

5. POTENTIAL FOR HUMAN EXPOSURE

5.1 OVERVIEW

DNOC can be released to the environment when it is manufactured, formulated, used as a pesticide, and disposed (EPA 1988a; Hauser and Bromberg 1982; Leuenberger et al. 1988; Spanggord et al. 1982a, 1982b). In the United States, the EPA canceled its registration as a pesticide agent starting in 1991 (EPA 1993b; Farm Chemicals Handbook 1993; HSDB 1994). DNOC also forms in the atmosphere when 2-methylphenol reacts with NO_x present in ambient air (Leuenberger et al. 1988; Tremp et al. 1986). Significant destruction of DNOC in the atmosphere due to photochemical or other chemical reactions is not likely. Dry and wet deposition of particulate DNOC are the two significant removal processes in the air (Alber et al. 1989; Leuenberger et al. 1988; Tremp et al. 1986). Neither photochemical nor other chemical processes have been identified that would be significant for the transformation/degradation of DNOC in natural waters (Capel et al. 1988; EPA 1979; Tratnyek and Holgne 1991). The loss of DNOC from water due to volatilization is negligible (EPA 1979). Adsorption will transport moderate amounts of DNOC from water to sediment and suspended solids (EPA 1979). Following an accidental spill, the estimated time for one-half the initial DNOC levels to disappear was 30 days (Capel et al. 1988). As in the case of water, no chemical process has been identified that would be significant for the removal of DNOC from soil. Biodegradation may be the most significant process for the removal of DNOC from soil (Kincannon and Lin 1985). The loss of DNOC from soil due to volatilization would not be significant. Although the mobility of DNOC in most soils will be low (Ammon 1985), it has been infrequently detected in groundwater from treated fields (Holden 1986). Therefore, loss of DNOC due to leaching may occur in some soils (e.g., sandy soils). The estimated persistence times of DNOC in soil ranged from 14 days to >1 month (Ammon 1985; Goring et al. 1975; Jensen and Lautrup-Larsen 1967; Loehr 1989).

Other than in workplace air, DNOC has not been detected in ambient air in the United States. In Europe, where DNOC has been extensively used as an herbicide, concentrations in ambient air or in rain or fog may be much higher. Tree foliage exposure to DNOC has been suggested as an important contributor to the phenomenon known as forest decline (Kloepffer 1992). DNOC has been detected in effluents from chemical industries (EPA 1976b), but it has not been detected in drinking water. DNOC has been identified in 50 of the 1,350 waste sites in the NPL (HazDat 1994). The frequency of these sites within the United States is summarized in Figure 5-1. No data are available regarding

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the levels of DNOC in food or total diet samples of the U.S. population. Applicators of DNOC pesticide are one group of the population formerly exposed to DNOC by dermal and inhalation routes (Batchelor et al. 1956; Durham and Wolfe 1962; Wolfe 1976).

5.2 RELEASES TO THE ENVIRONMENT

5.2.1 Air

DNOC can enter the atmosphere during mixing and use as a pesticide on plants and soil (Leuenberger et al. 1988). In the United States, the EPA canceled the registration of DNOC as a pesticide starting in 1991 (EPA 1993b; Farm Chemicals Handbook 1993; HSDB 1994). Some DNOC can enter the atmosphere during its manufacture and formulation (EPA 1988a). DNOC releases to air from U.S. facilities that manufactured or processed this compound during 1990 are reported in Table 5-1 (TR192 1994). According to TR192 (TR192 1994), an estimated 33 pounds (14.9 kg) were released to the air from manufacturing and processing facilities in 1990. The TRI data should be used with caution since only certain types of facilities were required to report. Table 5-1 is not an exhaustive list. DNOC also is formed in the atmosphere as a secondary pollutant via the reaction of toluene and 2-methylphenol with NO, and OH radicals (Leuenberger et al. 1988; Tremp et al. 1986) although such mechanisms are not expected to be a significant contribution. Atmospheric reactions may be a more significant source of DNOC in the air than pesticide application (Leuenberger et al. 1988; Tremp et al. 1986).

