutes, respectively (Chambers et al. 1963). In this experiment, the resistance of the nitrobenzenes to degradation seemed to decrease as the number of nitro groups on the benzene ring increased (Chambers et al. 1963).

The degradability of 1,3-DNB by microorganisms was studied in environmental samples and in laboratory cultures under aerobic conditions (Mitchell and Dennis 1982). After 21 days of incubation of 5 µg/mL 1,3-DNB with Tennessee River water samples taken downstream from the Volunteer Army Ammunition Plant (a munitions production facility in Chattanooga, Tennessee), the microbially mediated disappearance of 1,3-DNB was complete (Mitchell and Dennis 1982). The results showed that microorganisms from the Tennessee River could be grown on 1,3-DNB as a sole carbon source and could mineralize the compound. The half-life of 1,3-DNB in Tennessee River samples was estimated to be one day, assuming a total of one million total microorganisms per mL and a temperature of 25 °C. The half-life of 1,3-DNB in enrichment cultures grown on 1,3-DNB was 9.7 days. The authors concluded that the more rapid rate of 1,3-DNB removal seen during primary screening (one day) could result from enhanced biodegradation by microorganisms in a more natural state. Results also showed that the enrichment culture was specific for 1,3-DNB. The Tennessee River microorganisms grown on 1,3-DNB did not adapt to metabolize 1,3-TNB (Mitchell and Dennis 1982).

The transformation of 1,3-DNB was measured in sewage sludge effluent maintained for 28 days under aerobic and anaerobic conditions (Hallas and Alexander 1983). Under aerobic conditions, approximately 40% was degraded in 28 days, while under anaerobic conditions, approximately 80% was degraded in 28 days. Nitroaniline was the product formed from 1,3-DNB degradation under both aerobic and anaerobic conditions (Hallas and Alexander 1983).

5.3.2.3 Sediment and Soil

1,3-DNB was biodegraded under aerobic conditions to carbon dioxide by a microbial strain, *Candida pulcherrima*, isolated from soil contaminated with 1,3-DNB manufacture wastes (Dey and Godbole

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1986). Some biotransformation products detected in the metabolic pathway of biodegradation of 1,3-DNB included *m*-nitrophenol, *m*-aminophenol, resorcinol, fumaric acid, and some volatile fatty acids (Dey and Godbole 1986). A pure culture of *Rhodococcus sp.* isolated from soils contaminated with nitroaromatics was capable of using 1,3-DNB as a sole source of nitrogen. This culture metabolized 1,3-DNB to nitrite via a 4-nitrocatechol pathway even in the presence of high amounts of ammonia (Dickel and Knackmuss 1991).

Sixteen microorganisms isolated from soil exposed to the waste water effluent from 1,3-DNB manufacture had the ability to effectively degrade 1,3-DNB in synthetic media and 1,3-DNB waste under aerobic conditions (Dey et al. 1986). The percentage degradation of 1,3-DNB ranged from 32% to 87% and from 35% to 92% under stationary and shake culture conditions respectively, in a synthetic medium. *Streptomyces aminophilus* showed maximum degradation both under shake and stationary culture conditions, followed by *Streptomyces cacaoi*, *Micromonospora cabali* and *Micrococcus colpogenes*. Data on the percentage degradation of 1,3-DNB, based on the percentage reduction in chemical oxygen demand (COD) of the 1,3-DNB manufacture waste brought about by these organisms, showed that the percentage reduction ranged from 17 to 55% and from 19 to 53% under shake and stationary culture conditions, respectively. *M. colpogenes* gave maximum reduction in COD, followed by *S. aminophilus*, *S. cacaoi*, and *M. cabali*. The effects of different environmental conditions on 1,3-DNB degradation were also examined (Dey et al. 1986). The isolates were inoculated in a synthetic medium and incubated for 7 days under the following conditions: at different temperatures-22, 26, 37, and 40 °C; at different pH levels, ranging from 5 to 11; at different inoculum densities, from 0.3 to 9 million cells per mL of the medium; and with different periods of incubation at room temperature (26 °C) ranging from 3 to 35 days. Under conditions of varying temperature, results showed that for all microorganisms there was a rise in percentage degradation with a rise in temperature from 22 to 37 °C, followed by a steep fall in percentage degradation with a further rise in temperature from 37 to 40 °C. Data on the percentage degradation under different pH levels showed that 13 species belonging to the genera *Streptomyces*, *Micrococcus*, *Staphylococcus*, *Micromonospora*, *Candida*, *Klebsiella*, *Vibrio*, and *Aspergillus* showed maximum degradation ranging from 40 to 87% at pH 9. Only three species belonging to the genera *Bacillus* showed maximum degradation ranging from 38 to 47% at pH 8. Of all the species under study, *S. aminophilus* gave maximum degradation at all pH levels, followed by *S. cacaoi* and *M. colpogenes*. Under conditions of different inoculum densities, data showed that three million cells per mL of the medium as the inoculum density was the optimum for maximum degradation of 1,3-DNB. Under conditions of