5.2.2 Water

Dinitrocresols are released to water as effluents from chemical manufacturing industries, including pesticide and nitrotoluene manufacturing plants (EPA 1988a; Mhalas et al. 1989; Spanggord et al. 1982a, 1982b). DNOC releases in waste water from a pesticide plant and unspecified chemical manufacturing plants have been reported (EPA 1976b, 1988). The releases of DNOC to water from facilities that manufactured or processed this compound in the United States during 1990 are reported in Table 5-1 (TR192 1994). According to TRI, an estimated 4,910 pounds (2,224 kg) of DNOC were transferred to publicly owned treatment works (POTW); an additional 20 pounds (9 kg) were released to surface waters from direct industrial discharges. In addition, DNOC enters surface water and groundwater through runoff and leaching from fields and agricultural lands that have been treated with

Table 5-1. Releases to the Environment from Facilities that Manufacture or Process 4,6-dinitro-*o*-cresol

Reported amounts released in pounds per year									
State ^a	City	Facility	Air	Water	Underground Land Injection	Total Environment ^b	POTW Transfer	Offsite Waste Transfer	
LA	SAINT JAMES	CHEVRON CHEMICAL CO.		15		15			
MS	PASCAGOULA	FIRST CHEMICAL CORP.	3			3		1	
TX	PASADENA	AIR PRODUCTS MFG. CORP.					4,900	1,600	
TX	PASADENA	HUNTSMAN CHEMICAL CORP.					5	5	
TX	TEXAS CITY	STERLING CHEMICALS INC.	30			30	5	770	
TX	TEXAS CITY	SEA LION TECH. INC.		5		5		5,550	
Totals			33	20		53	4,910	7,926	

Source: TRI92 1994

^a Post office state abbreviations used

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

POTW = Publically Owned Treatment Works

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the pesticide; similar processes can transport DNOC from waste disposal sites that contain the compound (Cohen 1986; Hauser and Bromberg 1982). In the United States, the EPA canceled the registration of DNOC as a pesticide agent starting in 1991 (EPA 1993b; Farm Chemicals Handbook 1993; HSDB 1994). Small amounts enter water via deposition of atmospheric dinitrocresols (Leuenberger et al. 1988; Tremp et al. 1986).

5.2.3 Soil

DNOC is expected to be released to soil from the manufacture and formulation of the pesticide. More importantly, the pesticide would enter soil during its use in agricultural application for pest control. The release of DNOC to land from facilities that manufactured or processed the compound in the United States in 1990 is reported in Table 5-1 (TR192 1994). According to TRI, an estimated 7,926 pounds (3,590 kg) of wastes containing DNOC, amounting to 82% of the total environmental release of DNOC (see Table 5-1) from the manufacturing and processing facilities in the United States in 1990, was transported out of these facilities for disposal. Some may have been disposed in landfills and some may have been incinerated. Therefore, disposal of wastes containing the nitrocresols into landfills is another important source of these compounds in soil. Deposition of atmospheric dinitrophenols introduces small amounts to soil.

5.3 ENVIRONMENTAL FATE

5.3.1 Transport and Partitioning

In laboratory experiments, photolysis of o-cresol in the presence of nitrogen oxides produced dinitrocresols in the aerosol phase (Grosjean 1984, 1985). It was, therefore, presumed that dinitrocresols would be present in the ambient atmosphere in aerosol form (Grosjean 1984, 1985). The distance of atmospheric transport for DNOC depends on the half-life and the physical state of the compound in air. Residence times during atmospheric transport can be sufficiently long (see Section 5.3.2.1) so that such physical removal processes as wet or dry deposition may be important. The efficiency of both wet and dry precipitation is higher for particulate matter than for compounds that exist in the gas phase in the air (Schroeder et al. 1987). Therefore, atmospheric dinitrocresols, which exist predominantly in the particulate phase, may be removed by rain and snow, and these compounds may not be transported long distances from their source of emission. The detection of DNOC in rain and

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snow, and the observation that the ratio of concentrations of DNOC in rainwater to concentrations in air during a rain event was 5.6×10^4 , confirm the importance of these removal processes (Alber et al. 1989; Leuenberger et al. 1988; Tremp et al. 1986). Precipitation of atmospheric dinitrocresols transports the compound from air to land and water.