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different incubation periods, data showed that with the longest incubation period (35 days), 100% degradation was exhibited by *S. aminophilus*, *S. cacaoi*, *M. caballi*, *M. colpogenes*, *Micrococcus roseus*, *Micrococcus luteus*, *Staphylococcus saprophyticus*, and *Staphylococcus aureus*.

No studies were located regarding the transformation and degradation of 1,3,5-TNB in soil.

5.4 LEVELS MONITORED OR ESTIMATED IN THE ENVIRONMENT

No monitoring studies were located that gave levels of 1,3-DNB or 1,3,5-TNB in air.

5.4.2 Water

1,3-DNB and 1,3,5-TNB were detected in effluent (condensate water) from the production and purification of trinitrotoluene (TNT) (Spangord et al. 1982a). 1,3-DNB was detected in 97.5% of the 54 TNT samples collected over a period of 1 year at concentrations ranging from 0.2 to 8.5 mg/L (ppm) (detection limit not reported). 1,3,5-TNB was detected in 3.8% of the 54 TNT samples at concentrations ranging from 0.06 to 0.20 mg/L (ppm) (Spangord et al. 1982a).

1,3,5-TNB was detected in water from on-site and off-site wells at maximum concentrations of 352 and 114 ppb, respectively, at the Cornhusker Army Ammunition Plant (CAAP) near Grand Island, Nebraska (ATSDR 1989a). CAAP is an NPL site; CAAP is not currently producing or storing explosive materials. Present activities at the plant are limited to maintenance operations, leasing of property for agriculture and livestock grazing, storage building leasing, and wildlife management (ATSDR 1989a). On-site groundwater sampling at the Milan Army Ammunition Plant (MAAP) in Tennessee identified 1,3,5-TNB at concentrations ranging from non-detectable to 976 ppb (ATSDR 1989c). MAAP is an NPL site. From 1942 to 1978, waste water from a munitions demilitarization process line was discharged into unlined settling ponds (ATSDR 1989c). The Louisiana Army Ammunition Plant (LAAP) is a shell manufacturing and explosives load, assembly, and pack facility (Army 1988). From 1951 to 1980, waste waters were trucked to and discharged into a series of artificial leaching pits. This resulted in contamination of groundwater, soil, and sediments (Army 1988). Detectable levels of 1,3-DNB and 1,3,5-TNB measured in groundwater at LAAP ranged from

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1.2 to 195 µg/L (ppb) and from 0.8 to 7,720 µg/L (ppb), respectively (Army 1988). 1,3,5-TNB was also detected in surface water at LAAP at a concentration of 2 ppm (ATSDR 1989b).

5.4.3 Sediment and Soil

1,3,5-TNB has been detected in contaminated soil at the Alabama Army Ammunition Plant in Childersburg, Alabama (Army 1981; ATSDR 1987). The contaminants remain from World War II production activities. The levels of 1,3,5-TNB detected in soil were 614 ppb (smokeless powder manufacturing area), <368-2,540 ppb (magazine area), <368-3,920 ppb and 3,920 ppm (flashing ground), and 1,950 ppm (aniline sludge basin) (Army 1981; ATSDR 1987). 1,3,5-TNB was found on-site at the Savanna Army Depot (Illinois) in soil samples at a maximum concentration of 2,770 ppb (ATSDR 1989d). The Savanna Army Depot is an NPL site. It is an Army munitions plant engaged in munitions renovation, loading, demolition, and burning (ATSDR 1989d). 1,3,5-TNB was detected in soil samples collected from the Iowa Army Ammunition Plant in 1983 (Army 1985a; Jenkins and Grant 1987). Mean levels of 1,3,5-TNB in soil taken from an old ordnance-burning area that had not been used since 1981 ranged from 5.1 to 62 µg/g (Army 1985a; Jenkins and Grant 1987). Mean levels of 1,3,5-TNB taken from the surface of an old disposal lagoon ranged from 0.27 to 0.45 µg/g (Army 1985a; Jenkins and Grant 1987). Mean levels of 1,3-DNB detected in field-contaminated soil at an Army installation in Tennessee ranged from 0.77 to 1.5 µg/g (Jenkins et al. 1989).