The pK_a value of 4.4 (see Table 3-2) for DNOC suggests that in natural waters with a pH 5-9, >50% of the compound exists in the ionic state at pH 5 and the percent of ionic forms increases as the pH increases. In addition to this dissociation effect, DNOC may form H-bonds in water (EPA 1979), reducing its vapor pressure and chances of volatility from water. Using a Henry's law constant value of 1.4×10^{-6} atm-m³/mole (Shen et al. 1982a, 1982b) and an estimation method (Thomas 1990), the estimated volatilization half-life of DNOC from a typical river 1 meter deep, with a current speed of 1 m/second, and an overhead wind speed of 3 m/second, is 36 days. Therefore, direct volatilization from water will not be significant for DNOC.

The partitioning of DNOC from water to solids present in water transports the compound from the water phase to suspended solids and sediment. The adsorption of DNOC from water by suspended solids and sediment is pH dependent, and the adsorption increases as the pH of the solution decreases (Frissel and Bolt 1962; Jafvert 1990). The adsorption of DNOC also depends on the clay and organic carbon content of the suspended solids and sediment; an increase in either value increases adsorption (EPA 1979; Frissel and Bolt 1962; Jafvert 1990). This adsorption will decrease the concentration of DNOC in water. DNOC's adsorption coefficient (a Freundlich sorption parameter, K_p) of 590 mg/g (Dobbs et al. 1987; Dobbs et al. 1989) indicates that the compound moderately sorbs to suspended solids and sediment in water. However, in Rhine River water with a pH of 7.9 (Wanner et al. 1989), only an estimated 9.3% of DNOC accumulated in bottom sediment (Halfon and Bruggemann 1989). This low adsorption may be due to high water pH, lack of clay, or a low organic carbon content of the sediment, or a combination of these factors.

No experimental data regarding the bioconcentration potential of DNOC in aquatic organisms were located. Based on an estimated bioconcentration factor (BCF) of 40 (Kenaga 1980), the bioconcentration of DNOC in aquatic organisms may not be significant; however, based on an estimated log octanol/water partition coefficient [$\log(K_{ow})$] value of 2.85, DNOC may bioaccumulate in aquatic organisms (Loehr and Krishnamoorthy 1988). Given that DNOC exists predominantly in ionic

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forms in most natural waters (pH 5-9) and that the compound is markedly toxic to fish, bioconcentration is not expected to be important (EPA 1979).

Given the low values for vapor pressure (1.05×10^{-4} mm Hg) (see Table 3-2) and Henry's law constant (1.4×10^{-6} atm·m³/mol) (see Table 3-2), and the consideration that the majority of the compound will be either in an ionic state or tied up through H-bonds, volatilization as a significant transport process for DNOC from soil to the air. However, some loss of DNOC by volatilization via co-distillation with water may occur, as observed (Kaufman 1976) in the case of dinoseb, with its active ingredient 2,3-dinitro-6-sec-butyl-phenol. Volatilization is expected to occur more readily with an increase in soil acidity (which facilitates the formation of undissociated species DNOC), moisture content, and temperature (Kaufman 1976); however, a laboratory study of two types of soil found no loss of DNOC by volatilization in 65 days (Loehr 1989). The adsorption of DNOC to soil increases with a decrease in soil pH and an increase in clay and organic carbon contents of soil. The estimated soil sorption (K_{oc}) values ranging from 2.35 to 2.77 indicate that this compound is moderately adsorbed in soil. Therefore, DNOC shows moderate mobility in soil, but because of its short persistence in soil (<1 month), the compound may not leach beyond 5 cm (Ammon 1985). Similar conclusions were reached by other investigators. In spite of moderate mobility, DNOC leaching was not observed from soil columns with at least 16 bed volumes of leachate (Pohland et al. 1987). On the other hand, the water soluble salts of DNOC (sodium, potassium, calcium, and ammonium) might be expected to leach into soil. Although no experimental data were located, it seems likely that DNOC will transfer to adjacent surface water or land via runoff water from treated fields or waste sites.

5.3.2 Transformation and Degradation

5.3.2.1 Air

The two processes likely to remove dinitrocresols from the atmosphere are reactions with hydroxyl and nitrate radicals (Atkinson et al. 1992). No experimental kinetic data are available for these two reactions (Grosjean 1991). The rate constant for the gas phase reaction of dinitrocresols with OH radicals is 3.0×10^{-14} cm³/molecule-second (Grosjean 1991). Using the method of Atkinson (1988), the estimated rate constant for this reaction is 2.1×10^{-13} cm³/molecule-second. Based on an average ambient atmospheric concentration of OH radicals in the northern hemisphere of 5×10^5 radicals/cm³ (Atkinson 1988) and either of the rate constant values, the estimated half-life of the DNOC reaction

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with OH radicals is >77 days. Since dinitrocresols are expected to be present predominantly in the particulate phase in the atmosphere, the reaction rate will be even slower compared to the gas phase reaction rate (Grosjean 1991). The reactions of phenol and cresols with NO₃ radicals may be significant processes in the air (Atkinson et al. 1992). However, the products of these reactions with phenol or cresols are *o*- and possibly *p*-substituted nitrophenol and cresol compounds (Atkinson et al. 1992). Since both *o* and *p* positions are already occupied by nitro substituents, the reaction of DNOC with NO₃ radicals does not seem to be a significant atmospheric process.

Photolysis of dinitrocresols is another reaction that can be significant for the destruction of these compounds in the air. In water, the neutral DNOC species has a light absorption spectrum with a shoulder at 305 nm (Schwarzenbach et al. 1988). Therefore, it is possible that atmospheric DNOC will absorb sunlight and undergo a reaction such as nucleophilic displacement of the nitro group by a hydroxyl group. Experimental evidence of such transformation reactions is not available (Kaufman 1976). Photolysis of a structurally similar compound, dinoseb (which has a sec-butyl group in place of the *o*-methyl group), produced side-chain hydroxylation or unsaturation (of the sec-butyl group), but no nucleophilic substitution of nitro groups (Kaufman 1976).

5.3.2.2 Water

Both neutral and anionic species of DNOC show absorption shoulders at wavelengths >300 nm (Schwarzenbach et al. 1988). However, photolysis of DNOC in water involving nucleophilic displacement of the nitro group by the hydroxyl group does not seem likely (EPA 1979). The photochemical reduction of the nitro group in DNOC is possible in water in the presence of a reducing agent (e.g., ascorbic acid or ferrous ions) and a sensitizer, such as chlorophyll (EPA 1979). However, there is no experimental evidence of the photochemical reduction of DNOC in water.

The estimated rate constants for the reaction of DNOC and 2,6-dinitro-*p*-cresol with singlet oxygen in water at pH ≈7 are 1.25x10⁵/molecule-second and 1.43x10⁷/molecule-second, respectively (Tratnyek and Holgne 1991). Based on an average concentration of singlet oxygen in eutrophic freshwater of 4x10⁻¹⁴ M (Tratnyek and Holgne 1991) and the above reaction rate constants, this reaction may be insignificant for DNOC. The estimated half-life for 2,6-dinitro-*p*-cresol due to this reaction is 14 days, and it may be a significant process for the destruction of 2,6-dinitro-*p*-cresol in eutrophic freshwater.

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Several pure cultures of microorganisms isolated from soil or sediment, such as *Corynebacterium simplex* (Gundersen and Jensen 1956; Jensen and Gundersen 1955), *Rhizobium leguminosarum* (Hamdi and Tewfik 1970), *Veillonella alcalescens* (McCormick et al. 1976), unadapted or phenol-adapted *Pseudomonas* sp. (Chambers and Kabler 1964; Tewfik and Evans 1966), and *Azotobacter* sp. (Wallnoefer et al. 1978), can biodegrade DNOC. Above a certain concentration, DNOC may be toxic to organisms. For example, at concentrations >500 mg/L, DNOC may be toxic to *C. simplex* (Bollen 1961). The degradation pathway will depend on the microorganism. It has been shown that *C. simplex* releases nitro groups of DNOC as nitrite ions (Gundersen and Jensen 1956). *Pseudomonas* sp. may biodegrade DNOC by ring cleavage. Successive replacement of nitro groups with hydroxyl groups can also occur, forming trihydroxytoluene (Golovleva et al. 1992; Tewfik and Evans 1966). The biodegradation may proceed by the successive reduction of nitro groups to amino groups by *V. alcalescens* and a *Pseudomonas* sp. (McCormick et al. 1976; Williams 1977). The metabolites that have been isolated as biodegradation products are 6-amino-4-nitro-*o*-cresol; 6-acetamido-4-nitro-*o*-cresol; 2-methyl-6-nitro-catechol; 2-methyl-6-amino-catechol and 2,3,5-trihydroxytoluene (Tewfik and Evans 1966; Wallnoefer et al. 1978). Although these studies with pure cultures of microorganisms are important to establish degradative pathways, their relevance to environmental situations is uncertain.