5.4.4 Other Environmental Media

5.5 GENERAL POPULATION AND OCCUPATIONAL EXPOSURE

The general population is not likely to be exposed to 1,3-DNB or 1,3,5-TNB. Exposure is expected to be limited to populations in areas around Army ammunition plants where 1,3-DNB and 1,3,5-TNB have been produced. The most likely route of exposure for populations living in the vicinity of the Army ammunition plants is ingestion of contaminated drinking water. Dermal contact with contaminated soil is also a possible but unlikely route of exposure.

Occupational exposure to 1,3-DNB and 1,3,5-TNB can occur when workers handle the compounds in explosives plants and other industries, such as dyestuffs, plastics, and rubber, that use these compounds during manufacturing processes. The National Occupational Exposure Survey (NOES), conducted by

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NIOSH from 1981 to 1983, estimated that 2,489 workers were exposed to 1,3-DNB in 41 businesses and health services (NOES 1991). The workers included in this survey were chemists (except biochemists), geologists, geodesists, clinical laboratory technologists and technicians, and health aides (except nursing).

5.6 POPULATIONS WITH POTENTIALLY HIGH EXPOSURES

Persons living near Army ammunition plants may have a higher risk of exposure to 1,3-DNB and 1,3,5-TNB resulting from ingestion of contaminated drinking water or contact with contaminated soil.

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-DNB and 1,3,5-TNB is available. Where adequate information is not available, ATSDR, in conjunction with 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-DNB and 1,3,5-TNB.

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. 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.

5.7.1 Identification of Data Needs

Physical and Chemical Properties. The physical and chemical properties of 1,3-DNB and 1,3,5-TNB are sufficiently characterized to permit estimation of their environmental fate (Army 1987b; Merck 1989; DeNeer et al. 1987; HSDB 1994). Therefore, no additional studies are needed at this time.

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Production, Import/Export, Use, and Release and Disposal. 1,3-DNB has been produced and used commercially in the United States (HSDB 1994). The information that is available on production volumes of 1,3-DNB is neither complete nor current. DuPont reportedly generates 70,000-72,000 pounds of 1,3-DNB annually from production of nitro- and dinitro-benzenes (EPA 1991b). The production volumes of 1,3-DNB by other manufacturers are not known. Data on current and past production volumes for 1,3-DNB and 1,3,5-TNB needed for the discussion of production trends of these compounds are not available. In 1971, an estimated 10,100 pounds of 1,3-DNB was imported into the United States (EPA 1976). No data on either the past or current import/export volumes for 1,3,5-TNB were located. Therefore, the history of production and import/export data for both 1,3-DNB and 1,3,5-TNB are needed. Both 1,3-DNB and 1,3,5-TNB have been used for their explosive properties (HSDB 1994). 1,3-DNB has been suggested as a possible substitute for the explosive TNT (HSDB 1994). 1,3,5-TNB has been classified as a high explosive and used in explosive compositions (Merck 1989; Sax and Lewis 1987). Commercially, 1,3-DNB has been used in organic synthesis and dyes (McFarlane et al. 1987a). 1,3,5-TNB has been used as a vulcanizing agent in the processing of natural rubber and as an indicator in acid-base reactions in the pH range of 12.0-14.0 (HSDB 1994). Exposure to these compounds is limited to areas around Army ammunition plants. The most likely route of exposure for populations living near Army ammunition plants is ingestion of contaminated drinking water.

Data on the most commonly used disposal methods are sufficient (EPA 1981; HSDB 1994); however, estimates of amounts disposed of by each method are needed. 1,3-DNB, 1,3,5-TNB, and the wastes generated in the manufacture of 1,3-DNB and 1,3,5-TNB are classified as EPA hazardous wastes and disposal must be carried out according to EPA regulations (HSDB 1994).

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 1992, became available in May of 1994. This database will be updated yearly and should provide a list of industrial production facilities and emissions.