The biodegradation of DNOC was also tested with a mixture of microorganisms in activated sludge (Thorn and Agg 1975; Zahn and Wellens 1980), garden soil, compost, river mud, sediment of a waste lagoon (Tabak et al. 1964), and in settled domestic waste water (Tabak et al. 1981). These biodegradation studies with mixtures of microorganisms concluded that DNOC does not rapidly degrade under these conditions.

A patented waste treatment process that used activated sludge with added powdered activated carbon removed 99% of DNOC from influent that contained 11 µg/L of the compound (Patterson and Kodukala 1981). However, it is difficult to separate the contribution of the biological process from the adsorption effect of the activated carbon in removing DNOC from the influent. DNOC was resistant to anaerobic biodegradation under methanogenic conditions (O'Connor and Young 1989). Both laboratory die-away tests and experiments with natural marine plankton communities showed that DNOC was resistant to anaerobic biodegradation (Kuiper and Hanstveit 1988). Based on observations following a pesticide spill on the Rhine River involving DNOC, it was estimated that one-half the

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initial DNOC had disappeared (due to a combination of biotic and abiotic processes) within 30 days (Capel et al. 1988).

5.3.2.3 Sediment and Soil

The transformation and degradation pathways of DNOC in soil and sediment have not been studied thoroughly. The photolysis of DNOC in soil below the surface layer and in sediment is not significant due to the lack of available sunlight. DNOC does not contain any functional groups amenable to hydrolysis (EPA 1988a). It has been speculated that adsorbed DNOC may undergo hydrolysis on clay surfaces under acidic conditions (EPA 1979), but there is no experimental evidence. Biodegradation may be the most significant process for the transformation and of DNOC in soil.

Work reported in Bruinsma (1960) documents that above certain dosage levels, DNOC may be toxic to many types of soil microorganisms. These findings help explain a pattern in the available literature where the biodegradability of DNOC is widely taken for granted but where the results of different empirical studies on the persistence of DNOC in soils may show widely differing results. The effects of DNOC toxicity to soil flora also make it hard to interpret persistent (or disappearance) findings in terms of chemical kinetics and such concepts as half-lives.

In a soil column experiment, the estimated time for degradation on one-half the original amount of DNOC was 14 days (Kincannon and Lin 1985). These results are in line with findings from field plot analyses in Germany (Hurle and Rademacher 1970), where the disappearance of one-half the initial DNOC levels took 15 days. Other investigators have estimated that the persistence of DNOC in soil ranges from 14 days to >1 month (Ammon 1985; Goring et al. 1975; Jensen and Lautrup-Larsen 1967). However, in a study to determine the treatability potential of waste sludge from explosives production, no loss of DNOC was observed in two soil samples in 65 days (Loehr 1989). The soil in this experiment was not previously exposed to industrial chemicals, wastes, or any pretreatment to acclimate the microorganisms to the chemicals.

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5.4 LEVELS MONITORED OR ESTIMATED IN THE ENVIRONMENT

5.4.1 Air

Other than in workplace air (see Section 5.5), no data regarding the concentrations of DNOC in ambient air in the United States were located. From the concentration of DNOC in rainwater during a rain event in Dubendorf, Switzerland, the concentration of DNOC in air was estimated to be (from rainwater to air partition ratio) $0.05 \mu\text{g}/\text{m}^3$ (0.06 ppb) (Leuenberger et al. 1988).

5.4.2 Water

DNOC was detected at a concentration range of 8-400 $\mu\text{g}/\text{L}$ in waste water resulting from the production and purification of trinitrotoluene (Spanggord et al. 1982a). DNOC was also qualitatively detected in the waste waters of a plant in England that produced pest control chemicals (EPA 1988a) and in two effluents from unspecified chemical plants in the United States (EPA 1976b). In a project that monitored pollutant levels in urban runoff water of 1.5 cities in the United States, DNOC was not detected (detection limit unspecified) in any runoff water (Cole et al. 1984). The Great Lakes Water Quality Board has not viewed DNOC as a toxic substance of critical concern based on levels typically encountered in water from lakes Erie and Michigan (Great Lakes Water Quality Board 1983). DNOC was detected at a concentration of $<10 \mu\text{g}/\text{L}$ in water from the Potomac River near Quantico, Virginia (Hall et al. 1987). Following an accidental spill in 1986, the estimated concentration of DNOC in Rhine River water in Nauf, Switzerland, was $100430 \mu\text{g}/\text{L}$ (Capel et al. 1988). In California, where DNOC had been used as a pesticide, DNOC was detected in five groundwater samples at a maximum concentration of $35 \mu\text{g}/\text{L}$ (Cohen 1986; Holden 1986). In 1985, DNOC was detected in rainwater from Dubendorf, Switzerland, at concentrations ranging from 0.95 to $2.9 \mu\text{g}/\text{L}$ (Leuenberger et al. 1988; Tremp et al. 1986).