Environmental Fate. Based on its low vapor pressure and low value for Henry's law constant (HSDB 1994), it is unlikely that 1,3,5-TNB will partition to the air from soil or natural bodies of water (Lyman et al. 1982). The higher values for vapor pressure and Henry's law constant (HSDB

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1994) for 1,3-DNB suggest that it is likely to volatilize from shallow soil or water, but not from deep quiescent water or deep soil (Hine and Mookerjee 1975; Lyman et al. 1982). Both compounds are mobile in soil and can leach into groundwater. 1,3,5-TNB exhibits a higher mobility than 1,3-DNB (Army 1987b; Swann et al. 1983). Neither compound adsorbs to sediments in water to any great extent (Swann et al. 1983). Both compounds have the potential to undergo direct photolysis in air (EPA 1976; Mill and Mabey 1985); however, no direct atmospheric photolysis studies for either compound were located. Therefore, it would be useful to conduct further research to determine the effect of photolysis of these compounds in the vapor phase diluted with air. The reaction rate of 1,3,5-TNB in the presence of photochemically generated hydroxyl radicals is very slow, with an atmospheric half-life of 34 years (Atkinson 1985, 1987; HSDB 1994). No studies were located for 1,3-DNB regarding its reaction with hydroxyl radicals. Hydrolysis is not expected to be an important fate process for either compound (Lyman et al. 1982). Both compounds are expected to undergo photolysis in water; however, no experimental photolysis data were located for 1,3,5-TNB. Experimental data determining the effects of photolysis of 1,3,5-TNB in water would be useful. The experimental photolytic half-life of 1,3-DNB in water is 23 days, and the reaction is sensitized by humic substances (Simmons and Zepp 1986). 1,3-DNB can undergo biodegradation under aerobic and anaerobic conditions in water and soil (Chambers et al. 1963; Mitchell and Dennis 1982). 1,3,5-TNB is subject to biodegradation under aerobic conditions in water (Chambers et al. 1963); however, no data were located regarding anaerobic biodegradation in water or anaerobic and aerobic biodegradation in soil. Further research on the rates of biodegradation of 1,3,5-TNB in water and soil under anaerobic conditions, and of biodegradation of 1,3,5-TNB in soil under aerobic conditions would provide valuable information. Biodegradation half-life data in water and soil are needed for both compounds. This information will be helpful to better identify the most important pathways of human exposure to each compound.

Bioavailability from Environmental Media. Limited data indicate that 1,3-DNB is absorbed in humans following inhalation and dermal exposure (Ishihara and Ikeda 1979; Okubo and Shigeta 1982). No studies were located regarding absorption of 1,3-DNB following oral exposure. No studies were located regarding absorption of 1,3,5-TNB following inhalation, oral, or dermal exposure. More information regarding all absorption routes for both compounds, particularly on absorption following ingestion of contaminated drinking water and soil or plants grown in contaminated environments, are needed to better characterize the bioavailability of 1,3-DNB and 1,3,5-TNB.

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Food Chain Bioaccumulation. Based on low log K_{ow} values, both compounds have a low potential for bioaccumulation (Deneer et al. 1987). Based on a low experimental BCF for 1,3-DNB, bioaccumulation in aquatic organisms is not an important fate process (Deneer et al. 1987). No BCF data were located for 1,3,5-TNB. Data indicate that 1,3-DNB bioaccumulates in plants (McFarlane et al. 1987a). No studies were located regarding plant uptake of 1,3,5-TNB. Data are needed regarding the bioconcentration and biomagnification potential of both compounds in terrestrial food chains. This information would be useful to evaluate the importance of accumulation of these compounds in the food chain and on subsequent human exposure to 1,3-DNB and 1,3,5-TNB via the food chain.

Exposure Levels in Environmental Media. 1,3-DNB and 1,3,5-TNB were detected in groundwater and soil at Army ammunition plants (Army 1985a, 1988; ATSDR 1987, 1989a, 1989b, 1989c; Jenkins and Grant 1987; Jenkins et al. 1989). Data are needed regarding levels of 1,3-DNB and 1,3,5-TNB in air. No data were located regarding human intake estimates of 1,3-DNB and 1,3,5-TNB. This information would be helpful in evaluating human exposure from each medium. Reliable monitoring data for these compounds in contaminated media at ammunition plants/waste sites are needed so that the information obtained on their levels in the environment, and the resulting body burden caused, can be used to assess the potential risk of adverse health effects in populations living near ammunition plants/waste sites.

Exposure Levels in Humans. 1,3-DNB and 1,3,5-TNB have not been detected in human blood, urine, fat, or breast milk; however, 1,3-DNB has been detected in the urine and blood of rodents fed the compound (Bailey et al. 1988; McEuen and Miller 1991; Nystrom and Rickert 1987). Biological monitoring data for both 1,3-DNB and 1,3,5-TNB are needed for populations living near Army ammunition plants and for occupationally exposed populations. This information is necessary for assessing the need to conduct studies on these populations.

Exposure Registries. No exposure registries were located for 1,3-DNB and 1,3,5-TNB. 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 Ongoing Studies

No ongoing studies were located for either 1,3-DNB or 1,3,5-TNB.