5.4.3 Sediment and Soil

DNOC is expected to be found in soil near plants where the pesticide is produced and formulated, near disposal sites, and in agricultural and waste lands to which the pesticide was applied. No quantitative data regarding the levels of DNOC in soil were located. Similarly, DNOC is expected to be found in the sludge of waste treatment plants, such as pesticide manufacturing plants, trinitrotoluene production

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plants, and in the sediment of rivers where the pesticide has been discharged from manufacturing plants or carried by runoff water from treated lands or waste disposal sites. However, no quantitative data regarding the levels of DNOC in sludge were located. Studies on the lower Grand Calumet River around the Indian Harbor area (Hoke et al. 1993) has documented sediment concentration of 4,6-dinitro-*o*-cresol ranging from 0.24 to 2.08 mg/kg (dry weight).

5.4.4 Other Environmental Media

DNOC was not found in fish collected between 1980 and 1981 from Great Lakes harbors and tributaries (Devault 1985). DNOC was detected below the tolerance level on Rumanian plums at harvest time and in potatoes from treated fields in what was formerly East Germany (HSDB 1994).

5.5 GENERAL POPULATION AND OCCUPATIONAL EXPOSURE

The general population could be exposed to DNOC from inhaling air or ingesting food and drinking water. To estimate the daily intake of DNOC by the general population from inhaling ambient air or ingesting drinking water and food, the levels of DNOC in these media must be known, and these values were not located in the literature. There was no indication in the literature that DNOC is used in any consumer products that could lead to dermal exposure.

Workers involved in manufacturing and formulating, incinerating, or spraying the pesticide on agricultural products and waste lands, and possibly workers involved in remediating Superfund sites containing this pesticide could have been or might be occupationally exposed to DNOC. Of all the possible exposure scenarios, the level of dermal exposure of workers during spraying of DNOC in the field has actually been measured. During spray-thinning of apples with liquid sprays, the estimated average dermal exposure may range from 22.5 to 63.2 mg/hour, and the corresponding average inhalation exposure may range from <0.05 to 0.4 mg/hour (Batchelor et al. 1956; Durham and Wolfe 1962; Wolfe 1976). The DNOC levels in the urine of sprayers before, during, and after the exposure period were also determined, and DNOC was detected in 5 of 183 spray operators. The DNOC concentrations in urine in these 5 samples ranged from 0.6 to 1.3 mg/L, with an average of 0.8 mg/L (Batchelor et al. 1956). The concentration of DNOC in plasma of spray operators following a total exposure period of 5-48 hours ranged from <1 to 4.3 mg/kg (Batchelor et al. 1956).

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5.6 POPULATIONS WITH POTENTIALLY HIGH EXPOSURES

As discussed (see Section 5.5), spray operators are one group of people that could have experienced potentially high exposures (higher than background levels) to DNOC. Other occupational groups discussed in Section 5.5 have the potential to be exposed to DNOC at higher levels than the general population, but no experimental evidence of higher exposure among these occupational groups was located.

Within the general population, people who live near incinerators burning DNOC, DNOC disposal facilities, and DNOC manufacturing and formulating plants are potentially exposed to higher than background concentrations of DNOC. However, no study located in the literature provided evidence of higher than background exposure to DNOC among these groups of the population. Moreover, no study demonstrated the potential for higher than background exposure to DNOC from consuming excessive amounts of certain foods (e.g., sprayed apples or contaminated fish).

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 dinitrocresols is available. Where adequate information is not available, ATSDR, in conjunction with the NTP, is required to assure the initiation of a program of research designed to determine the health effects (and techniques for developing methods to determine such health effects) of dinitrocresols.

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

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5.7.1 Identification of Data Needs

Physical and Chemical Properties. Some of the physical and chemical properties (e.g., K_{ow} Henry's law constant), often useful in estimating environmental fate and transport processes, are available for DNOC but not for other isomers of dinitrocresols (see Table 3-2). Although not as important as DNOC, it would still be useful to develop such data for other commercially available isomers of dinitrocresols.

Production, Import/Export, Use, Release, and Disposal. The production and import/export data in recent years for the different isomers of dinitrocresols including DNOC are not available. These data are important for assessing the trend in use for these chemicals. It is known that exposure to DNOC primarily occurs in the workplace (Batchelor et al. 1956; Durham and Wolfe 1962; Wolfe 1976). Since DNOC has been used as a pesticide on certain trees and to control broad-leaved weeds (Worthing 1987), it may have entered certain foods (e.g., apples, cereals). Since DNOC has been primarily used as a pesticide for agricultural products and on land for locust control (Worthing 1987) and is inefficiently transported from soil to other media (Ammon 1985; Kaufman 1976; Loehr 1989), soil is the environmental medium in which DNOC is expected to be found most frequently. Although some data on the methods of DNOC disposal are available (HSDB 1994), more information on disposal methods and their efficiency in destroying DNOC would be helpful. EPA has regulations governing the disposal of DNOC wastes (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 (TR192 1994), which contains this information for 1988, became available in May of 1990. This database will be updated yearly and should provide a list of industrial production facilities and emissions.

Environmental Fate. The partition of DNOC from water to soil and sediment depends on the pH and organic carbon and clay content of soil and sediment (Frissel and Bolt 1962; Jafvert 1990). When soil and sediment have a low pH and high organic carbon and clay content, DNOC partitions from water to soil and sediment. DNOC has been detected infrequently in groundwater (Holden 1986), indicating that only under certain conditions (e.g., when sandy soil is treated with DNOC), will it transport from soil to groundwater. The abiotic reactions that may degrade/transform DNOC in air,

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water, and soil are not known with certainty. Therefore, studies of the natural chemical processes (e.g., photolysis, oxidation/reduction) that may degrade/transform DNOC would be helpful.

Bioavailability from Environmental Media. Available information regarding the absorption rate of DNOC after inhalation, oral, or dermal exposure is discussed in the Toxicokinetics Section (Section 2.3). No quantitative data regarding the bioavailability of DNOC from inhalation of, ingestion of, and dermal contact with contaminated water, or inhalation of and dermal contact with contaminated soil are available. It will be helpful to develop quantitative data for bioavailability of DNOC from environmental media. However, the bioavailability from these routes of exposure are expected to be <100%, because the compound may be present partially in the sorbed state in air, water, and soil.

Food Chain Bioaccumulation. No experimental data for the bioaccumulation potential of DNOC from water to aquatic organisms were located. However, according to one group of investigators, DNOC may bioaccumulate in terrestrial and aquatic organisms (Loehr and Krishnamoorthy 1988). An experimental determination of the bioaccumulation potential for DNOC in terrestrial or aquatic organisms would be helpful. Biomagnification potential for DNOC is unknown.

Exposure Levels in Environmental Media. Other than in workplace air, no data regarding the ambient level of DNOC in air were located. Similarly, no data regarding the levels of DNOC in drinking water and total diet sample were available that would permit an estimation of the daily intake of DNOC from these routes of exposure. Data regarding the levels of DNOC in air, drinking water, and total diet would be useful for estimating daily DNOC intake by the general population from the various environmental media.

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

Exposure Levels in Humans. Other than in a few instances arising from occupational exposure (Batchelor et al. 1956; Durham and Wolfe 1962; Wolfe 1976), the levels of DNOC in body tissues and fluids of humans are not available. To assess the severity of occupational exposure, it may be

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useful to determine the background levels of DNOC in the different tissues and body fluids of the general population. This information is necessary for assessing the need to conduct health studies on these populations.

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

5.7.2 Ongoing Studies

The United States Department of Agriculture's Cooperative State Research Service is funding studies at the Rutgers University Department of Biochemistry and Microbiology on the biodegradation of 13 mononitroaromatic compounds as well as DNOC (FEDRIP 1994). In addition to isolating natural or mutant strains of microorganisms capable of degrading nitroaromatic compounds, key controls on metabolic pathways and mechanisms will be explored along with determinations of the major degradation products.